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1 Vorwort / Foreword

Das Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS) (Mitglied der Leibniz-Gemeinschaft) legt hiermit Kollegen, Förderern und Kooperationspartnern des Instituts seinen Jahresforschungsbericht 2004 vor. Der Bericht gibt in seinem ersten Teil Auskunft über die gemachten Fortschritte und die erzielten Resultate, gegliedert nach Forschungsgebieten, Projekten und Einzelthemen. Im zweiten Teil wird ein Überblick über das wissenschaftliche Leben am WIAS gegeben.

The Weierstrass Institute for Applied Analysis and Stochastics (WIAS) (member of the Leibniz Association) herewith presents its Annual Scientific Report 2004 to its colleagues, supporters, and cooperation partners. In its first part, the report informs about the progress made and the results obtained in 2004, divided into research areas, projects, and single topics. The second part gives a general account of the scientific life at WIAS.

Das Berichtsjahr 2004 war — wie auch das Vorjahr — gekennzeichnet durch die externe Evaluierung des Instituts durch den Senat der Leibniz-Gemeinschaft. Nach dem Besuch der Evaluierungskommission im Juli 2003 am WIAS erhielt das Institut zu Anfang des Jahres 2004 den Bewertungsbericht der Evaluierungskommission, der in die schriftliche Stellungnahme des Senats der Leibniz-Gemeinschaft einging. Zentrale Aussage des Berichtes war:

The report year 2004 was——as the year 2003——marked by the institute's external evaluation by the Leibniz Association's Senate. After the visit of the evaluation team to WIAS in July 2003, the institute got its evaluation report in the beginning of 2004. This report is an inherent part of the Senate Report. The central statement in the evaluation report has been:

- „Das WIAS steht heute für erstklassige Forschung und anwendungsnahe Methodenentwicklung auf dem für die Praxis immer wichtiger werdenden Gebiet der Angewandten Mathematik. Es ist in der internationalen mathematischen Wissenschaftslandschaft sehr gut positioniert. Sowohl hinsichtlich seiner Mission als auch seiner wissenschaftlichen Einzelaktivitäten hat das WIAS einen sehr positiven Eindruck hinterlassen."

- *WIAS stands today for excellent research and application-related method development in Applied Mathematics, a field becoming more and more relevant in practice. WIAS is very well positioned in the mathematical-scientific community. Both with respect to its mission and to its separate scientific activities, it gave a very positive general impression.*

Ferner wurde die Arbeit mehrerer Forschungsgruppen als „sehr gut" bezeichnet; einer Forschungsgruppe wurde sogar bescheinigt, „exzellent" zu sein. Besonders wichtig in der gegenwärtigen forschungspolitischen Situation ist es auch, dass dem WIAS attestiert wurde, über „mehrere Alleinstellungsmerkmale" zu verfügen und in seiner forschungsstrategischen Ausrichtung national und international „einzigartig positioniert" zu sein.

Besides, the work of several research groups has been judged "very good", one research group was even referred to as "excellent". In the present scientifico-political situation, it is also of a special importance that WIAS has been attested to have "several unique features" and to be nationally and internationally "singularly positioned" as far as the strategic orientation of its research work is concerned.

Aufgrund dieser äußerst positiven Einschätzung der am Institut geleisteten Arbeit wurde von der Bund-Länder-Kommission für Bildungsplanung und Forschungsförderung beschlossen, das WIAS für weitere sieben Jahre gemeinsam zu fördern. Das WIAS sieht sich darin bestätigt, in den vergangenen Jahren hervorragende Arbeit geleistet zu haben. Gleichzeitig ist die hervorragende Bewertung des Instituts ein Ansporn, den beschrittenen Weg konsequent fortzusetzen.

Because of this extremely positive evaluation of the institute's work the German Bund-Länder Commission for Educational Planning and Research Promotion (BLK) has decided that the Federal and Länder governments will continue to finance WIAS jointly for another seven years. That confirms that WIAS has done very good work during the past years. At the same time, this excellent evaluation is an incentive for the institute to follow consistently its chosen path.

Im Berichtsjahr 2004 gab es im Institut weit reichende personelle und strukturelle Veränderungen. Mit Prof. Gajewski und Dr. Schneider gingen langjährige Forschungsgruppenleiter in den Ruhestand; mit Prof. Wilmański folgte zu Beginn des Jahres 2005 ein weiterer Forschungsgruppenleiter. Hinzu kam, dass der Leiter der Forschungsgruppe „Numerische Mathematik und Wissenschaftliches Rechnen", Prof. Bänsch, einem Ruf auf eine C4-Professur an die Universität Erlangen folgte. Erfreulicherweise gelang es dem Institut in einer gemeinsamen Berufung zusammen mit der Humboldt-Universität zu Berlin, Herrn Prof. Mielke von der Universität Stuttgart als Nachfolger von Herrn Prof. Gajewski zu gewinnen. Für die Nachfolge von Prof. Bänsch ist ein gemeinsames Berufungsverfahren mit der Freien Universität angelaufen.

The report year 2004 has seen far-reaching personal and structural changes in the institute. Two scientists who have been heading research groups for a long time, namely Prof. Gajewski and Dr. Schneider, went into retirement. The leader of another research group, Prof. Wilmański, followed them in January 2005. In addition, the head of the "Numerical Mathematics and Scientific Computing" Research Group, Prof. Bänsch, followed a call to a C4 professorship at the University of Erlangen. Fortunately, the institute succeeded in winning Prof. Mielke from Stuttgart University for the successorship to Prof. Gajewski in a joint appointment with the Humboldt University of Berlin. For the successorship to Prof. Bänsch, a joint appointment procedure has been started.

Die wesentliche strukturelle Veränderung des Jahres 2004 war die Zusammenlegung der bisherigen Forschungsgruppe „Kontinuumsmechanik" mit Teilen der Forschungsgruppe „Partielle Differentialgleichungen und Variationsgleichungen" zu einer neuen Forschungsgruppe „Thermodynamische Modellierung und Analyse von Phasenübergängen" unter der Leitung von Dr. Dreyer.

The most essential change in the institute's structure in 2004 has been the merging of the former Research Group "Continuum Mechanics" and parts of the Research Group "Partial Differential Equations and Variational Equations" into a new Research Group "Thermodynamic Modeling and Analysis of Phase Transitions", which is headed by Dr. Dreyer.

In wissenschaftlicher Hinsicht war das Jahr 2004 wiederum erfolgreich. Die Arbeiten am *Forschungsprogramm 2004–2006* schritten gut voran. Es gelang dem Institut, in Zeiten knapper werdenden Geldes und wachsender Kon-

From a scientific point of view, the year 2004 has again been successful. Work on the *Research Program 2004–2006* has made good progress. In spite of the growing shortness of money and a growing competition, WIAS

kurrenz seine Stellung als führende Institution im Bereich der mathematischen Behandlung konkreter Problemstellungen aus komplexen Anwendungsfeldern nicht nur zu halten, sondern weiter auszubauen. Dabei konnten wesentliche Beiträge sowohl zur Lösung konkreter Anwendungsprobleme als auch zu innermathematischen Problemstellungen geleistet werden, und die interne Verflechtung innerhalb des Instituts sowie die Anzahl der interdisziplinär bearbeiteten Aufgabenstellungen aus Industrie, Wirtschaft und Wissenschaft nahmen weiter zu.

succeeded in defending and even strengthening its position as a leading institution in the mathematical treatment of concrete problems from complex fields of applications. Essential contributions to the solution of both concrete application problems and purely mathematical problems could be made. There was an increase in the internal integration within the institute as well as in the number of tasks from industry, economy, and sciences that were treated interdisciplinarily.

Im Berichtsjahr wurden weitere Fragestellungen aus konkreten Anwendungssituationen in Medizin, Wirtschaft, Natur- und Ingenieurwissenschaften aufgegriffen, insbesondere in den sechs Schwerpunktthemen des Instituts,

In the report year, new problems were taken up from concrete applications in medicine, economy, natural sciences, and engineering, especially in the six main fields of WIAS

- Mikro-, Nano- und Optoelektronik,
- Optimierung und Steuerung technischer Prozesse,
- Phasenübergänge,
- Stochastik in Natur- und Wirtschaftswissenschaften,
- Strömungs- und Transportprobleme in Kontinuen,
- Numerische Methoden der Analysis und Stochastik.

- Micro-, nano-, and optoelectronics;
- Optimization and control of technological processes;
- Phase transitions;
- Stochastics in natural sciences and economics;
- Flow and propagation processes in continua;
- Numerical methods of analysis and stochastics.

Die positive Entwicklung spiegelt sich einerseits wider in der Drittmitteleinwerbung, die allerdings im Jahre 2004 wegen des Auslaufens des BMBF-Förderprogramms für die Mathematik leicht rückläufig war; andererseits war die Anzahl der in referierten Fachzeitschriften erschienenen Publikationen erfreulich.

The positive development is reflected by the third-party funds that have been raised, although there has been a slight decline compared to last year's funds due to the expiration of the BMBF funding program for mathematics; on the other hand, the number of publications that appeared in refereed journals was encouraging.

Besonders augenfällig wird der hohe Stellenwert, den die am WIAS geleistete Arbeit in der Scientific Community hat, weiterhin im Bereich der Berufungen: Mit der Berufung von Prof. Bänsch an die Universität Erlangen und

The high rank of WIAS's research work in the scientific community becomes again especially clear in the field of calls: With the calls that Prof. Bänsch received to the University of Erlangen and Dr. Rachinskii

von Dr. Rachinskii an die University of Cork sind nunmehr seit der Gründung des Instituts im Jahre 1992 schon 30 Rufe an Mitarbeiter/innen des Instituts auf Professuren erfolgt (davon 15 auf C4-Professuren im Inland und neun auf Professuren im Ausland), eine Bilanz, die sich bei einer Zahl von derzeit 54 etatisierten Wissenschaftlern wirklich sehen lassen kann.

to the University of Cork, since the institute's foundation in 1992, altogether 30 calls have been received by collaborators of WIAS (including 15 to C4 (full) professorships and nine to professorships abroad). This is a remarkable output, given a number of 54 scientists now in our budget.

Die an sich schon intensive Kooperation mit den mathematischen Institutionen im Raum Berlin wurde weiter vertieft. Besonderes Augenmerk galt weiterhin der Zusammenarbeit mit den Berliner Hochschulen. Derzeit sind fünf gemeinsame Berufungen auf C4-S-Professuren mit Berliner Universitäten realisiert; für eine sechste ist das Berufungsverfahren angelaufen. Es besteht damit gute Hoffnung, dass 2005/2006 insgesamt sechs gemeinsame Berufungen auf C4-S-Professuren mit den Berliner Universitäten realisiert sein werden.

The cooperation with the mathematical institutions in Berlin and its environs, having already been intensive, has been further strengthened. Our main attention was again directed to the cooperation with the Berlin universities. Now WIAS has altogether five joint appointments to C4 special professorships with the Berlin universities. The procedure for one further joint appointment has been started. With that, WIAS hopes that in 2005/2006 altogether six joint appointments to C4 special professorships will have been concluded with the Berlin universities.

Neben diesen Aktivitäten und neben der Zusammenarbeit mit den Hochschulen durch die vielfältigen von Mitarbeitern des WIAS abgehaltenen Lehrveranstaltungen, war das WIAS an Sonderforschungsbereichen, Schwerpunktprogrammen und Graduiertenkollegs der DFG beteiligt. So beteiligte sich das WIAS in größerem Umfang an der erfolgreichen Einwerbung des Graduiertenkollegs „Analysis, Numerics, and Optimization of Multiphase Problems“ an der Humboldt-Universität.

Besides these activities and besides the cooperation with the universities through manifold teaching activities by WIAS collaborators, WIAS participated in DFG Collaborative Research Centers, Priority Programs, and Graduate Colleges. For example, the institute participated on a large scale in the successful application for the DFG Graduate College "Analysis, Numerics, and Optimization of Multiphase Problems" at the Humboldt University of Berlin.

Zentrales Kooperationsprojekt mit den Berliner Hochschulen war aber weiterhin das DFG-Forschungszentrum MATHEON „Mathematik für Schlüsseltechnologien“ an der Technischen Universität Berlin, durch das bis zunächst Mai 2006 jährlich mehr als 5 Millionen Euro an DFG-Fördergeldern nach Berlin fließen, um in Berlin einen international sichtbaren „Leuchtturm“ der Forschung in angewandter Mathematik zu errichten. Das WIAS engagiert sich in erheblichem Maße finanziell und

The main cooperation project with the Berlin universities was also in 2004 the DFG Research Center MATHEON "Mathematics for Key Technologies" at the Technical University of Berlin. For the Center, more than five million euro in funding from the DFG go to Berlin in each year, for the time being until May 2006, in order to build an international beacon of research in applied mathematics. WIAS is committed to the success of the Center by providing considerable financial and personal

personell am Erfolg des Zentrums: Der Institutsdirektor ist Vorstandsmitglied des Zentrums, seine beiden Stellvertreter Mitglieder des Rates des Zentrums, und Mitarbeiter des Instituts sind an insgesamt 13 Teilprojekten des Forschungszentrums als Teilprojektleiter beteiligt. Insgesamt acht weitere wissenschaftliche Mitarbeiter und mehrere studentische Hilfskräfte konnten aus Zentrumsmitteln am WIAS eingestellt werden.

resources: The Director of WIAS is a member of the Center's Executive Board and both his deputies are members of its Council. WIAS collaborators participate in the management of 13 subprojects of the Center. Altogether, eight scientific collaborators and several student assistants were employed by WIAS from MATHEON funds in 2004.

Unverändert bleibt es das übergeordnete Ziel des Instituts, Grundlagenforschung und anwendungsorientierte Forschung miteinander zu verbinden und durch neue wissenschaftliche Erkenntnisse zur Fortentwicklung innovativer Technologien beizutragen. Die Erfüllung dieser Aufgabe wird angesichts der andauernden faktischen Absenkungen der Grundfinanzierung in den vergangenen Jahren immer schwieriger. Bisher ist es dem WIAS durch optimalen Einsatz seiner Ressourcen und Ausschöpfung seiner Kapazitäten gelungen, seine wissenschaftliche Gesamtleistung nicht nur auf hohem Niveau zu halten, sondern sogar zu steigern.

Our primary aim remains unchanged: to join fundamental research with application-oriented research, and, by new scientific insights, to contribute to the advancement of innovative technologies. The accomplishment of this mission becomes more and more difficult in view of the continued effective reduction in our basic funding during the last years. Thus far, WIAS has been able not only to keep up its scientific output on a high level but even to increase it by an optimal use of its resources and its capacities.

Allerdings ist hier nunmehr eine Grenze erreicht: Eine hinreichende Grundausstattung ist für das WIAS unerlässlich, um auch weiterhin erfolgreich im wissenschaftlichen Wettbewerb, insbesondere um Drittmittel und Industriekooperationen, aber auch um qualifizierte Mitarbeiter, bestehen zu können. Das Institut verfolgt daher mit großer Sorge die über viele Jahre hinweg fortgesetzte Aushöhlung des Institutshaushaltes.

But now a limit has been reached: A sufficient basic funding is imperative for the institute to remain successful in the scientific competition, particularly for third-party funding and industrial cooperation partners, but also for qualified collaborators. Therefore the institute views with much concern the erosion of the institute's budget that has been continued now for many years.

Wie in den vergangenen Jahren hoffen wir, dass dieser Bericht möglichst vielen Kollegen und Förderern aus Industrie, Wirtschaft und Wissenschaft zur Information dienen und Anregungen zur Zusammenarbeit geben möge.

As in the last years we hope that as many colleagues and supporters as possible from industry, economy, and sciences might find this report informative and might be encouraged to cooperate with us.

Berlin, im Mai 2005 / in May 2005

2 Wissenschaftlicher Beirat / Scientific Board

3 Aufgabenstellung und Struktur / Mission and Structure

3.1 Aufgabenstellung / Mission

Das *Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)* im Forschungsverbund Berlin e. V. verfolgt als Institut der Leibniz-Gemeinschaft (WGL) Forschungsziele, die von gesamtstaatlichem Interesse und überregionaler Bedeutung sind. Entsprechend den Empfehlungen des Wissenschaftsrats betreibt das WIAS *projektorientierte* Forschungen in Angewandter Mathematik, insbesondere in *Angewandter Analysis* und *Angewandter Stochastik*, mit dem Ziel, zur Lösung *komplexer Problemkreise aus Wirtschaft, Wissenschaft und Technik* beizutragen. Die Herangehensweise ist dabei ganzheitlich, d. h. am WIAS wird der gesamte Problemlösungsprozess von der interdisziplinären Modellierung über die mathematisch-theoretische Behandlung des Modells bis hin zur konkreten numerischen Simulation betrieben.

As a member of Leibniz Association (WGL), the *Weierstraß-Institut für Angewandte Analysis und Stochastik* (Weierstrass Institute for Applied Analysis and Stochastics/WIAS) in Forschungsverbund Berlin e.V. strives for research results of supraregional and national interest. Following the recommendations of the German Science Council, WIAS engages in *project-oriented* research in applied mathematics, particularly in *applied analysis* and *applied stochastics*, aiming at contributing to the solution of *complex economic, scientific, and technological problems*. WIAS approaches this aim integrally, pursuing the entire problem-solving process from the interdisciplinary modeling and the theoretical mathematical analysis of the model to concrete numerical simulations.

Die Forschungen am WIAS konzentrierten sich im Berichtsjahr auf die folgenden *Schwerpunktthemen*, in denen das WIAS besondere Kompetenz bezüglich Modellierung, Analysis und Simulation besitzt:

Research at WIAS focused, in the time under review, on the following *main fields*, in which the institute has a special competence in the modeling, analysis, and simulation:

- Mikro-, Nano- und Optoelektronik,
- Optimierung und Steuerung technischer Prozesse,
- Phasenübergänge,
- Stochastik in Natur- und Wirtschaftswissenschaften,
- Strömungs- und Transportprobleme in Kontinuen,
- Numerische Methoden der Analysis und Stochastik.

- Micro-, nano-, and optoelectronics;
- Optimization and control of technological processes;
- Phase transitions;
- Stochastics in natural sciences and economics;
- Flow and propagation processes in continua;
- Numerical methods of analysis and stochastics.

Dabei wurden u. a. mathematische Problemstellungen aus den folgenden Bereichen bearbeitet[1]:

Among others, mathematical problems from the following areas have been treated[2]:

3.1.1 Mikro-, Nano- und Optoelektronik / Micro-, nano-, and optoelectronics

- Mikroelektronische Bauelemente (Technologie- und Bauelementesimulation von Halbleiterbauelementen; in FG 1 und FG 3)
- Microelectronic devices (technology and device simulation of semiconductor devices, in FG 1 and FG 3)
- Simulation von mikroelektronischen Schaltkreisen und von Mikrowellenschaltungen (in FG 3)
- Simulation of microelectronic circuits and of microwave circuits (in FG 3)
- Modellierung und Simulation von Halbleiterlasern (in FG 1, FG 2 und FG 3)
- Modeling and simulation of semiconductor lasers (in FG 1, FG 2, and FG 3)
- Diffraktive Optik (Simulation und Optimierung optischer Gitter; in FG 4)
- Diffractive optics (simulation and optimization of optical gratings, in FG 4)

3.1.2 Optimierung und Steuerung technischer Prozesse / Optimization and control of technological processes

- Simulation und Steuerung chemischer Anlagen (in FG 3 und FG 4)
- Simulation and control of chemical plants (in FG 3 and FG 4)
- Robotik (Optimierung und inverse Modellierung von Mehrkörpersystemen; in FG 4)
- Robotics (optimization and inverse modeling of multi-body systems, in FG 4)
- Probleme des Optimal Shape Design (in FG 4 und FG 7)
- Problems of Optimal Shape Design (in FG 4 and FG 7)

3.1.3 Phasenübergänge / Phase transitions

- Wärmebehandlung und Schweißverfahren bei Stählen (Modellierung und Simulation; in FG 4)
- Heat treatment and welding processes for steels (modeling and simulation, in FG 4)
- Phasenfeldmodelle (Simulation von Formgedächtnislegierungen, flüssig-fest-Übergängen und Phasenseparation; in FG 1, FG 3 und FG 7)
- Phase-field models (simulation of shape-memory alloys, liquid-solid transitions and phase separation, in FG 1, FG 3, and FG 7)

[1] In Klammern sind die Forschungsgruppen (FG) angegeben, in denen das Thema jeweils behandelt wurde.
[2] The research groups (FG) involved in the respective research are indicated in brackets.

- Stochastische Modellierung von Phasenübergängen und Spingläsern (in FG 5)
- Verfahren der Züchtung von SiC- und GaAs-Einkristallen (in FG 7)

- Stochastic modeling of phase transitions and spin glasses (in FG 5)
- Growth processes of SiC and GaAs single crystals (in FG 7)

3.1.4 Stochastik in Natur- und Wirtschaftswissenschaften / Stochastics in natural sciences and economics

- Stochastische Teilchensysteme und kinetische Gleichungen (Modellierung und Simulation von Koagulationsprozessen und Gasströmungen; in FG 5, FG 6 und FG 7)
- Modellierung von Aktien-, Zins- und Wechselkursen (in FG 5 und FG 6)
- Bewertung von Derivaten, Portfolio-Management und Risikobewertung (in FG 6)
- Nichtparametrische statistische Methoden (Bildverarbeitung, Finanzmärkte, Ökonometrie; in FG 6)
- Datenanalyse (Cluster- und Diskriminanzanalyse, Credit-Scoring; in FG 6)

- Stochastic particle systems and kinetic equations (modeling and simulation of coagulation processes and gas flows, in FG 5, FG 6, and FG 7)
- Modeling of stock prices, interest rates, and exchange rates (in FG 5 and FG 6)
- Evaluation of derivatives, portfolio management, and evaluation of risk (in FG 6)
- Nonparametric statistical methods (image processing, financial markets, econometrics, in FG 6)
- Data analysis (clustering and discriminant analysis, credit scoring, in FG 6)

3.1.5 Strömungs- und Transportprobleme in Kontinuen / Flow and propagation processes in continua

- Navier-Stokes-Gleichungen (in FG 3)
- Strömungen und Massenaustausch in porösen Medien (Wasser- und Stofftransport in Böden und in porösen Gesteinen, Zweiphasenströmungen und Modellierung von Brennstoffzellen; in FG 3 und FG 7)
- Thermomechanik poröser Körper und granularer Stoffe (Schall- und Stoßwellen, Streuung und Beugung; in FG 7)

- Navier–Stokes equations (in FG 3)
- Flows and mass exchange in porous media (water and materials transport in soils and porous rocks, two-phase flows, and modeling of fuel cells, in FG 3 and FG 7)
- Thermomechanics of porous bodies and of granular materials (sound waves, shock waves, dispersion and diffraction, in FG 7)

3.1.6 Numerische Methoden der Analysis und Stochastik / Numerical methods of analysis and stochastics

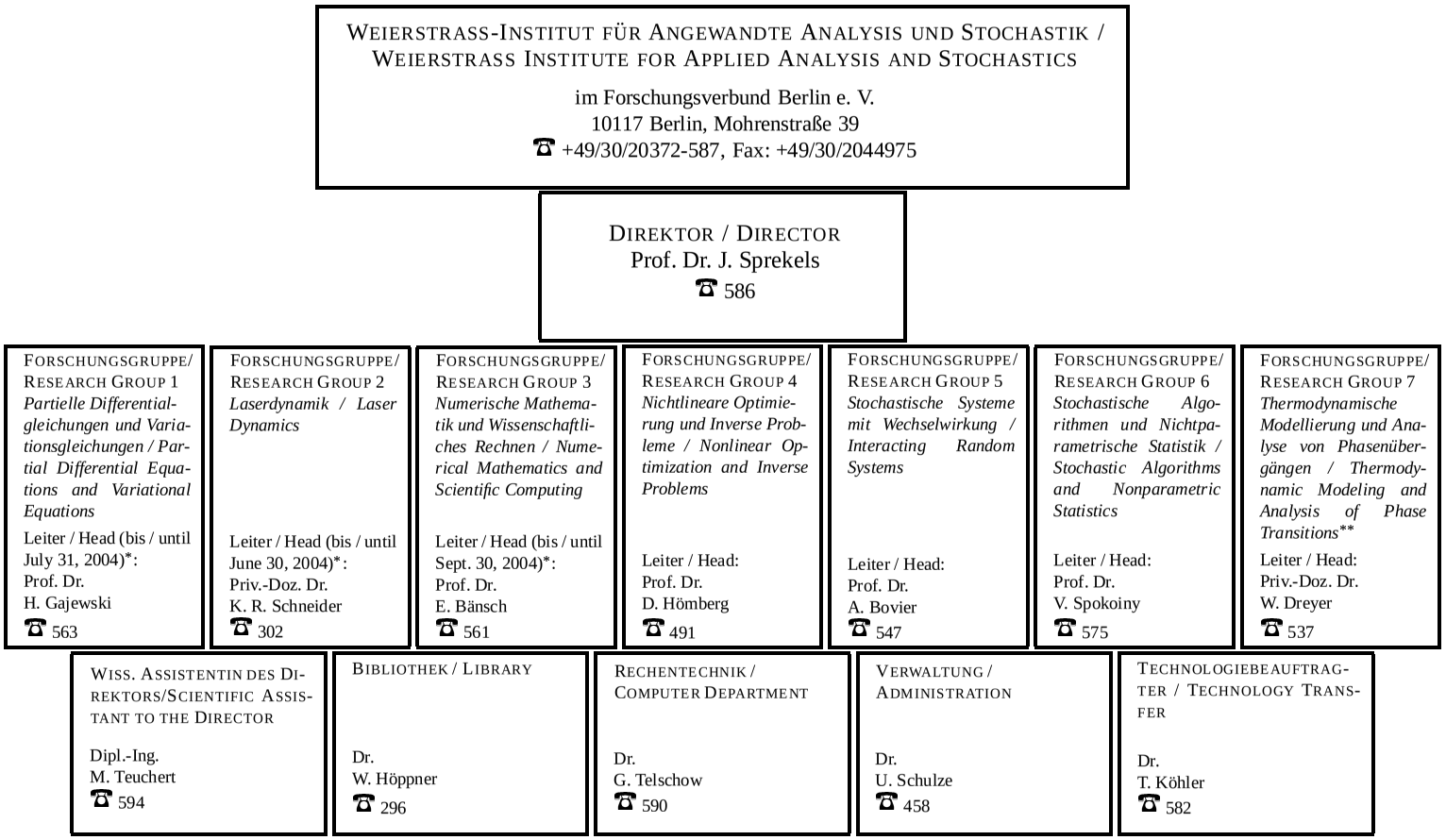
- Numerische Lösung partieller Differentialgleichungen (Finite-Volumen- und Finite-Element-Methoden, Vorkonditionierer, Gittergeneration, Fehlerschätzer und Adaptivität; in allen Forschungsgruppen, insbesondere in FG 3)
- Numerik von Algebro-Differentialgleichungen (in FG 3)
- Numerik von Integralgleichungen (Randelementmethoden, Waveletalgorithmen; in FG 4)
- Verfahren der nichtlinearen Optimierung (in FG 4 und FG 7)
- Stochastische Numerik (in FG 6)
- Monte-Carlo-Verfahren (kinetische Gleichungen, Koagulationsdynamik, Teilchensysteme; in FG 5, FG 6 und FG 7)
- Weiterentwicklung von Softwarepaketen des WIAS (`AWS`, `BOP`, `ClusCorr98`®, `DiPoG`, `gltools`, `WIAS-HiTNIHS`, `WIAS-TeSCA`, `LDSL-tool`, `pdelib`, `WIAS-SHarP` und `WIAS-QW`, siehe S. 265; in FG 1, FG 2, FG 3, FG 4, FG 6 und FG 7)

- Numerical solution of partial differential equations (finite volume and finite element methods, preconditioners, grid generation, error estimators, and adaptivity, in all research groups, especially in FG 3)
- Numerics of differential–algebraic equations (in FG 3)
- Numerics of integral equations (boundary element methods, wavelet algorithms, in FG 4)
- Nonlinear optimization techniques (in FG 4 and FG 7)
- Stochastic numerics (in FG 6)
- Monte Carlo processes (kinetic equations, coagulation dynamics, particle systems, in FG 5, FG 6, and FG 7)
- Further development of WIAS software packages (`AWS`, `BOP`, `ClusCorr98`®, `DiPoG`, `gltools`, `WIAS-HiTNIHS`, `WIAS-TeSCA`, `LDSL-tool`, `pdelib`, `WIAS-SHarP` and `WIAS-QW`, see page 265; in FG 1, FG 2, FG 3, FG 4, FG 6, and FG 7)

3.2 Organisatorische Struktur / Organizational Structure

Zur Erfüllung seiner wissenschaftlichen Aufgabenstellung war das WIAS im Berichtsjahr 2004 nach fachspezifischen Gesichtspunkten in sieben Forschungsgruppen gegliedert; hinzu kamen die wissenschaftlich-technischen Dienste. Im Folgenden sind die Aufgaben dieser Abteilungen angegeben.

In order to fulfil its scientific mission, WIAS has been divided, according to the mathematical fields treated there, into seven research groups and the scientific technical services. Please find in the following the tasks of these departments.



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* Leiterstelle bis Ende 2004 nicht besetzt / Head until end of 2004: N.N.

** Die FG 7 hieß bis 1.9.2004 *Kontinuumsmechanik* und wurde geleitet von Prof. Dr.-Ing. K. Wilmański. / The name of Research Group 7 until September 1, 2004 was *Continuum Mechanics.* It was headed by Prof. Dr.-Ing. K. Wilmański.

3.2.1 Forschungsgruppe Partielle Differentialgleichungen und Variationsgleichungen / Research Group Partial Differential Equations and Variational Equations

Die Arbeiten der Forschungsgruppe befassten sich mit der qualitativen Analyse von Systemen nichtlinearer partieller Differentialgleichungen und, darauf aufbauend, mit der Entwicklung von Verfahren zu ihrer numerischen Lösung. Speziell wurden Gleichungen betrachtet, die komplexe Phänomene und Prozesse aus der Physik, Chemie und Technik modellieren und die Grundlage zu deren numerischer Simulation bilden.

The group has been working on the qualitative analysis of systems of nonlinear partial differential equations and, on this basis, on the development of methods for their numerical solution. Especially equations were studied which model complex phenomena and processes from physics, chemistry, and technology and form the basis for their numerical simulation.

Die Forschungsschwerpunkte der Forschungsgruppe lagen im Jahr 2004 auf folgenden Anwendungsgebieten:

In 2004, the group's research work focused on the following application areas:

- Modelle zum Stoff-, Ladungs- und Energietransport in heterogenen Halbleiterstrukturen,
- Modellierung von optoelektronischen Bauelementen und nichtlinearen optischen Fasern,
- Quantenmechanische Modelle für Halbleiternanostrukturen,
- Nichtlokale Phasenseparationsmodelle mit Anwendungen in der Bildverarbeitung.

- Models describing mass, charge, and energy transport in heterogeneous semiconductor structures;
- Modeling of optoelectronical devices and nonlinear optical fibers;
- Quantum mechanical models for semiconductor nanostructures;
- Nonlocal phase separation models with application to image processing.

Im August 2004 wechselten fünf Mitarbeiter der Gruppe in die Forschungsgruppe „Thermodynamische Modellierung und Analyse von Phasenübergängen“. Über deren Arbeit wird im Abschnitt 3.2.7 berichtet.

In August 2004, five members of this group changed over to the Research Group "Thermodynamic Modeling and Analysis of Phase Transitions". Their work is reported upon in § 3.2.7.

3.2.2 Forschungsgruppe Laserdynamik / Research Group Laser Dynamics

Die Arbeiten dieser Forschungsgruppe befassten sich mit der Modellierung, der qualitativen Analyse, der numerischen Untersuchung und der Steuerung dynamischer Systeme, die Prozesse in der Optoelektronik, in der Reaktionskinetik und in der Biochemie beschreiben.

The research of this group was concerned with modeling, quantitative analysis, numerical study, and control of dynamical systems describing processes in optoelectronics, in reaction kinetics, and in biochemistry.

Das zentrale Forschungsthema der Gruppe war die

- Nichtlineare Dynamik von Mehrsektions-Halbleiterlasern.

The main topic of the group was the

- Nonlinear dynamics of multisection semiconductor lasers.

3.2.3 Forschungsgruppe Numerische Mathematik und Wissenschaftliches Rechnen / Research Group Numerical Mathematics and Scientific Computing

Die mathematische Modellierung naturwissenschaftlicher und technologischer Vorgänge erfordert die effiziente numerische Lösung von Systemen nichtlinearer gewöhnlicher und partieller Differentialgleichungen sowie von großen Systemen von Algebro-Differentialgleichungen. Die Hauptaufgabe der Forschungsgruppe bestand in der Entwicklung, theoretischen Begründung und Implementierung numerischer Methoden zur Lösung solcher Systeme. Die Untersuchungen konzentrierten sich auf die Themenkreise

- Numerische Verfahren und Softwarekomponenten für die Lösung von Systemen partieller Differentialgleichungen (insbesondere in der Mikro-, Nano- und Optoelektronik, bei Phasenübergängen und bei Strömungs- und Transportvorgängen),
- Simulation von Höchstfrequenzschaltungen,
- Dynamische Simulation chemischer Prozesse.

The mathematical modeling of scientific and technological processes requires the efficient numerical solution of systems of nonlinear ordinary and partial differential equations as well as of large systems of differential–algebraic equations. The main task of the research group was the development, the theoretical substantiation, and the implementation of numerical methods to solve such systems. The studies concentrated upon the topics

- Numerical methods and software components for the solution of systems of partial differential equations (particularly in micro-, nano- and optoelectronics, for phase transitions and for flow and propagation processes);
- Simulation of hyperfrequency circuits;
- Dynamical simulation of chemical processes.

3.2.4 Forschungsgruppe Nichtlineare Optimierung und Inverse Probleme / Research Group Nonlinear Optimization and Inverse Problems

Die Forschungsgruppe untersucht hochdimensionale Optimierungsaufgaben und inverse Probleme, die in aktuellen technischen und wirtschaftlichen Anwendungen auftreten. Die Ar-

The research group investigates large-scale optimization and inverse problems occurring in current engineering and economic applications. The tasks range from basic research on analysis

beit reicht von Grundlagenforschung zur Analysis und Numerik dieser Probleme über die Entwicklung effizienter Algorithmen und Software bis hin zur Lösung konkreter Praxisanwendungen.

and numerics and the development of efficient algorithms and software to the solution of tangible application problems.

Die Forschung konzentrierte sich im vergangenen Jahr auf zwei Anwendungsfelder:

Last year's research was focused on two application fields:

- Optimierung und inverse Probleme in der diffraktiven Optik und der Elektromagnetik,
- Optimale Steuerung von Produktionsprozessen.

- Optimization and inverse problems in diffractive optics and electromagnetics;
- Optimal control of production processes.

3.2.5 Forschungsgruppe Stochastische Systeme mit Wechselwirkung / Research Group Interacting Random Systems

Die mathematische Analyse sehr großer Systeme und Strukturen mit wechselwirkenden Komponenten ist in zahlreichen Bereichen der Naturwissenschaften und in vielen technischen Anwendungen von Bedeutung. Die Forschungsgruppe befasste sich in diesem Zusammenhang im Berichtsjahr mit Fragestellungen aus den Gebieten

The mathematical analysis of very large systems and structures with interacting components is important for various areas of the natural sciences and for many technical applications. In the year under review, the research group was concerned with problems from the following areas

- Gleichgewicht und Dynamik von ungeordneten Systemen,
- Katalytische Verzweigungsstrukturen und wechselwirkende Diffusionen,
- Stochastische Teilchensysteme und kinetische Gleichungen.

- Equilibrium states and dynamics of disordered systems;
- Catalytic branching processes and interactive diffusions;
- Stochastic particle systems and kinetic equations.

3.2.6 Forschungsgruppe Stochastische Algorithmen und Nichtparametrische Statistik / Research Group Stochastic Algorithms and Nonparametric Statistics

Die Forschungsgruppe befasste sich mit Arbeiten zur Angewandten Stochastik und Finanzmathematik.

The research group worked on problems from Applied Stochastics and Financial Mathematics.

Die Schwerpunkte lagen dabei auf den Bereichen

- Risikomessung, Bewertung und Simulation von Zinsderivaten sowie Portfolio-Optimierung,
- Stochastische Algorithmen und Turbulenztheorie,
- Nichtparametrische statistische Methoden der Bildverarbeitung und der Ökonometrie, Cluster- und Diskriminanzanalyse.

The main topics came from the areas

- Risk evaluation, interest rate modeling, calibration and pricing of non-standard derivatives, and portfolio optimization;
- Stochastic algorithms and turbulence modeling;
- Nonparametric statistical methods in image processing and econometrics, clustering and discriminant analysis.

3.2.7 Forschungsgruppe Thermodynamische Modellierung und Analyse von Phasenübergängen / Research Group Thermodynamic Modeling and Analysis of Phase Transitions

In ihrer jetzigen Zusammensetzung besteht die Forschungsgruppe seit dem 1. September 2004. Durch den Zusammenschluss der alten FG „Kontinuumsmechanik“ und mehrerer Mitarbeiter der FG „Partielle Differentialgleichungen und Variationsgleichungen“ wurde eine enge interdisziplinäre Zusammenarbeit auf den Gebieten Thermodynamik, Analysis und Simulation von Phasenübergängen in mechanischen Spannungsfeldern ermöglicht. Die aktuellen Schwerpunkte sind:

The research group exists since September 1, 2004, in its current composition. The integration of several former members of the Research Group “Partial Differential Equations and Variational Equations” into the the research group formerly called “Continuum Mechanics” made it possible to establish a tight interdisciplinary cooperation on thermodynamics, analysis, and simulations of phase transitions in mechanical stress fields. The ongoing research topics are:

- Diffusion in der Umgebung von flüssigen Ausscheidungen in einer kristallinen Matrix,
- Aufstellung neuer und thermodynamisch konsistenter Becker-Döring-Modelle zur Berechnung von Tropfenverteilungen,
- Phasenseparationsprozesse in Lotmaterialien,
- Kristallzüchtungsprozesse durch Sublimation,
- Modellierung und Analysis von Hysteresephänomenen,
- Dynamik dünner Filme.

- Diffusion in the vicinity of liquid precipitates in a crystalline matrix;
- Setting up of new and thermodynamically consistent Becker–Döring models.
- Phase separation in solder materials;
- Processes of crystal growth by sublimation;
- Modeling and analysis of hysteresis phenomena;
- Dynamics of thin films.

3.2.8 Wissenschaftlich-technische Dienste / Scientific Technical Services

Zur Versorgung der Forschungsgruppen mit Fachliteratur und Fachinformationen betreibt das WIAS eine *wissenschaftliche Bibliothek*, die den Charakter einer *Spezialbibliothek* hat, d. h. sie stellt aus eigenen Beständen und durch Mitnutzung fremder Bestände die Literatur für die wissenschaftliche Arbeit bereit. Dies geschieht in enger Zusammenarbeit mit der *Fachinformation*. Gehalten werden Zeitschriften, Serien, Monographien, Preprints, Reports und CD-ROMs.

In order to provide the research groups with specialized literature and with science information, WIAS has a *Scientific Library* with the character of a *specialized library*, making available the literature for the scientific work from its own stock or by using the stocks of other institutions, in close cooperation with the *Science Information*. The library offers journals, series, monographs, preprints, reports, and CD-ROMs.

Die Gruppe *Rechentechnik* ist zuständig für die Versorgung des Instituts mit den nötigen Kapazitäten im Bereich der EDV. Ihr obliegt neben der Hardware- und Software-Wartung das gesamte Systemmanagement und ferner die Betreuung des hausinternen Rechnernetzes.

The *Computer Department* is responsible for supplying the institute with the necessary electronical data processing facilities. Apart from maintaining the institute's hardware and software, the department is in charge of the management of the entire computer system and of the internal computer network.

Die *Verwaltung* erledigt die für die Arbeitsfähigkeit des Instituts notwendigen verwaltungstechnischen und organisatorischen Aufgaben. Das WIAS ist mit derzeit sieben weiteren naturwissenschaftlichen Forschungsinstituten im Forschungsverbund Berlin e. V. (FVB) rechtlich zusammengeschlossen. Administrative Aufgaben werden im FVB zwecks einer effizienten einheitlichen Verwaltungsleistung arbeitsteilig von der *Gemeinsamen Verwaltung des FVB* und den *Institutsverwaltungen* erbracht. Dem *Geschäftsführer* des FVB obliegt die Führung der Verwaltungsgeschäfte.

The *Administration* attends to the administrative and organizational tasks thus enabling the institute to fulfil its mission. WIAS has legally joined forces with seven other scientific research institutes in Forschungsverbund Berlin e.V. (FVB). Aiming at an efficient homogeneous administrative performance within FVB, the *FVB's Common Administration* and the *institutes' administrations* share the administrative tasks. The *Manager* of FVB is in charge of the administrative business.

4 Research Results and Applied Projects

4.1 Research Group Partial Differential Equations and Variational Equations

4.1.1 Overview

Im Einklang mit dem WIAS-Forschungsprogramm hat die Forschungsgruppe ihre Arbeiten zur mathematischen Modellierung und Analyse von Problemen aus der Mikro-, Opto- und Nanoelektronik sowie von Phasenseparationsproblemen fortgesetzt. Die Arbeiten betreffen grundlegende analytische Untersuchungen zur Existenz, Einzigkeit, Regularität und zu weiteren qualitativen Eigenschaften von Lösungen der Modellgleichungen, die Begründung, Entwicklung und Implementierung von numerischen Lösungsverfahren, und schließlich den Einsatz von Simulationsprogrammen zur Lösung von Anwendungsproblemen unserer Kooperationspartner.

According to the WIAS Research Program the research group has continued its work in mathematical modeling and analysis of problems arising in micro-, opto- and nanoelectronics as well as of phase separation problems. The work covers basic analytical investigations on existence, uniqueness, regularity, and on further qualitative properties of solutions to the model equations, foundation, development and implementation of numerical procedures, and finally, the application of simulation programs for solving problems of our cooperation partners.

Wichtige Arbeiten der Forschungsgruppe wurden durch Drittmittel finanziert. Im Rahmen des BMBF-Programms „Mathematik für Innovationen in Industrie und Dienstleistungen“ wurde folgendes Verbundprojekt gefördert:

- Anwendung eines nichtlokalen Phasenseparationsmodells zur Bildbewertung in der Rheumadiagnostik.

Some important research work of the group has been funded from external sources. The following joint project has been supported by the BMBF Program “Mathematics for Innovations in Industry and Services”:

- Application of a nonlocal phase separation model to optical diagnosis of rheumatic diseases.

Die DFG unterstützte folgende Forschungsprojekte:

- Energiemodelle für heterogene Halbleiterstrukturen (Normalverfahren),
- Spektralparameterabhängige Randwertprobleme und Hybridmodelle der Halbleitersimulation (Normalverfahren),

The DFG has sponsored the following research projects:

- Energy models for heterogeneous semiconductor structures (individual grant);
- Boundary value problems depending on the spectral parameter and hybrid models in semiconductor simulation (individual grant);

- Analytische und numerische Untersuchungen zur raum-zeitlichen Strukturbildung in Halbleiterlasern (Sonderforschungsbereich 555 „Komplexe nichtlineare Prozesse“),
- Mehrskalenmethoden zur Beschreibung elektronischer Zustände in Halbleiter-Nanostrukturen (Schwerpunktprogramm 1095 „Analysis, Modellierung und Simulation von Multiskalenproblemen“),
- Quantenmechanische und makroskopische Modelle optoelektronischer Bauelemente (Forschungszentrum MATHEON „Mathematik für Schlüsseltechnologien“).

- Analytical and numerical investigations on spatio-temporal formation of structures in semiconductor lasers (Collaborative Research Center 555 “Complex Nonlinear Processes”);
- Multiscale methods for the description of electronic states in semiconductor nanostructures (Priority Program 1095 “Analysis, Modeling, and Simulation of Multiscale Problems”);
- Quantum mechanical and macroscopic models for optoelectronic devices (Research Center MATHEON “Mathematics for Key Technologies”).

Im Rahmen des Verbundprojektes „Terabit Optics Berlin“ wurde folgendes Projekt finanziert:

- Simulation der Pulsausbreitung in nichtlinearen optischen Fasern.

The following project was funded in the framework of the Research Network Project “Terabit Optics Berlin”:

- Simulation of pulse propagation in nonlinear optical fibres.

Vom Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie (MBI), Berlin, wurde folgendes Projekt finanziert:

- Berechnung der elektronischen Bandstruktur von InAsSb-Quantenwells.

The Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy (MBI), Berlin has funded the project

- Calculation of electronic bandstructure of InAsSb multi-quantum wells.

Im August 2004 wurden fünf Mitarbeiter der Gruppe in die Forschungsgruppe „Thermodynamische Modellierung und Analyse von Phasenübergängen“ aufgenommen. Über deren Arbeit wird im Abschnitt 4.7.1 berichtet.

In August 2004 five members of this group have changed over to the Research Group “Thermodynamic Modeling and Analysis of Phase Transitions”. Their work is reported upon in Section 4.7.1.

4.1.2 Projects

Supercontinuum generation in nonlinear optical fibers

Collaborators: U. Bandelow, A. Demircan, M. Kesting

Cooperation with: M. Kroh, H.G. Weber (Fraunhofer-Institut für Nachrichtentechnik, Heinrich-Hertz-Institut (HHI) Berlin)

Supported by: Terabit Optics Berlin (project B4)

The propagation of short and intense optical pulses through a nonlinear optical fiber is described by the nonlinear Schrödinger equation (NLSE). Our model uses the following form of the NLSE for the complex envelope $A(z,\tau)$ of an optical pulse which includes group velocity dispersion up to fourth order as well as self-steepening and Raman scattering:

$$\begin{aligned}\frac{\partial A}{\partial z} &= -\frac{\mathrm{i}}{2}\beta_2\frac{\partial^2 A}{\partial\tau^2}+\frac{1}{6}\beta_3\frac{\partial^3 A}{\partial\tau^3}+\frac{\mathrm{i}}{24}\beta_4\frac{\partial^4 A}{\partial\tau^4}-\frac{1}{2}\alpha A\\ &\quad +\mathrm{i}\gamma|A|^2A-\frac{\gamma}{\omega_0}\frac{\partial}{\partial\tau}\left(|A|^2A\right)-\mathrm{i}\gamma T_R A\frac{\partial}{\partial\tau}\left(|A|^2\right). \qquad (1)\end{aligned}$$

The details of the derivation of this equation are given in [1]. The numerical investigation of Eq. 1 in view of the supercontinuum (SC) generation [3] requires a high accuracy as well as a high resolution. We use a de-aliased pseudospectral method with integration performed by an eighth-order Runge–Kutta integration scheme using adaptive stepsize control [1, 2] which is more precise than the widely-used split-step method. Experimental and numerical investigations [3, 4, 5] show the importance of higher-order dispersion terms. It turns out to be highly questionable whether the use of even higher-order dispersion terms resulting from a Taylor expansion in the Fourier domain is reasonable. This led us to a review of the modeling process to come up with more general equations. Concerning nonlinear Schrödinger equations, one may start with the following scheme:

$$\mathrm{i}u_z+\mathcal{N}(u)+\mathcal{L}u=0, \qquad (2)$$

where $u:\mathbb{R}\times\mathbb{R}^+\to\mathbb{C}$, $(\tau,z)\mapsto u(\tau,z)$. The linear operator $\mathcal{L}$ describing the dispersion is determined by the dispersion relation $\omega(\xi)$ in the Fourier domain as follows: $\widehat{\mathcal{L}(u)}(\xi)=\omega(\xi)\widehat{u}(\xi)$. In the case of ω being a polynomial (e.g., from a Taylor expansion), $\mathcal{L}$ is a differential operator and the equation is therefore local. Choosing non-polynomial functions for ω leads to pseudo-differential operators and nonlocal equations on which we focused our analysis. Similar to that it is worth to ask for generalizations of the nonlinearity $\mathcal{N}(u)$. We have investigated the case $\mathcal{N}(u)(\tau,z)=u(\tau,z)\left(R(\tau)*|u(\tau,z)|^2\right)$, which is suggested by the physical model. The convolution with R describes the response of the material and we have $R(\tau)=\delta_\tau$ in the standard case where only instantaneous response is considered ($\mathcal{N}(u)=u|u|^2$).

On the other hand, we validated our algorithm by the substantial example of supercontinuum generation [4, 5], which apparently comprises all physical effects modeled by Eq. 1. We demonstrate in [3] that the modulation instability (MI), which is a special four-wave-mixing process, can be responsible for ultrabroadband octave-spanning continua for pico- and subpicosecond

pulses in the anomalous as well as in the normal dispersion region. We illustrate the effect of MI in Figure 1.

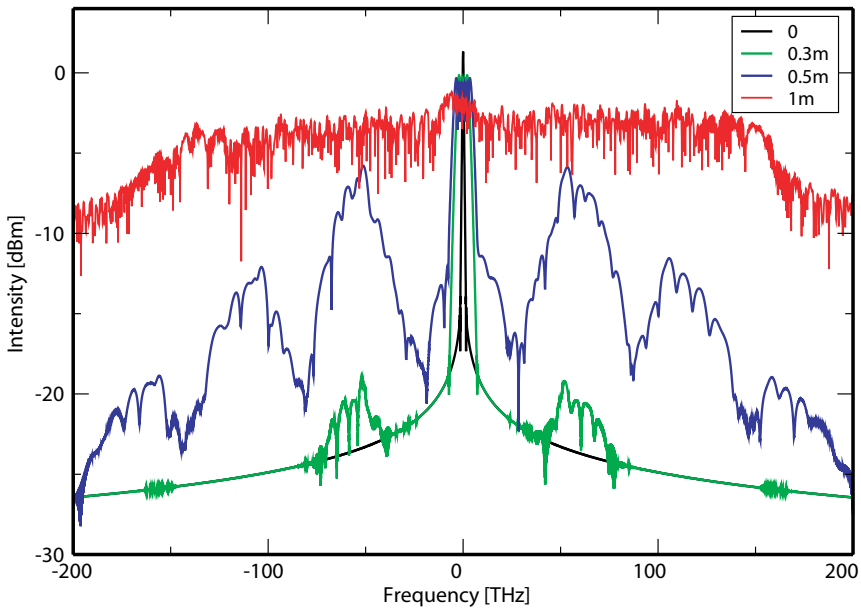

Fig. 1: Spectra of an initial sech pulse with $\tau_0 = 1ps$ with a peak input power $P_0 = 400\ W$ and $T_R = 3\ fs$ at different propagation distances. The initial spectrum has a sech profile (black). After 0.3 m (green), the MI generates two sidebands at $\mp 50\ THz$ (Stokes and anti-Stokes components), which are multiplied after 0.5 m (blue). Further phase-matched four-wave mixing then explosively excites new frequencies and hence broadens and completes the spectrum afterwards (red).

The MI can dominate higher-order effects such as third- and fourth-order dispersion, self-steepening, and Raman scattering, because it acts directly from the beginning on the high-order solitons. Therefore higher-order effects are not a prerequisite for the generation of SC, and it is hence not restricted only to ultrashort subpicosecond pulses, but appears for much longer pulses, too. The MI can also appear in the normal dispersion regime $\beta_2 > 0$, if the fourth-order dispersion coefficient β_4 is negative. In particular, we have verified quantitatively the experimental results in [4], where the MI sidebands are observed in the normal dispersion regime with negative β_4. For these calculations a resolution of 2^{19} frequencies is required. The calculated wavelenghts of the Stokes (λ_s) and anti-Stokes (λ_a) components are represented in the following table:

P_0 [W]	100	150	200	250	300	350	400
λ_a [nm]	503.84	502.9	502.26	501.37	501.45	501.51	501.48
λ_s [nm]	903.79	906.84	907.97	911.84	911.75	911.40	911.49

in dependence on the optical input power P_0.

In applications, the effect of spectral broadening of a pulse propagating through a fiber is used for pulse compression. A schematic of the experimental setup is shown in Figure 2. A highly nonlinear fiber (HNLF) is used to induce a linear chirp in the spectral broadening process and the chirped pulses are compressed by dispersion compensation in a subsequent standard single mode fiber (SMF). Applications require flat and wideband spectra without phase instabilities. This is achieved by the self-phase modulation $(i\gamma|A|^2A)$ in Eq. 1 as the main broadening mechanism. The corresponding spectral broadening is confirmed by the measurements. One example is shown in Figure 3.

The experimental investigations at the HHI as well as our numerical simulations indicate an optimal pulse compressor in the vicinity of the zero-dispersion wavelength in the normal dispersion regime leading to a linear up-chirp across the entire pulse width.

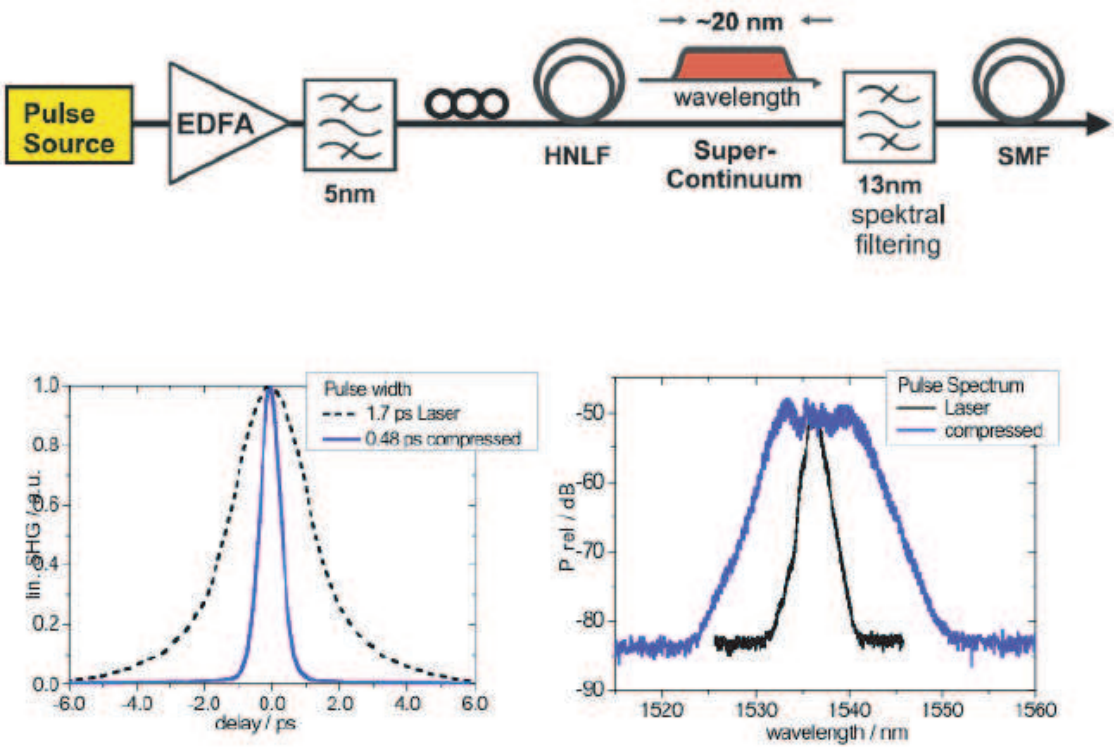

Fig. 2: Upper: Experimental setup used in the HHI for pulse compression using a HNLF. Lower left: measured pulse shape (black: before compression, blue: after compression). Lower right: measured pulse spectrum (black: before compression, blue: after compression). We acknowlegde the permission by Prof. Weber and M. Kroh (HHI) to show these figures.

We have simulated the spectral broadening for realistic fibers and have compared our results with measurements, results are plotted in Figure 3. A typical problem for such investigations is that the fiber coefficients of a realistic fiber are not exactly known. Therefore, we first used measurements at low optical power for a proper adjustment of the dispersion coefficients. The resulting spectrum is drawn in Figure 3, left. Then we used the simulation parameters obtained in this way for further simulations with higher optical input power. For medium input power (20.0 dBm sech input) we again obtained good agreement with the experiments. Furthermore, we could reconstruct the measured pulse compression down to 0.4 ps. We obtained good agreement with the measurements for even higher input power. Surprisingly, no further pulse compression could be achieved by increasing the input power, which is due to the occurrence of other disturbing nonlinearities. The latter can now be studied with our tools in order to design a proper HNLF.

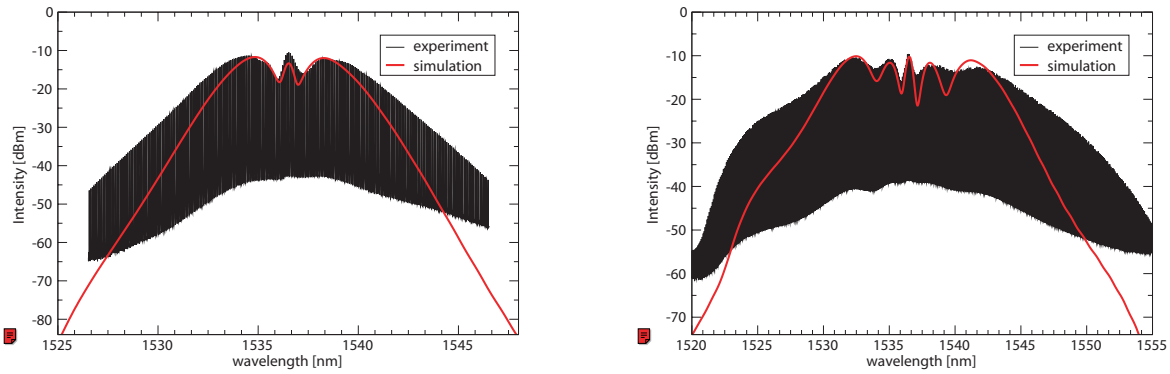

Fig. 3: Measured optical spectra (black, HHI, for a train of identical pulses) and calculated optical spectra for a single pulse (red, based on Eq. 1) after propagation over 510 meters along a HNLF; left: low input power, right: high input power.

References

1. U. BANDELOW, A. DEMIRCAN, M. KESTING, *Simulation of pulse propagation in nonlinear optical fibers*, WIAS Report no. 23, 2003.

2. N. SEEHAFER, A. DEMIRCAN, *Dynamo action in cellular pattern*, Magnetohydrodynamics, **39**(3) (2003), pp. 335–344.

3. A. DEMIRCAN, U. BANDELOW, *Supercontinuum generation by the modulation instability*, Optics Communications, **244**(6) (2005), pp. 181–185.

4. J.D. HARVEY, R. LEONHARDT, S. COEN, G.K.L. WONG, J.C. KNIGHT, W.J. WADSWORTH, P.S.J. RUSSEL, *Scalar modulation instability in the normal dispersion regime by use of a photonic crystal fiber*, Optics Letters, **28**(22) (2003), pp. 2225–2227.

5. W.J. WADSWORTH, N. JOLY, J.C. KNIGHT, T.A. BIRKS, F. BIANCALANA, P.S.J. RUSSEL, *Supercontinuum and four-wave mixing with q-switched pulses in endlessly single-mode photonic crystal fibres*, Optics Express, **12**(2) (2004), pp. 299–309.

Coupled Schrödinger drift-diffusion models

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Nowadays, quantum effects play an important role in semiconductor devices. The ongoing progress of industrial semiconductor device technologies permits to fabricate devices which inherently employ quantum phenomena in their operation, e.g., resonant tunneling diodes, quantum well laser, etc. The widely used drift-diffusion equation introduced by van Roosbroeck in 1950 is not capable of properly taking these quantum effects into account. A finer level of modeling has to be used which is achieved by Schrödinger's or equivalently Wigner's equation. However, the numerical treatment of these models is very expensive compared to the drift-diffusion model. In many semiconductor devices, quantum effects take place in a localized region, e.g., around the double barrier in a resonant tunneling diode, whereas the rest of the device is well described by classical models like the drift-diffusion model. Thus, it makes sense to follow a hybrid strategy: Use a quantum model in regions where quantum effects are strong and couple this model by proper interface conditions to a classical model in the rest of the device domain.
In this project we focus on hybrid models, more precisely, coupled Schrödinger drift-diffusion models, which describe the transport within a nanoscaled semiconductor device in a stationary and one-dimensional framework. The semiconductor domain $\Lambda = (0,L)$ is divided into a zone where quantum effects are dominant, called quantum zone $\Omega_q = (x_l, x_r)$, and a zone where they can be neglected, the so-called classical zone $\Omega_c = \Lambda \setminus \Omega_q$.
On Ω_c we consider a stationary drift-diffusion model, i.e. the current density J and particle density N are determined by the following system of equations

$$-\frac{d}{dx}J = 0, \qquad \text{continuity equation,} \tag{1a}$$

$$J = -\mu N \frac{d}{dx}\phi, \qquad \text{current density,} \tag{1b}$$

$$N = F(eV - e\phi - V_h), \qquad \text{particle density,} \tag{1c}$$

where μ denotes the mobility of particles, ϕ the electrochemical potential, $e > 0$ is the elementary charge, V the electrostatic potential, V_h the heterostructure potential describing the band-edge offset, and F is the Boltzmann distribution function

$$F(s) = N_0 \exp\left(\frac{s}{k_B T}\right),$$

with constant lattice temperature T, Boltzmann constant k_B, and density of states N_0.

In the quantum zone Ω_q the particle density n and current density j are given by means of a statistic f and the solutions ψ of Schrödinger's equation, i.e. we regard the following system of equations

$$\Big(-\frac{\hbar^2}{2}\frac{d}{dx}\frac{1}{m}\frac{d}{dx} - eV + V_h\Big)\psi_k = E(k)\,\psi_k, \qquad \text{Schrödinger equation,} \tag{2a}$$

$$j = \int f(k)\Im\left(\frac{\hbar}{m}\frac{d\psi_k}{dx}\overline{\psi_k}\right)dE, \qquad \text{current density,} \tag{2b}$$

$$n = \int f(k)|\psi_k|^2\,dE, \qquad \text{particle density,} \tag{2c}$$

where $m = m(x)$ denotes the effective mass and $\hbar$ the reduced Planck constant. ψ_k, $k > 0$, denote the right-going and ψ_k, $k < 0$, the left-going scattering states, respectively. $E(k)$ is the dispersion relation given by

$$E(k) = \begin{cases} \frac{\hbar^2 k^2}{2m(x_l)} + eV(x_l) - V_h(x_l), & \text{for } k > 0, \\ \frac{\hbar^2 k^2}{2m(x_r)} + eV(x_r) - V_h(x_r), & \text{for } k < 0. \end{cases}$$

As boundary conditions for the Schrödinger equation we chose either quantum transmitting boundary conditions ([3, 5]) or dissipative-type boundary conditions ([4, 6]).
The drift-diffusion (1) and Schrödinger model (2) are coupled by the following conditions:

1. The distribution function f in (2) is given by

$$f(k) = \begin{cases} f_0(E(k) + e\phi(x_l)), & \text{for } k > 0, \\ f_0(E(k) + e\phi(x_r)), & \text{for } k < 0, \end{cases}$$

   where ϕ is the electrochemical potential, f_0 is a reduced equilibrium distribution function of the two-dimensional carrier gas, e.g.,

$$f_0(\xi) = n_0 \exp\left(\frac{-\xi}{k_B T}\right),$$

   and n_0 denotes the integrated density of states.

2. We impose the continuity of the current densities, i.e.

$$J(x_l) = j = J(x_r),$$

   which is a condition for the coupling that is consistent with physics.

3. In order to have a meaningful description of the semiconductor device, the electrostatic potential V has to be computed self-consistently on the whole device domain Λ by Poisson's equation

$$-\frac{d}{dx}\varepsilon\frac{d}{dx}V = e\Big(D - \mathcal{N}\Big), \tag{3}$$

   where $\varepsilon = \varepsilon(x)$ is the dielectric permittivity function, D the density of ionized dopants in the semiconductor device, and $\mathcal{N}$ is the particle density, i.e.

$$\mathcal{N}(x) = \begin{cases} N(x), & \text{for } x \in \Omega_c, \\ n(x), & \text{for } x \in \Omega_q. \end{cases}$$

The coupled system is completed by imposing charge neutrality as boundary conditions for (1)

$$N(0) = D(0), \qquad N(L) = D(L),$$

and the applied bias V_b as boundary conditions for the Poisson equation (3), i.e.

$$V(0) = 0, \quad V(L) = V_b.$$

In [2], we show that the coupled system—with dissipative boundary conditions for the Schrödinger equation—is well posed and admits a solution. Moreover, we show that similar results hold for the bipolar system, where electrons and holes have to be considered.
The validity of the model is illustrated in [1], where the model is used to calculate current-voltage characteristics of resonant tunneling diodes. Resonant tunneling diodes are typical examples of devices whose functionality depends on quantum effects and thus cannot be described by the usual drift-diffusion model. We show that the hybrid model presented above is capable to describe the transport of electrons in a resonant tunneling diode and investigate the influence of the position of the quantum zone Ω_q. If the quantum zone is chosen properly, good results are obtained, see Figure 1. Additionally, collisions in the quantum zone have been taken into account by means of a Pauli master equation.

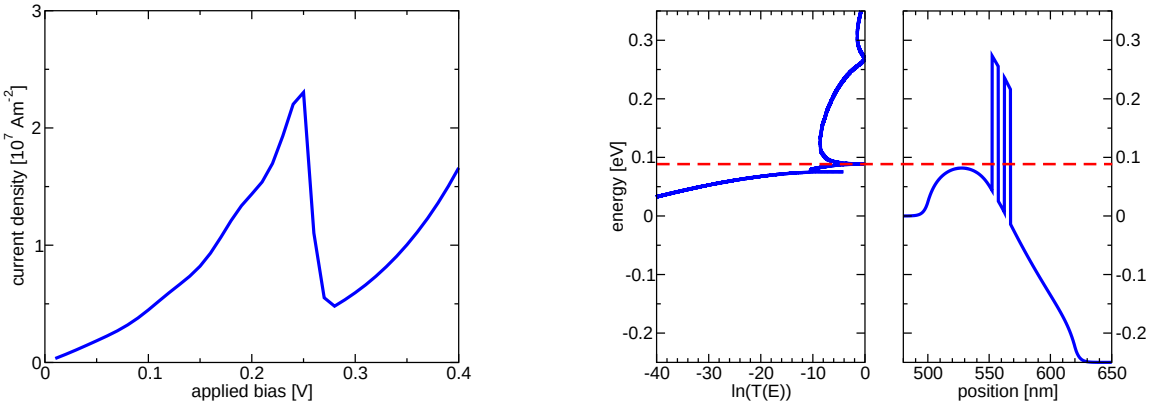

Fig. 1: The left figure shows the current-voltage characteristic of the device ([7]) calculated by means of the coupled Schrödinger drift-diffusion model.The calculated transmission coefficient and the potential profile for the current peak bias are depicted on the right figures.

References

1. M. BARO, N. BEN ABDALLAH, P. DEGOND, A. EL AYYADI, *A 1D coupled Schrödinger drift-diffusion model including collisions*, J. Comput. Phys., **203** (2005), pp. 129–153.

2. M. BARO, H. NEIDHARDT, J. REHBERG, *Current coupling of drift-diffusion models and dissipative Schrödinger–Poisson systems: Dissipative hybrid models*, WIAS Preprint no. 946, 2004, to appear in: SIAM J. Math. Anal.

3. M. BARO, H.-CHR. KAISER, H. NEIDHARDT, J. REHBERG, *A quantum transmitting Schrödinger–Poisson system*, Rev. Math. Phys., **16**(3) (2004), pp. 281–330.

4. ——, *Dissipative Schrödinger–Poisson systems*, J. Math. Phys., **45**(1) (2004), pp. 21–42.

5. N. BEN ABDALLAH, P. DEGOND, P.A. MARKOWICH, *On a one-dimensional Schrödinger–Poisson scattering model,* Z. Angew. Math. Phys., **48** (1997), pp. 135–155.

6. H.-CHR. KAISER, H. NEIDHARDT, J. REHBERG, *Macroscopic current induced boundary conditions for Schrödinger-type operators*, Integral Equations Operator Theory, **45** (2003), pp. 39–63.

7. P. MOUNAIX, O. VANBESIAN, D. LIPPENS, *Effect of space layer on the current-voltage characteristics of resonant tunneling diodes,* Appl. Phys. Lett., **57**(15) (1990), pp. 1517–1519.

Stationary energy models for semiconductor devices with incompletely ionized impurities

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The charge transport in semiconductor devices is described by the van Roosbroeck equations. They consist of two continuity equations for the densities n and p of electrons e and holes h, respectively, and a Poisson equation for the electrostatic potential φ. Physical parameters occurring in these equations depend on the device temperature T. Therefore, under nonisothermal conditions a balance equation for the density of total energy must be added, and a so-called energy model arises (see [1, 7]). Finally, if incompletely ionized impurities (for example, radiation-induced traps or other deep recombination centers) are taken into account, we have to consider further continuity equations for the densities of (in general immobile) species X_j, $j = 1,\dots,k$. These species exist in different charge states which are transformed into each other by ionization reactions. Let X_j be an acceptor-like impurity and let X^- be its ion. Then we have to consider the reactions

$$\mathrm{e}^- + \mathrm{X}_j \rightleftharpoons \mathrm{X}_j^-, \quad \mathrm{h}^+ + \mathrm{X}_j^- \rightleftharpoons \mathrm{X}_j. \tag{1}$$

If X_j is a donor-like impurity and X_j^+ denotes its ion, then the reactions are

$$\mathrm{e}^- + \mathrm{X}_j^+ \rightleftharpoons \mathrm{X}_j, \quad \mathrm{h}^+ + \mathrm{X}_j \rightleftharpoons \mathrm{X}_j^+. \tag{2}$$

Moreover, a (direct) electron-hole recombination-generation

$$\mathrm{e}^- + \mathrm{h}^+ \rightleftharpoons 0 \tag{3}$$

takes place. If X_j is a donor (an acceptor), we denote by u_{2j-1} the density of X_j (of X_j^-) and by u_{2j} the density of X_j^+ (of X_j). Furthermore, we define charge numbers as follows:

$$q_{2j-1} := \begin{cases} 0 & \text{if } \mathrm{X}_j \text{ is a donor} \\ -1 & \text{if } \mathrm{X}_j \text{ is an acceptor} \end{cases}, \qquad q_{2j} := 1 + q_{2j-1}, \quad j = 1,\dots,k.$$

Then the stationary energy model for devices with incompletely ionized impurities has the form

$$-\nabla\cdot(\varepsilon\nabla\varphi) = f_0 - n + p + \sum_{i=1}^{2k} q_i u_i, \quad \nabla\cdot j_e = 0, \tag{4}$$

$$\nabla\cdot j_n = R_0 + \sum_{j=1}^{k} R_{j1}, \quad \nabla\cdot j_p = R_0 + \sum_{j=1}^{k} R_{j2}, \tag{5}$$

$$R_{j1} = R_{j2}, \quad u_{2j-1} + u_{2j} = f_j, \quad j = 1,\dots,k. \tag{6}$$

Here j_n, j_p denote the particle flux densities of electrons and holes, R_{j1}, R_{j2}, and R_0 denote the reaction rates of the first and second reaction in (1) or in (2), respectively, and of the reaction

(3). Moreover, ε is the dielectric permittivity and f_0, f_j are a charge density and particle densities which must be prescribed. The system has to be completed by suitable state equations for the species *e, h,* $X_1,\dots,X_{2k}$ and kinetic relations.
Special isothermal models of this kind are presented in [6]. There also results of simulations with `WIAS-TeSCA` are compared with experimental results.
First, under reliable assumptions concerning the state equations and kinetic relations we eliminate the constraints from the system by evaluating the subsystem (6). We end up with a system of four strongly coupled equations with nonlinear source terms depending on φ, T, on the electrochemical potentials ζ_n, ζ_p of electrons and holes, on f_0, and on the local invariants f_j, $j=1,\dots,k$. The resulting stationary energy model can be written in the form

$$-\nabla\cdot\begin{pmatrix} \varepsilon & 0 & 0 & 0\\ 0 & \kappa+\widehat{\omega}_0 & \omega_1 & \omega_2\\ 0 & \widehat{\omega}_1 & \sigma_n+\sigma_{np} & \sigma_{np}\\ 0 & \widehat{\omega}_2 & \sigma_{np} & \sigma_p+\sigma_{np}\end{pmatrix}\begin{pmatrix}\nabla\varphi\\ \nabla T\\ \nabla\zeta_n\\ \nabla\zeta_p\end{pmatrix}=\begin{pmatrix}H\\0\\R\\R\end{pmatrix}\quad\text{in }\Omega, \tag{7}$$

where

$$\begin{pmatrix}\widehat{\omega}_1\\ \widehat{\omega}_2\end{pmatrix}=\begin{pmatrix}\sigma_n+\sigma_{np} & \sigma_{np}\\ \sigma_{np} & \sigma_p+\sigma_{np}\end{pmatrix}\begin{pmatrix}P_n\\P_p\end{pmatrix},\quad \widehat{\omega}_0=(\zeta_n+P_nT)\,\widehat{\omega}_1+(\zeta_p+P_pT)\,\widehat{\omega}_2,$$

$$\begin{pmatrix}\omega_1\\ \omega_2\end{pmatrix}=\begin{pmatrix}\sigma_n+\sigma_{np} & \sigma_{np}\\ \sigma_{np} & \sigma_p+\sigma_{np}\end{pmatrix}\begin{pmatrix}\zeta_n+P_nT\\ \zeta_p+P_pT\end{pmatrix},$$

$$H=H(\cdot,\varphi,T,\zeta_n,\zeta_p,f_0,f_1,\dots,f_m),\quad R=R(\cdot,\varphi,T,\zeta_n,\zeta_p,f_0,f_1,\dots,f_m)$$

with conductivities $\kappa>0$, $\sigma_n,\sigma_p>0$, $\sigma_{np}\geq 0$, and transported entropies P_n, P_p depending in a nonsmooth way on x and smoothly on the state variables. Let Γ be the boundary of the domain Ω, which is occupied by the heterogeneous semiconductor device. Γ_D and Γ_N denote disjoint, relatively open parts of Γ with $\mathrm{mes}(\Gamma\setminus(\Gamma_D\cup\Gamma_N))=0$. For (7) we suppose mixed boundary conditions of the form

$$\begin{array}{rrrrl}\varphi=v_{D1}, & T=v_{D2}, & \zeta_n=v_{D3}, & \zeta_p=v_{D4} & \text{on }\Gamma_D,\\ \nu\cdot(\varepsilon\nabla\varphi)=g_1, & -\nu\cdot j_e=g_2, & -\nu\cdot j_n=g_3, & -\nu\cdot j_p=g_4 & \text{on }\Gamma_N.\end{array} \tag{8}$$

We use the vectors $v=(\varphi,T,\zeta_n,\zeta_p)$, $v_D=(v_{D1},\dots,v_{D4})$, $g=(g_1,\dots,g_4)$, $f=(f_0,f_1,\dots,f_k)$, and the triplet of data $w=(v_D,g,f)$ and look for weak solutions of (7),(8) in the form $v=V+v^D$, where v^D is a function fulfilling the Dirichlet boundary conditions v_D and V represents the homogeneous part of the solution.
We assume that the boundary values v_{Di}, $i=1,2,3,4$, are traces of $W^{1,p}$ functions v_i^D, $p>2$ and find $W^{1,q}$ formulations ($q\in(2,p]$) for that system of equations,

$$F(V,w)=0,\quad V\in W_0^{1,q}(\Omega\cup\Gamma_N)^4,$$

$$w\in W^{1-1/p,p}(\Gamma_D)^4\times L^\infty(\Gamma_N)^4\times L^\infty(\Omega)\times\{h\in L^\infty(\Omega):\operatorname{essinf} h>0\}^k.$$

Using techniques from [5], the operator F turns out to be continuously differentiable. If $w^*=(v_D^*,g^*,f^*)$ is fixed such that $v_{Di}^*=\text{const}$, $i=2,3,4$, $v_{D3}^*+v_{D4}^*=0$, $v_{D2}^*>0$, and $g^*=(g_1^*,0,0,0)$, then there exists a solution V^* of $F(V^*,w^*)=0$ which represents a thermodynamic equilibrium. We prove that for suitable $q>2$ the linearization $\frac{\partial F}{\partial V}(V^*,w^*)$ is a linear isomorphism from

$W_0^{1,q}(\Omega\cup\Gamma_N)^4$ onto $W^{1,q'}(\Omega\cup\Gamma_N)^{*4}$. Here we use regularity results for strongly coupled elliptic systems with mixed boundary conditions stated in [4]. We apply the Implicit Function Theorem to obtain that for $w=(v_D,g,f)$ near w^*, the equation $F(V,w)=0$ has a unique solution V near V^*. Details and the precise assumptions of our investigations may be found in [3].
In [2], we investigated a more general energy model with m different species where all species were assumed to be mobile such that the stationary energy model corresponds to an elliptic system with $m+2$ equations.

References

1. G. ALBINUS, H. GAJEWSKI, R. HÜNLICH, *Thermodynamic design of energy models of semiconductor devices*, Nonlinearity, **15** (2002), pp. 367–383.

2. A. GLITZKY, R. HÜNLICH, *Stationary solutions of two-dimensional heterogeneous energy models with multiple species*, Banach Center Publ., **66** (2004), pp. 135–151.

3. ——, *Stationary energy models for semiconductor devices with incompletely ionized impurities*, WIAS Preprint no. 1001, 2005, submitted.

4. K. GRÖGER, *A $W^{1,p}$-estimate for solutions to mixed boundary value problems for second order elliptic differential equations*, Math. Ann., **283** (1989), pp. 679–687.

5. L. RECKE, *Applications of the implicit function theorem to quasi-linear elliptic boundary value problems with non-smooth data*, Comm. Partial Differential Equations, **20** (1995), pp. 1457–1479.

6. R. SIEMIENIEC, W. SÜDKAMP, J. LUTZ, *Determination of parameters of radiation induced traps in silicon*, Solid-State Electronics, **46** (2002), pp. 891–901.

7. G. WACHUTKA, *Rigorous thermodynamic treatment of heat generation and conduction in semiconductor device modelling*, IEEE Trans. CAD, **9** (1990), pp. 1141–1149.

Phenomenological modeling of drift-diffusion processes

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Drift-diffusion equations provide a powerful description of microscopic particle transport on the phenomenological level. However, the relation between the phenomenological description and the underlying microscopic transport phenomena, in general, is not clear-cut. Often only special solutions (the stationary solution), global properties (the free energy) or functionals of the solution (moments) are known. Therefore it is interesting to consider example problems which are non-trivial and the underlying microscopic processes are well known. We demonstrate this in two examples.

Ex. 1: A powerful thermodynamically consistent method for deriving drift-diffusion equations has been developed in the last years by H. Gajewski and others (see [1, 2, 3]). Looking for a phenomenological evolution equation for a concentration $u(x,t)$ with $u(x,t) \geq 0$, $\int_\Omega u(x,t) \equiv 1$ ($x \in \Omega \subset \mathbb{R}_n$, $t \geq 0$), we consider at first a microscopic picture. Let $u(x,t)$ be the solution of a Kolmogorov–Chapman equation

$$\frac{\partial}{\partial t} u \quad = \quad \mathbf{A}u, \tag{1}$$

where the linear operator $\mathbf{A}$ is of the form (+ suitable boundary conditions)

$$(\mathbf{A}f)(x) = \sum_{i,j=1}^{n} \frac{\partial^2}{\partial x_i \partial x_j} \Big(b_{ij}(x) f(x)\Big) - \sum_{i=1}^{n} \frac{\partial}{\partial x_i} \Big(a_i(x) f(x)\Big) + \int\!\!\!\!\!\!- _\Omega \Big(Q(x',x) f(x') - Q(x,x') f(x)\Big) dx'. \tag{2}$$

Here, $a_i(x)$, $b_{ij}(x)$, and $Q(x,x') \geq 0$ are suitable coefficient functions, and $\mathbf{B} = (b_{ij}(x))$ is a non-negative matrix. The integral is to be understood as a principle value integral. Let $u^*(x)$ be a stationary solution of $\mathbf{A}u^* = 0$. Equations (1)–(2) are the general form of a linear evolution equation conserving positivity $u(x,t) \geq 0$ and norm $\int_\Omega u(x,t)dx = 1$. Moreover, it can be shown, see [4], that every more or less arbitrary convex function $F : \mathbb{R} \longrightarrow \mathbb{R}$, normalized by $F(1) = 0$, generates a time-decreasing Lyapunov function,

$$H(t) = \Phi(u) = \int_\Omega F\left(\frac{u(x,t)}{u^*(x)}\right) u^*(x)dx \ , \quad H(t_1) \geq H(t_2) \geq 0, \ t_2 \geq t_1 \ . \tag{3}$$

Now we are going to derive a phenomenological equation for u by Gajewski's method, assuming that a free energy of type (3), with some reference concentration u^*, is given. This is a typical situation in applications.

We calculate the stationary state $u_s(x)$ by Lagrange's method, varying the functional $\Phi(u)$ under the constraint $\int_\Omega u(x,t)dx = 1$. This leads to the functional $L(u) = \Phi(u) - \lambda\,(\int_\Omega u(x)dx - 1)$. Thus, $u_s(x)$ is the solution to the Euler–Lagrange equation

$$\lambda = \varphi\left(\frac{u_s(x)}{u^*(x)}\right) \iff u_s(x) = \varphi^{-1}(\lambda) u^*(x)$$

with the monotone function $\varphi(z) = F'(z)$. From $\int_\Omega u^*(x)dx = \int_\Omega u_s(x)dx = 1$ we get $\lambda = \varphi(1)$. It follows $u_s = u^*$, as expected.
For deriving an evolution equation, we assume that the Lagrange multiplier λ is the chemical potential depending on x and t, and

$$u(x,t) = \varphi^{-1}(\lambda(x,t))u^*(x)$$

is the state equation. Let $\mathbf{D}$ be a linear operator with $\mathbf{D}1 = 0$. We assume that $bfD\lambda$ is the driving force of the diffusion vanishing in the stationary state $\lambda =$ const., and postulate an equation for u of the form

$$\frac{\partial}{\partial t}u(x,t) = -\mathbf{D}^*\sigma\mathbf{D}\lambda \tag{4}$$

with some suitable operator σ. Equations of this type satisfy some desired basic properties: All solutions are normalized

$$\frac{d}{dt}\langle 1, u(t)\rangle = \langle 1, \dot{u}(t)\rangle = -\langle 1, \mathbf{D}^*\sigma\mathbf{D}\lambda\rangle = -\langle \mathbf{D}1, \sigma\mathbf{D}\lambda\rangle = 0$$

($\langle\cdot,\cdot\rangle$ is the dual pairing) and the free energy is monotone

$$\frac{d}{dt}\Phi\big(u(t)\big) = \left\langle \varphi\left(\frac{u(t)}{u^*}\right), \dot{u}(t)\right\rangle = -\langle\lambda, \mathbf{D}^*\sigma\mathbf{D}\lambda\rangle = -\langle\sigma\mathbf{D}\lambda, \mathbf{D}\lambda\rangle \le 0\,,$$

if σ is positive definite. Moreover, to prove the positivity of the solution of such equations can be a hard problem. Since σ can depend on u or the gradient of u, equation (4) can be nonlinear. We have to choose $\mathbf{D}$ and σ in such a manner that the equations (4) and (1) describe the same physical problem. As usual, $\mathbf{D}$ is taken as a gradient $\mathbf{D} = \mathbf{G}\nabla$ with an $n\times n$ matrix $\mathbf{G}(x)$. There is good reason, see [3] and the references there, to take σ similar to the inverse Hessian of Φ

$$\sigma = \mu\, u^*\varphi'\left(\frac{u}{u^*}\right)^{-1}$$

with some positive function $\mu(x)$. Then (4) becomes

$$\frac{\partial}{\partial t}u(x,t) = \nabla\mathbf{G}^*\mu\mathbf{G}\left(\nabla u - u\nabla\log u^*\right)\ , \tag{5}$$

a typical drift-diffusion equation widely used in semiconductor analysis, chemotaxis, and phase separation, [1, 2, 3]. On the other hand, this is the Fokker–Planck equation, a special case of (1)–(2) with $Q = 0$, $\mathbf{B} = \mathbf{G}^*\mu\mathbf{G}$, and $a_i(x) = \sum_j \frac{\partial}{\partial x_j}b_{ij}(x) + \frac{1}{u^*(x)}\frac{\partial}{\partial x_j}u^*(x)$, and therefore it conserves positivity. This and the linearity of equation (5) favor the inverse Hessian among other choices for σ.
Ex. 2: An other typical situation is the following: We want to derive an equation for $u(x,t)$ of type (4) for the diffusion of particles in a space-homogeneous medium. However, for an exact description of the problem we have to take into account more state parameters than x, e.g., the velocity v, too. Let $v\in\mathbb{R}$ and $x\in\mathbb{R}$. Let us assume that the trajectory in phase space is Markovian with the probability density $W(v,x,t)$. Then the Kolmogorov–Chapman equation describing the time evolution of $W(v,x,t)$ has the form

$$\frac{\partial}{\partial t}W(v,x,t) = \mathbf{A}W - v\frac{\partial}{\partial x}W,\ W(v,x,0) = w_0(v)u_0(x)\ , \tag{6}$$

where $\mathbf{A}$ is a linear operator of type (2) acting only on the parameter v.
Ultimately, we are only interested in the concentration (space density) $u(x,t) = \int_{\mathbb{R}} W(v,x,t)dv$. A typical method to calculate u is to derive a system of equations for the v-moments of W and close this system in a heuristic way. In the case of the general Brownian motion, governed by equation (6) and

$$(\mathbf{A}f)(v) = \frac{\partial}{\partial v}\big(avf\big) + b\frac{\partial^2}{\partial v^2}f + \fint_{\mathbb{R}} \big(Q(v-v')f(v') - Q(v'-v)f(v)\big)dv',$$

with constants a and $b > 0$, this can be done rigorously without further heuristic arguments (see [5]). For simplicity, let us assume that the velocity is already relaxed. This means the initial value w_0 is the stationary velocity density, i.e., $\mathbf{A}w_0 = 0$. It turns out that $u(x,t)$ is the solution of the non-autonomous equation

$$\frac{\partial}{\partial t}u(x,t) = \frac{b}{a^2}\big(1-e^{-at}\big)\frac{\partial^2}{\partial x^2}u(x,t) + \fint_{\mathbb{R}} \frac{a}{(1-e^{-at})^2}\, Q\left(\frac{ax'}{1-e^{-at}}\right)\big(u(x-x',t)-u(x,t)\big)dx'$$

with initial data $c(x,0) = c_0(x)$, whereas the original physical problem is autonomous.
In the limit $t \longrightarrow \infty$ we get the equation

$$\frac{\partial}{\partial t}u(x,t) \;=\; \frac{b}{a^2}\frac{\partial^2}{\partial x^2}u(x,t) + \fint_{\mathbb{R}} aQ(ax')\big(u(x-x',t)-u(x,t)\big)dx' \;.$$

For $Q = 0$ this is the diffusion equation which is parabolic.
In the limit $t \longrightarrow 0$ we get the second-order hyperbolic equation

$$\frac{\partial^2}{\partial t^2}u(x,t) = \frac{b+q}{2a}\frac{\partial^2}{\partial x^2}u(x,t)\;,$$

where $Q(v) = Q(-v)$ and $q = \int v^2 Q(v)dv$.

References

1. G. ALBINUS, H. GAJEWSKI, R. HÜNLICH, *Thermodynamic design of energy models of semiconductor devices*, Nonlinearity, **16** (2002), pp. 367–383.

2. H. GAJEWSKI, K. ZACHARIAS, *Global behaviour of a reaction-diffusion system modelling chemotaxis*, Math. Nachr., **195** (1998), pp. 77–114.

3. J.A. GRIEPENTROG, *On the unique solvability of a phase separation problem for multicomponent systems*, Banach Center Publ., **66** (2004), pp. 153–164.

4. H. STEPHAN, *Lyapunov functions for positive linear evolution problems*, WIAS Preprint no. 978, 2004, submitted.

5. ——, *A dimension-reduced description of general Brownian motion by non-autonomous diffusion-like equations*, WIAS Preprint no. 994, 2004, submitted.

4.2 Research Group Laser Dynamics

4.2.1 Overview

Der Arbeitsschwerpunkt der Forschungsgruppe besteht in der Weiterentwicklung mathematischer Methoden und Theorien auf dem Gebiet der Nichtlinearen Dynamik anhand konkreter Anwendungen aus der Optoelektronik.

Die durchgeführten Forschungsarbeiten reichen von einer effizienten Modellierung der maßgeblichen physikalischen Effekte in konkreten optoelektronischen Bauelementen über die Entwicklung und Implementierung von Verfahren zur numerischen Simulation bis hin zur Untersuchung der analytischen Eigenschaften der Modelle und zur Weiterentwicklung von mathematischen Methoden im Hinblick auf die vorliegenden Fragestellungen.

Auf der Seite der Anwendungen waren die Arbeitsschwerpunkte

- Dynamik von gekoppelten Lasersystemen und Lasern mit Rückkopplung,
- Mode-locking in Lasern mit saturierbaren Absorbern,

die in enger Kooperation mit den Anwendungspartnern Fraunhofer-Institut für Nachrichtentechnik – Heinrich-Hertz-Institut (HHI), Berlin, Ferdinand-Braun-Institut für Höchstfrequenztechnik (FBH), Berlin, und Forschungszentrum COM der Technischen Universität Dänemark durchgeführt wurden. In diesem Zusammenhang bestehen Drittmittelprojekte im Rahmen des DFG-Forschungszentrums MATHEON, des Sonderforschungsbereiches 555 „Komplexe Nichtlineare Prozesse“ und des Verbundforschungsvorhabens Terabit Optics Berlin (gemeinsam mit der Forschungsgruppe „Partielle Differentialgleichungen und Variationsgleichungen“). Eine wichtige Rolle spielt dabei auch die Weiterentwicklung des Softwarepakets `LDSL-tool` zur Simulation der raumzeitlichen Dynamik von Halbleiterlasern.

The research of this group was focused on the development of mathematical methods and theories in the field of Nonlinear Dynamics, related to concrete applications in optoelectronics.

The performed research includes the efficient modeling of the relevant physical effects in certain optoelectronic devices and the development and implementation of methods and algorithms for a numerical simulation, as well as the investigation of analytical properties of these models, and the development of mathematical methods related to the application problems.

In the field of applications, the main subjects of research were

- Dynamics of coupled laser systems and lasers with feedback;
- Mode-locking in lasers with saturable absorption.

The investigations were performed in close cooperation with the partners from Fraunhofer-Institut für Nachrichtentechnik – Heinrich Hertz Institute (HHI), Berlin, Ferdinand-Braun-Institut für Höchstfrequenztechnik (FBH), Berlin, and the Research Center COM of the Technical University of Denmark. In this context there exist funded projects, supported by the DFG Research Center MATHEON, the Collaborative Research Centre 555 “Complex Nonlinear Processes” and the research network project Terabit Optics Berlin (together with the Research Group “Partial Differential Equations and Variational Equations”). An important contribution to this work consists in the development of the software package `LDSL-tool` for the simulation of spatio-temporal dynamics in semiconductor lasers.

Aus mathematischer Sicht standen die folgenden Themen im Vordergrund:

- Theorie singulärer Störungen für Gleichungen mit Delay und partielle Differentialgleichungen,
- Synchronisation,
- Numerische Verzweigungsanalyse in unendlichdimensionalen Systemen.

From a mathematical point of view, the main focus was on the following topics

- Singular perturbation theory for delay differential equations and partial differential equations;
- Synchronization;
- Numerical bifurcation analysis for infinite-dimensional systems.

4.2.2 Projects

Dynamics and synchronization for laser systems with feedback or coupling

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Cooperation with: L. Recke (Institut für Mathematik, Humboldt-Universität zu Berlin (HU)), A. Samoilenko (Institute of Mathematics, National Academy of Sciences of Ukraine, Kiev), H.-J. Wünsche (Institut für Physik, Humboldt-Universität zu Berlin (HU)) T. Kapitaniak and A. Stefanski (Technical University of Lodz, Poland)

Supported by: DFG: Collaborative Research Centre "Complex Nonlinear Processes" (SFB 555), DFG Research Center MATHEON, project D8

It is well known that in various experimental situations where semiconductor lasers interact by coupling or feedback, they tend to develop instabilities and complicated dynamical behavior on a time scale of GHz. A qualitative and quantitative understanding of such dynamical effects is essential for the development of optoelectronic components in modern telecommunications systems. Using methods from the theory of dynamical systems, one can effectively study and describe such dynamical features.
The performed research in this field was focused to the following topics:

- Feedback lasers with large delay time;
- Systems of coupled lasers and synchronization;
- Entrainment of the modulation frequency.

For delay differential equations (DDE) with large delay time we were able to develop a new theoretical approach, using multiple-scale methods, to investigate the eigenvalue problem for stationary and periodic solutions, [3, 4]. In particular, the set of eigenvalues can be splitted into two parts. The first part corresponds to instantaneous instabilities and can be found as zeros of some polynomials. The other set is organized in branches and accounts for contributions from delayed feedback.
Applying this method to the Lang–Kobayashi model for lasers with delayed feedback, we were able to classify the occurring instabilities (see Figure 1): weak stability (first column), weak modulational instability (second column), and strong instability (the last two columns).

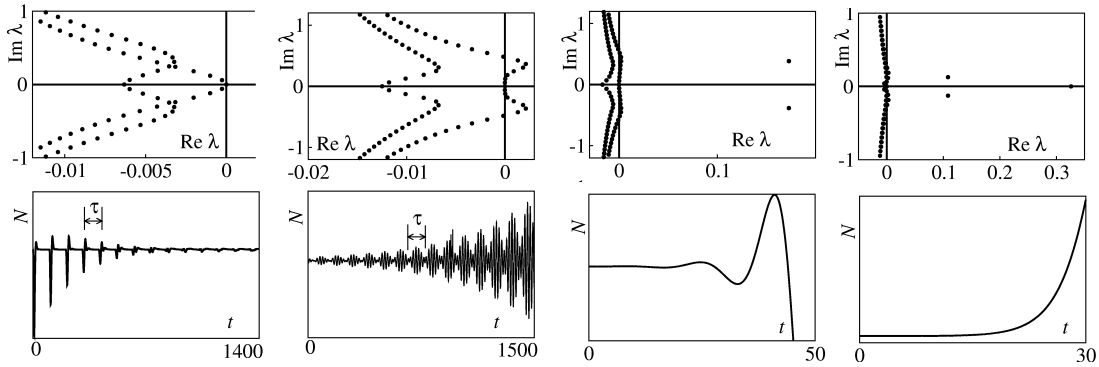

Fig. 1: Different types of local (in-)stability for laser with large feedback. Top: Eigenvalues with largest real parts. Bottom: Typical orbit in the vicinity of the corresponding stationary state.

In [6,7], we investigate the synchronization properties of a system of two optically face-to-face coupled lasers. In particular, we observe a highly sensitive dependence of the locking regions and the bifurcation scenario on the coupling phase parameter φ (see Figure 2)

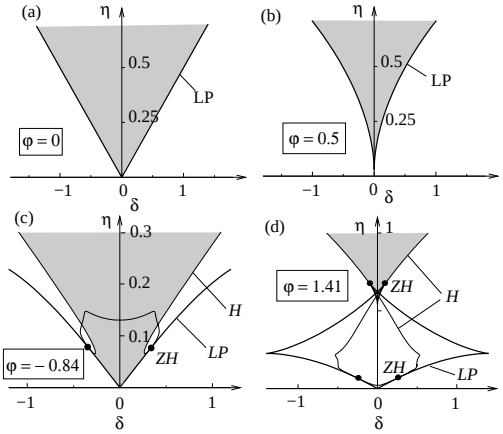

Fig. 2: Bifurcations and locking regions (gray) for two coupled lasers. H – Hopf and LP – saddle-node bifurcation lines. ZH – zero-Hopf bifurcation point.

In [5], we contribute to the development of the general theory of synchronization of coupled systems of the form

$$\dot{x}_j = f(x_j) + \sum_{j=1}^{n} D_{ij}(x_j - x_i), \quad x_j \in R^k.$$

We have shown how the synchronization threshold can be estimated for chaotic systems which are coupled via all components by an arbitrary coupling structure.

A classical problem in the theory of synchronization is the problem of frequency entrainment of an oscillatory system by an external force. We were able to extend a result from [9], showing how an entrainment of the modulation frequency can take place even for different wave frequencies, if the frequencies of the carrier wave are sufficiently fast with respect to the modulation. This is an essential feature of pulsating lasers locking to an external optical signal with optical frequency different to that of the laser.

Using the software `LDSL-tool`, we have analyzed the performance of several types of devices which are developed and produced at the Heinrich Hertz Institute (HHI) as components for optical telecommunications systems. In particular, we have considered a phase-controlled mode-beating (PhaseCOMB) laser consisting of two active sections and a passive section in between and an active feedback laser (AFL) where a single laser section is followed by a passive section for phase tuning and an active amplifier section, [2].

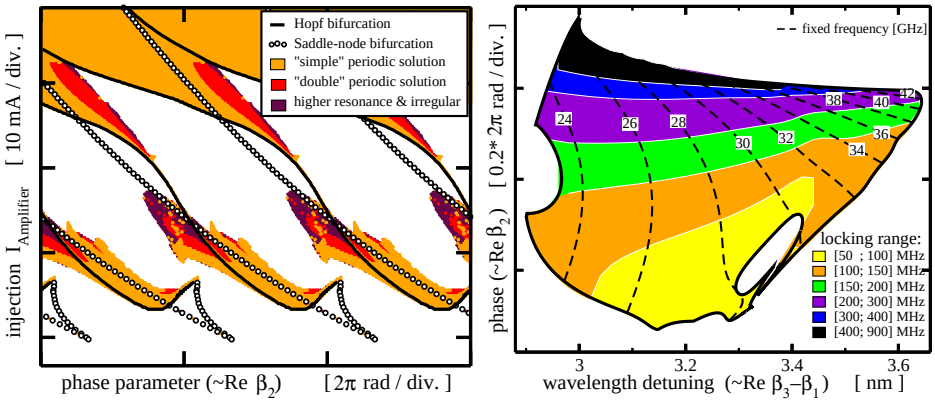

Fig. 3: Using `LDSL-tool` for investigation of laser structures from HHI. Left: AFL. Right: Electrically modulated PhaseCOMB.

References

1. S. BAUER, O. BROX, J. KREISSL, B. SARTORIUS, M. RADZIUNAS, J. SIEBER, H.-J. WÜNSCHE, F. HENNEBERGER, *Nonlinear dynamics of semiconductor lasers with active optical feedback*, WIAS Preprint no. 866, 2003, Phys. Rev. E, **69** (2004), 016206.

2. N. KORNEYEV, M. RADZIUNAS, H.-J. WÜNSCHE, F. HENNEBERGER, *Mutually injecting semiconductor lasers: Simulations for short and zero delay*, in: Proceedings of SPIE: Semiconductor Lasers and Laser Dynamics Conference “Photonics Europe”, Strasbourg, France, April 26–30, 2004, vol. 5452, SPIE, Washington, USA, 2004, pp. 63–70.

3. S. YANCHUK, M. WOLFRUM, *Instabilities of stationary states in lasers with long-delay optical feedback*, WIAS Preprint no. 962, 2004.

4. S. YANCHUK, *Properties of stationary states of delay equations with large delay and applications to laser dynamics*, WIAS Preprint no. 944, 2004.

5. A. STEFANSKI, J. WOJEWODA, T. KAPITANIAK, S. YANCHUK, *Simple estimation of synchronization threshold in ensembles of diffusively coupled chaotic systems*, Phys. Rev. E, **70** (2004), 026217.

6. S. YANCHUK, K.R. SCHNEIDER, L. RECKE, *Dynamics of two mutually coupled semiconductor lasers: Instantaneous coupling limit*, Phys. Rev. E, **69** (2004), 056221.

7. ——, *Dynamics of two F2F coupled lasers: Instantaneous coupling limit*, in: Proceeding of SPIE: Semiconductor Lasers and Laser Dynamics Conference “Photonics Europe”, Strasbourg, France, April 26–30, 2004, vol. 5452, SPIE, Washington, USA, 2004, pp. 51–62.

8. M. RADZIUNAS, *Numerical bifurcation analysis of traveling wave model of multisection semiconductor lasers*, WIAS Preprint no. 985, 2004.

9. L. RECKE, D. PETERHOF, *Abstract forced symmetry breaking and forced frequency locking of modulated waves*, J. Differential Equations, **144** (1998), pp. 233–262.

Mode-locking and Q-switching in semiconductor lasers with saturable absorber

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Supported by: Terabit Optics Berlin: project “Modeling and simulation of mode-locked semiconductor lasers” (together with Research Group 1)

Semiconductor lasers operating in mode-locking (ML) regime are efficient, compact, low-cost sources of short optical pulses with high repetition rates (tens and hundreds of GHz), suitable for applications in telecommunication technology. Similarly to other types of lasers, these lasers can be passively mode-locked by incorporating an intracavity saturable absorber section into the laser.

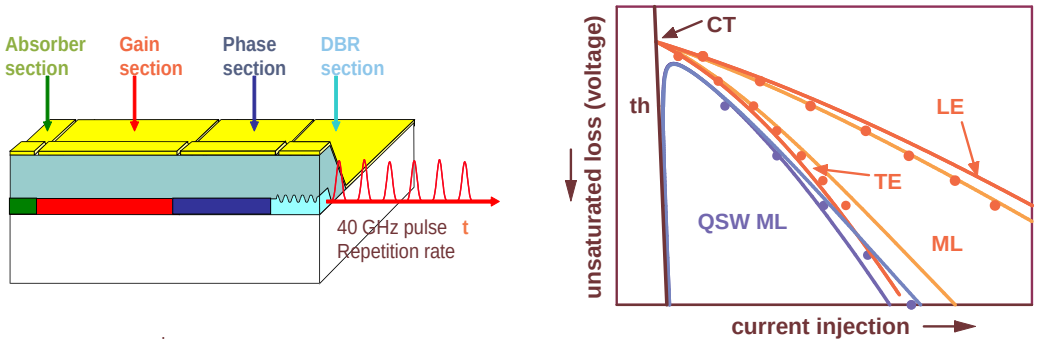

Fig. 1: Left: Schematic view of monolithic mode-locked semiconductor laser. Right: QSW ML – domain of Q-switched mode-locking. ML – stable fundamental mode-locking regime. Solid lines – analytical results. Dots – numerical results.

After the development of a new model for passive ML——a set of differential equations with time delay, [1, 2]——we have obtained a simple and efficient method to analyze the stability of ML pulses and their bifurcations. Reducing the delay differential model to a map that describes the transformation of the ML pulse parameters after one round trip in the cavity, one can study bifurcations of this map, [3, 4]. The continuous-wave (CW) ML regimes correspond to nontrivial fixed points of this map. In this way, we have described the stability domains and bifurcations of ML regimes in monolithic semiconductor lasers. Some of the results are shown in Figure 1.

It is well known that lasers with a saturable absorber have a tendency to exhibit undamped Q-switching (QSW) pulsations. In a mode-locked laser, QSW instability leads to a transition from CW-ML regime to a so-called Q-switched ML regime. It is characterized by a pulse amplitude modulated by the QSW oscillations frequency, which is typically of the order of a few GHz, for semiconductor lasers. Since fluctuations of the ML pulse amplitude are undesirable in most applications, it is an important question how to avoid this type of instability in real devices.

Using the approaches described above, we have suggested analytical approximations for the QSW instability boundary of the fundamental ML regime, [4]. We have studied the dependence of this boundary on several laser parameters and compared it with the results of direct numerical analysis of the original delay differential model (see Figure 1). The results are in good agreement with the experimental data and with the results of direct numerical simulations using the traveling wave model (see Figure 2).

Mode-locking pulsations in the TW model. Mode-locked pulsations in semiconductor lasers with saturable absorber can also be recovered by the traveling wave (TW) model. Additionally to the delay differential equations (DDE) model discussed above, this model includes the effects of the linear configuration as well as spatial hole burning of carriers, nonlinear gain compression, and spontaneous emission. After adjusting the parameters, the model equations were integrated numerically by our software `LDSL-tool` over some transient time. The sampling of the computed pulse trains and the corresponding RF-spectra [8] allow to distinguish different operating regimes of the laser and to characterize the quality of the pulses. By repeating this for different values of the control parameters, we can characterize the dynamical behavior of the laser in the parameter space (see Figure 2).

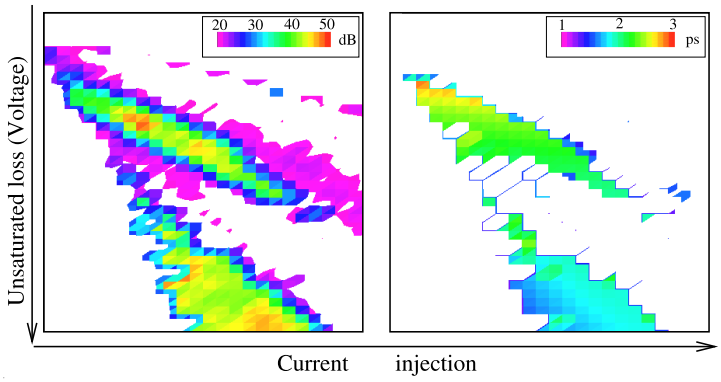

Fig. 2: Mode-locked pulsations in current injection / unsaturated loss (voltage) plane. Left: Signal-to-noise ratio. Right: Pulse width.

Q-switching pulsations in a blue semiconductor laser. Blue-violet semiconductor lasers are very attractive for high-density optical storage applications. In particular, laser diodes operating at 400 nm are required for CD or DVD systems to increase the disk storage capacity up to 25 Gbytes. A number of other applications, such as full color electroluminescent displays, laser printers, and many others in biology and medicine have increased the interest in such lasers. Recently, specific interest has been focused on the Q-switching operation of blue-emitting devices [5–7]. QSW can significantly increase the laser performance for certain applications and is considered, for example, to be important for the reduction of feedback noise. Figure 3 shows the structure of the InGaN laser (lasing wavelength 395 nm) with saturable absorber that has been investigated. To model the laser properties, we used the Yamada model adapted to the specific case of the InGaN laser with saturable absorber incorporated as a layer parallel to the active region. The region of QSW in the plane of cavity length vs. injected current parameters is shown in Figure 3. As the cavity length is increased, the Q-switching range becomes wider. However, this spread is accompanied by a shift of the threshold current to higher values. Figure 3 also shows quite good agreement between the experimental data (dotted lines terminated by symbols) and the regions of QSW predicted by numerical calculation.

Finally, two different possibilities to obtain excitable behavior of the blue laser with saturable absorber have been discussed.

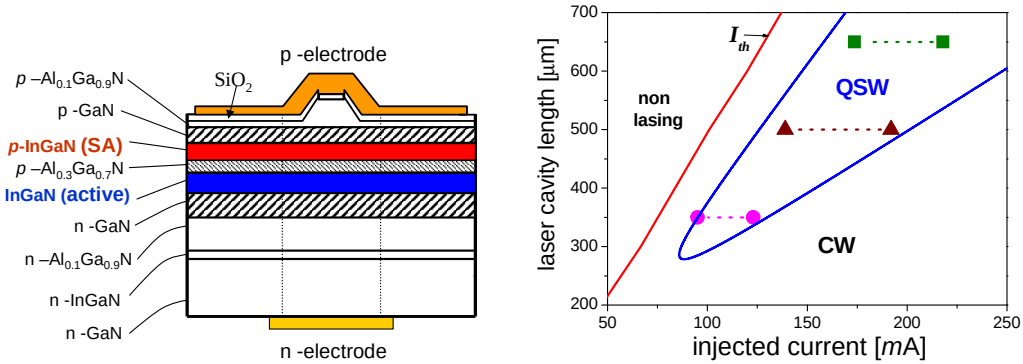

Fig. 3: Left: Schematic view of a blue InGaN laser. Right: Numerical (blue line) and experimental (dotted lines) regions of Q-switching. Red line – threshold current.

References

1. A.G. VLADIMIROV, D. TURAEV, G. KOZYREFF, *Delay differential equations for mode-locked semiconductor lasers*, Opt. Lett., **29** (2004), pp. 1221–1223.

2. A.G. VLADIMIROV, D. TURAEV, *A new model for a mode-locked semiconductor laser*, to appear in: Radiophysics and Quantum Electronics, **47** (2004).

3. ——, *Passive mode-locking with slow saturable absorber: A delay differential model*, WIAS Preprint no. 947, 2004.

4. D. RACHINSKII, A.G. VLADIMIROV, *Q-switching instability in a mode-locked semiconductor laser*, WIAS Preprint no. 975, 2004.

5. V.Z. TRONCIU, M. YAMADA, R.A. ABRAM, *Analysis of the dynamics of a blue-violet InGaN laser with a saturable absorber*, Phys. Rev. E, **70** (2004), 026604.

6. V.Z. TRONCIU, M. YAMADA, T. KAWAKAMI, S. ITO, T. OHNO, M. TANEYA, R.A. ABRAM, *A theoretical and experimental investigation of the dynamics of tandem blue-violet lasers*, Opt. Commun., **235** (2004), pp. 409–414.

7. V.Z. TRONCIU, M. YAMADA, R.A. ABRAM, T. KAWAKAMI, S. ITO, T. OHNO, M. TANEYA, *Self-pulsation and excitability of blue-violet InGaN lasers*, WIAS Preprint no. 940, 2004.

8. M. RADZIUNAS *Sampling techniques applicable for the characterization of the quality of self pulsations in semiconductor lasers*, WIAS Technical Report no. 2, 2002.

Numerical methods for laser dynamics

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Supported by: DFG Reseach Center MATHEON, project D8

Our software `LDSL-tool` is a comprehensive toolkit to simulate and to analyze the spatio-temporal dynamical behavior of a broad range of edge-emitting multisection semiconductor lasers, including lasers with dispersive or amplified feedback, mode-locked lasers with saturable absorbers, ring lasers, and the interaction of several lasing sections. It is based on the traveling wave (TW) model

$$\begin{aligned} \frac{\partial}{\partial t}E(z,t) &= H\left(\partial_z, \beta(z) + \tilde{\beta}(n, \varepsilon|E|^2, z), z\right) E(z,t), \qquad E(z,t) \in \mathbb{C}^4, \\ \frac{d}{dt}n(z,t) &= I(z,t) - R(n,z) - \Re e\langle E, G(n, \varepsilon|E|^2, z)E\rangle, \quad n(z,t) \in \mathbb{R}, \end{aligned} \tag{1}$$

supplied with reflectivity / transmission / injection conditions for the field E at the edges of each part of the device. Well-posedness and smoothness properties for different types of the TW model have been investigated in [3, 6].
In order to obtain information about different dynamical effects and their sensitive dependence on the various design and control parameters in an efficient way, the further development of `LDSL-tool` has been focused on the combination of the existing tools for simulations and spectral analysis [4] with the path-following software AUTO [1] for numerical bifurcation analysis. In the case of the TW model, the application of such techniques is based on an effective central manifold reduction, [6], leading to a low-dimensional mode approximation (MA) system of ODEs.

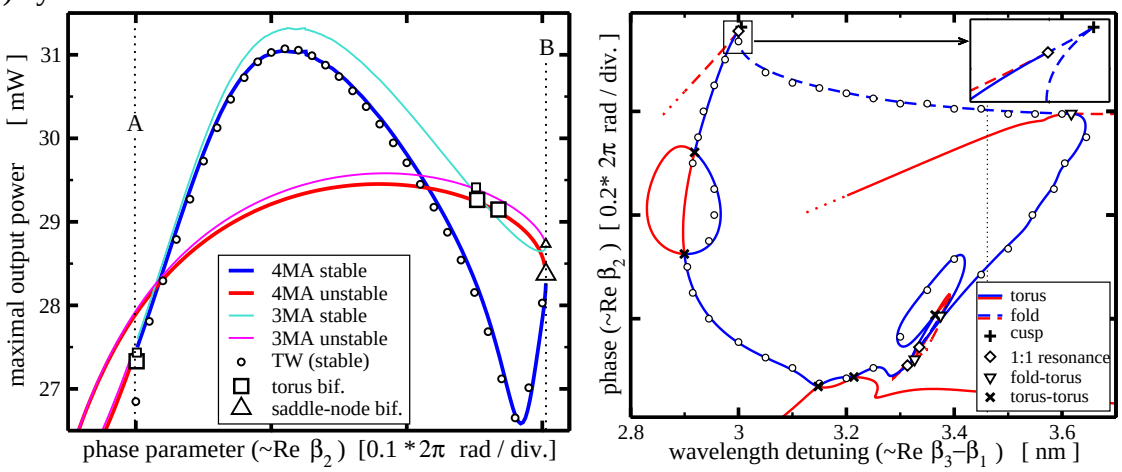

Fig. 1: Bifurcations of periodic solutions for a laser with two active sections. Left: One parameter. Right: Two parameters.

Figure 1 shows the result of a numerical bifurcation analysis for a laser with two active sections after reduction to mode approximation (MA) systems, [5]. Empty bullets, obtained by integration of the full TW model, show the good precision for MA systems with sufficiently high dimension.
For a numerical bifurcation analysis of the delay differential model for mode-locking in monolithic semiconductor lasers, we have used also the software package DDE-BIFTOOL [2]. Using this package, we have calculated Hopf bifurcations of continuous-wave (CW) solutions (laser modes) of the laser equations and analyzed bifurcations of the solutions with periodic laser intensity. These bifurcate from the CW solutions at Hopf bifurcations and correspond to mode-locking regimes with different repetition rates. An example of a bifurcation diagram is shown in Figure 2.

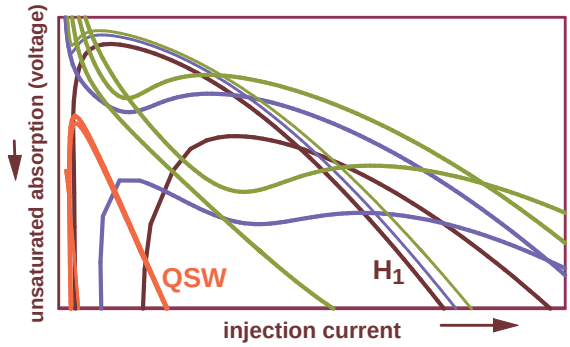

Fig. 2: Curves of Hopf bifurcations for CW solutions of a mode-locked laser. QSW: Q-switching. H_1: Hopf bifurcations to fundamental mode-locked solution regime.

References

1. E.J. DOEDEL, A.R. CHAMPNEYS, T.F. FAIRGRIEVE, YU.A. KUZNETSOV, B. SANDSTEDE, X. WANG, *AUTO97: Continuation and bifurcation software for ordinary differential equations (with HomCont)*, Technical Report, Concordia University, Montreal, Canada, 1997.

2. K. ENGELBORGHS, T. LUZYANINA, G. SAMAEY, *DDE-BIFTOOL V. 2.00: A Matlab package for bifurcation analysis of delay differential equations*, Technical Report TW-330, Department of Computer Science, Catholic University of Leuven, 2001.

3. M. LICHTNER, M. RADZIUNAS, *Well posedness and smooth dependence for a semilinear hyperbolic system with nonsmooth data*, Preprint no. 174 of DFG Research Center MATHEON, Berlin, 2004.

4. M. RADZIUNAS, H.-J. WÜNSCHE, *Multisection lasers: Longitudinal modes and their dynamics*, WIAS Preprint no. 939, 2004, in: "Optoelectronic Devices – Advanced Simulation and Analysis", J. Piprek, ed., Springer Verlag, New York, 2005, pp. 121–150, ISBN: 0-387-22659-1.

5. M. RADZIUNAS, *Numerical bifurcation analysis of traveling wave model of multisection semiconductor lasers*, WIAS Preprint no. 985, 2004.

6. J. SIEBER, M. RADZIUNAS, K.R. SCHNEIDER, *Dynamics of multisection semiconductor lasers*, Math. Model. Anal., **9** (2004), pp. 51–66.

Periodic processes

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Localization of periodic orbits is one of the basic problems in the analysis and control of dynamical systems. Using methods of topological degree theory, we have developed new analytic approaches to nonlocal problems on periodic solutions of systems with nonlinearities of saturation type, which are typical particularly for problems of laser dynamics.
We have studied bifurcations of periodic solutions from infinity and obtained estimates for the number of, and asymptotic formulas for, solution branches, [1, 2]. It was proved that generically there are two branches of forced periodic oscillations. However, many (any even number of) branches may appear in degenerate situations, which are standard for problems on subharmonic solutions. We have derived sufficient conditions for the existence of subharmonics (periodic solutions of multiple periods $2\pi n$) with arbitrarily large amplitudes and periods for higher-order ordinary differential equations

$$L\left(\frac{d}{dt},\lambda\right)x = f(x) + b(t), \tag{1}$$

depending on a scalar parameter λ, with a 2π-periodic forcing term b and a nonlinearity f with saturation. This type of a subharmonic bifurcation from infinity occurs ([3]) whenever a pair of simple roots $\eta(\lambda) \pm \xi(\lambda)i$ of the characteristic polynomial L crosses the imaginary axis at points $\pm\alpha i$ with an irrational α. Under some further assumptions, we have estimated the parameter intervals of frequency locking, where subharmonics with amplitudes and periods increasing to infinity appear sporadically as the parameter approaches a bifurcation value λ_0. These assumptions relate the quality of the rational Diophantine approximations of α, the rate of convergence of the nonlinearity to its limits at infinity, and the smoothness of the forcing term. Actually, our results provide estimates for the width and length of the Arnold tongues in the problem of bifurcation of subharmonics from infinity (see Figure 1).

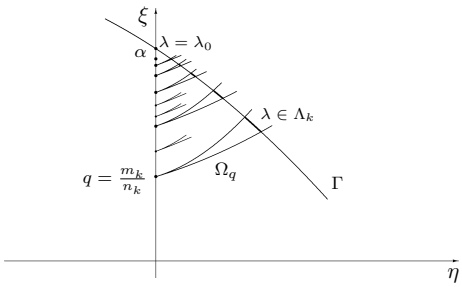


Fig. 1: Frequency-locking intervals Λ_k are obtained as preimages of the intersections of the Arnold tongues with the trajectory Γ of a root of L

In [4], we applied our method to a Hopf bifurcation problem with a multiple resonance. Some numerical aspects of the problems were considered in [5].
A separate research direction was aimed at understanding the dynamics of systems where hysteresis plays an important role. Using the theory of closed systems with hysteresis operators as a framework for our studies, and concentrating mostly on periodic and cyclic processes, their stability and bifurcations, we have observed that hysteresis may be a source of several specific effects. For example, systems with hysteresis may have attractors consisting of a continuum of periodic or quasiperiodic orbits in generic situations. The results were tested with hysteresis models of different types.

We have studied the structure and stability of nontrivial connected clusters of periodic orbits that appear from an asymptotically stable periodic trajectory as a result of a hysteresis perturbation of the system, [6], as well as Hopf bifurcations of such attracting clusters from equilibria and from infinity, [7, 8]. A variety of dynamic and bifurcation scenarios (see, for example, Figure 2) was analyzed for the Duffing-type forced oscillator

$$x'' + x = \sin(\sqrt{2}t) + \lambda P(x)(t) \tag{2}$$

with the hysteresis friction modeled by the Preisach operator P, on the basis of new topological approaches developed in [9], which combine analytic and rigorous computer-aided methods. Global stability of some complex hysteresis models, including that with the so-called ratchetting effect (unclosed hysteresis loops), was studied in [10, 11].

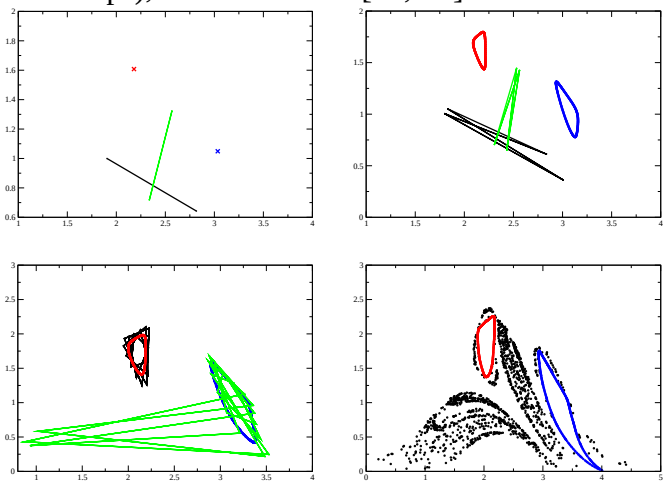


Fig. 2: Bifurcations of stable periodic orbits of the Poincaré map for Eq. (2) for different values of the parameter λ: Two equilibria and two period-2 points (upper left); bifurcations of the equilibria to clusters of invariant curves (quasiperiodic orbits) and period doubling bifurcation of the period-2 orbits to period-4 orbits (upper right); further bifurcations of the periodic orbits to higher-order subharmonics (lower left); bifurcation to chaos (lower right)

References

1. A.M. KRASNOSEL'SKII, D.I. RACHINSKII, *Branching at infinity of solutions to equations with degeneration of multiplicity two*, Doklady Math., **69**(1) (2004), pp. 79–83.

2. ——, *On a number of unbounded solution branches near the asymptotic bifurcation point*, to appear in: Funct. Anal. Appl.

3. V.S. KOZYAKIN, A.M. KRASNOSEL'SKII, D.I. RACHINSKII, *Subharmonic bifurcation from infinity*, submitted.

4. A.M. KRASNOSEL'SKII, D.I. RACHINSKII, *Remark on the Hopf bifurcation theorem*, Math. Nachr., **272** (2004), pp. 95–103.

5. A.M. KRASNOSEL'SKII, A.V. POKROVSKII, D.I. RACHINSKII, *On guaranteed estimates of convergence rate for one class of iteration procedures*, Autom. Remote Control, **65**(10) (2004), pp. 1635–1640.

6. M. BROKATE, A.V. POKROVSKII, D.I. RACHINSKII, *Asymptotic stability of continual sets of periodic solutions to systems with hysteresis*, WIAS Preprint no. 902, 2004.

7. M. BROKATE, D.I. RACHINSKII, *Hopf bifurcations and simple structures of periodic solution sets in systems with the Preisach nonlinearity*, WIAS Preprint no. 921, 2004.

8. D.I. RACHINSKII, *On a bifurcation of stable large-amplitude cycles for equations with hysteresis*, Autom. Remote Control, **65**(12) (2004), pp. 1915–1937.

9. M. BROKATE, A.V. POKROVSKII, D.I. RACHINSKII, O. RASSKAZOV, *Differential equations with hysteresis in examples*, to appear in: The Science of Hysteresis, I. Mayergoyz, G. Bertotti, eds., Elsevier Science, 150 pages.

10. M. BROKATE, D.I. RACHINSKII, *On global stability of the scalar Chaboche models*, Nonlinear Anal. Real World Appl., **6** (2005), pp. 67–82.

11. ——, *Global stability of Armstrong–Frederick models with periodic uniaxial inputs*, to appear in: NoDEA Nonlinear Differential Equations Appl.

Multiscale systems

Collaborators: M. Radziunas, D. Rachinskii, K.R. Schneider, M. Wolfrum, S. Yanchuk

Cooperation with: V.F. Butuzov, N.N. Nefedov, A.B. Vasil'eva (Moscow State University, Russia)

Supported by: DFG: Cooperation Project "Singularly perturbed systems and exchange of stability" of German and Russian scientists in the framework of the *Memorandum of Understanding* between DFG and RFFI

Delayed loss of stability for singularly perturbed systems. We have studied the phenomenon of delayed loss of stability for singularly perturbed systems of ordinary differential equations in case that the associated autonomous system undergoes a Hopf bifurcation at the zero equilibrium as some parameter changes. In that case, the system "notices" that the equilibrium has lost its stability only after some delay. In contrast to the well-known standard situation, we were interested in a class of systems where the linearization of the associated system is independent of the slowly changing parameter. For this class, superlinear positive homogeneous terms in the expansion of the right-hand parts at zero define the bifurcation points and the stability of the equilibrium and the cycles. We have derived simple formulas to estimate the asymptotic delay for the delayed loss of stability phenomenon. More precisely, we found conditions which ensure that the zeros of a simple function ψ defined by the positive homogeneous nonlinear terms are the Hopf bifurcation points of the associated system, the sign of ψ at other points determines the stability of the zero equilibrium, and the asymptotic delay equals the distance between a bifurcation point and a zero of a primitive of ψ.

Alternating contrast structures. We consider the scalar singularly perturbed parabolic differential equation

$$\varepsilon^2 \left(\frac{\partial^2 u}{\partial x^2} - \frac{\partial u}{\partial t} \right) = f(u,x,t),\ x \in (0,1),\ t > 0, \tag{1}$$

where ε is a small parameter, with the initial condition

$$u(x,0,\varepsilon) = u^0(x,\varepsilon) \quad \text{for} \quad 0 \le x \le 1, \tag{2}$$

and the boundary conditions of Neumann type

$$\frac{\partial u}{dx}(0,t,\varepsilon) = \frac{\partial u}{\partial x}(1,t,\varepsilon) = 0 \quad \text{for} \quad t > 0. \tag{3}$$

It is well known that the boundary value problem (1), (3) in general has solutions exhibiting for small ε boundary layers (i.e., there are small regions near the boundaries $x = 0$ and $x = 1$, where the solutions rapidly change) and/or interior layers (i.e., there are small regions in the interval $0 < x < 1$, where the solutions rapidly change). We call solutions of (1), (3), which have only boundary layers pure boundary layer solutions, solutions possessing an interior layer are called contrast structures.
The case that the type of the solution changes with increasing time is called alternating contrast structures, [3].

The focus of this paper is on the analytical investigation of the initial-boundary value problem (1)–(3) with periodic right-hand side in the case that a solution with a step-type interior layer exists, which moves to the boundary $x = 1$ or $x = 0$ and changes its type to a pure boundary layer solution when the interior layer arrives at the boundary. The analytical investigations are based on the method of lower and upper solutions. We distinguish three transition cases: (i) Slow transition, (ii) Fast transition, (iii) Fast-slow transition. All cases have also been investigated numerically. The case of slow transition is represented in Figure 1 for a special equation. The solution $u(x,t,\varepsilon)$ is represented for fixed t by a boldface curve.

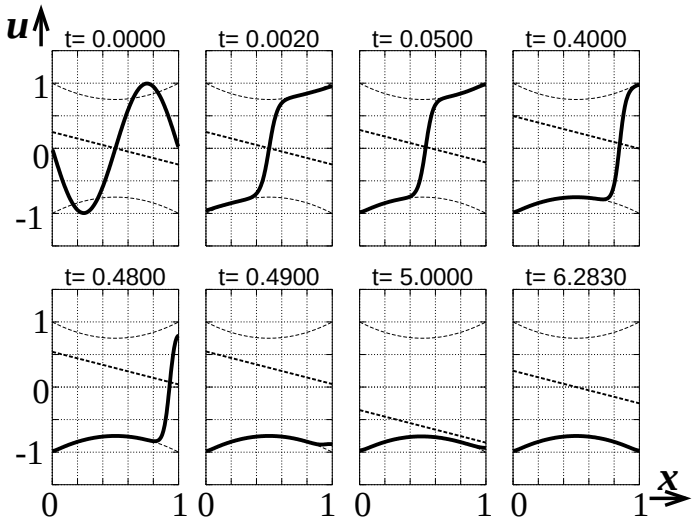


Fig. 1: Slow passage

References

1. D.I. RACHINSKII, K.R. SCHNEIDER, *Dynamic Hopf bifurcations generated by nonlinear terms*, to appear in: J. Differential Equations.

2. N.N. NEFEDOV, M. RADZIUNAS, K.R. SCHNEIDER, A.B. VASIL'EVA, *Change of the type of contrast structures in parabolic Neumann problems*, WIAS Preprint no. 984, 2004, to appear in: Comput. Math. Math. Phys., **45** (1) (2005).

3. A.B. VASIL'EVA, A.P. PETROV, A.A. PLOTNIKOV, *On the theory of alternating contrast structures*, Comput. Math. Math. Phys., **38** (1998), pp. 1534–1543.

4. M. WOLFRUM, J. HÄRTERICH, *Describing a class of global attractors via symbol sequences*, Discrete Contin. Dyn. Syst., **12** (2005), pp. 531–554.

4.3 Research Group Numerical Mathematics and Scientific Computing

4.3.1 Overview

Die Gruppe entwickelt, analysiert und implementiert numerische Verfahren für Systeme partieller Differentialgleichungen und von Algebro-Differentialgleichungen und wendet diese auf praktische Problemstellungen an.

Externe Kooperationspartner der Gruppe sind Forschungsinstitute der Max-Planck-Gesellschaft und der Leibniz-Gemeinschaft sowie ALSTOM (Switzerland) Ltd.

Im Jahre 2004 konzentrierte sich die Gruppe auf Forschungen und Anwendungen auf folgenden Gebieten:

- Numerische Lösung nichtlinearer Systeme von Konvektions-Diffusions-Reaktionsgleichungen auf der Basis des Finite-Volumen-Verfahrens. Ein Beitrag der Gruppe zu diesem Gebiet war ein neuer Weg zur Herleitung von Finite-Volumen-Schemata für diese Problemklasse (siehe S. 55).

  Die Methode wurde erfolgreich in verschiedenen Kontexten angewendet, insbesondere für Halbleitergleichungen für das Design von DEPFET-Sensoren (siehe S. 57) und – in Kooperation mit der Forschungsgruppe „Partielle Differentialgleichungen und Variationsgleichungen” – für Phasenseparationsprobleme (siehe S. 182).

- Lösung von sehr großen Systemen von Algebro-Differentialgleichungen für die Konstruktion von Gasturbinen. Der Simulator `BOP` wird für die industrielle Gasturbinen-Simulation durch ALSTOM (Switzerland) Ltd. genutzt (siehe S. 71).

The group develops and implements numerical methods for systems of partial differential equations and differential–algebraic equations, analyzes these methods, and applies them to practical problems of interest.

External cooperation partners of the group are research institutes of the Max Planck Society and the Leibniz Association as well as ALSTOM (Switzerland) Ltd.

During 2004, the group focused on research and applications for several problem classes:

- Numerical solution of nonlinear systems of convection-diffusion-reaction equations based on the finite volume method. A new way for deriving finite volume schemes for problems of this class (see page 55) has been a contribution of the group to this field in 2004.

  The method has been successfully applied in various settings, namely in semiconductor device equations for DEPFET sensor design (see page 57) and—in cooperation with the Research Group “Partial Differential Equations and Variational Equations”—phase separation problems (see page 182).

- Solution of large-scale DAE systems in gas turbine engineering. The simulator `BOP` is in commercial use for industrial gas turbine simulation at ALSTOM (Switzerland) Ltd. (see page 71).

- Numerische Lösung der Navier-Stokes-Gleichungen auf der Basis der Finite-Elemente-Methode. Die hauptsächlichen Anwendungen waren Flüssigkeiten mit freien Oberflächen in Tanks (siehe S. 60) und die Simulation der Strömungsverhältnisse in der Schmelze bei der Czochralski-Kristallzüchtung (siehe S. 63).

  Weiterhin wurde die Robustheit des gemischten Finite-Elemente-Verfahrens für eine verallgemeinerte Stokes-Gleichung untersucht (siehe S. 66).

- Numerische Simulation von Wellenleitern für Laser und Mikrowellen (siehe S. 68).

- Berechnung der elektronischen Bandstruktur von InAsSb-Multi-Quantum-Well-Lasern in Kooperation mit der Forschungsgruppe „Partielle Differentialgleichungen und Variationsgleichungen" (siehe S. 175).

- Dreidimensionale Delaunay-Gittergenerierung. Dieses Gebiet ist eng mit den Finite-Volumen-Verfahren verbunden. Verschiedene Verbesserungen wurden an dem Netzgenerator TetGen vorgenommen (siehe S. 74).

- Lineare Löser für schwach besetzte lineare Gleichungssysteme sind wesentlich für alle oben genannten Probleme. Beträchtliche Anstrengungen wurden unternommen, um den parallelen direkten Löser PARDISO zu verbessern. (siehe S. 76).

Die Integration einzelner Komponenten für die numerische Lösung von Systemen partieller Differentialgleichungen in eine konsistente Softwareumgebung ist das Ziel des `pdelib`-Projekts (siehe S. 77).

- Numerical solution of the Navier–Stokes equations based on the finite element method. The two main applications have been fluids with free surfaces in tanks (see page 60) and melt flow simulation in Czochralski crystal growth (see page 63).

  Furthermore, the robustness of mixed finite element methods for a generalized Stokes equation has been investigated (see page 66).

- Numerical simulation of microwave and laser waveguides (see page 68).

- Calculation of the electronic bandstructure of InAsSb multi quantum wells of in cooperation with the Research Group "Partial Differential Equations and Variational Equations" (see page 175).

- Three-dimensional Delaunay mesh generation. This field is closely linked to the finite volume method. Several improvements have been contributed to the mesh generator TetGen (see page 74).

- Linear solvers for sparse matrix problems. These are a key component in all applications mentioned above. Considerable effort went into the improvement of the parallel sparse direct solver PARDISO (see page 76).

The integration of particular components for the numerical solution of systems of partial differential equations into a consistent software environment is the aim of the `pdelib` project (see page 77).

Verschiedene Anwendungsprojekte benutzen inzwischen die neuentworfene Programmierschnittstelle `pdelib2` (siehe S. 66 und S. 90, MATHEON/C1) oder Teile davon (siehe S. 57 und S. 74). Dieses Projekt ist ein Schlüsselprojekt der Gruppe. Es vereinigt neue Entwicklungen aus den oben genannten Forschungsgebieten und ist damit ein schneller Weg, diese Resultate innerhalb und außerhalb des WIAS anwendbar zu machen.

Die Gruppe unterstützt andere Projekte des Instituts mit ihrem Wissen zur Visualisierung (siehe S. 79) und numerischen Analysis.

Prof. E. Bänsch, Leiter der Gruppe seit 2000, hat einen Ruf an die Friedrich-Alexander-Universität Erlangen-Nürnberg angenommen.

Several projects now use the newly designed `pdelib2` API (see pages 66 and 90, and MATHEON/C1) or parts of it (see pages 57 and 74). The `pdelib` project is a key project of the group. It incorporates achievements of the research topics listed above. It is a direct and fast way to make these results applicable in and outside WIAS.

The group supports other projects of the institute with know-how concerning visualization (see page 79) and numerical analysis.

Prof. E. Bänsch, head of the group since 2000, accepted a call to the Friedrich-Alexander-Universität Erlangen-Nürnberg.

4.3.2 Projects

Finite volume methods for nonlinear parabolic problems

Collaborators: J. Fuhrmann, K. Gärtner

Cooperation with: R. Eymard (Université de Marne-la-Vallée, Champs-sur-Marne, France)

We propose a new method to compute the numerical flux of a finite volume scheme, used for the approximation of the solution of the nonlinear partial differential equation

$$u_t + \nabla(\vec{q} f(u) - \nabla\phi(u)) = 0$$

in a 1D, 2D or 3D domain Ω.

Here, $\vec{q} \in C^1(\bar{\Omega}, \mathbb{R}^d)$ is such that $\mathrm{div}\vec{q} = 0$. Furthermore, we assume $\phi \in C^1(\mathbb{R}^d, \mathbb{R}^d)$ to be Lipschitz continuous and strictly monotonically increasing, and $f \in C^0(\mathbb{R}^d, \mathbb{R}^d)$.
The method is based on the solution of the nonlinear elliptic two-point boundary value problem

$$\begin{cases} [-\phi(v)' + qf(v)]' & = 0 \text{ on } (0,h), \\ v(0) & = a, \\ v(h) & = b, \end{cases} \tag{1}$$

where q is the normal projection of $\vec{q}$ onto the line connecting the centers of the control volumes.
We define a function $g(a,b,q,h)$ by setting its value to the constant value $-[\phi(v(x))]' + qf(v(x))$ for all $x \in (0,h)$ for given a,b,q,h.
This function then is used to describe the numerical flux between two adjacent control volumes in a finite volume method, where a,b are the values of this solution in the adjacent control volumes.
We prove the existence of a solution to this two-point boundary value problem. We show that the expression for the numerical flux can be yielded without referring to this solution. Furthermore, we prove that the so designed finite volume scheme has the expected stability properties and that its solution converges to the weak solution of the continuous problem.
We have proven that the value of $g(a,b,q,h)$ is given by the following relation:

if $a \le b$ then, setting $G^\flat_{a,b} = \min_{s\in[a,b]} (qf(s))$,

if $\forall \varepsilon > 0$, $\displaystyle\int_a^b \frac{\phi'(s)ds}{qf(s) - G^\flat_{a,b} + \varepsilon} \le h$, then

$\boxed{g(a,b,q,h) = G^\flat_{a,b}}$

else

$\boxed{g(a,b,q,h) = G \in (-\infty, G^\flat_{a,b}) \text{ such that } \displaystyle\int_a^b \frac{\phi'(s)ds}{qf(s) - G} = h}$

else if $a > b$ then

$\boxed{g(a,b,q,h) = -g(b,a,-q,h).}$

This approach generalizes known discretization schemes like the Scharfetter–Gummel scheme to the nonlinear case.

Except in special cases, the calculation of the numerical fluxes involves the solution of nonlinear equations. To illustrate the method, we take $\Omega = (0,1)$, $\phi : s \mapsto s^2$, $f : s \mapsto s$, $q \in [0,+\infty)$, the initial value $u_0 = 0$. For a given $v \in (q,+\infty)$, we use the boundary conditions at $x = 0$ $\overline{u}(0,t) = (v-q)vt/2$ and set $\overline{u}(1,t) = 0$ for $t < 1/v$ and $\overline{u}(1,t) = (v-q)(vt-1)/2$, otherwise. The unique weak solution of this problem is then given by

$$u(x,t) = \begin{cases} (v-q)(vt-x)/2 & \text{if } x < vt, \\ 0 & \text{if } x \geq vt. \end{cases}$$

The numerical scheme has to approximate the moving kink by a nonnegative discrete solution. The observed experimental order of convergence is shown in the following figures.

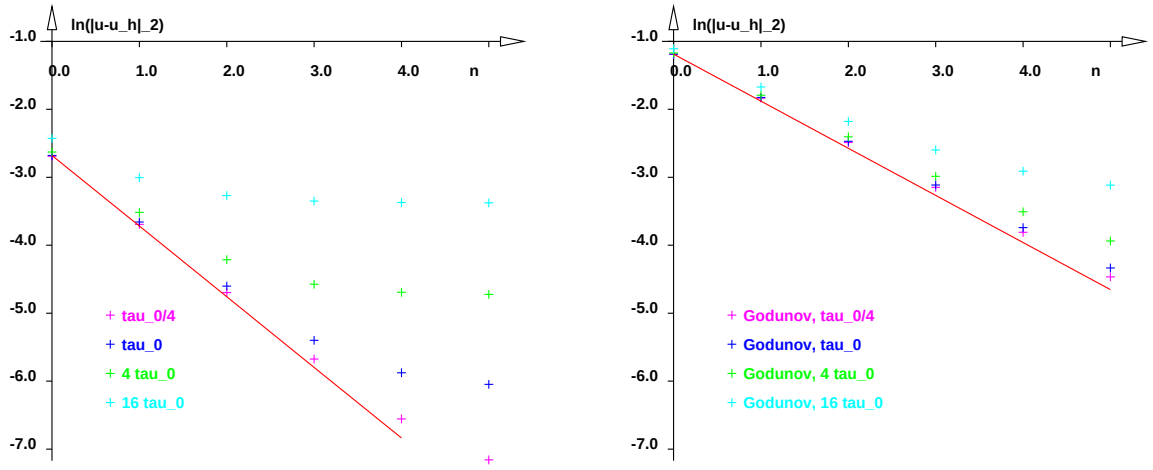


Fig. 1: Proposed scheme (left): Experimental order of convergence (EOC)=$h^{3/2}$, Godunov scheme (right): EOC=h^1

References

1. R. EYMARD, J. FUHRMANN, K. GÄRTNER, *A finite volume scheme for nonlinear parabolic equations derived from one-dimensional local Dirichlet problems*, WIAS Preprint no. 966, 2004, submitted.

Algorithms for the solution of the semiconductor device equations in three dimensions with application to DEPFET sensor design

Collaborator: K. Gärtner

Cooperation with: R. Richter (Halbleiterlabor (Semiconductor Laboratory), Max-Planck-Institut für Physik, München, and Max-Planck-Institut für extra-terrestrische Physik, Garching)

Supported by: HP Integrity for Research Program

A short progress report is presented, for details, links, etc., compare WIAS Annual Report 2003[1].
The focus is on algorithms and the X-ray sensor prototypes. Satellite-based X-ray astronomy and high energy physics are the primary applications. Detailed simulations of the detectors are necessary.

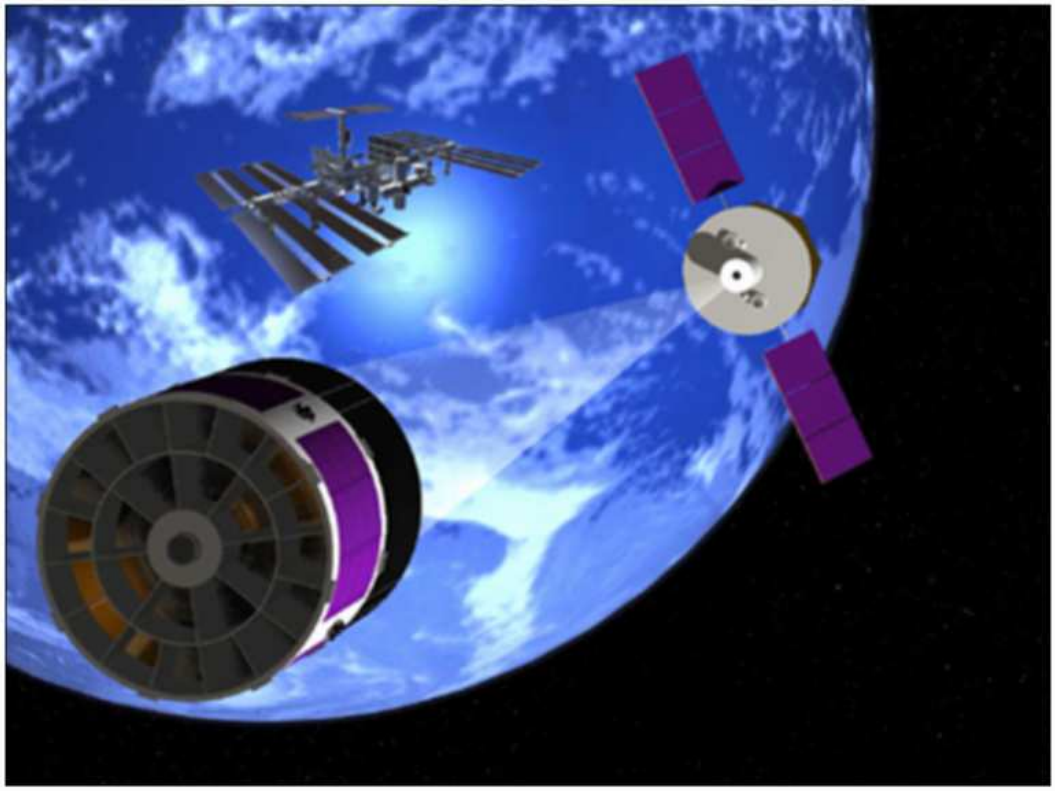


Fig. 1: ESA-XEUS project: A mirror satellite reflects X-rays into the detector satellite, distance 50 m to reach the spacial resolution

The sensor design goals are:

- very low noise operation (3 electrons equivalent noise charge);
- best amplification and low power;
- high data rates.

[1] http://www.wias-berlin.de/publications/annual-reports/2003/node43.html

The most interesting results 2004 are:

a) Time integration added;

b) 2D computed doping profiles interpolated to 3D and

c) Qualitative agreement of simulations and experiments for two prototype designs was reached.

We are in the position to start parameter variations to study the first amplifier stage in detail by solving the 3D problem on a very regular basis. The steps considered are:

1. Depletion of the sensor volume;
2. Removal of the electrons in the internal gate (clear process);
3. Collection process of the electrons generated by a single interaction of one Mn K_α X-ray photon with the silicon crystal;
4. Check of the “read-out” time (thermal generation creates electrons, too; these electrons limit the measurement time and force a new clear process).

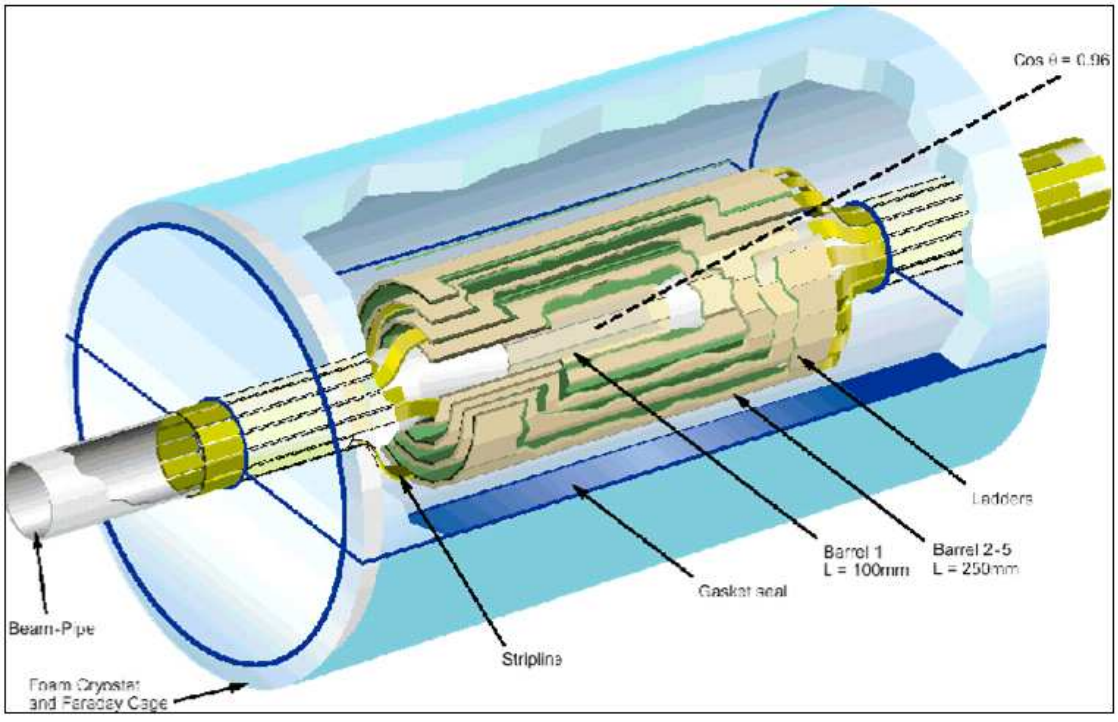


Fig. 2: Detector chamber, the green areas are made up by millions of detector cells

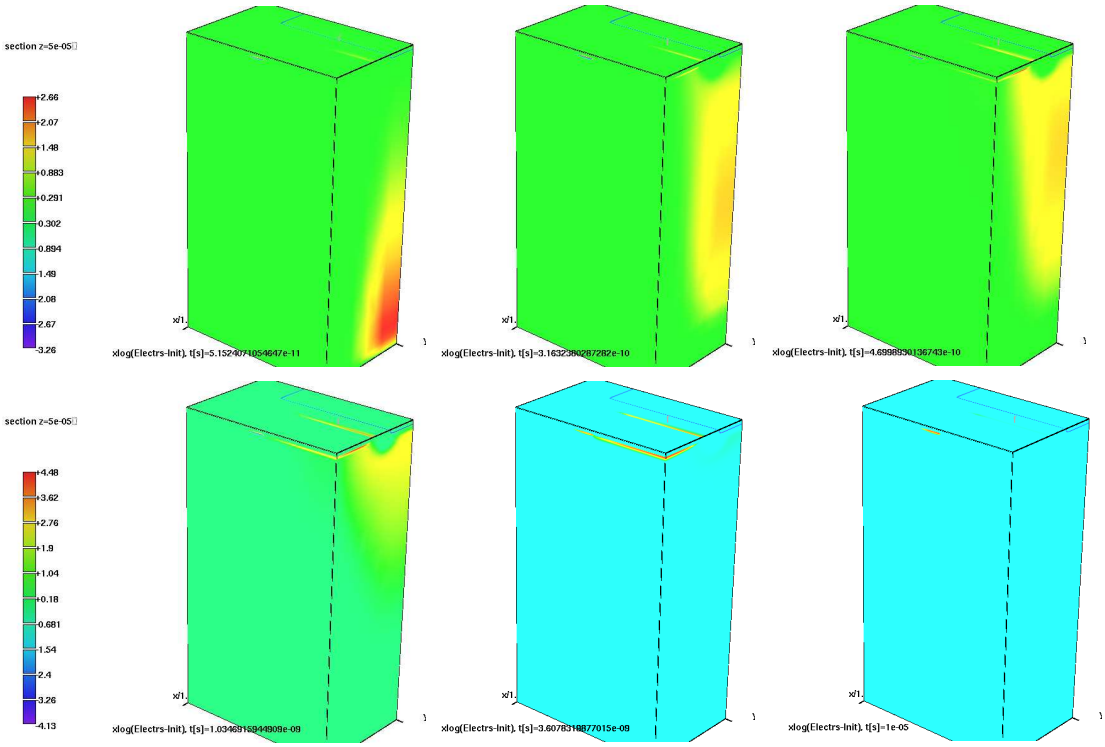


Fig. 3: A computed detection processes (half-cell) is shown in the following sequence ($n(t) - n(0)$, $n(t)$ electron density):
1600 electrons created 50 ps (upper left), electrons move to the top 300 ps, 400 ps;
horizontal diffusion supported by small fields 1 ns, 3 ns, 10 μs

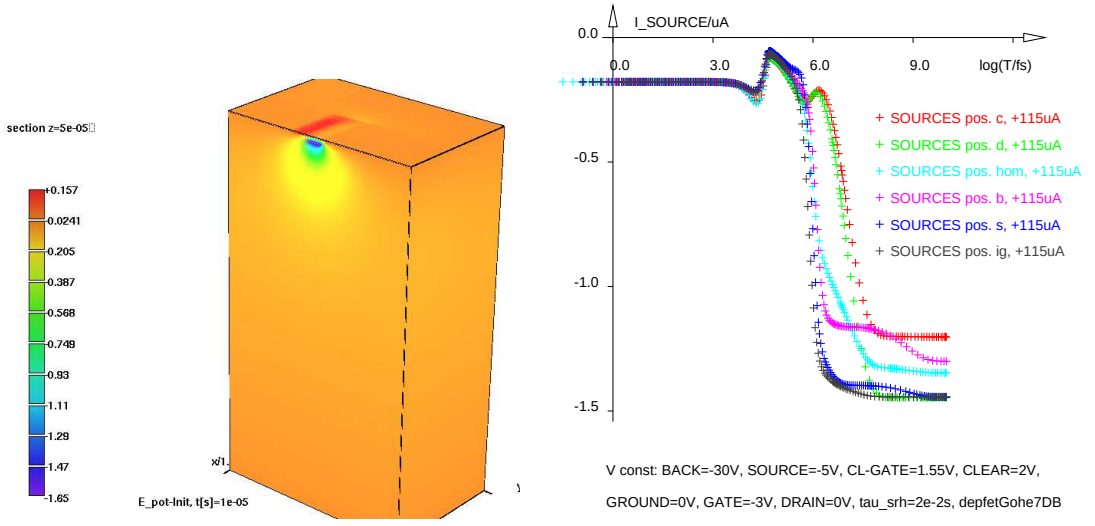


Fig. 4: Approximately 1296 electrons arrive at the internal gate and cause a potential (left) and a source contact current difference (right); contact current signals for different starting positions show the amplification per electron and the position-dependent losses at the clear contact.

Numerical investigation of the non-isothermal contact angle

Collaborators: R. Krahl, E. Bänsch

Cooperation with: M. Dreyer (Universität Bremen, ZARM)

Supported by: BMBF-DLR: „Treibstoffverhalten in Tanks von Raumtransportsystemen — Comportement des Ergols dans les Réservoirs”

It is known that thermal effects have a considerable impact on the shape of a gas-liquid phase boundary and on the angle between this surface and a solid wall at the contact line. Gerstmann et al. investigated in [1] the reorientation of such a phase boundary upon step reduction of gravity in the non-isothermal case experimentally. Our aim is similar, but we want to focus on the effect of Marangoni convection on the shape of the phase boundary. Therefore, we limit ourselves to the case where no external body forces act on the fluid.

Consider a circular cylinder, partly filled with liquid. We assume isothermal initial conditions. In the absence of gravity, the liquid surface is spherical due to surface tension. Now, the upper part of the cylinder walls, starting from a point below the liquid surface, is going to be heated.

The temperature gradient at the gas-liquid phase boundary induces a Marangoni stress, exciting a flow in the liquid and a deformation of the free surface (Figure 1). As indicator for the deformation of the phase boundary, we study the vertical coordinate of the center of the free surface z_c and of the contact point of the surface with the cylinder wall z_w. The initial deformation caused by the raise of temperature in the heated part of the wall is characterized by a raise of z_c and a recede of z_w. The angle of contact between the free surface and the wall appears to be larger. After this deformation, the shape of the free surface changes only slowly in time, so that one may speak of a quasi-stationary state.

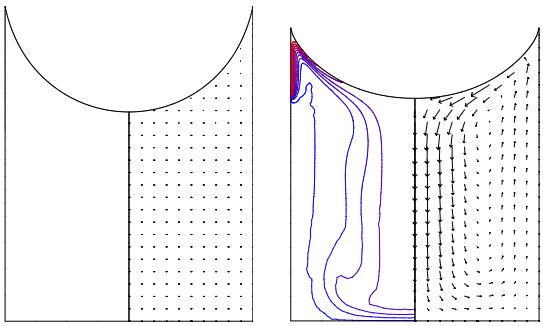


Fig. 1: Shape of the free surface, isolines of temperature and velocity field in the isothermal initial configuration (left) and after the onset of thermocapillary convection (right)

The shape of the non-isothermal phase boundary has been evaluated. It is significantly flattened near the center compared to the isothermal initial configuration, resulting in a higher (flatter) angle between the tangent to the surface and the vertical cylinder wall (Figure 2, center). While the curvature of the free surface is constant in the isothermal configuration, it becomes much larger close to the cylinder wall in the non-isothermal case (Figure 2, right). One might assume that this strong variation in curvature within a small layer close to the wall is hardly visible to the eye. This could explain why the contact angle in the non-isothermal configuration *appears* to be higher than in the isothermal case, although the same contact angle was prescribed in both cases.

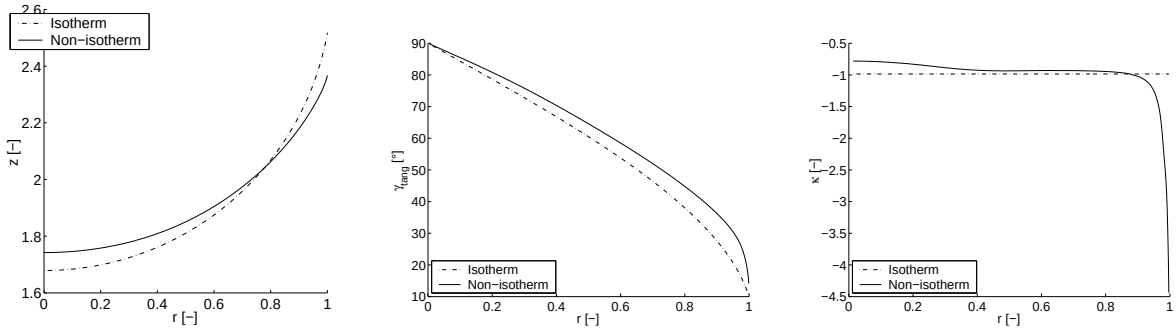


Fig. 2: Free surface (left). Angle of the tangent to the free surface and the vertical cylinder wall (center). Curvature of the free surface (right).

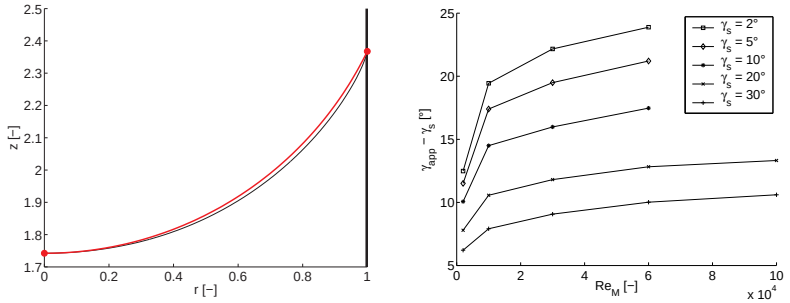


Fig. 3: Definition of the apparent contact angle: Approximation of the free surface by the circle connecting the center and the contact point (left). Deviation of the apparent contact angle from the prescribed static contact angle vs. Re_M for different static contact angles (right).

In order to get a notion of a contact angle that corresponds to what may be observed in experiments, we define an "apparent contact angle" as follows: We approximate the free surface by the circle connecting the center and the contact point (Figure 3, left). Now the *apparent contact angle* γ_{app} is defined to be the angle between the tangent of this circle and the vertical cylinder wall at the contact point. Using this definition, the apparent contact angle is given by

$$\gamma_{app} = 90^\circ - 2\tan^{-1}(z_w - z_c). \tag{1}$$

Figure 3 (left) shows the deviation of γ_{app} from the prescribed static contact angle γ_s for different thermocapillary Reynolds numbers and for different values of γ_s. The trend of a larger apparent contact angle with increasing Re_M, as observed in the experiments, is confirmed by the numerical simulations. But also the static contact angle γ_s turns out to play an important role: In case of a small γ_s, the convection role is more confined due to the narrower layer at the meniscus. In turn, the direction of the flow induced by the Marangoni stress that is pointing away from the wall forms a larger angle with the tangent of the surface, thus having a stronger effect on its shape. For larger contact angles, the situation is opposite. The flow direction is more parallel to the surface and thus has a weaker influence on its shape.

From our numerical investigations we can conclude that the enlargement of the apparent contact angle as observed in experiments in the scenario of a cold liquid meniscus on a hot solid wall is confirmed. We would like to emphasize that this effect does not depend on the specific model of a dynamic contact angle, since in our simulations a fixed static contact angle as boundary condition for the shape of the free surface has been used.

References

1. J. GERSTMANN, M. MICHAELIS, M.E. DREYER, *Capillary driven oscillations of a free liquid interface under non-isothermal conditions*, to appear in: J. Appl. Math. Mech.

2. R. KRAHL, E. BÄNSCH, *Numerical investigation of the non-isothermal contact angle*, WIAS Preprint no. 972, 2004, submitted.

Three-dimensional unsteady melt-flow simulation in Czochralski crystal growth

Collaborators: D. Davis, H. Langmach, G. Reinhardt

Cooperation with: K. Böttcher, W. Miller, U. Rehse (Institut für Kristallzüchtung, Berlin)

In 2004 we continued a collaborative project with the Institute for Crystal Growth (IKZ) in Berlin, involving the numerical unsteady flow simulation of semiconductor (GaAs) melt in a vapor-pressure-controlled Czochralski crucible (cf. previous two annual reports; also [1], [2]). As explained in the above references, the melt-flow behavior and temperature distribution in the crucible are pivotal features which ultimately determine the shape of the crystallization front (see also [3], [4]). Our previous work on GaAs melt-flow simulation concentrated on fully transient flows and their associated time-averaged properties (WIAS Annual Report 2002[2], [2]). More recently, we have been concerned with understanding the underlying instability mechanisms, including weakly-nonlinear mode interaction, to provide a more rational explanation for the complex unsteady processes hitherto observed. (A similar procedure has been used in our InP study (WIAS Annual Report 2003[3])). After first establishing that the critical Reynolds number (marking the onset of unsteady flow) occurred in the range (1700, 1800), we focused on five cases $(Re = 1800, 1900, 2000, 2100, 2200)$, which all demonstrated oscillatory flow behavior. A Fourier mode analysis was applied to determine the time evolutions of individual azimuthal modes, whereas the dominant frequencies were found by means of discrete Fourier transformations. In Table 1, the dominant frequencies are shown; here we have also included the results from some fully transient cases $(Re = 2500, 3000)$, where pointwise frequencies were no longer discernible, reflecting the relatively "chaotic" flow behavior in these cases.

Reynolds no. Re	crystal–crucible rotation frequency (Hz)	dominant frequency/significant other frequencies (Hz)	first active 3D mode/main 3D modes at endtime $t = t_E$	Endtime t_E (mins.)
0 – 1700	0 – 0.022	—/—	–/–	—–
1800	0.024	0.181/0.004; 0.021; 0.361	4/8; 16	22.499
1900	0.025	0.191/0.006; 0.020; 0.382	4/8; 16	21.315
2000	0.026	0.201/0.007; 0.023; 0.402	4/8; 16	20.249
2100	0.028	0.211/0.005; 0.024; 0.105	4/8; 4	19.285
2200	0.029	0.221/0.005; 0.025; 0.112	4/8; 4	18.408
2500	0.033	0.123 – 0.247/ 0 – 0.010; 0.027 – 0.033	4/ –	72.898
3000	0.039	0.173 – 0.309/ 0 – 0.017; 0.025 – 0.040	4/ –	33.749

Table 1: Major frequency responses and principal azimuthal modes for three-dimensional numerical simulations in flat-based crucibles; for the transient cases ($Re = 2500,\ 3000$) the major frequency *clusters* are noted. For the oscillatory cases ($Re = 1800$ – 2200) the dominant frequency stems from the $m = 8$ mode, and the significant other frequencies (in order of size, smallest first) from the axisymmetric mode, the $m = 1$ mode (which solely dominates the horizontal-velocity behavior near the axis), and either the first higher harmonic or subharmonic of the $m = 8$ mode. The dimensional values in the table are determined using a crucible radius $R_C = 0.077$ m, and kinematic viscosity $\nu = 4.88 \times 10^{-7} \mathrm{m}^2\mathrm{s}^{-1}$ (Rehse et al. [4]).

[2] http://www.wias-berlin.de/publications/annual-reports/2002/node46.html

[3] http://www.wias-berlin.de/publications/annual-reports/2003/node50.html

It is clear from the oscillatory cases that the most unstable linear mode is $m = 4$, but as demonstrated in Figure 1, the dominance of this mode is short-lived, and it quickly gives way to the (nonlinearly-induced) modes $m = 8$ and $m = 16$; in this figure, we have focused on the temperature at the point (0.75*R_C, 0.33*H), where R_C is the radius of the crucible and H is the height of the melt ($H = 0.3 \times R_C$), but we note that the general pattern of behavior observed here is essentially unchanged for other quantities and at other non-axial locations within the crucible.

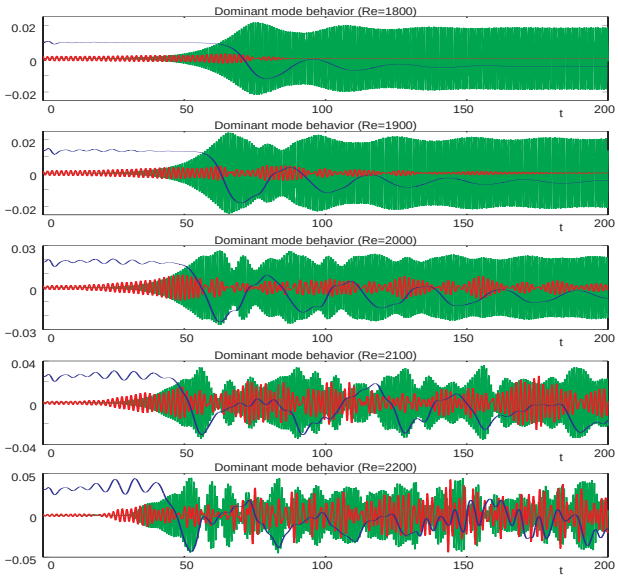


Fig. 1: Time histories of the Fourier cosine modes $m = 0$ (dark), 4 (medium dark), 8 (light) of the temperature at $(0.75 \times R_C,\ 0.33 \times H)$ for $Re = 1800 - 2200$ with $Gr = 1.36 \times Re^2$ in each case

In Figure 2, a snapshot of the temperature is given for the case $Re = 1800$, where the importance of the $m = 8$ mode can clearly be seen. (Some higher harmonics——$m = 8k_i,\ i = 1, \ldots, r$, say——are also active we note, but these do not affect the observed 8-fold azimuthal symmetry, since the greatest common divisor of the dominant modes is 8, i.e. gcd$(8, 8k_1, \ldots, 8k_r)$=8.) In contrast, for $Re = 2500$ no such simple periodic behavior can be observed (see Figure 3).

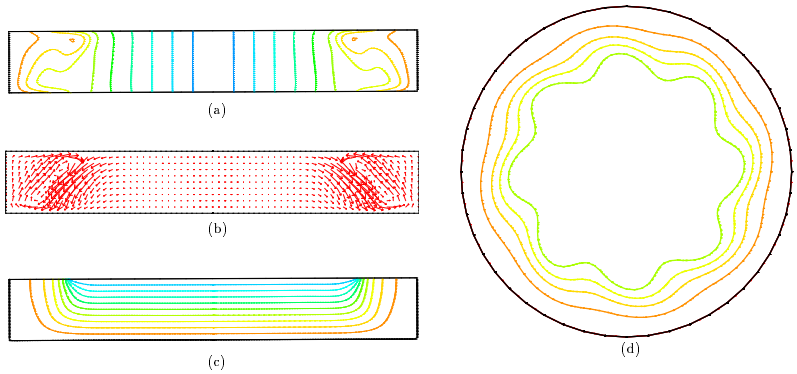


Fig. 2: Snapshots at $t = 193.2$ for iso-rotation with $Re = 1800$, $Gr = 4.4064 \times 10^6$. Results show (a) azimuthal velocity component, (b) velocity projection, (c) temperature contours, all in the same vertical plane, and (d) temperature contours in the midheight plane $(0.5 \times H)$. In (a) the contours range from 0 (axis) to 1 (wall), in (c) from 0 (crystal) to 1 (wall/base), and in (d) decrease in value inwards from wall (value 1), in each case in intervals of 0.1.

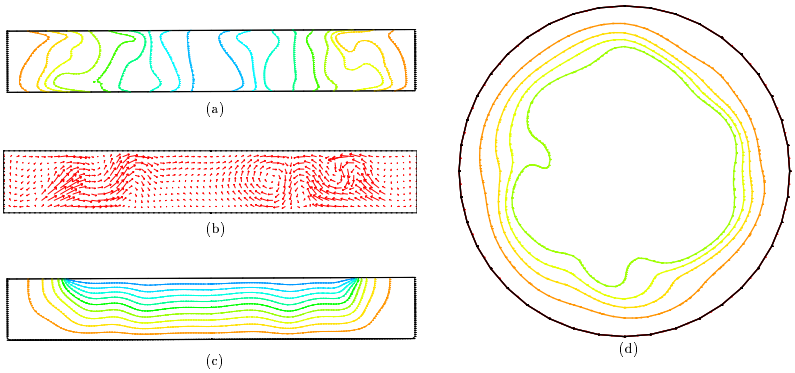


Fig. 3: Snapshots at $t = 535$ for iso-rotation with $Re = 2500$, $Gr = 8.5 \times 10^6$. Results show (a) azimuthal velocity component, (b) velocity projection, (c) temperature contours, all in the same vertical plane, and (d) temperature contours in the midheight plane ($0.5 \times H$). In (a) the contours decrease in value from 1 (wall), in (c) they range from 0 (crystal) to 1 (wall/base), and in (d) they decrease in value inwards from wall (value 1), in each case in intervals of 0.1.

References

1. E. BÄNSCH, D. DAVIS, H. LANGMACH, W. MILLER, U. REHSE, G. REINHARDT, M. UHLE, *Axisymmetric and 3D calculations of melt-flow during VCz growth*, J. Crystal Growth, **266** (2004), pp. 60–66.

2. E. BÄNSCH, D. DAVIS, H. LANGMACH, G. REINHARDT, M. UHLE, *Two- and tree-dimensional transient melt-flow simulation in vapour-pressure-controlled Czochralski crystal growth*, 2004, submitted.

3. W. MILLER, U. REHSE, *Numerical simulation of temperature and flow field in the melt for the vapour-pressure-controlled Czochralski growth of GaAs*, Crys. Res. Technol., **36** (2001), pp. 685–694.

4. U. REHSE, W. MILLER, CH. FRANK, P. RUDOLPH, M. NEUBERT, *A numerical investigation of the effects of iso- and counter-rotation on the shape of the VCz growth interface*, J. Crystal Growth, **230** (1997), pp. 143–147.

Robustness of mixed FE methods for a generalized Stokes equation

Collaborator: H. Langmach

Cooperation with: A. Linke (Freie Universität Berlin (DFG Research Center MATHEON))

Supported by: DFG Research Center MATHEON, project C2

One important application for solving the Navier–Stokes equation at WIAS has been the flow simulation of crystal melts in Czochralski crystal growth. This research is continued by the project C2 at the DFG Research Center MATHEON.

The simulation of crystal growth makes very high demands on available computing time. Typically, the three-dimensional simulation of small model problems for industrial crystal growth with our efficient Navier–Stokes solver NAVIER needs computing time in the order of weeks.

This has to be reduced by new software techniques delivered by `pdelib2` and new mathematical methods and algorithms.

On the mathematical side the focus lies on robust discretization and robust iterative solvers for the Navier–Stokes equations. As shown below, the standard Taylor–Hood ($P^{k+1} - P^k$) discretization for the Navier–Stokes equation does not fully accomplish these robustness requirements. Therefore, we consider alternative discretization methods. We started with the implementation and investigation of the stabilized P1-P1 element. This element is used for preconditioning purposes.

Non-robustness of the Taylor–Hood element Let us look at the following simple model problem, a stationary generalized Stokes problem:

$$\begin{aligned} -\frac{1}{Re}\Delta\mathbf{u} + \nabla p &= f \quad \text{in } \Omega, \\ \nabla \cdot u &= 0 \quad \text{in } \Omega, \\ u &= 0 \quad \text{on } \partial\Omega. \end{aligned} \tag{1}$$

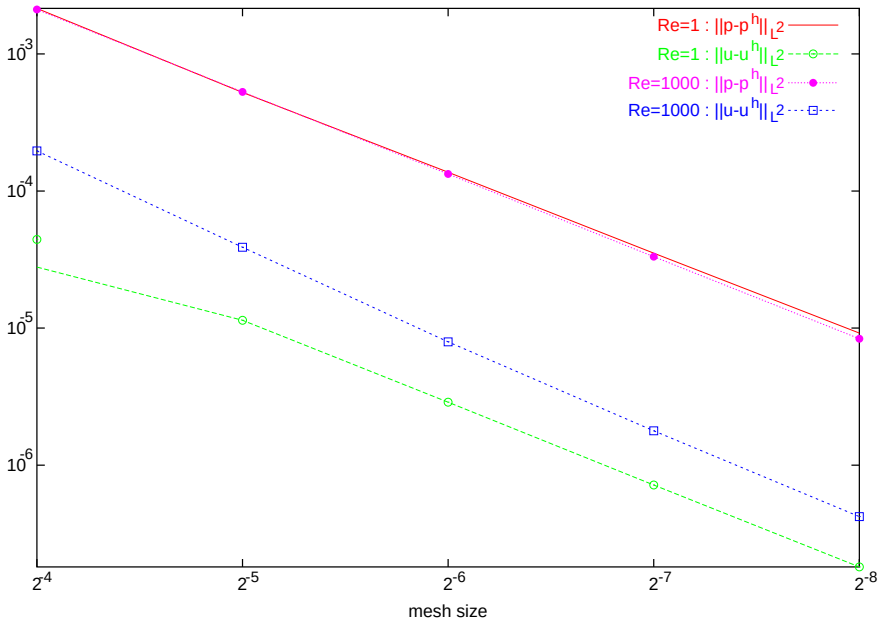
Let $(\mathbf{u}^h, p^h)$ denote the discrete solution of (1) obtained by the Taylor–Hood ($P^{k+1} - P^k$) mixed finite element method. Then one can derive the following a priori FEM error estimate 1

$$h|\mathbf{u} - \mathbf{u}^h|_{H^1} + ||\mathbf{u} - \mathbf{u}^h||_{L^2} \leq Ch^2(|\mathbf{u}|_{H^2} + Re|p|_{H^1}), \tag{2}$$

where C depends on Ω. In the case that Re is high, the second term in the error estimate possesses a large weighting factor. This effect can be reproduced numerically ([1]) and is not limited to the Taylor–Hood element family. For the Navier–Stokes equation, one can make a similiar observation.

Robustness of the P1-P1-stab element In 2004, the implementation of a stabilized P1-P1 element for Stokes equations using `pdelib2` has been completed. This will be used for preconditioning by algebraic multigrid methods. Stabilized P1-P1 elements have interesting robustness properties in respect of high Reynolds number flow ([2]), but have a low approximation order. The robustness is shown by the following numerical study. The example is taken from [1] and is typical for the kind of investigated problems. We look for a numerical solution of [1] with $Re = 1$ and $Re = 1000$ in the unit square $\Omega = [0,1]^2$. δ is the respective optimal stability parameter. We prescribe the solution to $\mathbf{u} = (u_1, u_2)$ and p given by

$$\begin{aligned} u_1(x,y) &= 2x^2(1-x)^2(y(1-y)^2 - y^2(1-y)) \\ u_2(x,y) &= -2y^2(1-y)^2(x(1-x)^2 - x^2(1-x)) \\ p(x,y) &= x^3 + y^3 - \frac{1}{2}. \end{aligned}$$



References

1. S. GANESAN, V. JOHN, *Pressure separation — A technique for improving the velocity error in finite element discretisations of the Navier–Stokes equations*, to appear in: Appl. Math. Comput.

2. G. LUBE, M.A. OLSHANSKII, *Stable finite-element calculation of incompressible flows using the rotation form of convection*, IMA J. Numer. Anal., **22** (2002), pp. 437–461.

Simulation of microwave and semiconductor laser structures including perfectly matched layer by means of FIT

Collaborators: G. Hebermehl[4], R. Schlundt

Cooperation with: W. Heinrich, Th. Tischler (Ferdinand-Braun-Institut für Höchstfrequenztechnik, Berlin (FBH))

The electromagnetic simulation plays an indispensable part in the development of microwave circuits as well as in diode laser design, [6, 7]. Commonly the electromagnetic characteristics of the structures are described by their scattering matrix which is extracted from the orthogonal decomposition of the electric field at a pair of neighboring cross-sectional planes on each waveguide, [2]. The electric field is the solution of a two-dimensional eigenvalue and a three-dimensional boundary value problem for Maxwell's equations in the frequency domain, [4]. The surface of the computation domain is assumed to be an electric or a magnetic wall. Open-region problems require uniaxial Perfectly Matched Layer (PML) absorbing boundary conditions. At the ports, p the transverse mode field is given by superposing transmission line modes.

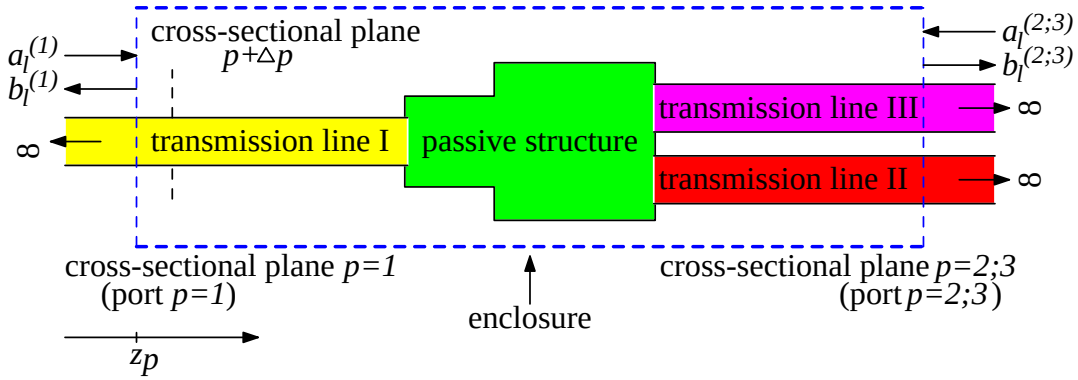


Fig. 1: The basic structure under investigation

The subject under investigation can be represented by the basic description shown in Figure 1, a structure of arbitrary geometry which is connected to the remaining circuit by transmission lines. The passive structure (discontinuity) forms the central part of the problem. Short transmission line sections are attached to it in order to describe its interaction with other circuit elements, [4].

A three-dimensional boundary value problem can be formulated using the integral form of Maxwell's equations in the frequency domain, [1]. The Maxwell equations are discretized with orthogonal grids using the Finite Integration Technique (FIT), [1, 3, 9].

$$\oint_{\partial\Omega} \vec{E}\cdot d\vec{s} = -j\omega \int_{\Omega} \vec{B}\cdot d\vec{\Omega}, \qquad \oint_{\Omega} \vec{B}\cdot d\vec{\Omega} = 0,$$

$$\oint_{\partial\Omega} \frac{1}{(\mu)}\vec{B}\cdot d\vec{s} = j\omega \int_{\Omega} (\varepsilon)\vec{E}\cdot d\vec{\Omega}, \qquad \oint_{\Omega} (\varepsilon)\vec{E}\cdot d\vec{\Omega} = 0,$$

$$\vec{D} = (\varepsilon)\vec{E}, \quad \vec{B} = (\mu)\vec{H}, \quad (\varepsilon) = \mathrm{diag}\,(\varepsilon_x, \varepsilon_y, \varepsilon_z), \quad (\mu) = \mathrm{diag}\,(\mu_x, \mu_y, \mu_z).$$

[4]Former staff member of WIAS

For the PML region in x direction, the effective permittivity and permeability are represented as follows:

$$(\varepsilon) = \begin{pmatrix} \varepsilon_x & 0 & 0 \\ 0 & \varepsilon_y & 0 \\ 0 & 0 & \varepsilon_z \end{pmatrix} \quad \longrightarrow \quad (\varepsilon)[\Lambda]_x = \begin{pmatrix} \varepsilon_x & 0 & 0 \\ 0 & \varepsilon_y & 0 \\ 0 & 0 & \varepsilon_z \end{pmatrix} \begin{pmatrix} \frac{1}{\lambda_\varepsilon} & 0 & 0 \\ 0 & \lambda_\varepsilon & 0 \\ 0 & 0 & \lambda_\varepsilon \end{pmatrix},$$

$$(\mu) = \begin{pmatrix} \mu_x & 0 & 0 \\ 0 & \mu_y & 0 \\ 0 & 0 & \mu_z \end{pmatrix} \quad \longrightarrow \quad (\mu)[\Lambda]_x = \begin{pmatrix} \mu_x & 0 & 0 \\ 0 & \mu_y & 0 \\ 0 & 0 & \mu_z \end{pmatrix} \begin{pmatrix} \frac{1}{\lambda_\mu} & 0 & 0 \\ 0 & \lambda_\mu & 0 \\ 0 & 0 & \lambda_\mu \end{pmatrix},$$

with $\lambda_\varepsilon = 1 - j\dfrac{\kappa_\varepsilon}{\varepsilon_0\omega}$, $\lambda_\mu = 1 - j\dfrac{\kappa_\mu}{\mu_0\omega}$, and $\dfrac{\kappa_\varepsilon}{\varepsilon_0} = \dfrac{\kappa_\mu}{\mu_0}$.
For edges, for example, an edge in z direction, the values (ε) and (μ) should be chosen so that $(\varepsilon) \longrightarrow (\varepsilon)[\Lambda]_x[\Lambda]_y$ and $(\mu) \longrightarrow (\mu)[\Lambda]_x[\Lambda]_y$, respectively. For corners, the (ε) and (μ) will be the product of the tensors in all three directions.

• Eigenmode problem [2]: In order to compute the three-dimensional boundary value problem, the transverse mode fields at the ports *p* (see Figure 1) have to be known. The transverse mode fields are the solutions of an eigenvalue problem. The sparse matrix is generally complex. The solutions of the eigenvalue problem correspond to the propagation constants of the modes. Using a conformal mapping, it can be shown that the eigenvalues corresponding to the few interesting modes of smallest attenuation are located in a region bounded by two parabolas. Because of the high wavenumber we can find, in general, the interesting modes only covering the region with *s* circles and calculating the eigenvalues located in these circles.

Especially, for diodes, laser frequencies of several hundred THz are common. That means, a significantly higher number of high-dimensional eigenvalue problems has to be solved with our algorithm. Additionally, using PML, the number of eigenmodes to be calculated and the iteration number of the applied Arnoldi algorithm increase. Thus, the number *s* of modified eigenvalue problems to be solved is controlled ([5]) restricting the number of required eigenvalues in one circle, the number of iterations of the Arnoldi method, and the overlapping size of the circles. The *s* eigenvalue problems can be solved in parallel.

• Boundary value problem [1]: The electromagnetic fields are computed by the solution of large-scale systems of linear equations with indefinite, complex symmetric coefficient matrices. Independent set orderings, Jacobi and SSOR preconditioning using Eisenstat's trick are applied to accelerate the speed of convergence of the used Krylov subspace method [4, 8] for the systems of linear algebraic equations.
The PML layers have a significant influence on computational efforts, which is demonstrated in Table 1 for a quasi-TEM waveguide.

References

1. K. BEILENHOFF, W. HEINRICH, H.L. HARTNAGEL, *Improved finite-difference formulation in frequency domain for three-dimensional scattering problems*, IEEE Transactions on Microwave Theory and Techniques, **40** (1992), pp. 540–546.

2. A. CHRIST, H.L. HARTNAGEL, *Three-dimensional finite-difference method for the analysis of microwave-device embedding*, IEEE Transactions on Microwave Theory and Techniques, **35** (1987), pp. 688–696.

3. G. HEBERMEHL, R. SCHLUNDT, H. ZSCHEILE, W. HEINRICH, *Improved numerical methods for the simulation of microwave circuits*, Surveys Math. Indust., **9** (1999), pp. 117–129.

4. G. HEBERMEHL, F.-K. HÜBNER, R. SCHLUNDT, TH. TISCHLER, H. ZSCHEILE, W. HEINRICH, *Simulation of microwave and semiconductor laser structures including absorbing boundary conditions*, in: Challenges in Scientific Computing – CISC2002, E. Bänsch, ed., vol. 35 of Lecture Notes Comput. Sci. Eng., Springer, Berlin, 2003, pp. 131–159.

5. ——, *Eigen mode computation of microwave and laser structures including PML*, in: Scientific Computing in Electrical Engineering, W.H.A. Schilders, S.H.M.J. Houben, E.J.W. ter Maten, eds., Mathematics in Industry, Springer, 2004, pp. 196–205.

6. G. HEBERMEHL, J. SCHEFTER, R. SCHLUNDT, TH. TISCHLER, H. ZSCHEILE, W. HEINRICH, *Simulation of microwave circuits and laser structures including PML by means of FIT*, Advances in Radio Science, **2** (2004), pp. 107–112.

7. ——, *Simulation of microwave and semiconductor laser structures including PML: Computation of the eigen mode problem, the boundary value problem, and the scattering matrix*, WIAS Preprint no. 987, 2004.

8. R. SCHLUNDT, G. HEBERMEHL, F.-K. HÜBNER, W. HEINRICH, H. ZSCHEILE, *Iterative solution of systems of linear equations in microwave circuits using a block quasi-minimal residual algorithm*, in: Scientific Computing in Electrical Engineering, U. van Rienen, M. Günther, D. Hecht, eds., vol. 18 of Lecture Notes Comput. Sci. Eng., Springer, Berlin, 2001, pp. 325–333.

9. T. WEILAND, *A discretization method for the solution of Maxwell's equations for six-component fields*, Electronics and Communication (AEÜ), **31** (1977), pp. 116–120.

Table 1: Influence of the PML layers on computational efforts. The value ω denotes the relaxation parameter of the Krylov subspace method. The order of the system of linear algebraic equations is 40 824.

	Number of Iteration					
	$\omega = 1.00$			$\omega = 1.58$		
f/GHz / Structure	10	50	100	10	50	100
no PML	63	72	127	45	53	91
z-PML	649	647	716	431	452	543
yz-PML	13 912	27 924	32 298	16 457	44 824	104 642
xyz-PML	12 307	44 723	213 358	15 983	111 965	$> 10^6$
xyz-PML (nonov.)	628	591	742	493	436	624

Process simulation in gas turbine engineering

Collaborators: J. Borchardt, F. Grund, D. Horn

Cooperation with: D. Zeitz (ALSTOM (Switzerland) Ltd., Baden)

Supported by: ALSTOM (Switzerland) Ltd., Baden

In today's gas turbine engineering, it is not only needed to increase the capacity and the efficiency of the turbines, but also to reach the highest possible reliability and to ensure a safe, economic, and environmentally acceptable operation of heavy duty industrial turbines. In modern gas-fired combined-cycle power stations, a new generation of advanced gas turbines (Figure 1) is used. These turbines use the sequential combustion technology. With this technology, the fuel is injected twice into the gas turbine, and the capacity and efficiency are increased without increasing the fire temperature. Power augmentation can be achieved, among other things, by inlet cooling and high fogging. The processes which proceed within these turbines are highly integrated, leading to complex and highly nonlinear process models. In this context, large-scale process simulation problems may arise. Using concentrated physical models, high-dimensional systems of nonlinear or differential–algebraic equations (DAEs) have to be solved in steady state or dynamic process simulation, respectively. For their solution, robust, fast, and reliable numerical simulation tools are needed.

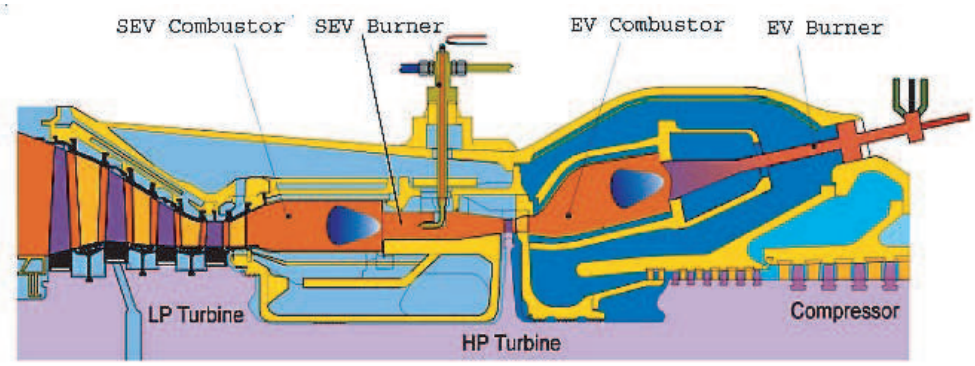


Fig. 1: Gas turbine for power stations (source: www.power.alstom.com)

To handle those large-scale process simulation problems, we have developed a simulation approach that is based on "divide and conquer" techniques. Within this approach, the modular structure of the process is exploited for an efficient numerical solution of the resulting equation system. Because the modular process structure corresponds to the hierarchical unit structure of the underlying plant, the corresponding system of equations can be structured into subsystems according to the units. Based on this structure, it can then be portioned into blocks

$$F_j(t, Y_j(t), \dot{Y}_j(t), U_j(t), \dot{U}_j(t), u(t)) = 0, \quad j = 1(1)p,$$

$$F_j : \mathbb{R} \times \mathbb{R}^{m_j} \times \mathbb{R}^{m_j} \times \mathbb{R}^{n-m_j} \times \mathbb{R}^{n-m_j} \times \mathbb{R}^q \to \mathbb{R}^{m_j}, \quad \sum_{i=1}^{p} m_j = n, \quad t \in [t_0, t_{end}],$$

where the vectors $Y_j(t)$ and $U_j(t)$ denote the unknown and coupling variables of the blocks, respectively, and $u(t)$ the parameter functions. In the steady state case, the system of DAEs degenerates to a block-structured system of nonlinear equations. To exploit the hierarchical subsystem structure of the equation system during its numerical solution, we have considerably

modified and adapted the standard methods BDF, Newton, and sparse Gaussian elimination. At the other hand, we have appropriately extended the block-partitioned system of equations, so that the approach can be efficiently parallelized on shared memory computers. Within this parallel approach, the equation blocks can be treated almost concurrently, both in the model evaluation as well as in the solution. The key part of parallelization is realized within so-called block-structured Newton-type methods, [1]. Among other things, these methods enable a controlled relaxation decoupling between blocks.

The approach has been implemented in the Block Oriented Process simulator BOP [2] that uses an own compiler to generate a hierarchically structured data interface from a process description with its modeling language MLPE (Modeling Language for Process Engineering).
In the period under report, we have continued our cooperation with ALSTOM (Switzerland) Ltd., a leading gas turbine producer. We have delivered BOP Version 2.0 to ALSTOM, where the simulator is now used for the process simulation of industrial gas turbines. It runs under the Windows XP operating system on PCs, where it is called by ALSTOMs graphical user interface *ALPEG*. Compared to the previous version, Version 2.0 of BOP contains a number of new features. Among other things, it enables a binary input/output and a direct data transfer between the Java GUI and the simulator via the Java Native Interface (JNI) and a dynamic link library. The scope of the process description possibilities has been considerably extended. The combination *ALPEG*-BOP is now in successful business use. Different versions of this simulation tool can be used by process designers or sells managers, respectively.
In continuation of this work and based on a new license agreement with ALSTOM, we have started the development of BOP Version 2.1. In this context, we have made changes to the control strategy of the steady state solver within BOP to improve its reliability and performance even in critical regions of the modeling, as, e.g., for the problem of anti-icing and the problem of discontinuous modeling with respect to the turbine operation at low part-load. Competitive simulation runs for those critical problems have shown that BOP still converges where the Aspen Custom Modeler^{TM} (ACM), a worldwide leading commercial simulation tool of Aspen Technology (USA), fails.
Additionally, we continued the implementation of advanced elements of the modeling language of ACM, whose functionality goes far beyond the scope of MLPE. With it, we have considerably enlarged the application area of BOP. These achievements will finally make it possible to use BOP for the simulation of processes described with the modeling language of ACM, without the necessity to make extensive changes in the process description. The realized language extension covers in particular complex IF-statements which can contain multiple instructions as well as procedure calls, the usage of different actions if a variable is fixed or free, the possibility of defining a new model by extending or modifying an existing one, and the possibility to include source code from a library. Beside this, new standard functions have been implemented and it is now possible to use integer, string, and logical parameters as well as global parameter-type definitions. All these new language elements can now be treated by our three-step compiler, which first analyzes the process description statements, then links the entire system, and finally generates the data and the program interface to the BOP solver. Their practicability has been tested for process descriptions of different industrial gas turbines.
Finally, we have written a documentation [2] for BOP.
For the near future it is planned to add a Monte Carlo simulation mode to the simulator BOP. It should enable probabilistic statements about the process, as, e.g., probability curves for engine power, engine efficiency, or engine exhaust energy.

References

1. J. BORCHARDT, *Newton-type decomposition methods in large-scale dynamic process simulation*, Computers and Chemical Engineering, **25** (2001), pp. 951–961.

2. J. BORCHARDT, D. HORN, *Process Simulator BOP (Version 2.0) — Documentation*, WIAS, Berlin, 2004, pp. 1–74.

3. ——, *The block oriented process simulator BOP*, submitted.

4. F. GRUND, K. EHRHARDT, J. BORCHARDT, D. HORN, *Heterogeneous dynamic process flowsheet simulation of chemical plants*, in: Mathematics — Key Technology for the Future. Joint Projects Between Universities and Industry, W. Jäger, H.J. Krebs, eds., Springer, Berlin, 2003, pp. 184–193.

Three-dimensional conforming Delaunay mesh generation

Collaborators: H. Si, J. Fuhrmann, K. Gärtner

Mesh generation is one of the crucial points for many applications of numerical methods to real-world problems. Delaunay meshes have many optimal mathematical properties which are favorite for finite element and finite volume methods. Automatically generating conforming Delaunay meshes from arbitrary 3D geometries is a problem far from having been solved in computational geometry. Our work focuses on both theoretical and practical aspects of this problem. Algorithms are needed to generate Delaunay meshes. We are developing provable and efficient algorithms. On the other hand, the program TetGen for computing 3D Delaunay meshes is continuously developing and has been improved significantly. In the year 2004, a new algorithm [1] for generating constrained Delaunay tetrahedralization has been developed and implemented. A new version (v 1.3) of TetGen [2] with many new features was released.

Constrained Delaunay tetrahedralizations A fundamental problem in mesh generation is to decompose a 3D domain Ω into tetrahedra which should respect the boundary Γ of Ω. *Constrained Delaunay tetrahedralizations* (CDTs) are variations of the Delaunay tetrahedralizations which are perfect structures for the problem. Furthermore, they are essential for getting the conforming Delaunay meshes. We have developed an algorithm [1] for triangulating any *piecewise linear complex* (PLC) into a CDT. It has two advantages over other available methods: (1) it efficiently explores the available locally geometrical information to construct the Steiner points, hence it uses less additional points, and the creation of unnecessarily short edges can be avoided; and (2) it handles small input angles automatically, there is no need to preprocess sharp corners. This algorithm has been implemented in our 3D Delaunay mesh generator TetGen [2]. The implementation shows that this algorithm can be made robust and efficient. Moreover, there is no restriction on the size and complexity of the input geometries. Two examples with complicated geometrical shapes are shown in Figure 1.

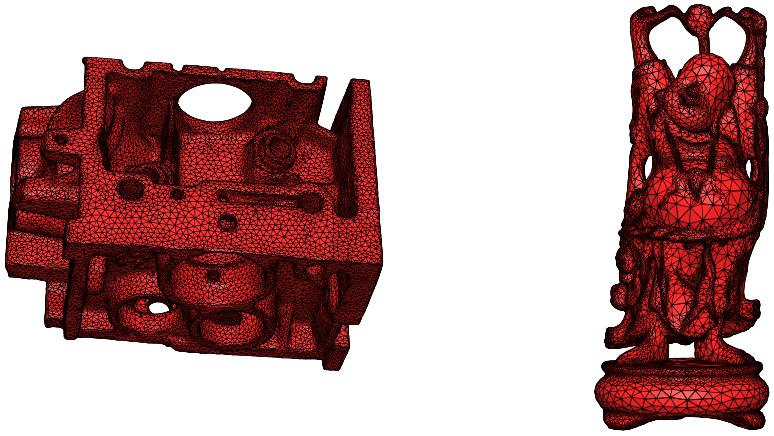


Fig. 1: Examples of constrained Delaunay tetrahedralizations. Left: A CAD model of a mechanical part. The surface mesh has 57270 nodes, 114680 triangles. Right: A computer-reconstructed model of the statue of a happy buddha. It has 31881 nodes, 65561 triangles.

TetGen Version 1.3 TetGen is a 3D tetrahedral mesh generator. It generates exact Delaunay tetrahedralizations, constrained Delaunay tetrahedralizations, and quality conforming Delaunay meshes. TetGen is written in C++ and includes a suite of state-of-the-art algorithms. It can be compiled into an executable program or a library which can be integrated into other applications. The code is highly portable and has been successfully compiled and tested on all major operating systems, e.g., Unix/Linux, MacOS, Windows, etc. It is publicly available for non-commercial use at http://tetgen.berlios.de.
Version 1.3 introduced some re-design. The year 2004 was focused on enhancing the ability to mesh geometries with arbitrarily complicated shapes. Version 1.3 includes our new constrained Delaunay tetrahedralization algorithm [1] and many other useful features such as refining pre-generated meshes, automatically detecting incorrect inputs, and so on.
Figure 2 is an example created by `pdelib2`: Adaptive mesh generation for a heat conduction problem. The pictures show a sequence of meshes refined by using the -i switch and the corresponding solutions.

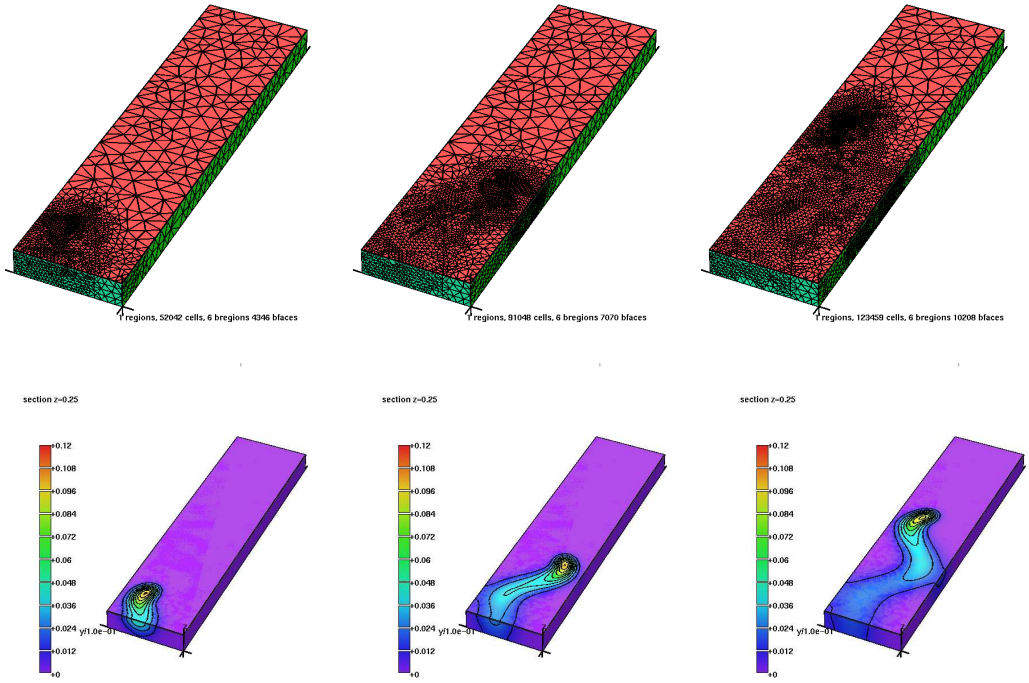


Fig. 2: Examples of adaptive mesh refinement by TetGen (use -i switch). The grid is coarse and refined again in some regions corresponding to the moving hot spot.

References

1. H. SI, K. GÄRTNER, *An algorithm for three-dimensional constrained Delaunay tetrahedralizations*, in: Proceedings of the Forth International Conference on Engineering Computational Technology, B. Toppings, C.M. Soares, eds., Civil-Comp Press, Stirling, 2004, p. 16. ISBN 0-948749-97-0 CD-ROM.

2. H. SI, *TetGen, a quality tetrahedral mesh generator and three-dimensional Delaunay triangulator, v1.3*, WIAS Technical Report no. 9, 2004.

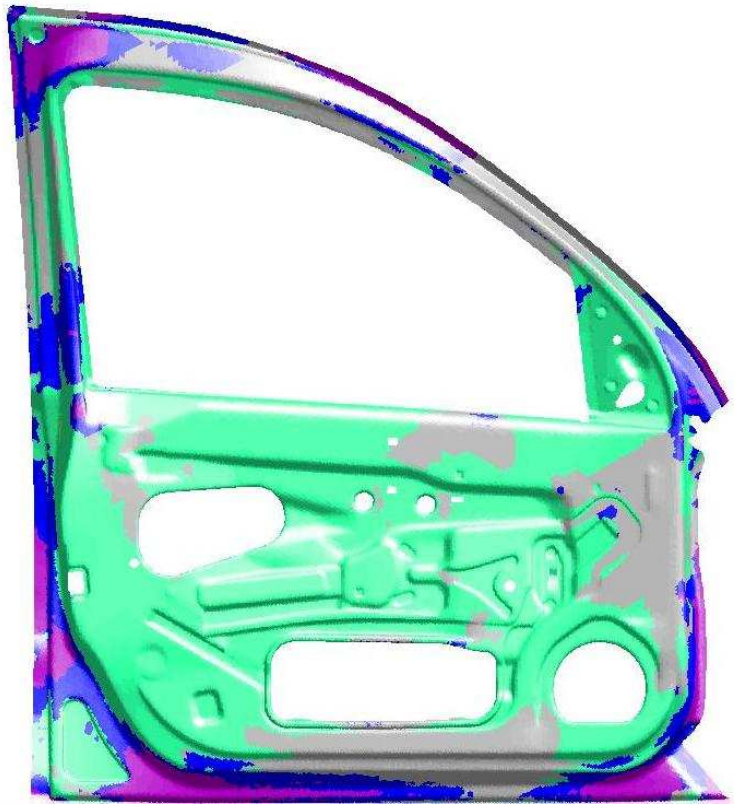
PARDISO, improvements for symmetric indefinite linear systems

Collaborator: K. Gärtner

Cooperation with: O. Schenk (Universität Basel, IFI, Switzerland)

Supported by: HP Integrity for Research Program

The work on PARDISO continued with respect to different topics, the central one was the introduction of matching algorithms and Bunch–Kaufman pivoting for indefinite symmetric linear systems. The problem is to enlarge the pivoting possibilities without introducing extraordinarily large fill-in or loosing the advantages of precomputed data dependency graphs during the parallel factorization. The present implementation uses two strategies (more exist) to construct a permutation to reduce fill-in and to make Bunch–Kaufman pivoting within the supernodes an efficient method: The permutation due to matching is split into cycles, and the cycles are broken up into smaller ones. The final permutation guarantees that supernodes are formed with respect to fill-in but include at least a cycle of length 2 or 3. Solving a symmetric linear system consisting of a two-cyclic matrix requires Bunch–Kaufman pivoting. In special circumstances regular matrices will still result in zero pivots and static pivoting. But for large classes of problems, serious progress was made. Users are now able to apply the proper level of stabilization according to the requirements of the special problem class.
With these extensions, a lot of new applications, especially optimization problems using interior point methods, can benefit from the faster factorization algorithm.
For personal academic use, the code is distributed now for many architectures via the net (see http://www.computational.unibas.ch/cs/scicomp/software/pardiso/).



A classical PARDISO application area: Sheet metal forming, Audi-TT door, green: acceptable plastic stretching, problem requires the solution of symmetric indefinite linear systems.

References

1. O. SCHENK, K. GÄRTNER, *On fast factorization pivoting methods for sparse symmetric indefinite systems*, Technical Report CS-2004-004, Universität Basel, submitted.

`pdelib` – Algorithms and software components for the numerical solution of partial differential equations

Collaborators: J. Fuhrmann, K. Gärtner, H. Langmach, M. Uhle, T. Streckenbach

Cooperation with: A. Linke, J. Bloch (Freie Universität Berlin (DFG Research Center MATHEON)), D. Hömberg (FG 4)

Supported by: DFG Research Center MATHEON, project C1, project C2

The purpose of this project is the further development of `pdelib`, a toolbox of software components for the numerical solution of partial differential equations. The re-design of the API and the code internals have reached the goal of first application projects.

Main features

- Solver kernel Application Programming Interface (API) targeted at ease of use with OpenMP or pthreads on SMP computers. User callback routines operate on *zones* consisting of a certain number of elements rather than one element;
- APIs for time step control, iterative solvers, preconditioners, bifurcation analysis;
- *fvsys* API for implementing a solver for nonlinear systems of reaction-diffusion-convection equations using the finite volume method on simplicial grids;
- Integration of the Delaunay mesh generators triangle [1] (2D) and TetGen (3D). This allows to describe geometries in the extension language Lua or in the C code and thus offers a large amount of flexibility for grid adaptation and geometry modification;
- Grid partitioning for parallel computing and cache efficiency based on the METIS [4] code;
- Parameter input and solver control can use the Lua [3] extension language;
- Online visualization of the solution process based on OpenGL using the visualization tool `gltools`.
- Components for medium complexity graphical user interfaces based on the FLTK GUI toolkit.

Focus during 2004

- In close cooperation with project C1 “Coupled systems of reaction-diffusion equations and application to the numerical solution of direct methanol fuel cell (DMFC) problems” of the DFG Research Center MATHEON, we continued the development of tools for path following and bifurcation detection for systems of partial differential equations. The methods developed in this project have been successfully integrated with the `pdelib2` solver kernel and the fvsys problem class. First benchmarks for two-dimensional problems have been run successfully.

- The `pdelib` design was extended in order to allow the implementation of solvers using higher-order finite elements on simplices, focusing on second- and third-order elements. This new API in `pdelib` was applied and tested in the implementation of an experimental solver for the Oseen problem (see page 66).
- The build system was restructured using `autoconf` and `automake`. This was motivated by the fact that, despite of some drawbacks, this is the standard build system used in the Open Source Community. Based on this work, porting to MacOS X and Microsoft Windows is now possible.
- Together with a general grid-to-grid interpolation code, Delaunay mesh generators have been tested successfully for implementing local adaptivity (see pages 74 and 90).

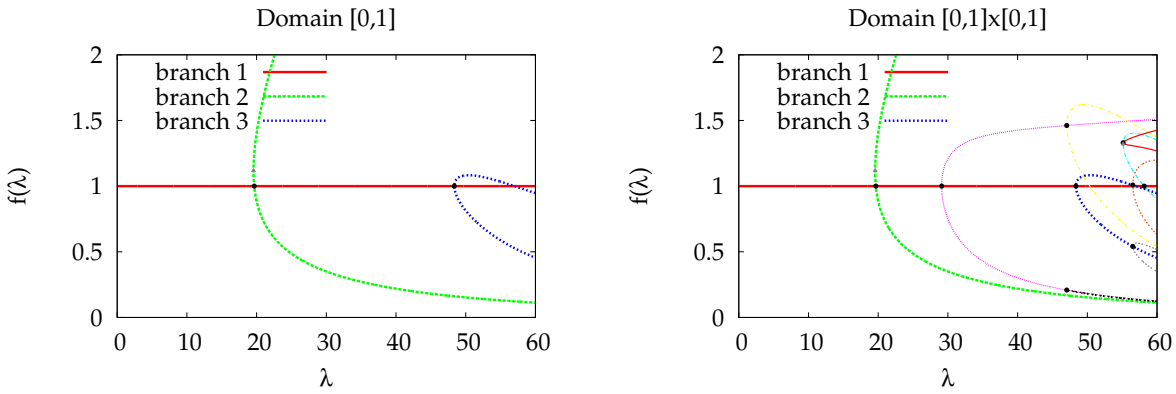


Fig. 1: Bifurcation analysis of a Brusselator model: one-dimensional domain (left) vs. two-dimensional domain (right)

References

1. J.R. SHEWCHUK, *Triangle: Engineering a 2D quality mesh generator and Delaunay triangulator*, in: Applied Computational Geometry: Towards Geometric Engineering, M.C. Lin, D. Manocha, eds. Springer, Berlin, 1996, pp. 203–222.
2. B. SPITZAK ET AL., *FLTK - the Fast Light Toolkit*. URL:http://www.fltk.org.
3. R. IERUSALIMSCHY, *Programming in Lua*, Lua.org, 2003, ISBN 85-903798-1-7. URL: http://www.lua.org.
4. G. KARYPIS, V. KUMAR, *METIS – Family of Multilevel Partitioning Algorithms*. URL: http://www-users.cs.umn.edu/ karypis/metis/

Visualization of numerical simulations and production of presentations

Collaborator: G. Reinhardt

In accordance with the scientific orientation of WIAS to engage in project-oriented research in applied mathematics with the aim of solving complex problems, the amount of data generated by (mostly three-dimensional) computer simulations is ever increasing. A typical example is unsteady weakly supercritical flow simulation of semiconductor melt in a crucible, where large computational times are needed due to the slow evolution of the flow, but also sufficiently small time steps to accurately capture underlying instability features. The visual interpretation is only possible with software tools that do not require the whole data to be stored in the main memory. Hence, in our institute the use of the visualization tool "AVS/Express" was increased significantly.

The production of VHS/SVHS videos is now essentially redundant, due to the growing efficiency of the software and hardware of computers (notably laptops) which has led to a markedly improved quality of animations.

For presentation purposes, it has been necessary to complete the design of the new corporate identity of WIAS. New flyers were produced for two research groups, while English versions of all existing flyers were created. Active support in the preparation and the realization of a so-called "Parlamentarischer Abend" ("Parliamentary Evening") was provided (creation of posters). This event involved participation by all institutes of Forschungsverbund Berlin e.V.

As a new visualization technique, the transformation of a pixel graphic to a vector graphic was required for some cases, in particular for the graphical display of mathematical functions. It led to an improved quality of the graphical display, while the required storage size was considerably decreased. For this purpose eligible software was sought and a suitable software-tool for purchase was selected. In Figure 1, the advantages of this visualization technique are demonstrated.

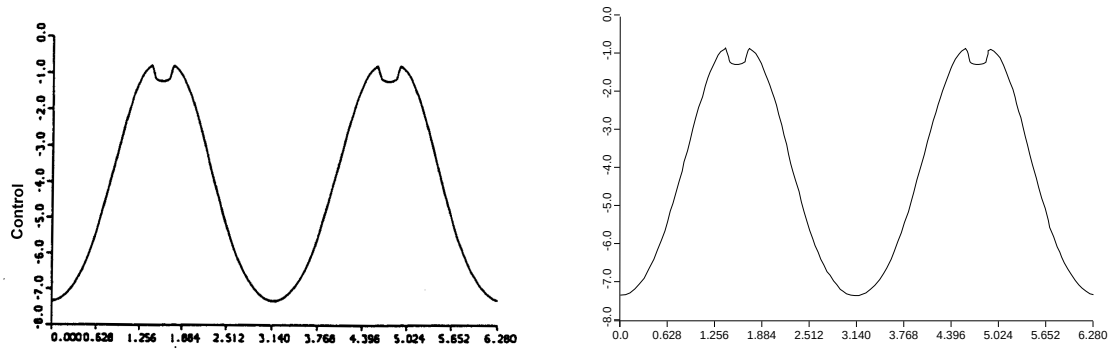


Fig. 1: Left: The pixel graphic (20 MByte). Right: The corresponding vector graphic (6.5 KByte).

4.4 Research Group Nonlinear Optimization and Inverse Problems

4.4.1 Overview

Die Forschungsgruppe untersucht hochdimensionale Optimierungsaufgaben und inverse Probleme, die in aktuellen technischen und wirtschaftlichen Anwendungen auftreten. Die Arbeit reicht von Grundlagenforschung zur Analysis und Numerik dieser Probleme über die Entwicklung effizienter Algorithmen und Software bis hin zur Lösung konkreter Praxisanwendungen. Sie wird finanziell durch Industriepartner, das BMBF und die DFG gefördert.

Die Forschung konzentrierte sich 2004 auf zwei Anwendungsfelder:

- Optimierung und inverse Probleme in der diffraktiven Optik und der Elektromagnetik,
- Optimale Steuerung von Produktionsprozessen.

Kennzeichnend für die Arbeit der Gruppe ist, dass sie in ihren Projekten langfristige Kooperationen mit Industriepartnern aufgebaut hat, die durch direkte Industriemittel, gemeinsame Drittmitteleinwerbungen und Kooperationsvereinbarungen abgesichert sind.

Weiterhin hat die Forschungsgruppe an den folgenden gruppenübergreifenden Projekten am WIAS mitgearbeitet:

- Optoelektronische Sensoren (mit Forschungsgruppe „Partielle Differentialgleichungen und Variationsgleichungen“),
- Optimale Regularität für elliptische Operatoren mit nichtglatten Daten (mit Forschungsgruppe „Partielle Differentialgleichungen und Variationsgleichungen“),

The research group investigates large-scale optimization and inverse problems occurring in current engineering and economic applications. The tasks range from basic research on analysis and numerics and the development of efficient algorithms and software to the solution of tangible application problems. Our work is financially supported by industrial partners, BMBF, and DFG.

Our research was focused in 2004 on two application fields:

- Optimization and inverse problems in diffractive optics and electromagnetics;
- Optimal control of production processes.

A characteristic feature of this group is that it has strived to build up long-term cooperations with partners from industry, which are supported by direct industrial fundings, the joint acquisition of third-party funds and the conclusion of cooperation agreements.

Moreover, the group has collaborated on the following joint projects with other research groups at WIAS:

- Optoelectronic sensors (in cooperation with Research Group “Partial Differential Equations and Variational Equations”),
- Optimal regularity for elliptic operators with non-smooth data (in cooperation with Research Group “Partial Differential Equations and Variational Equations”),

- Enveloppenfunktionsapproximation für elektronische Zustände in Halbleiter-Nanostrukturen (mit den Forschungsgruppen „Partielle Differentialgleichungen und Variationsgleichungen“ und „Numerische Mathematik und Wissenschaftliches Rechnen“).

- Envelope function approximation for electronic states in semiconductor nanostructures (in cooperation with Research Groups “Partial Differential Equations and Variational Equations” and “Numerical Mathematics and Scientific Computing”).

4.4.2 Projects

Optimization and inverse problems in diffractive optics and electromagnetics

Collaborators: J. Elschner, K. Eppler, A. Rathsfeld, G. Schmidt

Cooperation with: G. Bao (Michigan State University, East Lansing, USA), F. Courty (Technische Universität Berlin), A. Erdmann (Frauenhofer-Institut IISB, Erlangen), R. Güther (Ferdinand-Braun-Institut für Höchstfrequenztechnik, Berlin), H. Harbrecht (Christian-Albrechts-Universität zu Kiel), B. Kleemann (Carl Zeiss AG Oberkochen), R. Schneider (Christian-Albrechts-Universität zu Kiel), M. Yamamoto (University of Tokyo, Japan)

Supported by: Carl Zeiss AG Oberkochen

1. Efficient simulation and optimization tools for the diffraction by optical gratings (A. Rathsfeld and G. Schmidt).

If the periodic cross-section structure of an optical grating is determined by one or two simple profile curves, then the best method of computation for the electromagnetic field is likely to be the integral equation method. The program package IESMP (cf. [16]) of our cooperation partner Carl Zeiss Oberkochen realizes the boundary element field simulation and the subsequent determination of efficiencies and phase shifts corresponding to the reflected and transmitted modes. Last year we have started to extend the package by a spline collocation method adapted to corner profiles and thin coated layers, and this year we have finished the new version of IESMP. Now, together with `DiPoG`, we have at our disposal two independent software packages for the efficient simulation of optical gratings.

The *new version of IESMP* can deal with general polygonal profiles and is robust with respect to the thickness of the coated layer. To combine the short computing times of the old trigonometric Nyström method with the higher accuracy of the cubic spline algorithm, we have designed a hybrid discretization. Finally, we succeeded in developing a preconditioner of circulant pattern such that the preconditioned GMRES converges even in the difficult case of coated gratings of finite conductivity. Thanks to the iterations, the solution of the linear systems is faster than their assembling.

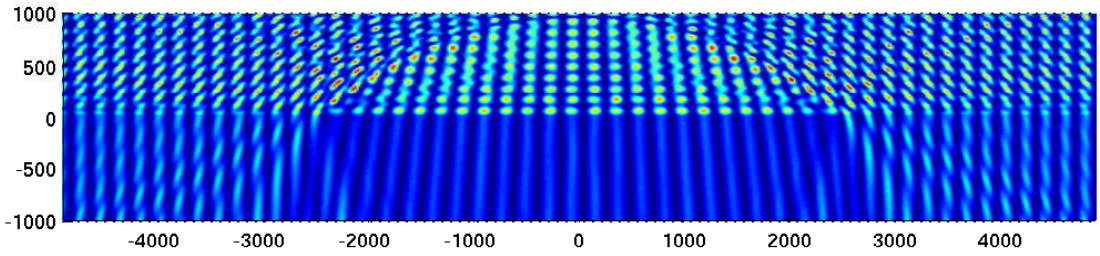


Fig. 1: Light intensity around a bubble between fluid and resist

In addition, we have continued to improve our *FEM package* `DiPoG` (cf. [17, 18]). In accordance with the requirements of our cooperation partners in Oberkochen, we have extended the class of echelle gratings. For application in lithography, a new code to simply generate gratings determined by an arbitrary set of profile curves has been added to the package. Moreover, we have included into our FEM package a code for the computation and the display

of the light intensity in periodic diffractive structures if the latter is illuminated by coherent plane waves from multiple directions.

Using DiPoG, we have performed *simulations of lithographic examples*. Figure 1 shows the 2D simulation of the intensity distribution around a bubble (shape: segment of a circle) located between an immersion fluid and a resist area. In accordance with observations and with the FDTD simulation of A. Erdmann (Erlangen), there is a dark shadow region behind the bubble which is bounded by brighter rays. Figure 2 (left) shows a silicon bridge with square shaped cross section and with a thin layer of silicon oxide (1nm) around the bridge in the case of TM polarization, and Figure 2 (right) shows the difference of the intensity compared to the bridge without oxide layer. The lithographic applications of DiPoG are to be continued next year.

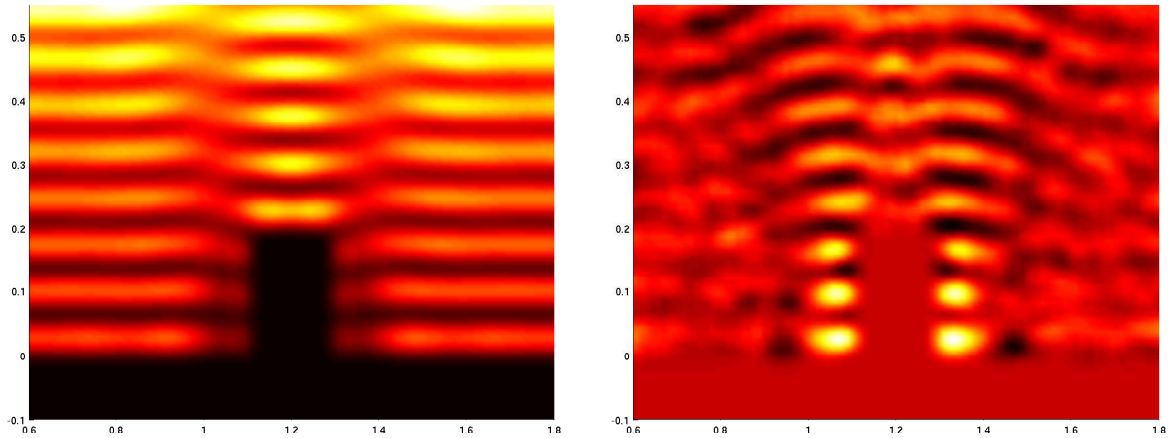


Fig. 2: Silicon bridge with oxide layer and intensity disturbance due to the oxide

For the *optimization of grating profiles* we have tested the global method of simulated annealing. Unfortunately, there is no fixed set of parameters working efficiently for general objective functions and profiles. Therefore and since our cooperation partners are mainly interested in small modifications of given scenarios, we now concentrate on local optimization methods. For the case of conical diffraction, we have implemented the computation of the gradient with respect to the parameters of general polygonal profile curves. The code is based upon the finite element representation developed in [3]. Currently, we are incorporating these gradient representations into conjugate gradient as well as into interior-point optimization algorithms.

2. Uniqueness results for inverse diffraction problems (J. Elschner).

In inverse scattering one is trying to reconstruct an object (an obstacle D) from observations of the scattered field generated by plane incident waves of frequency k. The field itself (acoustic or electromagnetic), in the simplest situation of scattering by a two-dimensional obstacle D, is a solution to the Helmholtz equation $\Delta u + k^2 u = 0$ in $\mathbb{R}^2 \setminus \overline{D}$ satisfying the homogeneous Dirichlet boundary condition $u = 0$ on ∂D (soft obstacle) or the Neumann condition $\partial_\nu u = 0$ on ∂D (hard obstacle). This solution is assumed to be the sum of a plane incident wave $u^i = \exp(ikx \cdot d)$ and a scattered wave u^s which is required to satisfy the usual Sommerfeld radiation condition at infinity. Moreover, u^s admits the representation

$$u^s(x) = r^{-1/2} u_\infty(x/r) \exp(ikr) + O(r^{-3/2}), \quad r = |x| \to \infty,$$

where u_∞ is called the *far-field pattern*.

The *inverse scattering problem* is to determine the obstacle D from the far-field pattern u_∞ for a given frequency k and possibly several incident directions d. This problem is fundamental for exploring bodies by acoustic or electromagnetic waves, and its uniqueness (in the general 2D and 3D cases) presents important and challenging open questions since many years (see, e.g., [15]). An essential progress on uniqueness results has recently been made for polygonal and polyhedral obstacles ([2], [1]).

In [5], we considered the two-dimensional inverse scattering problem of determining a sound-hard obstacle by the far-field pattern. We established the uniqueness within the class of polygonal domains by two incoming plane waves without further geometric constraints on the scatterers. This improves the uniqueness result by Cheng and Yamamoto [2]. Refining the approach of [5], it is possible to prove uniqueness in this problem for one incident wave only, which corresponds to the result of [1] for the inverse Dirichlet problem in 2D.

Combining the methods developed in [7] and [5], we were also able to prove more general uniqueness results for inverse periodic diffraction problems. The problem of recovering a periodic structure from knowledge of the scattered field occurs in many applications in diffractive optics. We continued to study the scattering of monochromatic plane waves by a perfectly reflecting diffraction grating in an isotropic lossless medium, which is modeled by the Dirichlet problem (transverse electric polarization) or the Neumann problem (transverse magnetic polarization) for the periodic Helmholtz equation. First uniqueness theorems for 2D inverse periodic transmission problems appeared in [4]; see also Annual Research Report 2003, p. 102, for a preliminary version.

Let the profile of the diffraction grating be given by a 2π-periodic curve Λ, and suppose that a plane wave given by

$$u^i := \exp(i\alpha x_1 - i\beta x_2), \quad (\alpha,\beta) = k(\sin\theta,\cos\theta)$$

is incident on Λ from the top, where the wave number k is a positive constant and $\theta \in (-\pi/2,\pi/2)$ is the incident angle. The *inverse problem* or the *profile reconstruction problem* can be formulated as follows:

Determine the grating profile Λ from the wave number k, possibly several incident directions θ and the scattered field on a straight line $\{x \in \mathbb{R}^2 : x_2 = b\}$ above the structure.

Extending the results of [7] to general piecewise linear grating profiles (which are not necessarily given by the graph of a function), we proved that a polygonal interface Λ is always uniquely determined by two different incident directions in the Dirichlet case and by four incident waves in the Neumann case, [6]. Here we exclude the standard non-uniqueness examples of two parallels to the x_1 axis, which are not relevant for applications. Contrary to bounded obstacle scattering, it can be shown by appropriate counter examples that a smaller number of measurements is not sufficient in general. However, if one avoids the Rayleigh frequencies, then one incident direction is enough to determine the profile in the inverse Dirichlet problem.

3. Shape optimization for elliptic problems by integral equation methods (K. Eppler).

The main aim of the present work is to develop and test efficient optimization algorithms for the minimization of integral functionals, depending on the solution of an elliptic boundary value problem with a special emphasis on second-order methods. Contrary to classical control problems, the domains themselves, resp. their boundary serve as the variable or unknown in shape optimization problems. Based on a related shape calculus, complete boundary integral

representations for the shape gradient and the shape Hessian provide update rules directly for the boundary. In some specific cases, integral equation methods using wavelet compression techniques for the numerical computation of the state turn out to be a powerful tool. We refer to [8], [9] for basic concepts of the proposed method. In particular, the following applications have been investigated.

- *Exterior electromagnetic shaping of liquid metals.* For a given external magnetic field, generated by conductors, the aim is to compute the free surface of liquid metal by means of shape optimization techniques.

  The 2D problem: A cylindrical vertical column of molten metal with a prescribed area for the cross section is falling down in a magnetic field, generated by conductors (Dirac masses or circular conductors with finite radii ε). The algorithm computes the unknown surface of the cross section (see [10]). Within an overall computational time of about 90 sec., the underlying PDE is solved on several dozens (≈ 50) of different exterior domains in the test cases.

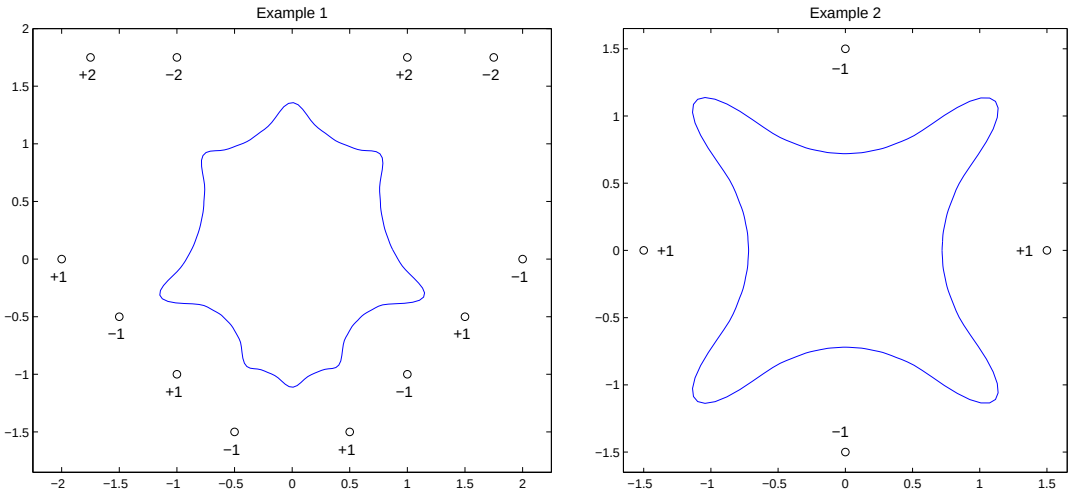


Fig. 3: Computed cross sections for Example 1 (left) and Example 2 (right)

The 3D analog: The algorithm computes the shape of a bubble $\Omega \subset R^3$ ($|\Omega| = V_0$) of liquid metal, levitating in a magnetic field generated by polygonal wires (see [11]).

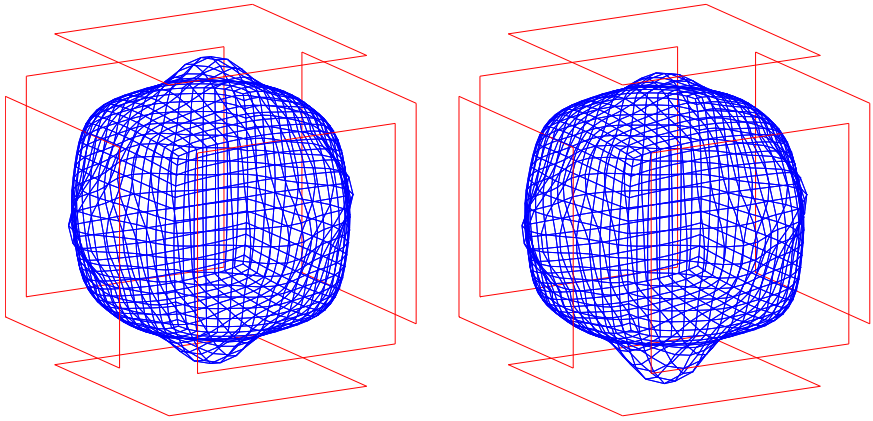


Fig. 4: Resulting bubbles of liquid metal without (left) and with (right) gravitational force

- *A shape identification problem from electrical impedance tomography.* We implemented and tested the method for identifying a perfectly conducting obstacle within a background material of constant conductivity by measuring simultaneously voltage and current on the outer boundary. We proved the compactness of the shape Hessian at the optimal shape, which is strongly related to the known exponential illposedness of the underlying identification problem, [12]. In particular, a regularization technique for the shape Hessian provides more stability for the second-order method. We refer to [13] for the extension to 3D and related numerical results.

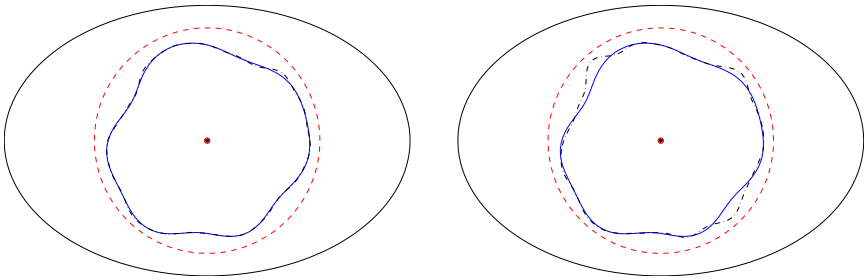


Fig. 5: Initial guess (red) and final approximation (blue) of the inclusion for 33 Fourier coefficients in case of the regularized Newton method (left) and the quasi-Newton method (right). The black line indicates the outer boundary.

- Finally, we investigated *free boundary problems*, arising, for example, in chemical processing, [14]. In particular, we proved strong coercivity estimates w.r.t. $H^{1/2}(\Gamma^\star)$ for the shape Hessian of stationary domains, implying the validity of sufficient second-order optimality conditions. Moreover, such estimates ensure numerical stability for related optimization algorithms and are important ingredients towards a convergence proof, if related finite-dimensional auxiliary optimization problems are appropriately chosen.

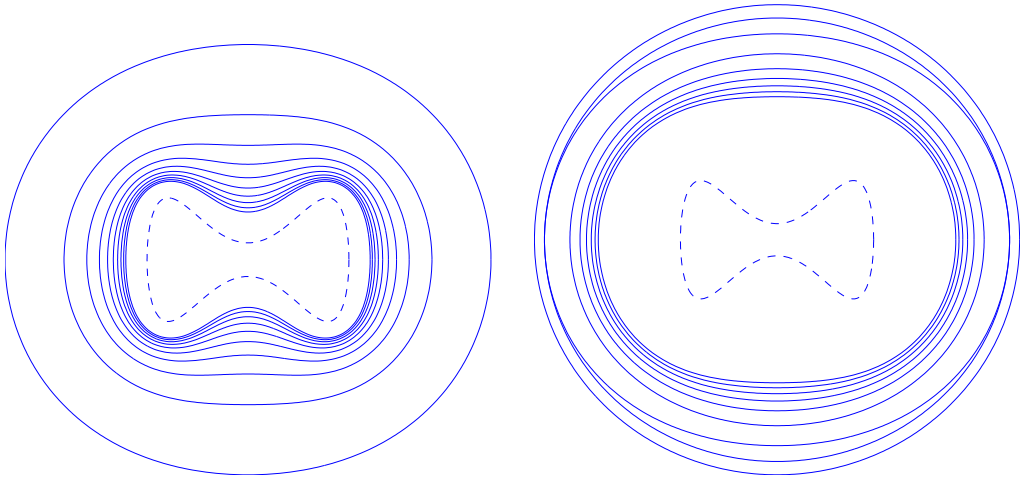


Fig. 6: Computed free boundaries for Example 1 (left) and Example 2 (right)

References

1. G. ALESSANDRINI, L. RONDI, *Determining a sound-soft polyhedral scatterer by a single far-field measurement*, to appear in: Proc. Amer. Math. Soc.

2. J. CHENG, M. YAMAMOTO, *Uniqueness in an inverse scattering problem within non-trapping polygonal obstacles with at most two incoming waves*, Inverse Problems, **19** (2003), pp. 1361–1384.

3. J. ELSCHNER, G. SCHMIDT, *Conical diffraction by periodic structures: Variation of interfaces and gradient formulas*, Math. Nachr., **252** (2003), pp. 24–42.

4. J. ELSCHNER, M. YAMAMOTO, *Uniqueness results for an inverse periodic transmission problem*, Inverse Problems, **20** (2004), pp. 1841–1852.

5. ——, *Uniqueness in determining polygonal sound-hard obstacles*, to appear in: Appl. Anal.

6. ——, *Uniqueness in determining polygonal periodic structures*, in preparation.

7. J. ELSCHNER, M. YAMAMOTO, G. SCHMIDT, *An inverse problem in periodic diffractive optics: Global uniqueness with a single wave number*, Inverse Problems, **19** (2003), pp. 779–787.

8. K. EPPLER, H. HARBRECHT, *Numerical solution of elliptic shape optimization problems using wavelet-based BEM*, Optim. Methods Softw., **18** (2003), pp. 105–123.

9. ——, *2nd order shape optimization using wavelet BEM*, to appear in: Optim. Methods Softw.

10. ——, *Exterior electromagnetic shaping using wavelet BEM*, to appear in: Math. Methods Appl. Sci.

11. ——, *Fast wavelet BEM for 3D electromagnetic shaping*, to appear in: Appl. Numer. Math.

12. ——, *A regularized Newton method in electrical impedance tomography using shape Hessian information*, WIAS Preprint no. 943, 2004, to appear in: Control Cybernet.

13. ——, *Shape optimization for 3D electrical impedance tomography*, WIAS Preprint no. 963, 2004, submitted.

14. ——, *Efficient treatment of stationary free boundary problems*, WIAS Preprint no. 965, 2004, submitted.

15. V. ISAKOV, *Inverse Problems for Partial Differential Equations*, vol. 127 of Appl. Math. Sci., Springer, New York, 1998.

16. B. KLEEMANN, *Elektromagnetische Analyse von Oberflächengittern von IR bis XUV mittels einer parametrisierten Randelementmethode: Theorie, Vergleich und Anwendungen*, Forschungsberichte aus den Ingenieurwissenschaften, Mensch & Buch Verlag, Berlin, 2003.

17. A. RATHSFELD, *DIPOG-2.0, User guide, Direct problems for optical gratings over triangular grids*, WIAS Technical Report no. 7, 2004.
URL: http://www.wias-berlin.de/software/DIPOG

18. G. SCHMIDT, *Handbuch DIPOG-1.4*, WIAS Technical Report no. 8, 2004.
URL: http://www.wias-berlin.de/software/DIPOG

Optimal control of production processes

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Supported by: DFG-Forschungszentrum MATHEON, projects C7 & C11; Rücker GmbH; Volkswagen AG

1. Mean risk models for electricity portfolio management (R. Henrion).

Continuing the work initiated in this project, the focus was on scenario reduction in stochastic optimization. The multistage decision/observation structure of optimization problems with random data (like electricity demands or prices in power generating systems) is usually reflected in a scenario tree. Figure 1 (upper part) shows an example of a 4-stage tree with 7 branches at each node where branching probabilities are visualized by different gray values.

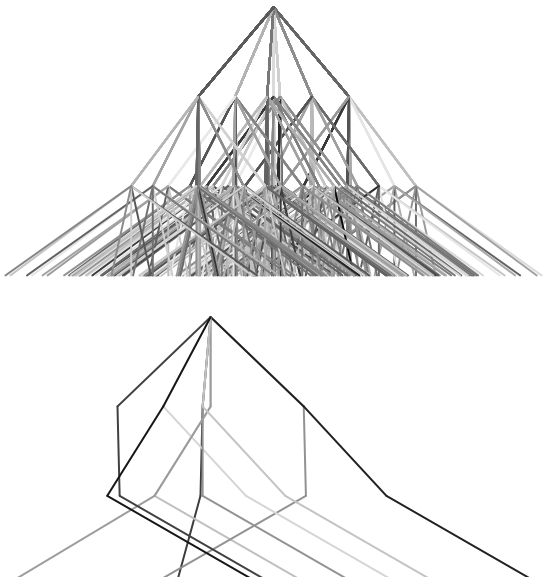

Fig. 1: Reduction of a scenario tree based on discrepancy distances

The optimization problem induced by such trees may become too large to be solved efficiently. Hence, a careful reduction of such trees is a crucial prerequisite for their solution. The modification of a scenario tree can be interpreted as a perturbation of the underlying probability measure. A theoretically sound approach of carrying out such reduction relies on the use of suitable probability metrics which are well adapted to the problem class, [11]. Efficient scenario reduction algorithms have been obtained before in the case of purely continuous

decision variables, [3]. A new challenge arises in case of additional discrete decision variables (e.g., on/off decisions for power generating units). The class of probability metrics to be considered then, in order to ensure that the reduced tree stays close to the original one, is given by discrepancy distances based on rectangles or cells. A solution method based on linear programming and capable of dealing with all discrepancy-type distances has been developed and implemented. Figure 1 (lower part) shows a reduced set of 10 out of originally 343 scenarios (again with gray values corresponding to probabilities) which minimizes the (cell-) discrepancy distance to the original tree.

Further works related to this project were concerned with solution stability in stochastic optimization ([4]), error bounds in nonlinear optimization ([5, 1]), and structural properties of quasi-concave probability measures ([6]).

2. Optimal control of surface heat treatments (D. Hömberg, W. Weiss).

In [12], a simplified version of a thermomechanical model of phase transitions in steel ([7]) has been considered. Disregarding the transformation plasticity, numerical simulations with density depending on temperature and phase volume fractions show that the model is capable of reproducing the typical thermomechanical behavior of materials exhibiting phase transitions. Figure 2 shows the results of a numerical simulation where the lateral boundary of a steel cylinder has been cooled so fast that only martensite is produced. On top, one can see the evolution of temperature in the core and at the boundary of the cylinder. In the middle, the growth of the martensitic phase is depicted. The picture at the bottom shows the evolution of thermal stresses. Especially two stress reversals can be seen, which is a typical feature of materials exhibiting phase transitions during cooling.

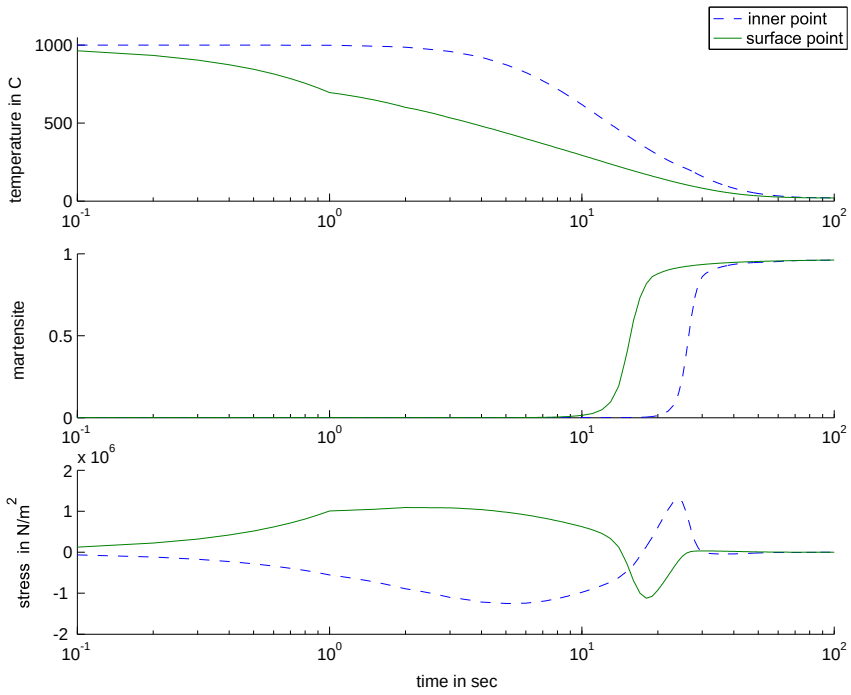

Fig. 2: Evolution of temperature (top), phase volume fractions (middle), and thermal stress (bottom) for core and boundary of a cylinder cooled at the lateral boundary

Disregarding furthermore the temperature dependency of the density of the different phases and assuming instead that the main effect stems from the different thermal expansions of the

respective phases, control problems for the resulting thermomechanical problem have also been investigated in [12].

Another natural approach is to generalize the usual equations of linearized thermoelasticity for the case of materials with phase transition by incorporating phase-dependent thermal expansion coefficients via a mixture ansatz. While in [8] a contact problem for such a model has been investigated, the aim of [2] is to investigate the related control problem.

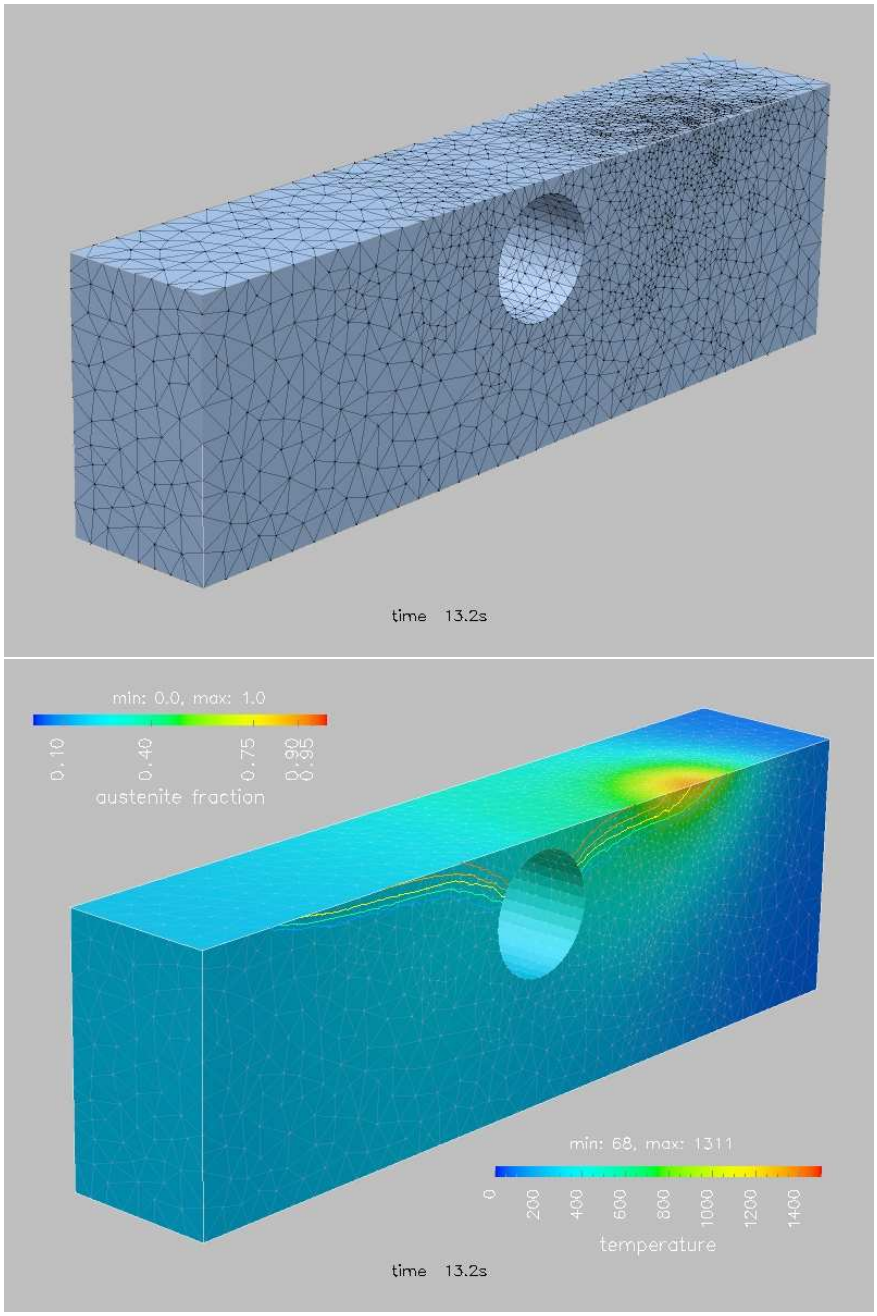

Fig. 3: Snapshot of a simulation of laser surface hardening: adaptively refined grid (top), temperature and isolines of austenite volume fraction (bottom)

Concerning laser surface treatments, we have started to exploit the adaptivity features of `pdelib2` in collaboration with Research Group 3 (see page 77). As a first result, Figure 3 shows a snapshot of a laser hardening simulation. On top, the adaptively refined grid which

moves with the laser focus is depicted. At the bottom, one can see the temperature and isolines of the austenite volume fraction. To resolve the thin austenitic layer, a second grid had to be introduced.

As has been described in last year's report, an efficient PID algorithm has been developed for controlling laser material treatments. As a partial justification for this approach we could prove the exact controllability of a linear parabolic equation along a curve. The result can also be extended to a semilinear heat equation (cf. [10]).

3. Path planning for industrial robots and human models in automotive industry (I. Bremer, R. Henrion, W. Weiss).

According to the demands of our cooperation partner, our work last year was centered around three tasks: time-optimal path-planning avoiding collisions, path-planning and simulation of cooperative robots, and a comparison between virtual reality and real world, to assure that robotic movements in a virtual shop-floor environment take the same time as in reality.
An additional challenge in this project is to maintain the real-time capabilities of complete shop-floor simulations including more than 100 active robots and further components.

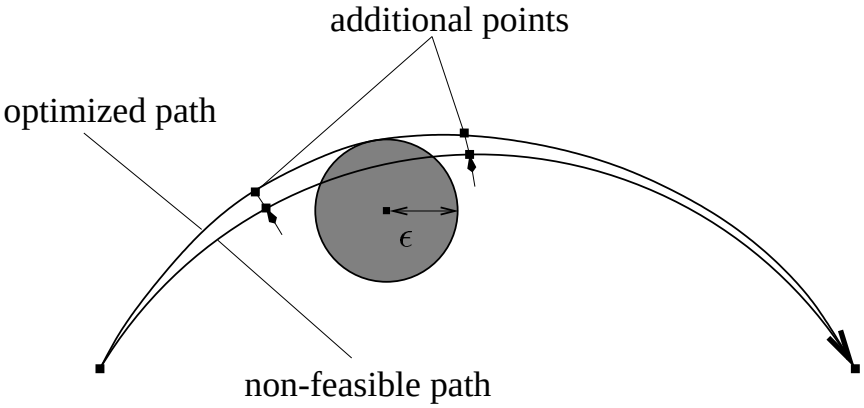

Fig. 4: Avoidance of collisions with ε tolerance by including additional auxiliary points in the robot path

To avoid collisions between a robot and its surrounding, one has to compute a time-optimal path respecting a prescribed minimal distance to all objects in the scene. The circumvention of barriers is realized by introducing additional points in the robot path. If one uses the real geometry of theses barriers, the problem is high-dimensional and time-consuming. Instead, the geometries of the barriers are approximated by simple geometries, e.g., balls. Then the problem is reduced to computing the coordinates of additional auxiliary points in the robot path to obtain a time-optimal path which respects the minimal distance to a given point (cf. Figure 4).

A typical situation in which the employment of cooperative robots is beneficial is the case of one robot moving a workpiece with a gripper while another one performs some spot-welding tasks on that workpiece (cf. Figure 5). Compared to the usual inverse kinematics problem for one robot, the number of degrees of freedom is increased by 1 to 6, depending on prescriptions for the path of the partner robot. To compute a common pair of positions, an SQP method is used to minimize the position error subject to angle constraints in the robotic joints.

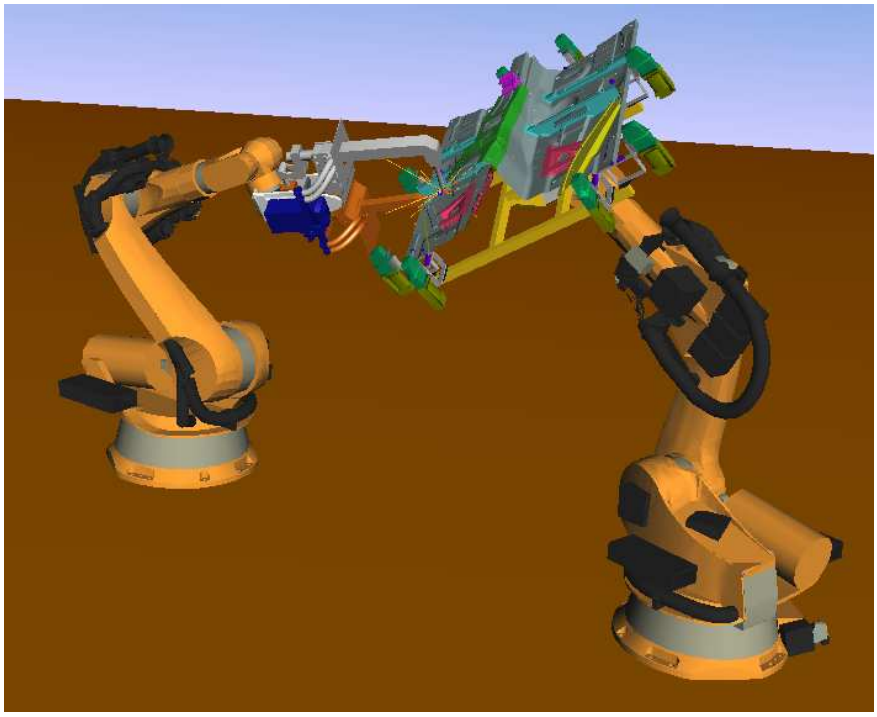

Fig. 5: Spot-welding of a car component using two cooperative robots

4. Modeling and parameter identification for cost parameters of car factories (D. Hömberg, W. Weiss).

The aim of the project is the development of cost models in cooperation with our partner Volkswagen AG. The investments for the building of a car factory depend on a number of different variables, for example, the size of the cars, the produced number of cars per day, and the size of that part of the car which is really assembled in the respective factory. The typical number of variables is small, e.g., five. If the investment is known as a function of these variables, it is possible to optimize the costs for building a factory.

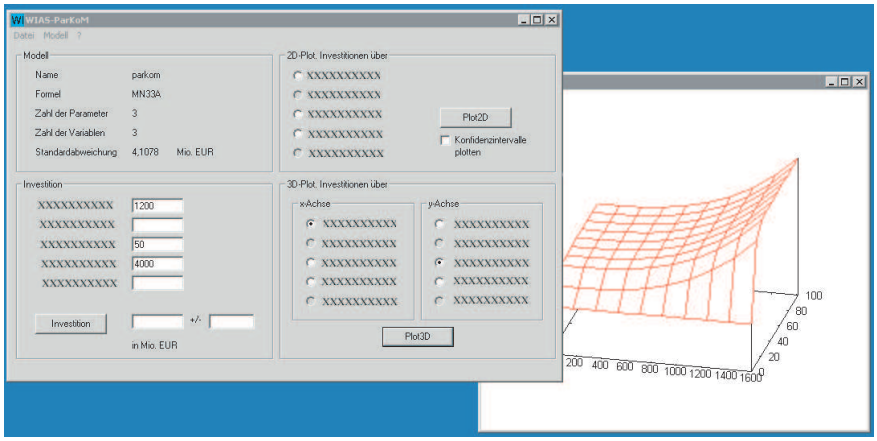

Fig. 6: Screenshot of `WIAS-ParKoM`. Here "$X\ldots$" represent different confidential variables.

Unfortunately, there exist only few data sets of really existing factories in order to determine a decent cost model. Therefore, the desired formula should contain only a small number of free parameters, which may be determined by using the data of the really existing factories. Thus the most important part of the project was to find appropriate cost models based on plausible

assumptions which are able to reproduce the given data with only few parameters and on the other hand allow for an extrapolation outside the given range of parameter values.

To solve the nonlinear regression problem, the software `WIAS-ParKoM` has been developed (cf. Figure 6). The free parameters in the model are determined by a hybrid optimization strategy. First a random search is used to find different possible local solutions, and then a conjugate gradient method is used to single out the best global solution. The software `WIAS-ParKoM` allows for calculating and plotting costs for arbitrary values of the variables together with the corresponding confidence intervals.

References

1. P. BOSCH, A. JOURANI, R. HENRION, *Sufficient conditions for error bounds and applications*, Appl. Math. Optim., **50** (2004), pp. 161–181.

2. C. CHELMINSKI, D. HÖMBERG, *Optimal control of a thermomechanical phase transition model*, in preparation.

3. J. DUPAČOVA, N. GRÖWE-KUSKA, W. RÖMISCH, *Scenario reduction in stochastic programming: An approach using probability metrics*, Math. Program., **95** (2003), pp. 493–511.

4. R. HENRION, W. RÖMISCH, *Hölder and Lipschitz stability of solution sets in programs with probabilistic constraints*, Math. Program., **100** (2004), pp. 589–611.

5. R. HENRION, J. OUTRATA, *Calmness of constraint systems with applications*, WIAS Preprint no. 929, 2004, to appear in: Math. Program.

6. R. HENRION, W. RÖMISCH, *Lipschitz and differentiability properties of quasi-concave and singular normal distribution functions*, 2005, submitted.

7. D. HÖMBERG, *A mathematical model for induction hardening including mechanical effects*, Nonlinear Anal. Real World Appl., **5** (2004), pp. 55–90.

8. D. HÖMBERG, A. KHLUDNEV, *A thermoelastic contact problem with a phase transition*, WIAS Preprint no. 914, 2004.

9. D. HÖMBERG, S. VOLKWEIN, W. WEISS, *Optimal control strategies for the surface hardening of steel*, in: Proceedings of the 2nd International Conference on Thermal Process Modelling and Computer Simulation, Nancy, France, March 31 – April 2, 2003, S. Denis, P. Archambault, J.-M. Bergheau, R. Fortunier, eds., vol. **120** of J. Physique IV, EDP Sciences, 2004, pp. 324–335.

10. D. HÖMBERG, M. YAMAMOTO, *Exact controllability on a curve for a parabolic equation*, in preparation.

11. W. RÖMISCH, *Stability of stochastic programming problems*, in: Stochastic Programming, A. Ruszczyński, A. Shapiro, eds., Handbooks Oper. Res. Management Sci., **10**, Elsevier, Amsterdam, 2003, pp. 483–554.

12. M. SEIBOLD, *Optimale Steuerung thermomechanischer Phasenübergänge in Stahl*, diploma thesis, Technische Universität Berlin/Universität Karlsruhe, 2004.

4.5 Research Group Interacting Random Systems

4.5.1 Overview

Das Hauptinteresse unserer mathematischen Forschung galt weiterhin den stochastischen dynamischen Systemen. Die erzielten Resultate betreffen klassische Diffusionen in Potentialen, zufällige Störungen von schnell-langsamen Systemen, unendlichdimensionale Diffusionsprozesse sowie wechselwirkende Verzweigungsprozesse. Von besonderem Interesse waren Prozesse in zufälligen Umgebungen, motiviert durch Anwendungen in der Physik (ungeordnete Materialien) und Biologie (Entwicklung in räumlich inhomogenen Umgebungen). Das Konzept der Koagulations- und Fragmentationsprozesse gewinnt in den verschiedensten Anwendungen in zunehmendem Maße an Bedeutung und ist von uns aus verschiedenen Perspektiven untersucht worden, von der theoretischen Analyse bis hin zur Entwicklung leistungsfähiger Algorithmen für die Lösung der Smoluchowski-Koagulationsgleichung.

The focus of our mathematical research has continued to be on stochastic dynamical systems. The results obtained concern classical diffusions in potential drift fields, stochastic perturbations of slow-fast dynamical systems, infinite-dimensional diffusion processes, and interacting branching diffusions. Of special interest were processes in random environments, motivated by applications both in physics (disordered materials) and biology (evolution in spatially inhomogeneous environments). The concept of coagulation and fragmentation processes appears increasingly in several of the applications and has been investigated from various perspectives ranging from theoretical analysis to the development of efficient algorithms for the solution of Smoluchowski's coagulation equation.

Sowohl die Aktivitäten im Zusammenhang mit der DFG-NWO Deutsch-Niederländischen Forschergruppe als auch mit dem RDSES-Programm der ESF hatten im Jahr 2004 einen hohen Stellenwert. Zwei Workshops (in Eindhoven und Wien) wurden im Rahmen der regelmäßigen Treffen der Mitglieder der bilateralen Forschergruppe organisiert. Eine bedeutende Konferenz zum Thema Spin-Gläser auf dem Monte Veritá in Ascona im April wurde von A. Bovier und E. Bolthausen im Zusammenhang mit dem RDSES-Programm organisiert. Diese Konferenz, die sowohl von Mathematikern als auch von theoretischen Physikern sehr gut besucht wurde, verdeutlichte den derzeitigen großen mathematischen Fortschritt im Verständnis von Spin-Gläsern.

Both the activities in the context of the DFG-NWO Dutch-German bilateral research group and in the ESF program RDSES have taken a high place in the last year. Two workshops (in Eindhoven and in Vienna) were organized as meetings of the members of the bilateral research group. A major conference on spin glasses was organized by A. Bovier and E. Bolthausen in the context of RDSES on the Monte Verità, Ascona, in April. This conference highlighted recent mathematical progress in the understanding of spin glasses and was very well attended by both mathematicians and theoretical physicists.

Auf den folgenden Seiten werden die wissenschaftlichen Ergebnisse des vergangenen Jahres ausführlicher dargestellt.

The following pages report on the scientific achievements of the past year in more detail.

4.5.2 Projects

Stochastic dynamics

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Supported by: DFG: Dutch-German Bilateral Research Group "Mathematics of random spatial models from physics and biology", DFG Research Center MATHEON, project E1

The central issue that is addressed in this project is how to adequately describe a complex system whose dynamics is specified on a microscopic scale, on spatially coarsened macro- or mesoscopic scales in terms of an effective dynamics on different time scales inherent to the system. The emphasis here is to be put on the fact that these effective dynamics must depend, in general, on the time-scale considered. For example, while even in microscopic stochastic systems one expects generally deterministic limit dynamics for the spatially coarsened system on *short* time scales (homogenization), on much longer time scales, stochastic effects may again become relevant and may even *appear* in deterministic systems as a residual effect of the integrated short-wavelength degrees of freedom.

One of the central concepts in this context is that of *metastability* [1]. It applies to situations where the state space of a system can be decomposed into several ("quasi-invariant") subsets in which the process remains for a very long time before transiting from one such set into another. In a collaboration with F. den Hollander and F. Nardi, [3], we have studied the problem of nucleation in a model of conservative dynamics of a lattice gas ("Kawasaki dynamics"). The issue is to obtain precise information on the time it takes to form a supercritical droplet, and thus to initiate a vapor-liquid phase transition, in a super-saturated gas in some finite volume at low temperatures. This problem has been analyzed rigorously in the last few years by den Hollander, Olivieri, and Scoppola [5] and den Hollander, Nardi, Olivieri, and Scoppola [4] in dimensions two and three, respectively, using the conventional large deviation-type methods. The shortcoming of these methods is the limited precision that usually allows only to obtain the exponential rate of the nucleation times. In [3], we slightly refine the analysis of the energy landscape in the vicinity of the saddle points (critical droplets) and apply the machinery developed in [2]. As a result we obtain, as expected, striking improvements of all the estimates and are able to compute (at least for large Λ) essentially the precise values of the prefactors of the exponential rates. Interestingly, the variational problems arising in the computation of the relevant capacities are seen to be closely related to classical capacity estimates involving the free diffusion of a single particle.

A challenge for the coming years will be the extension of this analysis to finite temperatures and larger volumes.

The investigation of more complex systems with an infinity of metastable states leading to the phenomenon of "ageing" has continued rather intensely.

Work in the past year has been focused on the analysis of trap models.

The first objective was to prove some fine properties of the one-dimensional Bouchaud trap model, i.e. finding asymptotic properties of the behavior of ageing two-point functions on

time scales that are different from the right ageing scales. These properties were observed numerically, Bouchaud and Bertin [10]. Černý [11] extended the methods used in Fontes, Isopi, and Newman [12] and Ben Arous and Černý [7] to give a rigorous analytic derivation of these properties. The refined methods have also allowed to partially justify the concept of the local equilibrium introduced in Rinn, Maass, and Bouchaud [13].
Another goal was to formalize the main properties of Markov chains that lead to ageing behavior. Together with G. Ben Arous, [8], we tried to isolate several conditions that should be verified in order to prove ageing. These conditions were then used to give different, and much shorter, proofs of ageing in the Random Energy Model (first proved by Ben Arous, Bovier, and Gayrard [6]) and on the cubic lattice (proved by Ben Arous, Černý, and Mountford [9]). To verify the conditions in the REM case, we developed some new potential-theoretic methods for the simple random walk on the hypercube. The results obtained by these methods can be of independent interest.
One of the desiderata in the field is a better understanding of the relation between ageing and spectral properties of the generator of the process, as this may lead to attractive methods for the numerical analysis of such systems. As a first step we have concentrated in [14] on the Bouchaud REM-like trap model. Here the generator can be diagonalized explicitly, and precise expressions for eigenvalues and eigenfunctions were obtained. From these it was possible to derive the dynamical properties of the system on all relevant time scales. A clear connection between ageing exponents and the singularity of the limiting spectral density at the bottom of the spectrum can be traced. As a second example, we have started to analyze Sinai's random walk in a random environment. In this case, an exact diagonalization of the generator is not possible, but it is possible to compute perturbatively the eigenvalues at the bottom of the spectrum, as well as the corresponding eigenfunctions.

In another line of research, we continued our investigation of noise-induced phenomena in non-autonomous dynamical systems. Over the last years, we developed a novel approach to the mathematics of small random perturbations of singularly perturbed dynamical systems, providing a constructive method to describe typical sample-path behavior, and yielding precise estimates on atypical behavior at the same time.
One of the key applications was the phenomenon of stochastic resonance which plays an eminent rôle in many applications. Examples include climate models and neural models as well as technical applications such as ring lasers and Schmitt triggers. Studying stochastic resonance in a periodically modulated double-well potential, we had so far focused on the parameter regime in which noise-induced synchronization is observed, [15]. In this regime, with high probability, inter-well transitions are concentrated near the first instant of minimal barrier height.
One of the popular means to quantify stochastic resonance is the distribution of residence times. It can be derived from the distribution of inter-well transitions which are characterized by passage through the unstable periodic orbit separating the domains of attraction of the potential wells. While the exponential asymptotics, accessible to the classical Wentzell–Freidlin theory, is trivial, the sub-exponential asymptotics reflects the fact that the unstable orbit is generally not uniformly repelling. As first observed by Day [19], "cycling" occurs, i.e., a periodic dependence on the logarithm of the noise intensity. Generalizing results obtained last year for a class of model equations [16], the first-passage density is derived in [17], [18]. Remarkably, the density is close to an exponential one, modulated by a universal *cycling profile*, the profile depending only on the product of the period of the unstable orbit with its Lyapunov exponent. This representation holds in a large parameter regime, ranging from noise-induced synchronization to the general stochastic resonance regime.

References

1. A. BOVIER, *Metastability and ageing in stochastic dynamics*, to appear in: Proceedings of the II Workshop on Dynamics and Randomness, Santiago de Chile, Dec. 9–13, 2002, A. Maas, S. Martínez, J. San Martin, eds., Kluwer Acad. Publishers (2004).

2. A. BOVIER, M. ECKHOFF, V. GAYRARD, M. KLEIN, *Metastability and low-lying spectra in reversible Markov chains*, Comm. Math. Phys., **228** (2002), pp. 219–255.

3. A. BOVIER, TH.W.F. DEN HOLLANDER, F. NARDI, *Sharp asymptotics for Kawasaki dynamics on a finite box with open boundary*, WIAS Preprint no. 920, 2004, submitted.

4. F. DEN HOLLANDER, F.R. NARDI, E. OLIVIERI, E. SCOPPOLA, *Droplet growth for three-dimensional Kawasaki dynamics*, Probab. Theory Related Fields, **125** (2003), pp. 153–194.

5. F. DEN HOLLANDER, E. OLIVIERI, E. SCOPPOLA, *Metastability and nucleation for conservative dynamics*, J. Math. Phys., **41** (2000), pp. 1424–1498.

6. G. BEN AROUS, A. BOVIER, V. GAYRARD, *Glauber dynamics of the random energy model. II. Aging below the critical temperature*, Comm. Math. Phys., **236** (2003), pp. 1–54.

7. G. BEN AROUS, J. ČERNÝ, *Bouchaud's model exhibits two aging regimes in dimension one*, to appear in: Ann. Appl. Probab, 2005.

8. ——, *Aging on general graphs*, in preparation.

9. G. BEN AROUS, J. ČERNÝ, T. MOUNTFORD, *Aging for Bouchaud's model in dimension two*, to appear in: Ann. Appl. Probab., 2005.

10. E. BERTIN, J.-P. BOUCHAUD, *Sub-diffusion and localisation in the one dimensional trap model*, Phys. Rev. E, **67** (2003), p. 026128.

11. J. ČERNÝ, *The behaviour of aging functions in one-dimensional Bouchaud's trap model*, WIAS Preprint no. 961, 2004.

12. L.R.G. FONTES, M. ISOPI, C.M. NEWMAN, *Random walks with strongly inhomogeneous rates and singular diffusions: Convergence, localization and aging in one dimension*, Ann. Probab., **30** (2002), pp. 579–604.

13. B. RINN, P. MAASS, J.-P. BOUCHAUD, *Multiple scaling regimes in simple aging models*, Phys. Rev. Lett., **84** (2000), pp. 5403–5406.

14. A. BOVIER, A. FAGGIONATO, *Spectral characterisation of ageing: The REM-like trap model*, WIAS Preprint no. 927, to appear in: Ann. Appl. Probab., 2005.

15. N. BERGLUND, B. GENTZ, *A sample-paths approach to noise-induced synchronization: Stochastic resonance in a double-well potential*, Ann. Appl. Probab., **12** (2002), pp. 1419–1470.

16. ——, *On the noise-induced passage through an unstable periodic orbit I: Two-level model*, J. Statist. Phys., **114** (2004), pp. 1577–1618.

17. ——, *Universality of residence-time distributions in non-adiabatic stochastic resonance*, WIAS Preprint no. 957, 2004.

18. ——, *On the noise-induced passage through an unstable periodic orbit II: The general case*, in preparation.

19. M.V. DAY, *Conditional exits for small noise diffusions with characteristic boundary*, Ann. Probab., **20** (1992), pp. 1385–1419.

Disordered systems and combinatorial optimization problems

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Supported by: ESF Programme RDSES, DFG Research Center MATHEON, project E1

It has long been noted that many problems of combinatorial optimization are structurally similar to disordered systems in statistical mechanics. The maybe simplest of these problems is the *number partitioning problem*. The connection of this problem to statistical mechanics, and in particular to the random energy model, has been pointed out by St. Mertens [1], 2]. The number partitioning problem is a classical optimization problem: Given N numbers $n_1, n_2, \ldots, n_N$, find a way of distributing them into two groups, such that their sums in each group are as similar as possible. What is needed in practice is an algorithm that, when presented with the N numbers, finds the optimal partitioning as quickly as possible. Since the number of possible partitions is 2^N, simply trying them all out is not going to be a very clever way of doing this. Rather surprisingly, however, it is quite hard to do very much better, as this problem is (believed) to be $N-P$-hard, i.e. no algorithm can be found that is sure to solve the problem in a time that is polynomial in the size N!
As pointed out by Mertens, this fact can to some extent be understood by realizing that the problem is rather closely related to mean-field spin glasses, and in particular the random energy model. Of course, the occurrence of the number 2^N should already have made us suspect that. Indeed, any partition of the set $\{1,\ldots,N\}$ into two disjoint subsets, Λ_1, Λ_2, is equivalent to a spin configuration $\sigma \in \mathcal{S}_N$ via $\Lambda_1 \equiv \{i : \sigma_i = +1\}$ and $\Lambda_2 = \equiv \{i : \sigma_i = -1\}$. Moreover, the quantity to be minimized is

$$\left| \sum_{i\in\Lambda_1} n_i - \sum_{i\in\Lambda_2} n_i \right| = \left| \sum_{i=1}^{N} n_i \sigma_i \right| \equiv H_N(\sigma).$$

This is a spin-system Hamiltonian depending on the parameters n_i. While statistical mechanics will not provide algorithms that solve this problem, they will say something about the solutions, i.e. the minimum, and more generally, the energy landscape. This should then be useful to people who want to find algorithms.
The properties of the optimal solutions conjectured by Mertens can be described as follows:

(i) Optimal partitions have a discrepancy of the order $C(N) = 2^{-N+1}\sqrt{\frac{2\pi N}{12}}$.

(ii) The discrepancies of the best, second best, etc. partitions, when divided by $C(N)$, converge to the standard Poisson process on $\mathbb{R}_+$.

(iii) The k best partitions are independently and uniformly distributed in the space of partitions, and, in particular, have maximal distance from each other.

Borgs et al [4], [3] proved that this conjecture is true.
In [5], we proved an analogous result in the generalized case when N numbers are to be partitioned into $k \geq 2$ groups (of equal cardinality) in such a way that the sums in each group are to be as similar as possible. We considered the successive differences of the sums in each

group, and showed that the properly rescaled vector of these differences converges to a Poisson point process on $\mathbb{R}^{k-1}$. This problem turned out to be much harder than expected, due to the possibility of linear relations. A key element in the proof is a very general theorem that established criteria for the convergence of extremal processes to Poisson processes that is of independent interest and that we expect to be useful in many related problems.

References

1. S. MERTENS, *A physicist's approach to number partitioning. Phase transitions in combinatorial problems (Trieste, 1999)*, Theoret. Comput. Sci., **265** (2001), pp. 79–108.

2. H. BAUKE, S. FRANZ, S. MERTENS, *Number partitioning as random energy model*, J. Stat. Mech.: Theor. Exp., (2004), P04003.

3. C. BORGS, J.T. CHAYES, S. MERTENS, B. PITTEL *Phase diagram for the constrained integer partitioning problem*, Random Structures Algorithms, **24** (2004), pp. 315–380.

4. CH. BORGS, J.T. CHAYES, B. PITTEL, *Phase transition and finite-size scaling for the integer partitioning problem*, Random Structures Algorithms, **19** (2001), pp. 247–288.

5. A. BOVIER, I. KURKOVA, *Poisson convergence in the restricted k-partitioning problem*, WIAS Preprint no. 964, 2002, submitted.

Microscopic modeling of financial assets

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Supported by: DFG Research Center MATHEON, project E1

The goal of this project is to develop and investigate more realistic models of order book dynamics that take into account the actual trading mechanisms involved in the price evolution. In this way, one hopes to bring methods and ideas from the theory of interacting random systems to bear on the fundamental theory of price processes in finance. Our modeling ansatz is to consider a Markovian time evaluation on the "virtual order book", i.e. the space of opinions on the value of an asset of all traders on the market (a trader, by definition, has the opinion that the value of an asset is p if he is willing to buy resp. sell the asset at the price p). An opinion is of the ask type if the trader wants to sell at this price, and of the bid type if he wants to buy at this price. An opinion state is stable iff no trades can be performed, i.e. if the lowest ask price exceeds the highest bid price. The current price is then the midpoint between these two values. In our model, traders change their opinion according to some random mechanism, and transactions are performed instantly to always keep the opinion state stable.
While the price formation mechanism in this model is realistic, the difficulty is to find suitable rules for the opinion changes of the traders. Simulations show that realistic price processes can only be achieved if the updating rules take a time-dependent environment (optimism/pessimism) into account. A reasonable scenario is a process of events (news/information) that trigger periods of optimism/pessimism of random strength and duration. Without much effort, this produces processes whose correlation structure has properties similar to real data.

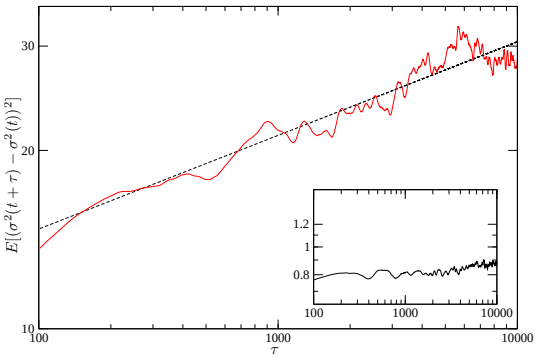

Fig. 1: Volatility clustering in model with external influence. In the inset the same quantity for the original model.

Mathematically, one would like to obtain limit theorems that allow to characterize the properties of the price process resulting from such a model. This can at first only be done in rather simple versions of the model. A popular one is the $B+S \to \emptyset$ model, introduced earlier by Bak et al. [3].
Here, the traders take opinions that belong to the set $B_L = \{-L, -L+1, \ldots, L\}$. The opinion of any trader performs a time-continuous simple random walk (possibly with a drift) in this set. If the opinion leaves B_L, then it disappears from the game. On the other hand, the buyers and sellers are injected at L, resp. $-L$ with rates ρ_+ and ρ_-. If a buyer meets a seller, they

interchange the stock, and they both change their opinion in such a way that they leave B_L and are no longer considered.
In this context we could prove convergence of the empirical order book, in the limit when the number of traders goes to zero, under proper rescaling, to the solution of a nonlinear diffusion equation,

$$\begin{aligned}
\frac{\partial}{\partial t}\rho(t,x) &= \frac{\partial^2}{\partial x^2}\rho(t,x) + \delta \mathrm{sign}(\rho(t,x))\frac{\partial}{\partial x}\rho(t,x) \qquad x \in (-1,1), t > 0,\\
\rho(0,x) &= \rho_0(x) \qquad x \in [-1,1],\\
\rho(t,-1) &= -c_- \qquad t > 0,\\
\rho(t,+1) &= c_+ \qquad t > 0.
\end{aligned}$$

The proofs use techniques from the theory of hydrodynamic limits and large deviations [2].

References

1. A. BOVIER, J. ČERNÝ, O. HRYNIV, *The opinion game: Stock price evolution from microscopic market modelling*, WIAS Preprint no. 903, 2004, submitted.

2. ——, *$A+B \to \emptyset$ interface problems arising from a model of trading agents*, in preparation.

3. P. BAK, M. PACZUSKI, M. SHUBIK, *Price variations in a stock market with many agents*, Physica A: Statistical and Theoretical Physics, **246** (1997), pp. 430-453.

Stochastic models for biological populations — Genealogies and spatial structures

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Supported by: DFG: Dutch-German Bilateral Research Group "Mathematics of random spatial models from physics and biology"

The general aim is to understand mathematical properties of models for randomly reproducing, possibly spatially extended populations. In particular, we are interested in describing the genealogy and, in scenarios with explicit spatial distribution, the spatial distribution of individuals in an "old" population (i.e. in an equilibrium). See, e.g., [7] for an overview over this area.
An important problem for biological applications (e.g., estimation of mutation rates) is to describe the distribution of the genealogy connecting a finite sample from a population. For the "classical" finite variance superprocess, it is well known that the genealogy is, up to a time change, depending on the total mass, given by the so-called Kingman coalescent (which was originally introduced in connection with a simpler class of models where the population size is artificially kept fixed), see [8]. In joint work with several co-authors ([3]) we could clarify for which general continuous state branching processes the genealogy is given by a time change of a general coalescent: This is exactly the case for the stable continuous state branching processes.
This project is connected with the studies of the renormalized spatial Neveu branching process by K. Fleischmann and V. Vakhtel: The Neveu process is a special example of a stable continuous branching process, and the methods developed in [3] could in fact be adapted to settle a technical question of Fleischmann and Vakhtel, see [4].
Stochastic models for spatially extended populations with local self-regulation (in particular in two spatial dimensions) which remove the strong independence assumptions inherent in classical branching random walks and at the same time are able to predict a non-trivial long-time behavior, are desirable from the point of view of ecological modeling. In order to do this, one introduces a "feedback", rendering individual reproduction super- oder subcritical in dependence on the "local" configuration. Up to now, such models have been mostly studied via computer simulation, among the first mathematically rigorous papers are [5], [6]. [5] studied the phenomenon using continuous masses, i.e. in a limit with many particles with small individual masses.
In collaboration with A. Depperschmidt, we are studying a particle-based analog of the model in [5] in discrete time: In a preliminary investigation, we could rigorously show that long-time survival is possible in an appropriate part of the parameter space.
Branching random walks in random environments can be viewed as another step to remove the strong independence assumptions in "classical" branching random walks. Non-spatial branching processes in random environment have a rich variety of possible limit behaviors, a similar (and exhaustive) classification in the spatial setting is still missing. Some steps in this direction were taken in [2] where we could give conditions for extinction and for supercritical growth of a single family by analyzing the genealogy of a sampled individual under the annealed measure.

Notably, space facilitates survival in this model: There are constellations in which the spatial population grows exponentially even though its non-spatial analog would die out almost surely. The so-called directed polymer in random environment, a model known from statistical physics, appears as a conditional mean of the (local) population size, given the environment. Methods established in the field of branching processes, namely representations of size-biased laws, could be adapted to yield an improved criterion for weak disorder, see [1].

References

1. M. BIRKNER, *A Condition for Weak Disorder for Directed Polymers in Random Environment*, Electron. Comm. Probab., **9** (2004), pp. 22–25.

2. M. BIRKNER, J. GEIGER, G. KERSTING, *Branching processes in random environment – A view on critical and subcritical cases*, in: Interacting Stochastic System, J.-D. Deuschel, A. Greven, eds., Springer, Berlin/Heidelberg, 2005, pp. 269–291.

3. M. BIRKNER, J. BLATH, M. CAPALDO, A. ETHERIDGE, M. MÖHLE, J. SCHWEINSBERG, A. WAKOLBINGER, *Alpha-stable branching and beta-coalescents*, WIAS Preprint no. 979, 2004.

4. M. BIRKNER, J. BLATH, *Non-tightness of the rescaled α-spatial Neveu process for the case $\alpha < 2$*, in preparation.

5. A. ETHERIDGE, *Survival and extinction in a locally regulated population*, Ann. Appl. Probab., **14** (2004), pp. 188–214.

6. N. FOURNIER, S. MÉLÉARD, *A microscopic probabilistic description of a locally regulated population and macroscopic approximations*, Ann. Appl. Probab., **14** (2004), pp. 1880–1919.

7. R. DURRETT, *Probability models for DNA sequence evolution*, Springer, New York, 2002.

8. E. PERKINS, *Conditional Dawson–Watanabe processes and Fleming–Viot processes*, in: Seminar on Stochastic Processes, 1991 (Los Angeles, CA), Progr. Probab., **29** (1992), pp. 143–156.

Branching processes in random media

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Branching models describe the evolution of materials, which randomly move, split, and possibly disappear in space. Typically, a random medium is additionally involved, often called the catalyst.
Essential progress has been made in the understanding of the *spatial version of Neveu's continuous-state branching process* constructed in [3]. In this super-α-stable motion X in $\mathbb{R}^d$ $(0 < \alpha \leq 2)$ in a constant medium, the nonlinear term in the related log-Laplace equation is the locally non-Lipschitz function $u \log u$, hence the branching has infinite expectation. Clearly, in supercritical super-α-stable motions of finite mean, one expects a spread out of mass in space according to a profile described by the α-stable density function. But here in the infinite mean case, at macroscopic scales, the mass renormalized to a (random) probability measure is concentrated in a *single* space point which *randomly fluctuates* according to the underlying symmetric α-stable motion, see [4]. In the Brownian case $\alpha = 2$, convergence is shown on the Skorohod path space, whereas for $\alpha < 2$ only convergence of finite-dimensional distributions is established. Tightness on the Skorohod space is actually violated in the latter case, this is verified in Birkner and Blath [1] using lookdown constructions. Surprisingly, the macroscopic single-point concentration is shown by asymptotic calculations using only the first two moments of the randomly renormalized process, which can be computed based on a remarkable log-Laplace product formula which holds just by the occurrence of the logarithm in the branching term.
Superprocesses under a Brownian flow had been introduced by Skoulakis and Adler [12]. A conditional log-Laplace (CLL) approach was founded by Xiong [14]. Many of the properties of former super-Brownian motions were derived by using the log-Laplace transform which is the unique solution to a nonlinear partial differential equation (PDE). Although the nonlinear stochastic partial differential equation (SPDE) satisfied by the CLL transform is much harder to handle than the PDE, it can be expected that many properties of this superprocess under a Brownian flow can be derived using the CLL transform. As a first step in this direction, in [15] the long-term behavior of this superprocess is investigated by means of the CLL transform. Then, in [10], the CLL transform for a more general model driven by a *space-time white noise* is studied, and additionally the *immigration* of particles is allowed. Again, the long-term behavior of the superprocess is obtained. Finally in [11], a conditional excursion representation for the process from [10] is established by making use of the CLL approach.

The *particle system representations* [7], [8] due to Kurtz and Xiong for a class of SPDEs have been completed in [9]. This method has found applications in filtering theory. It turns out that the derivation of the filtering equation based on this method is much simpler than the classical one. Further, it is applicable to a much broader class of filtering models (cf. Kouritzin and Xiong [6] and Xiong and Zhao [17]). As a further application, in [16] a utility maximization problem in selecting optimal investment portfolio is considered when the appreciation rate for the stock is unobserved. Filtering technique is used to estimate this appreciation rate. Note that models as in [6], [16], [17] arise naturally from real-world problems, and classical filtering methods do not apply to these models.
Further understanding has been achieved for the *single point catalytic super-Brownian motion*. In [5], a large deviation principle is established when the branching rate tends to zero. The representation formula of [2] plays a key role. In the related model of single point catalytic branching random walk, interesting new long-term effects have been discovered, see [13].

References

1. M. BIRKNER, J. BLATH, *Non-tightness of rescaled α-spatial Neveu process for the case $\alpha < 2$*, in preparation.

2. K. FLEISCHMANN, J.-F. LE GALL, *A new approach to the single point catalytic super-Brownian motion*, Probab. Theory Related Fields, **102** (1995), pp. 63–82.

3. K. FLEISCHMANN, A. STURM, *A super-stable motion with infinite mean branching*, Ann. Inst. H. Poincaré Probab. Statist., **40** (2004), pp. 513–537.

4. K. FLEISCHMANN, V. VAKHTEL, *Large scale localization of a spatial version of Neveu's branching process*, WIAS Preprint no. 951, 2004.

5. K. FLEISCHMANN, J. XIONG, *Large deviation principle for the single point catalytic super-Brownian motion*, WIAS Preprint no. 937, 2004, submitted.

6. M. KOURITZIN, J. XIONG, *Nonlinear filtering: From Ornstein–Uhlenbeck to white noise*, to appear in: SIAM J. Control Optim., 2005.

7. T.G. KURTZ, J. XIONG, *Particle representations for a class of nonlinear SPDEs*, Stochastic Process. Appl., **83** (1999), pp. 103–126.

8. ——, *Numerical solutions for a class of SPDEs with application to filtering*, in: Stochastics in Finite and Infinite Dimensions, T. Hida, R. Karandikar, H. Kunita, B. Rajput, S. Watanabe, J. Xiong, eds., Birkhäuser, Boston, MA, 2001.

9. ——, *A stochastic evolution equation arising from the fluctuation of a class of interacting particle systems*, Commun. Math. Sci., **2** (2004), pp. 325–358.

10. Z. LI, H. WANG, J. XIONG, *Conditional log-Laplace functionals of immigration superprocesses with dependent spatial motion*, WIAS Preprint no. 900, 2004, to appear in: Acta Appl. Math., 2005.

11. ——, *Conditional excursion representation for a class of interacting superprocesses*, WIAS Preprint no. 935, 2004.

12. G. SKOULAKIS, R.J. ADLER, *Superprocesses over a stochastic flow*, Ann. Appl. Probab., **11** (2000), pp. 488–543.

13. V. VATUTIN, J. XIONG, *Some limit theorems for a particle system of single point catalytic branching random walks*, WIAS Preprint no. 919, 2004.

14. J. XIONG, *A stochastic log-Laplace equation*, Ann. Probab., **32** (2004), pp. 2262–2388.

15. ——, *Long-term behavior for SBM over a stochastic flow*, Electron. Comm. Probab., **9** (2004), pp. 36–52.

16. J. XIONG, Z.J. YANG, *Optimal investment strategy under saving/borrowing rates spread and under partial information*, WIAS Preprint no. 908, 2004.

17. J. XIONG, X. ZHAO, *Nonlinear filtering with fractional Brownian motion noise*, to appear in: Stochastic Anal. Appl., 2005

Stochastic models for Boltzmann-type equations

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Supported by: DFG: "Einfluss räumlicher Fluktuationen auf das Gelationsverhalten von Koagulationsprozessen" (Influence of spatial fluctuations on the gelation behavior of coagulation processes)

Rarefied gas flows play an important role in applications like aerospace design (space shuttle reentry), vacuum engineering (material processing, pumps), or, more recently, nanotechnology. Mathematically such flows are described (in the simplest case of a monatomic gas) by the Boltzmann equation

$$\frac{\partial}{\partial t} f(t,x,v) + (v,\nabla_x) f(t,x,v) = \int_{\mathcal{R}^3} dw \int_{\mathcal{S}^2} de B(v,w,e) \Big[f(t,x,v^*) f(t,x,w^*) - f(t,x,v) f(t,x,w) \Big], \tag{1}$$

where $v^* = v + e(e, w-v)$, $w^* = w + e(e, v-w)$, and $\mathcal{S}^2$ denotes the unit sphere in the Euclidean space $\mathcal{R}^3$. The solution $f(t,x,v)$ represents the relative amount of gas molecules with velocity v at position x and time t. The quadratic nonlinearity in (1) corresponds to the pairwise interaction between gas particles, which consists in the change of velocities of two particles. The collision kernel B contains information about the assumed microscopic interaction potential.
A nonlinear equation of similar structure as equation (1) is Smoluchowski's coagulation equation

$$\frac{\partial}{\partial t} c(t,x) = \frac{1}{2} \sum_{y=1}^{x-1} K(x-y,y)\, c(t,x-y)\, c(t,y) - \sum_{y=1}^{\infty} K(x,y)\, c(t,x)\, c(t,y), \tag{2}$$

where $t \geq 0$ and $x = 1,2,\ldots$. It describes the time evolution of the average concentration of particles of a given size in some spatially homogeneous physical system. The concentration of particles of size x increases as a result of coagulation of particles of sizes $x-y$ and y. It decreases if particles of size x merge with any other particles. The intensity of the process is governed by the coagulation kernel K representing properties of the physical medium. The phenomenon of coagulation occurs in a wide range of applications, e.g., in physics (aggregation of colloidal particles, growth of gas bubbles), meteorology (merging of drops in atmospheric clouds, aerosol transport), chemistry (reacting polymers, soot formation), and astrophysics (formation of stars and planets).
The purpose of the project is to study the relationship between stochastic interacting particle systems and solutions of equations of type (1) or (2). On the one hand, results on the asymptotic behavior of the particle system (when the number of particles increases) provide insight into properties of the solution. On the other hand, appropriate stochastic particle systems are used for the numerical treatment of the macroscopic equation.

Significant progress in the development and justification of stochastic algorithms for the Boltzmann equation (1) has been achieved in recent years. Various aspects of this development are described in [1], which is based on an invited lecture presented at the 24th International Symposium on Rarefied Gas Dynamics (Bari, Italy, 07/2004). This paper concentrates on applied and numerical issues. Theoretical and convergence aspects are emphasized in [2], which is an extended version of a plenary talk given at the Fifth International Conference on Monte Carlo and Quasi-Monte Carlo Methods in Scientific Computing (Singapore, 11/2002). First steps towards another field of application were taken in [3], where a Boltzmann-type equation describing charge transport in semiconductors is considered. In particular, the time-step discretization error of several direct simulation Monte Carlo algorithms is studied.
The topic of studying stochastic models for Smoluchowski's coagulation equation (2) has attracted much interest in recent years. A challenging direction of research is the phenomenon of gelation, which occurs for sufficiently fast increasing coagulation kernels. At the level of the macroscopic equation, the gelation effect is represented by a loss of mass of the solution. An appropriate interpretation of this phenomenon in terms of stochastic particle systems is of both theoretical and practical interest. Some conjectures based on detailed numerical observations have been stated in [4]. Interesting new results contributing to this direction of research are obtained in [5]. First we establish explosion criteria for jump processes with an arbitrary locally compact separable metric state space. Then these results are applied to two stochastic coagulation-fragmentation models——the direct simulation model and the mass flow model. In the pure coagulation case, there is almost sure explosion in the mass flow model for arbitrary homogeneous coagulation kernels with exponent bigger than 1. In the case of pure multiple fragmentation with a continuous size space, explosion occurs in both models provided the total fragmentation rate grows sufficiently fast at zero. However, an example shows that the explosion properties of both models are not equivalent. Finally, some numerical issues related to Smoluchowski's coagulation equation are studied in [6]. Convergence for a quasi-Monte Carlo scheme is proved and error estimates are obtained.

References

1. W. WAGNER, *Monte Carlo methods and numerical solutions*, WIAS Preprint no. 954, 2004.

2. ——, *Stochastic models and Monte Carlo algorithms for Boltzmann type equations*, in: Monte Carlo and Quasi-Monte Carlo Methods 2002, H. Niederreiter, ed., Springer, New York, 2004, pp. 129–153.

3. O. MUSCATO, W. WAGNER, *Time step truncation error in direct simulation Monte Carlo for semiconductors*, WIAS Preprint no. 915, 2004.

4. W. WAGNER, *Stochastic, analytic and numerical aspects of coagulation processes*, Math. Comput. Simulation, **62** (2003), pp. 265–275.

5. ——, *Explosion phenomena in stochastic coagulation-fragmentation models*, Preprint no. NI04006-IGS, Isaac Newton Institute for Mathematical Sciences, Cambridge, UK, 2004.

6. C. LÉCOT, W. WAGNER, *A quasi-Monte Carlo scheme for Smoluchowski's coagulation equation*, Math. Comp., **73** (2004), pp. 1953–1966.

4.6 Research Group Stochastic Algorithms and Nonparametric Statistics

4.6.1 Overview

Die Forschungsgruppe bearbeitet innerhalb der Forschungsprojekte *Statistische Datenanalyse, Angewandte Finanzmathematik* und *Numerische Methoden* Probleme aus der angewandten Stochastik und der Finanzmathematik.

Die Forschung der Forschungsgruppe konzentriert sich auf Fragestellungen aus der angewandten algorithmisch orientierten Wahrscheinlichkeitstheorie und Mathematischen Statistik, die konstruktive und theoretische Aspekte statistischer und numerischer Aufgabenstellungen beinhalten und durch Komplexitätsuntersuchungen ergänzt werden. Im Vordergrund stehen dabei Anwendungen in den Wirtschafts-, Ingenieur- und Lebenswissenschaften. Insbesondere geht es um die Modellierung komplexer Zusammenhänge mit Methoden der nichtparametrischen Statistik, um die Risikobewertung für Finanzmärkte mit Hilfe stochastischer Differentialgleichungen und um die Effizienz stochastischer Algorithmen.
Auf diesen Gebieten, die sowohl bei der Lösung von Problemen in Technologie und Umweltforschung als auch bei der Risikomessung und Bewertung von Finanzderivaten Anwendung finden, hat sich die Forschungsgruppe in den vergangenen Jahren mit wichtigen mathematischen Beiträgen und mit der Entwicklung anerkannter statistischer Software eine führende Stellung erworben.

Für das vergangene Jahr wurden in der Forschungsgruppe folgende Schwerpunkte für die Arbeit gesetzt:

The research group works on problems from applied stochastics and financial mathematics within the research projects *Statistical data analysis, Applied financial mathematics* and *Numerical methods*.

The research of the research group centers on topics in applied and algorithmic probability theory and mathematical statistics that include methodological and theoretical aspects of statistical and numerical problems. This is complemented by investigations of their complexity. The focus is on applications in economics, engineering, and life sciences. Of special interest are modeling of complex systems using methods from nonparametric statistics, risk assessments in financial markets using stochastic differential equations and the efficiency of stochastic algorithms. In these fields, which find applications in solving problems in technology and environmental research as well as in risk measurement and the evaluation of financial derivatives, the research group has reached a leading position with important mathematical contributions and with the development of statistical software.

For the last year the following main topics were set:

- Nichtparametrische statistische Methoden der Bildverarbeitung (Entrauschen, Segmentierung, Thresholding, Kompression), Analyse von Finanzdaten, Ökonometrie, Diskriminanzanalyse, Dimensionsreduktion, Wavelet Shrinkage und Clusteranalyse; Anwendungen auf medizinische Bildverarbeitung (funktionale und dynamische MRI, Positron-Emission-Tomographie, EEG-Zeitreihen), Analyse von Finanzzeitreihen, Klassifikation,
- Angewandte Finanzmathematik, speziell Risikobewertung, Risikomanagement, Zinsmodellierung, Kalibration und Preisfestsetzung für Nicht-Standard-Derivate sowie Portfolio-Optimierung unter Transaktionskosten, stochastische Modelle der numerischen Mathematik und Monte-Carlo-Methoden mit Anwendungen auf turbulenten Transport, Nukleations- und Koagulationsprozesse, und Lösung von Randwertproblemen in deterministischer und stochastischer Form.

- Nonparametric statistical methods in imaging processing (denoising, segmentation, thresholding, compression), analysis of financial data, econometrics, discriminant analysis, dimension reduction, wavelet shrinkage, clustering; applications to medical imaging (functional and dynamic MRI, positron emission tomography, EEG time series), analysis of financial time series, classification;
- Applied financial mathematics, especially risk evaluation, risk management, interest rate modeling, calibration and pricing of non-standard derivatives, and portfolio optimization in the presence of transaction costs, stochastic models in numerical mathematics and Monte Carlo methods with applications to turbulent transport, nucleation and coagulation processes, and to the solution of boundary value problems in deterministic and stochastic formulations.

Ein wichtiges Kennzeichen der Forschung in der Gruppe ist ihr interdisziplinärer Charakter, der ständige Kooperation und Interaktion zwischen den verschiedenen Projekten voraussetzt. So erfordert zum Beispiel die effektive Lösung von Problemen des Risikomanagements die statistische Analyse und das Schätzen von Parametern für Finanzzeitreihen und den Einsatz numerischer Monte-Carlo-Algorithmen zur Bewertung komplexer stochastischer Funktionale. Weitere Beispiele sind die Anwendung von Monte-Carlo-Methoden wie Bootstrap zum Einstellen von Parametern statistischer Verfahren oder die Anwendung statistischer Methoden zur Verbesserung der Effizienz von Monte-Carlo-Verfahren zur numerischen Lösung von stochastischen Differentialgleichungen.

An important feature of the research in the group is its interdisciplinary character that requires permanent cooperation and interaction between the different projects. For instance, the problem of risk management effectively involves a statistical analysis and parameter estimation for financial time series and numerical Monte Carlo algorithms for the evaluation of complex stochastic functionals. Some more examples are given by applications of Monte Carlo methods like bootstrap for parameter tuning in statistical procedures, while statistical methods can be effectively applied for improving the efficiency of many Monte Carlo procedures for the numerical solving of stochastic differential equations.

4.6.2 Projects

Statistical data analysis

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The project *Statistical data analysis* focuses on the development, theoretical investigation and application of modern nonparametric statistical methods, designed to model and analyze complex data structures. WIAS has, with main mathematical contributions, obtained authority for this field, including its applications to problems in technology, medicine, and environmental research as well as risk evaluation for financial products.
Methods developed in the institute within this project area can be grouped into the following main classes.

1. Adaptive smoothing procedures (D. Belomestny, V. Essaoulova, J. Polzehl, V. Spokoiny).

Research on adaptive smoothing methods is driven by challenging problems from imaging and time series analysis. Applications to imaging include reconstruction of 2D and 3D images from Magnetic Resonance Tomography or microscopy, signal detection in functional Magnet Resonance Imaging (fMRI) experiments, or edge recovery from Positron Emission Tomography (PET) data.

The models and procedures proposed and investigated at WIAS are based on three main approaches: pointwise adaptation, originally proposed in [57] for estimation of regression

functions with discontinuities and extended to images in [38], propagation-separation or adaptive weights smoothing, proposed in [39] in the context of image denoising, and stagewise aggregation, introduced in [3].

The main idea of the pointwise adaptive approach is to search, in each design point, for the largest acceptable window that does not contradict the assumed local model, and to use the data within this window to obtain local parameter estimates. This allows for estimates with nearly minimal variance under controlled bias.

Stagewise aggregation, see [3], is defined as a pointwise adaptation scheme based on an ordered sequence of "weak" local likelihood estimates $\tilde{\theta}^{(k)}(x)$ of the local parameter $\theta(x)$ at a fixed-point x ordered due to decreased variability. Starting from the most variable and least biased estimate $\tilde{\theta}^{(1)}(x)$, the procedure sequentially defines the new estimate $\hat{\theta}^{(k)}$ as a convex combination of the next "weak" estimate $\tilde{\theta}^{(k)}(x)$ and the previously computed estimate $\hat{\theta}^{(k-1)}(x)$ in the form

$$\hat{\theta}^{(k)}(x) = \gamma_k \tilde{\theta}^{(k)}(x) + (1-\gamma_k)\hat{\theta}^{(k-1)}(x),$$

where the coefficient γ_k may depend on the location x and is defined by comparing two estimates $\hat{\theta}^{(k-1)}(x)$ and $\tilde{\theta}^{(k)}(x)$. The proposed method yields a new aggregated estimate whose pointwise risk does not exceed the smallest risk among all "weak" estimates multiplied by some logarithmic factor. The paper [3] establishes a number of important theoretical results concerning optimality of the aggregated estimate and shows a good performance of the procedure in simulated and real-life examples.

The general concept behind the propagation-separation approach, see [43, 44], is structural adaptation. The procedure attempts to recover for each point the largest neighborhood where local homogeneity with respect to a prespecified model is not rejected. This is achieved in an iterative process by extending regions of local homogeneity (propagation) as long as this does not contradict the structural information obtained in previous iteration steps. Points are separated into different regions if their local parameter estimates become significantly different within the iteration process. This class of procedures is derived from adaptive weights smoothing, as introduced in [39, 41, 42], by adding stagewise aggregation as a control step. This allowed to put the procedures from [41, 42] into a unified and slightly simpler concept and to prove theoretical properties for the resulting estimates.

The propagation-separation approach possesses a number of remarkable properties like preservation of edges and contrasts and nearly optimal noise reduction inside large homogeneous regions. It is almost dimension free and applies in high-dimensional situations. Moreover, if the prespecified model is valid globally, both stagewise aggregation and the propagation-separation approach yield the global estimate. Both procedures are rate optimal in the pointwise and global sense.

2. Imaging (A. Hutt, J. Polzehl, V. Spokoiny).

The propagation-separation approach enables us to handle locally smooth images [43], see Figure 1 for an example, and local constant likelihood estimation for exponential family models [44] in a unified way. The latter allows, e.g., for images containing Poisson counts, binary or halftone images, or images with intensity-dependent gray value distributions. We now expect to have the necessary understanding and tools to extend the approach to locally smooth exponential family models.

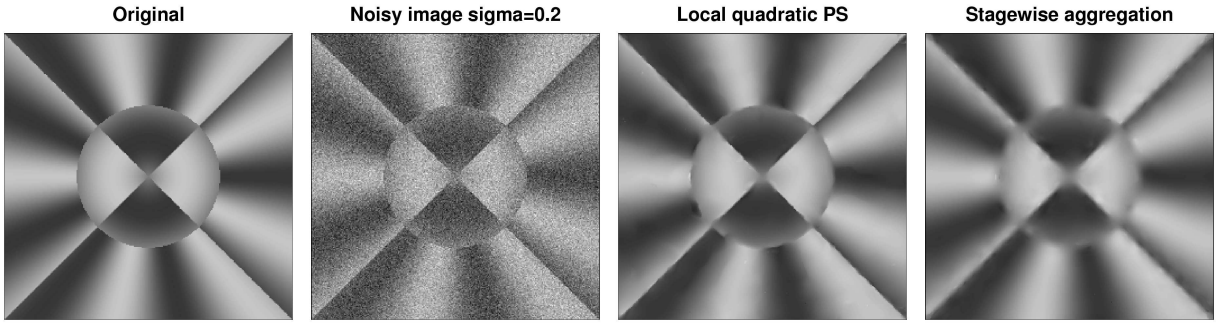

Fig. 1: Reconstruction of a piecewise smooth image by local quadratic propagation-separation and stagewise aggregation

Stagewise aggregation turns out to be more suitable for smooth images. It is less sensitive to edges, see again Figure 1, but on the other hand less dependent on the prespecified local model. Due to its less involved structure it allows for much faster implementations and therefore different classes of applications.

3. Classification and density estimation (D. Belomestny, J. Polzehl, V. Spokoiny).

In [44], the propagation-separation approach is used to derive a class of classification procedures based on a binary response model. This allows to improve on classical nonparametric procedures like kernel regression and the nearest-neighbor by weakening the problem of optimal parameter choice.

The equivalence of Poisson regression and density estimation allows to extend both the propagation-separation approach and stagewise aggregation to the problem of density estimation. The applicability of the propagation-separation approach from [44] is, being based on a local constant structural assumption, currently restricted to densities with pronounced discontinuities. This limitation will be removed with the extension of the approach to generalized linear models.

Stagewise aggregation allows for excellent estimates for smooth densities. Figure 2 illustrates the density estimates obtained for the Old Faithful Geyser data set.

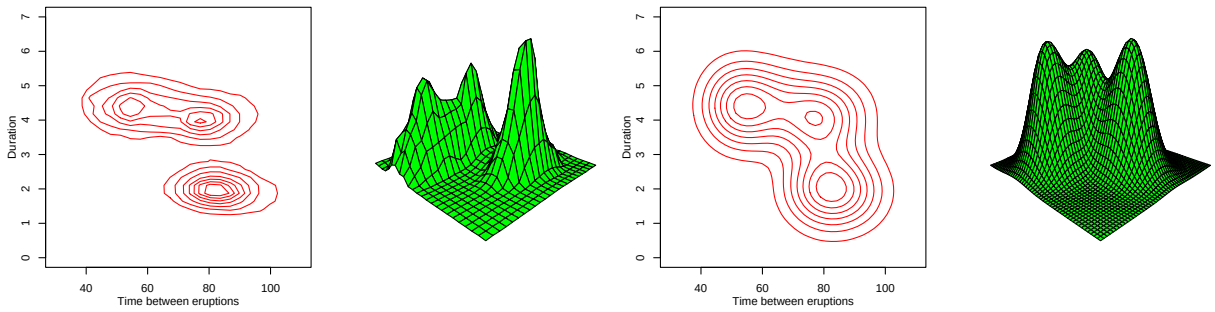

Fig. 2: Contour and perspective plots of density estimates obtained by the stagewise aggregation procedure (top) and bivariate kernel smoothing (bottom) for the Old Faithful Geyser data set

4. Analysis of biosignals (A. Hutt, J. Polzehl, V. Spokoiny).

A growing number of real-life problems in medicine and biosciences lead to the statistical analysis of large data sets with unknown complex structure. The well-developed statistical theory for traditional parametric models or for uni-(low-)dimensional functional data cannot

directly be applied for many of these data sets. We aim to develop novel methods for biomedical signal processing based on neural networks and nonlinear nonstationary time series models. In addition, we tried to combine these methods with microscopic models of biomedical activity to further improve the developed methods. We attack the problem of analysis and modeling of biomedical signals. In one part, the synchronization of multivariate brain signals is investigated by a fixed-point clustering algorithm. It turns out that functional brain processes generate transient signal states, which exhibit global phase synchronization on a dramatically decreased time scale. In a second part, the project aims to model these signal states by neural activity models. Here, we study the spatiotemporal dynamics of neural population activity concerning its stability [1, 18, 19, 20, 22].

5. Modeling of financial time series and volatility estimation (D. Mercurio, J. Polzehl, V. Spokoiny).

Our approach for time series focuses on local stationary time series models. These methods allow for abrupt changes of model parameters in time. Applications for financial time series include volatility modeling, volatility prediction, risk assessment.

ARCH and GARCH models gained a lot of attention and are widely used in financial engineering since they have been introduced in [4, 11]. The simple GARCH(1,1) model is particularly popular suggesting a very natural and tractable model with only three parameters to be estimated. Moreover, this model allows to mimic many important stylized facts of financial time series like volatility clustering (alternating periods of small and large volatility) and persistent autocorrelation (slow decay of the autocovariance function of the absolute or squared returns). The GARCH models are successfully applied to short term forecasting of the volatility and particularly to Value-at-Risk problems, see also the project *Applied mathematical finance*.

However, it appears that the most crucial problem in the GARCH approach is that GARCH models are not robust w.r.t. violation from the stationarity assumption. If the stationarity assumption is violated, GARCH modeling is essentially reduced to exponential smoothing of the last observed squared returns. [33, 34] also argued that the other stylized facts of financial time series like long-range dependence, persistent autocorrelation, and the integration GARCH effect can be well explained by nonstationarity in the observed data.

Our approach to model local stationary time series is based on the assumption of local homogeneity: For every time point there exists an interval of time homogeneity in which the volatility parameter can be well approximated by a constant. The pointwise adaptive procedure from [32] recovers this interval from the data using local change-point analysis. Then the estimate of the volatility can be simply obtained by local averaging. The performance of the procedure is investigated both theoretically and through Monte Carlo simulations. A comparison with the LAVE procedure from [31] and with a standard GARCH model is provided.

In [45], a general class of GARCH models with time-varying coefficients is introduced. The adaptive weights approach is extended to estimate the GARCH coefficients as a function of time. This is based on a localization of the GARCH model by local perturbation of the likelihood function that allows to test for equivalence of two local models. A simpler semiparametric model in which the nonlinear parameter is fixed is discussed. The performance of the parametric, time-varying non- and semiparametric GARCH(1,1) models and the local constant model from [41] is assessed by means of simulated and real data sets using different forecasting criteria. Our results indicate that the simple local constant model outperforms the other models in almost all cases. The GARCH(1,1) model demonstrates a relatively good

forecasting performance as far as the short-term forecasting horizon is considered. However, its application to long-term forecasting seems questionable because of possible misspecification of the model parameters.

In [46], a non-parametric, non-stationary framework for business-cycle dating is developed based on the adaptive weights smoothing techniques from [41, 42]. The methodology is used both for the study of the individual macroeconomic time series relevant to the dating of the business cycle as well as for the estimation of their joint dynamics. Since the business cycle is defined as the common dynamics of *some* set of macroeconomic indicators, its estimation depends fundamentally on the group of series monitored. Our dating approach is applied to two sets of US economic indicators including the monthly series of industrial production, nonfarm payroll employment, real income, wholesale-retail trade, and gross domestic product (GDP). We find evidence of a change in the methodology of the NBER's Business-Cycle Dating Committee: In the dating of the largest recession, an extended set of five monthly macroeconomic indicators replaced the set of indicators emphasized by the NBER's Business-Cycle Dating Committee in recent decades. This change seems to seriously affect the continuity in the outcome of the dating of business cycles. Had the dating been done on the traditional set of indicators, the last recession would have lasted one year and a half longer. We find that, independent of the set of coincident indicators monitored, the last economic contraction began in November 2000, four months before the date of the NBER's Business-Cycle Dating Committee.

6. Inference for partly linear regression (V. Spokoiny).

In [55], the authors proposed a new method of analysis of a partially linear model whose nonlinear component is completely unknown. The target of analysis is the indentification of the set of regressors which enter in a nonlinear way in the model function, and the complete estimation of the model including slope coefficients of the linear component and the link function of the nonlinear component. The procedure also allows for selecting the significant regression variables. We also develop a test of linear hypothesis against a partially linear alternative, or, more generally, a test that the nonlinear component is M-dimensional for $M = 0, 1, 2, \ldots$. The method of analysis goes back to the idea of structural adaptation from [16, 17], where the problem of dimension reduction was considered for a single and multiple index model, respectively. The new approach is very general and fully adaptive to the model structure. The only restrictive assumption is that the dimensionality of the nonlinear component is relatively small. The theoretical results indicate that the procedure provides a prescribed level of the identification error and estimates the linear component with the accuracy of order $n^{-1/2}$. A numerical study demonstrates a very good performance of the method even for small or moderate sample sizes.

7. Search of non-Gaussian components of a high-dimensional distribution (V. Spokoiny).

Suppose $X_1, \ldots, X_n$ is an i.i.d. sample in a high-dimensional space $\mathbb{R}^d$ drawn from an unknown distribution with density $f(x)$. A general multivariate distribution is typically too complex to be recovered from the data, thus dimension reduction methods need to be used to decrease the complexity of the model [2, 8, 54, 56, 60]. Many such dimension reduction techniques rely on some linear representation of data. For instance, PCA projects the data into the orthogonal principal component basis that are defined via the eigenvalue decomposition of the covariance matrix of the vector X. This method is well suited for the case of a normal distribution, because orthogonality implies independence of components for a multivariate Gaussian distribution. However, in practical situations, especially if the assumption of normality is violated, PCA can easily reach its limits.

An alternative approach, the *Independent Component Analysis*, assumes that the data is a linear transformation of a d-dimensional vector with independent components. Usually these components are assumed to be strictly non-Gaussian except for one Gaussian component to ensure their identifiability [6, 23]. Note that independent components do not necessarily form an orthogonal basis.

In [58], a new approach that allows to bridge these two completely different modeling approaches is developed. The model assumption is that the random vector X can be decomposed into a product of multivariate Gaussian and purely non-Gaussian components leading to the semiparametric class of densities

$$f(x) = g(Tx)\phi_{\theta,\Gamma}(x)$$

where T is a linear mapping from $\mathbb{R}^d$ to another space $\mathbb{R}^m$ with $m \le d$, g is an unknown function in $\mathbb{R}^m$, and $\phi_{\theta,\Gamma}$ is a normal density with the mean θ and the covariance matrix Γ. Note that this model includes as particular cases both the pure parametric ($m = 0$) and pure nonparametric ($m = d$) models. The first numerical results indicate a very reasonable performance of the method, while the theoretical results show that the procedure provides a prescribed level of the identification error.

8. Inverse problems (P. Mathé, J. Polzehl, M. Reiß, V. Spokoiny).

Ill-posed equations arise frequently in the context of inverse problems, where it is the aim to determine some unknown characteristics of a physical system from data corrupted by measurement errors.

An estimation method based on pointwise recovering of the support function of a planar convex set from noisy observations of its moments is developed in [13]. Intrinsic accuracy limitations in the shape-from-moments estimation problem are shown by establishing a lower bound on the rate of convergence of the mean squared error. The proposed estimator is near-optimal in the sense of the order. [14] considers the problem of recovering edges of an image from noisy Positron Emission Tomography (PET) data. The original image is assumed to have a discontinuity jump (edge) along the boundary of a compact convex set. The Radon transform of the image is observed with noise, and the problem is to estimate the edge. We develop an estimation procedure which is based on recovering the support function of the edge. It is shown that the proposed estimator is nearly optimal in order in a minimax sense. Numerical examples illustrate reasonable practical behavior of the estimation procedure.

For ill-posed problems it is often impossible to get sensible results unless special methods, such as Tikhonov regularization, are used. Work in this direction is carried out in collaboration with

S.V. Pereverzev, RICAM Linz. We study linear problems where an operator A acts injectively and compactly between Hilbert spaces, and the equation is disturbed by noise. Under a priori smoothness assumptions on the exact solution x, such problems can be regularized. Within the present paradigm, smoothness is given in terms of general source conditions, expressed through the operator A as x = $\varphi(A*A)v, \|v\| \leq R$, for some increasing function φ, $\varphi(0) = 0$. This approach allows to treat regularly and severely ill-posed problems in a unified way. The study [25] provides a general approach to determine the degree of ill-posedness for statistical ill-posed problems and thus the intrinsic complexity for such problems. Moreover, in [28] the numerical analysis could be extended to statistical ill-posed problems, including the issue of discretization and adaptation, when the smoothness of the true solution is not known *a priory*.

Adaptive parameter choice strategies date back to the original paper by Phillips [30] and it became an important issue how this can be given a sound mathematical basis. Based on new tools for variable Hilbert scales, as developed in [27], the *discrepancy principle* is thoroughly analyzed in [26] while in [29], its extension to discretization was considered. The analysis results in a new algorithm, which allows to take into account the advantages of the discrepancy principle while classical projection methods do not.

Ergodic scalar diffusion processes of the type

$$dX(t) = b(X(t))dt + \sigma dW(t), \quad t \in [0,T], \tag{1}$$

form an archetype model for time-dependent data. The nonparametric estimation problem for b based on continuous or high-frequency observations is well studied, cf. [24], and the asymptotic results for long-time asymptotics $T \to \infty$ resemble those for standard regression models. In [9], this relationship has been corroborated in the strong sense of Le Cam's equivalence for statistical experiments. This allows an immediate transfer of asymptotic statistical theory between these two models and yields a more profound understanding of the model itself.

It is shown that the above diffusion model is asymptotically equivalent to the Gaussian white noise model given by the observation of

$$dZ(x) = b(x)\sqrt{\mu_0(x)}\,dx + T^{-1/2}dB(x), \quad x \in I\!R, \tag{2}$$

where μ_0 is the invariant density of X under the central parameter of the localization. The technical conditions imposed to obtain this result are basically a uniform ergodicity property and a minimal regularity of order $1/2$ for the function b. The method of proof relies on a coupling scheme on the diffusion space using the local time of the process to obtain the analogue of a deterministic design. Based on the principal local result, a global asymptotic equivalence result is obtained and extensions into several directions like constructive equivalence, time discretization, and more general diffusion coefficients are possible.

Nonparametric estimation for diffusion processes based on low-frequency data is an intricate problem and had first been considered in [12] for compact state spaces. In [52], this approach has been generalized to diffusion processes with natural boundary conditions on the state space $I\!R$. This extension poses many new difficulties: On the probabilistic side, the corresponding infinitesimal generator is usually not compact anymore and its eigenfunctions are unbounded, while statistically the highly degenerate observation design causes a heteroskedastic noise structure.

Using warped wavelet bases and imposing conditions on the underlying Dirichlet form, some of the difficulties can be overcome and mathematical efficiency results are obtained. The

procedure is based on projection estimators for the invariant density and the Markov transition operator and on spectral decomposition results. Numerical simulation results, implementing the method with an adaptive wavelet thresholding approach, support the feasibility of this estimation procedure.

Inverse problems appear naturally in all areas of quantitative science, cf. the calibration problem described in the applied finance section. A statistical formulation is needed when modeling the error stochastically or when solving statistical inference problems for stochastic processes. An instance of the latter is the estimation of the delay length r in the affine stochastic differential equation

$$dX(t) = \Big(\int_{-r}^{0} X(t+u) g(u)\, du \Big)\, dt + \sigma\, dW(t), \quad t \in [0,T].$$

In [52], an estimator for r from the observation $(X(t), t \in [0,T])$ in the stationary case has been proposed. Assuming $g(-r) \neq 0$, the estimation procedure is based on a change-point detection algorithm for a closely related inverse problem involving the empirical covariance operator, see also [50]. It consists of a two-step procedure using a cumulative sum (CUSUM) change-point detection for suitable wavelet coefficients. The rate of convergence for $T \to \infty$ corresponds to change point detection for a statistical inverse problem with degree one of ill-posedness.

The problem of an error in the operator, e.g., due to uncertainty about certain parameter values or due to numerical approximation errors, has been considered more fundamentally in [15]. The problem of recovering $f \in L^2$ from the observation

$$\begin{cases} g_\varepsilon = Kf + \varepsilon \dot{W} \\ K_\delta = K + \delta \dot{B} \end{cases}$$

is studied, where $\dot{W}$ denotes an L^2-Gaussian white noise and $\dot{B}$ is a canonical operator Gaussian white noise. Assuming ellipticity and a degree t of ill-posedness, a nonlinear adaptive wavelet approach is developed, which generalizes the linear approach by [10] and the wavelet-Galerkin method of [5]. Minimax rates are obtained for the joint asymptotics $\delta, \varepsilon \to 0$. For functions f in d-dimensional Besov spaces $B^s_{p,p}$, the optimal rate of the integrated mean square error is $\max\{\delta, \varepsilon\}^{\frac{4s}{2s+2t+d}}$, provided $1/p \leq 1/2 + s/(2t+d)$ under certain minimal regularity conditions. Interestingly, the error in the operator does not yield a significant deterioration of the estimator as long as its level is below the error level in the data.

SIMEX was introduced in [7, 59] as a simulation-type estimator in errors-in-variables models. The idea of the SIMEX procedure is to compensate for the effect of the measurement errors while still using naive regression estimators. In [47, 48], a symmetrized version of this estimator is defined. Now [49] establishes some results relating these two simulation-extrapolation-type estimators to well-known consistent estimators like the total least squares estimator (TLS) and the moment estimator (MME) in the context of errors-in-variables models. We further introduce an adaptive SIMEX (ASIMEX). The main result of this paper is that SYMEX, ASIMEX are equivalent to total least squares. Additionally, we see that SIMEX is equivalent to the moment estimator.

9. Cluster analysis and data mining (H.-J. Mucha).

Easy-to-understand graphical output of cluster analysis would be appreciated in the reality of a high-dimensional setting. To supply this need, new graphical outputs of hierarchical clustering are under development. Hierarchical cluster analysis is a well-known method of stepwise

data compression. As a result one gets a dendrogram, that is, a special binary tree with a distinguished root and with all the data points (observations) at its leaves. Unfortunately, both the real or potential order of the objects and the potential quantitative locations of the objects are not reflected in the dendrogram. Often, neighboring objects in the dendrogram are quite distinct from one another in the reality of a heterogeneous, high-dimensional setting. Therefore, the reading of conventional dendrograms as well as their interpretation becomes difficult and it is often confusing. In [35], some dendrogram drawing and reordering techniques are recommended that reflect the total order in the one-dimensional case (univariate case) and, in the multivariate case, an order that corresponds approximately to a total order in some degree. The result, a so-called ordered dendrogram, is recommended because it makes the interpretation of hierarchical structures much easier.

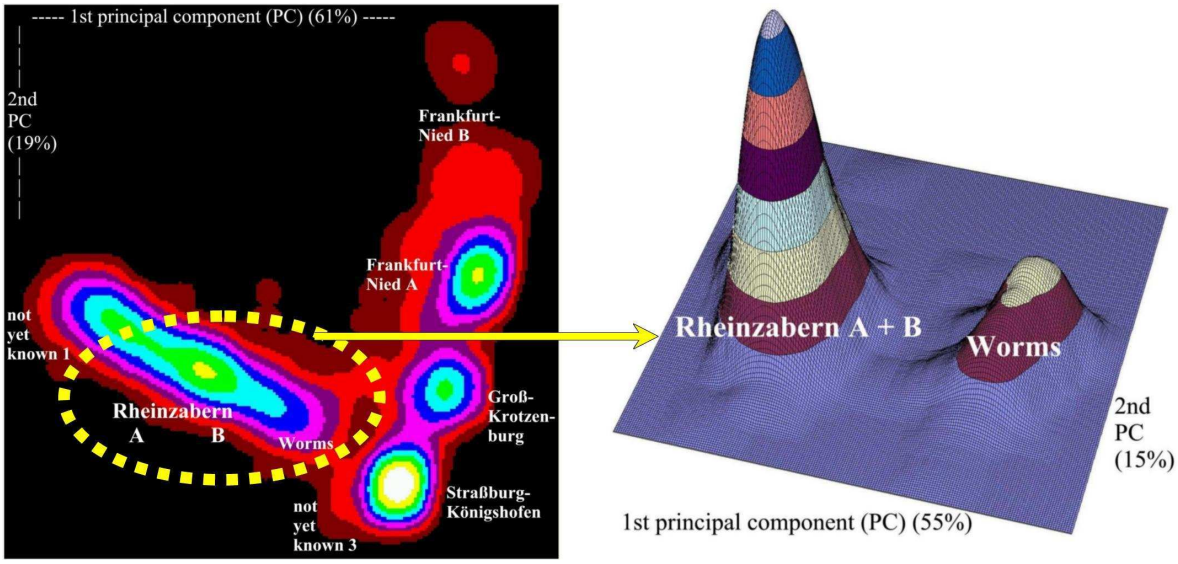

Fig. 3: From global to local adaptive clustering: A graphical exemplification

Another focus is on the development of stable clustering techniques. Usually, a (global) cluster analysis model is applied first in order to find homogeneous subsets in data. As a result, ten or more clusters are detected in a heterogeneous data set. Often subsequent (or iterative) local cluster analyses perform better. This can be confirmed by using validation techniques [36]. By doing so, both the appropriate number of clusters can be validated and the stability of each cluster can be assessed. Figure 3 shows a successful application in archeometry. At the left-hand side, the overall cluster analysis result is presented based on the first two principal components. The clusters correspond to the high-density areas of the nonparametric bivariate density estimation. Several cuts of the density at different levels are shown. At the left-hand side of the figure, the local adaptive cluster analysis result corresponds to the two well-separated peaks of the bivariate density surface.

References

1. F. ATAY, A. HUTT, *Stability and bifurcations in neural fields with axonal delay and general connectivity*, to appear in: SIAM J. Appl. Math.

2. M. BELKIN, P. NIYOGI, *Laplacian eigenmaps for dimensionality reduction and data representation*, Neural Computation, **15** (2003), pp. 1373–1396.

3. D. BELOMESTNY, V. SPOKOINY, *Local likelihood modeling via stagewise aggregation*, WIAS Preprint no. 1000, 2004.

4. T. BOLLERSLEV, *Generalized autoregressive conditional heteroscedasticity*, J. Econometrics, **31** (1986), pp. 307–327.

5. A. COHEN, M. HOFFMANN, M. REISS, *Adaptive wavelet Galerkin methods for linear inverse problems*, to appear in: SIAM J. Numer. Anal.

6. P. COMON, *Independent component analysis – A new concept ?*, Signal Processing, **36** (1994), pp. 287–314.

7. J.R. COOK, L.A. STEFANSKI, *Simulation-extrapolation estimation in parametric measurement error models*, J. Amer. Statist. Assoc., **89** (1994), pp. 1314–1328.

8. T.F. COX, M.A.A. COX, *Multidimensional Scaling*, Chapman & Hall, London, 2001.

9. A. DALALYAN, M. REISS, *Asymptotic statistical equivalence for scalar ergodic diffusion processes*, WIAS Preprint no. 916, 2004, to appear in: Probab. Theory Related Fields.

10. S. EFROMOVICH, V. KOLTCHINSKII, *On inverse problems with unknown operators*, IEEE Trans. Inform. Theory, **47** (2001), pp. 2876–2894.

11. R.F. ENGLE, *Autoregressive conditional heteroscedasticity with estimates of the variance of UK inflation*, Econometrica, **50** (1982), pp. 987–1008.

12. E. GOBET, M. HOFFMANN, M. REISS, *Nonparametric estimation of scalar diffusions based on low frequency data*, Ann. Statist., **32** (2004), pp. 2223–2253.

13. A. GOLDENSHLUGER, V. SPOKOINY, *On the shape-from-moments problem and recovering edges from noisy Radon data*, Probab. Theory Related Fields, **128** (2004), pp. 123–140.

14. ——, *Recovering edges of an image from noisy tomographic data*, WIAS Preprint no. 909, 2004.

15. M. HOFFMANN, M. REISS, *Nonlinear estimation for linear inverse problems with error in the operator*, WIAS Preprint no. 990, 2004.

16. M. HRISTACHE, A. JUDITSKY, J. POLZEHL, V. SPOKOINY, *Structure adaptive approach for dimension reduction*, Ann. Statist., **29** (2001), pp. 1537–1566.

17. M. HRISTACHE, A. JUDITSKY, V. SPOKOINY, *Direct estimation of the index coefficient in a single-index model*, Ann. Statist., **29** (2001), pp. 595–623.

18. A. HUTT, *Effects of nonlocal feedback on traveling fronts in neural fields subject to transmission delay*, WIAS Preprint no. 953, 2004, Phys. Rev. E, **70** (2004), 052902, 4 pages.

19. A. HUTT, F. ATAY, *Analysis of nonlocal neural fields for both general and gamma-distributed connectivities*, WIAS Preprint no. 969, 2004.

20. A. HUTT, A. DAFFERTSHOFER, U. STEINMETZ, *Detection of mutual phase synchronization in multivariate signals and application to phase ensembles and chaotic data*, Phys. Rev. E, **68** (2003), 036219, 10 pages.

21. A. HUTT, T.D. FRANK, *Stability, critical fluctuations and* $1/f^{\alpha}$*-activity of neural fields involving transmission delays*, Preprint no. 140 of DFG Research Center MATHEON, Technische Universität Berlin, 2004.

22. A. HUTT, M. SCHRAUF, *Detection of transient generalized and mutual phase synchronization by clustering and application to single brain signals*, WIAS Preprint no. 925, 2004.

23. A. HYVARINEN, J. KARHUNEN, E. OJA, *Independent Component Analysis*, Wiley, New York, 2001.

24. Y. KUTOYANTS, *Statistical Inference for Ergodic Diffusion Processes*, Springer, London [u.a.], 2004.

25. P. MATHÉ, *Degree of ill-posedness of statistical inverse problems*, WIAS Preprint no. 954, 2004.

26. ——, *What do we learn from the discrepancy principle?*, manuscript written at RICAM, 2004.

27. P. MATHÉ, S.V. PEREVERZEV, *Discretization strategy for linear ill-posed problems in variable Hilbert scales*, Inverse Problems, **19** (2003), pp. 1263–1277.

28. ——, *Regularization of some linear ill-posed problems with discretized random noisy data*, 2004, submitted.

29. ——, *The discretized discrepancy principle under general source conditions*, manuscript, 2005.

30. D.L. PHILLIPS, *A technique for the numerical solution of certain integral equations of the first kind*, J. Assoc. Comput. Mach., **9** (1962), pp. 84–97.

31. D. MERCURIO, V. SPOKOINY, *Statistical inference for time-inhomogeneous volatility models*, Ann. Statist., **32** (2004), pp. 577–602.

32. ——, *Estimation of time dependent volatility via local change point analysis*, WIAS Preprint no. 904, 2004.

33. T. MIKOSCH, C. STĂRICĂ, *Is it really long memory we see in financial returns?*, in: Extremes and Integrated Risk Management, P. Embrechts, ed., Risk Books, 2000.

34. ——, *Non-stationarities in financial time series, the long range dependence and the IGARCH effects*, Rev. Econom. Statist., **86** (2004), pp. 378–390.

35. H.-J. MUCHA, H.-G. BARTEL, J. DOLATA, *Techniques of rearrangements in binary trees (dendrograms) and applications*, to appear in: Match.

36. H.-J. MUCHA, E. HAIMERL, *Automatic validation of hierarchical cluster analysis with application in dialectometry*, to appear in: Proceedings of the 28th Annual Conference of GfKl, Springer, Berlin.

37. H.-J. MUCHA, H.-G. BARTEL, J. DOLATA, *Model-based cluster analysis of Roman bricks and tiles from Worms and Rheinzabern*, to appear in: Proceedings of the 28th Annual Conference of GfKl, Springer, Berlin.

38. J. POLZEHL, V. SPOKOINY, *Image denoising: Pointwise adaptive approach*, Ann. Statist., **31** (2003), pp. 30–57.

39. ——, *Adaptive weights smoothing with applications to image restoration*, J. Roy. Statist. Soc. Ser. B, **62** (2000), pp. 335–354.

40. ——, *Functional and dynamic magnetic resonance imaging using vector adaptive weights smoothing*, J. Roy. Statist. Soc. Ser. C, **50** (2001), pp. 485–501.

41. ——, *Local likelihood modeling by adaptive weights smoothing*, WIAS Preprint no. 787, 2002.

42. ——, *Varying coefficient regression modeling by adaptive weights smoothing*, WIAS Preprint no. 818, 2003.

43. ——, *Spatially adaptive regression estimation: Propagation-separation approach*, WIAS Preprint no. 998, 2004.

44. ——, *Propagation-separation approach for local likelihood estimation*, manuscript, 2004.

45. ——, *Varying coefficient GARCH versus local constant volatility modeling. Comparison of the predictive power*, WIAS Preprint no. 977, 2004.

46. J. POLZEHL, V. SPOKOINY, C. STĂRICĂ, *When did the 2001 recession really start?*, WIAS Preprint no. 934, 2004.

47. J. POLZEHL, S. ZWANZIG, *On a symmetrized extrapolation estimator in linear errors-in-variables models*, Comput. Statist. Data Anal., **47** (2004), pp. 675–688.

48. ——, *On a comparison of different simulation extrapolation estimators in linear errors-in-variables models*, U.U.D.M. Report no. 17, 2003, Uppsala University.

49. ——, *SIMEX and TLS: An equivalence result*, WIAS Preprint no. 999, 2004.

50. M. REISS, *Adaptive estimation for affine stochastic delay differential equations*, to appear in: Bernoulli.

51. ——, *Estimation of the delay length in affine stochastic delay differential equations*, Internat. J. Wavelets Multiresolut. Inf. Process., **2** (2004), pp. 525–544.

52. ——, *Nonparametric volatility estimation on the real line from low-frequency observations*, WIAS Preprint no. 911, 2004.

53. B. RÖHL-KUHN, J. POLZEHL, P. KLOBES, *Simultaneous confidence and prediction bands in the certification of pressure-volume curves for the pore analysis of solids*, manuscript, 2004.

54. S. ROWEIS, L. SAUL, *Nonlinear dimensionality reduction by locally linear embedding*, Science, **290** (2000), pp. 2323–2326.

55. A. SAMAROV, V. SPOKOINY, C. VIAL, *Component identification and estimation in nonlinear high-dimensional regression models by structural adaptation*, WIAS Preprint no. 828, 2003.

56. B. SCHÖLKOPF, A.J. SMOLA, K.-R. MÜLLER, *Nonlinear component analysis as a kernel eigenvalue problem*, Neural Computation, **10** (1998), pp. 1299–1319.

57. V. SPOKOINY, *Estimation of a function with discontinuities via local polynomial fit with an adaptive window choice*, Ann. Statist., **26** (1998), pp. 1356–1378.

58. V. SPOKOINY, G. BLANCHARD, M. SUGIYAMA, M. KAWANABE, K.-R. MÜLLER, *In search of non-Gaussian components of a high-dimensional distribution*, manuscript, 2004.

59. L.A. STEFANSKI, J.R. COOK, *Simulation-extrapolation: The measurement error jackknife*, J. Amer. Statist. Assoc., **90** (1995), pp. 1247–1256.

60. J.B. TENENBAUM, V. DE SILVA, J.C. LANGFORD, *A global geometric framework for nonlinear dimensionality reduction*, Science, **290** (2000), pp. 2319–2323.

Applied mathematical finance and stochastic simulation

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The central theme of the project *Applied mathematical finance and stochastic simulation* is the quantitative treatment of problems raised by industry, based on innovative methods and algorithms developed in accordance with fundamental stochastic principles. The project concentrates on two main areas: Applications in financial industry (A) and the development of basic stochastic models and algorithms in computational physics (B). The problems in area (A) include stochastic modeling of financial data, valuation of complex derivative instruments (options), risk analysis, whereas in area (B), stochastic algorithms for boundary value problems of electrostatic and elasticity potentials, random velocity field simulation, transport in porous media, and behavior of complex particle systems like the formation of charged nanoparticles in a combustion process are studied.

A: Stochastic modeling in finance

1. Methods for pricing and hedging of derivatives with early exercise opportunities (D. Belomestny, Ch. Bender, A. Kolodko, J. Schoenmakers).

The valuation of financial derivatives based on abritrage-free asset pricing involves non-trivial mathematical problems in martingale theory, stochastic differential equations, and partial differential equations. While its main principles are established (Harrison, Pliska, 1981), many numerical problems remain such as the numerical valuation of (multidimensional) American

equity options and the valuation of Bermudan-style derivatives involving the term structure of interest rates (LIBOR models), [11]. The valuation and optimal exercise of American and Bermudan derivatives is one of the most important problems both in theory and practice, see e.g., [1]. American options are options contingent on a set of underlyings which can be exercised at any time in some prespecified future time interval, whereas Bermudan options may be exercised at a prespecified discrete set of future exercise dates. A new development is the valuation of multiple callable products. In general, the fair price of an American- or Bermudan-style derivative can be represented as the solution of an optimal stopping problem.

- *Iterative methods for Bermudan-style products*

  In Kolodko and Schoenmakers (2004), a new iterative procedure for solving the discrete optimal stopping problem is developed. The method is based on improving a canonical suboptimal policy for Bermudan options: Exercise as soon as the cash flow dominates all underlying Europeans ahead. An iteration of this policy produces monotonically increasing approximations of the Snell envelope from below, which coincide with the Snell envelope after finitely many steps. The method may be sketched as follows:

  The Bermudan option: Let $\{0,1,\ldots,k\}$ be the set of Bemudan exercise dates. At one of these dates, say i, the Bermudan option holder may exercise a cash flow Z_i.

  Construction of the optimal stopping time: Take a fixed integer κ, $1 \le \kappa \le k$, and an input stopping family $\tau = (\tau_i, 0 \le i \le k)$; τ_i is the stopping (exercise) time due to policy τ at exercise date i provided the Bermudan option was not exercised before date i. Then consider the intermediate process

  $$\widetilde{Y}_i := \max_{p:\, i \le p \le \min(i+\kappa,k)} E^i Z_{\tau_p} \quad .$$

  Using $\widetilde{Y}_i$ as an exercise criterion, we define a new family of stopping indexes

  $$\begin{aligned} \widehat{\tau}_i : &= \inf\{j : i \le j \le k,\ \widetilde{Y}_j \le Z_j\} \\ &= \inf\{j : i \le j \le k,\ \max_{p:\, j \le p \le \min(j+\kappa,k)} E^j Z_{\tau_p} \le Z_j\}, \quad 0 \le i \le k, \end{aligned}$$

  and consider the process

  $$\widehat{Y}_i := E^i Z_{\widehat{\tau}_i}$$

  as a next approximation of the Snell envelope. Iterating this procedure gives then an increasing sequence of stopping families which rapidly converges to the optimal one.

  By duality, the iterative method induces a convergent sequence of upper bounds as well. Contrary to backward dynamic programming, the presented iterative procedure allows to calculate approximative solutions with only a few nestings of conditional expectations and is, therefore, tailor-made for a plain Monte Carlo implementation. The power of the procedure is demonstrated for high-dimensional Bermudan products, in particular, for Bermudan swaptions in a full factor Libor market model.

- *Iterative methods for multiple callable products*

  In a subsequent study, Bender and Schoenmakers (2004), the iterative procedure of Kolodko and Schoenmakers is extended for multiple callable options. Moreover, the stability of the algorithm is proved.

- *Modeling American options by consumption processes*

  An approach for pricing both continuous-time and discrete-time American options, which is based on the fact that an American option is equivalent to a European option with a consumption process involved, is developed in Belomestny and Milstein (2004). This approach admits the construction of an upper bound (a lower bound) on the true price using some lower bound (some upper bound). The method requires the ability of computing the price of a lower bound at every position, for instance, by a Monte Carlo procedure. As an example, let $f(t,x)$ be the payoff function of an American option, then a lower bound $v(t,x)$ is given by

  $$v(t,x) = \max\{f(t,x), u_{eu}(t,x)\},$$

  where $u_{eu}(t,x)$ is the price of the underlying European option which, in principle, can easily be computed by Monte Carlo. Then, by the Monte Carlo method, an upper bound $V(t,x)$ due to this lower bound is constructed at position (t,x). A number of effective estimators of the upper and lower bounds with reduced variance are proposed. The results obtained are supported by numerical experiments which look promising.

- *Pricing Libor Bermudans by Greenian kernel expansions*

  In a research cooperation with J. Kampen at Heidelberg University we aim to value Bermudan-style derivatives in the Libor market model based on higher order approximation of Greenian kernels. Greenian kernels are connected with the (high-dimensional) Libor process and integration with respect to these kernels will be implemented on sparse grids.

- *Option pricing under constraints*

  The classical theory of option pricing presupposes a frictionless market. For example, the market is assumed to be liquid, fractions of shares can be traded, and there are no restrictions on short selling stocks and borrowing money from the money market account. To incorporate constraints into a model, one can penalize violations of the constraints or prohibit violations completely. In Bender and Kohlmann (2004), several constructions of penalization processes for different classes of constraints are presented in the context of a generalized Black–Scholes market, which yield arbitrage-free, nonlinear pricing systems. The constraints may be time-dependent, random, and nonconvex. It is shown that with increasing weight of the penalization the option prices monotonically tend to the superhedging price (i.e. the seller's price, when violation of the constraint is prohibited) due to the monotonic limit theorem for BSDEs.

- *Arbitrage with fractional Brownian motion:*

  Fractional analogues of the Black–Scholes model have been proposed in recent years in order to incorporate long memory into market models. In Bender and Elliot (2004), a binary version of the Wick-fractional Black–Scholes model is considered and an arbitrage is constructed in the binary model. It is explained within the binary model why the no-arbitrage results in continuous time rather stem from replacing the self-financing condition by an economically doubtful condition than by the use of the Wick product in the stock price modeling.

2. General interest rate modeling (J. Schoenmakers).

- *Book project: Robust Libor modeling and pricing of derivative products* The research on Libor modeling, robust calibration, and pricing of exotic products has continued and has led to the monograph of Schoenmakers (2005). This book contains also much recent work on Bermudan-style derivatives.

- *Interest rate modeling in intrinsic Black–Scholes economies* In the research of Reiß, Schoenmakers, and Schweizer (2004), the following result is established. If an economy follows a Black–Scholes dynamics with respect to intrinsic values, on may define a natural intrinsic asset index, called spherical index, and with respect to this index there is a testable relationship between the correlation of index and short rate, and the slope of the yield curve. This relationship may be used, for example, for determination of a volatility function in a short rate model.

3. Calibration of Lévy-based financial models (D. Belomestny, M. Reiß, V. Spokoiny).

Nowadays, the main focus of financial engineering is the development and application of probabilistic models that at the same time capture the main stylized facts of financial time series and allow robust and fast calibration and pricing methods. Soon after the introduction of the classical Black & Scholes model for asset prices, Merton (1976) proposed a more realistic model incorporating random jumps of the price process. Since then, the idea of incorporating jumps into the models has become very popular in mathematical finance, see, e.g., Cont and Tankov (2004), but the empirical work only concentrated on some very specific parametric models.

In the work of Reiß and Belomestny (2004), a calibration method is developed for the classical exponential Lévy model of the asset price

$$S_t = S_0 \exp(L_t), \quad t \geq 0,\ L \text{ a process with stationary, independent increments.}$$

From observations of European put and call option prices, the Lévy–Khinchin characteristic (b, σ^2, ν) of the process L is estimated, which is a nonparametric statistical problem due to the unknown jump measure ν. In contrast to the Black–Scholes model, there is in general no unique equivalent martingale measure in the exponential Lévy model such that a model fit purely based on historical asset price data is not meaningful and the main pricing information can only be obtained from liquid options traded at the market. Cont and Tankov (2004b) have proposed a penalized nonlinear least squares method to tackle this calibration problem, which relies on a rather time-consuming iterative optimization procedure and does not yield provably optimal convergence results.

Our method is based upon an explicit nonlinear inversion formula for the price function in the spectral domain and uses the FFT algorithm. Due to the ill-posedness of the inversion, a spectral cut-off scheme is employed as regularization method. For an increasing number of observations the method is provably rate-optimal, but the rates, even for the parametric drift and diffusion part, correspond in general to a severely ill-posed problem. Although this seems discouraging for practical purposes, simulation studies show that for realistic model assumptions and observation designs, the calibration works reasonably well and captures the main features of the underlying parameters; see picture.

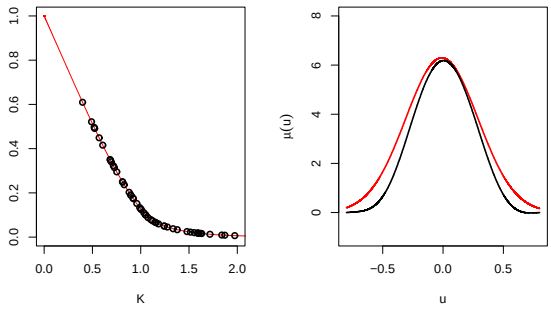

Fig. 1: Merton model. Left: Simulated 50 call option prices as a function of strike K together with the true price curve (red). Right: True and estimated Lévy densities.

4. Volatility modeling by local change-point analysis (D. Mercurio, V. Spokoiny).

Since the seminal papers of [66] and [70], modeling the dynamic features of the variance of financial time series has become one of the most active fields of research in econometrics. New models, different applications and extensions have been proposed as it can be seen by consulting, for example, the monographs [71]. The main idea behind this strain of research is that the volatility clustering effect that is displayed by stock or exchange rate returns can be modeled globally by a stationary process. This approach is somehow restrictive and it does not fit some characteristics of the data, in particular the fact that the volatility process appears to be "almost integrated" as it can be seen by usual estimation results and by the very slow decay of the autocorrelations of squared returns. Other global parametric approaches have been proposed by [65] and by [72] in order to include these features in the model. Furthermore, continuous time models, and in particular diffusions and jump diffusions, have also been considered; see, for example, [69] and [64].

However, [79] showed that long memory effects of financial time series can be artificially generated by structural breaks in the parameters. This motivates another modeling approach which borrows its philosophy mainly from the nonparametric statistics. The main idea consists in describing the volatility clustering effect only by a locally stationary process. Therefore, only the most recent data are considered and weighting schemes, which can be themselves either global or local and data driven, are suggested in order to decrease the dependence of the estimate on the older observations. Some examples of this approach can be found in [67], in [68], and in [73]. Furthermore, [76] proposes a new locally adaptive volatility estimation (LAVE) of the unknown volatility from the conditionally heteroskedastic returns. The method is based on pointwise data-driven selection of the interval of homogeneity for every time point. The numerical results demonstrate a reasonable performance of the new method. In particular, it slightly outperforms the standard GARCH(1,1) approach. [74] extend this method to estimating the volatility matrix of the multiple returns and [78] apply the same idea in the context of a regression problem.

Mercurio and Spokoiny (2004b) developed another procedure which, however, applies a similar idea of pointwise adaptive choice of the interval of homogeneity. The main differences between the LAVE approach and the new procedure is in the way of testing the homogeneity of the interval candidate and in the definition of the selected interval. The new approach is based on the local change-point analysis. This means that every interval is tested on homogeneity against a change-point alternative. If the hypothesis is not rejected, a larger interval candidate is taken. If the change point is detected, then the location of the change point is used for

defining the adaptive interval while [76] suggested to take the latest non-rejected interval. The modified procedure allows to improve the sensitivity of the method to changes of volatility by using the more powerful likelihood ratio test statistic with the careful choice of the critical level. In addition, the use of the additional information about the location of the change point which is delivered by the change-point test, helps to reduce the estimation bias. Finally, the interpretation of the procedure as a multiple test against a change-point alternative leads to a very natural method of tuning the parameters of the procedure.

Another important feature of the proposed procedure is that it can be easily extended to multiple volatility modeling, cf. [74]. Suppose that a number of financial time series is observed and the goal is to estimate the corresponding time-depending volatility matrix. We again assume that the volatility matrix is nearly constant within some historical time interval which we identify from the data. The volatility matrix is estimated in a usual way from the observations which belong to the detected interval.

The new procedure is shown to be rate-optimal in detecting the volatility changes and in estimating the smoothly varying volatility function. The numerical results indicate quite reasonable performance of the procedure.

The assumption of a local constant volatility is very useful in applications to Value-at-Risk analysis. Indeed, the volatility matrix is assumed nearly constant in some historical interval and this value of volatility can be extrapolated on some short time interval of ten working days in the future which is only relevant in the VaR analysis. Mercurio and Spokoiny (2004) systematically applied this approach and compared the results with what the standard GARCH (1,1) modeling delivers, see [75]. It turns out that the local constant method delivers better accuracy in volatility forecasting leading to a better fit of the prescribed excess rate.

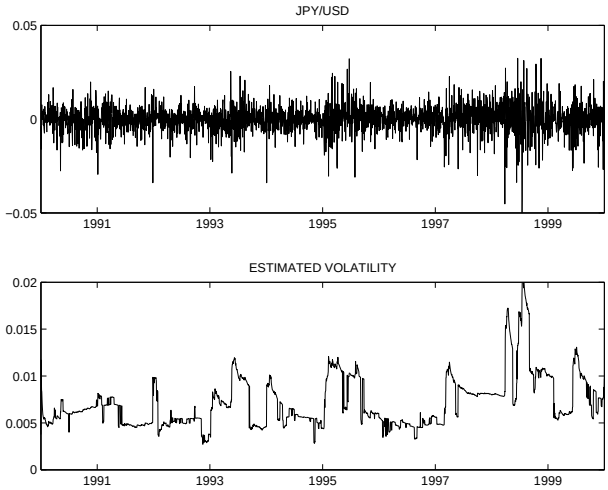

Fig. 2: Returns and estimated volatility for the JPY/USD exchange rate

5. Variance reduction and stratification in risk management (P. Mathé).

Many financial portfolios are influenced by a variety of underlyings, but which are only locally correlated. The valuation of such products leads to high-dimensional integration, but the integrands possess a small effective dimension. Prototypically, we exhibit the following situation, describing a portfolio of a set $\{S_1, S_2, ..., S_m\}$, of m underlyings with respective shares $\omega_1, \omega_2, ..., \omega_m$, determining the present value

$$V_t = \sum_{j=1}^{m} \omega_j S_j.$$

There are many numerical schemes for the valuation of such financial products. Often a reasonable approximation is obtained using the Δ-Γ-normal method for the forecast of V_{t+1} at a future time, knowing V_t, given by

$$V_{t+1} \approx V_t + \theta + \Delta y + \langle \Gamma y, y \rangle,$$

with θ, Δ, and Γ completely determined by the structure of the portfolio, and y Gaussian innovations, see [11]. In this case we obtain a quadratic functional in the underlyings. This remains quadratic when turning to the independent risk factors. Normally, Γ is sparse.

In cooperation with S. Jaschke, Bundesanstalt für Finanzdienstleistungsaufsicht Bonn, previous analysis of valuation of the Δ-Γ-normal approximation by means of stratification, in particular using *randomized orthogonal arrays*, of large portfolios was extended to risk analysis. It could be shown that stratification is a general tool for enhancing known algorithms. This holds true for randomized orthogonal arrays and also for randomized digital nets, where recently codes became available for high dimensions. Specifically, the authors introduce a numerical quantity $\kappa(meth, x, n)$, which describes the speedup of any chosen method "meth", using sample size n, against plain Monte Carlo sampling at location x. For specific methods, this quantity can be shown to be less than 1; thus such methods enhance Monte Carlo simulations.

In Jaschke and Mathé (2004), the theoretical results are combined with an extensive case study, see Figure 3, based on a portfolio of a German mid-sized bank.

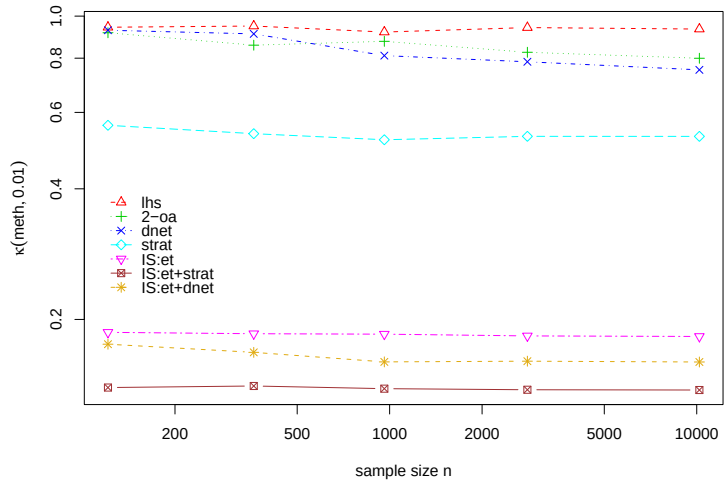

Fig. 3: Comparison of the efficiency of different sampling strategies at the 1 % quantile

6. Estimating environmental risk in shallow waters by forward-reverse simulation (J. Schoenmakers).

The method of Milstein, Schoenmakers and Spokoiny [41] developed in cooperation with the project *Statistical data analysis* provides a new transition density estimator for diffusion processes which is basically root-N consistent for any dimension of the diffusion process. This estimator,

$$\hat{p}(t,x,T,y) = \frac{1}{MN\delta^d} \sum_{m=1}^{M} \sum_{n=1}^{N} K\left(\frac{X_{t,x}^{(n)}(t_1) - Y_{t_1,y}^{(m)}(T)}{\delta} \right) \mathcal{Y}_{t_1,y}^{(m)}(T), \tag{1}$$

which does not suffer from the "curse of dimensionality", is based on forward simulation of the given process X and reverse simulation of an adjoint process $(Y, \mathcal{Y})$ which can be constructed via the (formal) adjoint of the generator of the original process.

The forward-reverse density estimator in this year was successfully applied to pollution particle models in the North Sea environment by Spivakovskaya, Heemink, Milstein and Schoenmakers (2004). In this work, particle models are used to simulate the spreading of a pollutant in coastal waters in case of a calamity at sea. Many different particle trajectories starting at the point of release are generated to determine the particle concentration at some critical locations after the release. A standard Monte Carlo method for this essentially density problem would consume a long CPU time. However, here it is shown that the forward-reverse estimator gives superior results, see the figure below.

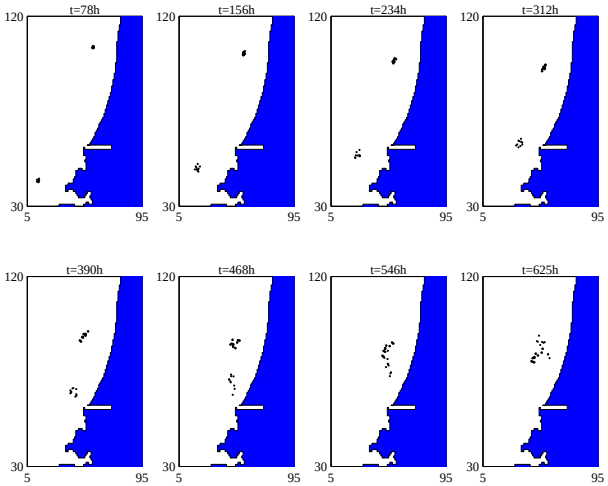

Fig. 4: Forward and reverse pollution particle simulation near the cost of Holland

B: Stochastic models and algorithms in computational physics

In 2004, the research concentrated on the development of new stochastic models and simulation techniques for solving high-dimensional boundary value problems with random coefficients related to the transport in porous media, potential and elasticity problems, and to the numerical solution of the Smoluchowski equation governing ensembles of interacting charged particles generated in a combustion process. New fundamental results were obtained in the random field simulation: Novel spectral randomization methods and Fourier/wavelet-based representations for divergenceless random fields were developed. These models have nice ergodic properties and can be efficiently implemented in numerical calculations.

The results are presented in the published papers [25], [28], [55], [63], in the papers [13], [29], [30] in press, and in five talks at international conferences.

1. Random fields simulation (K.K. Sabelfeld).

We analyze and compare the efficiency and accuracy of two simulation methods for homogeneous random fields with multiscale resolution: the Fourier-wavelet method and three variants of the randomization method: (A) without any stratified sampling of wavenumber space, (B) stratified sampling of wavenumbers with equal energy subdivision, (C) stratified sampling with a logarithmically uniform subdivision. We focus on fractal Gaussian random fields with Kolmogorov-type spectra. As known from the previous work [52], variants (A) and (B) of the randomization method are only able to generate a self-similar structure function over three to four decades with reasonable computational effort. By contrast, variant (C), along with the Fourier-wavelet method, is able to reproduce accurate self-similar scaling of the structure function over a number of decades increasing linearly with computational effort (for our examples we show that twelve decades can be reproduced). We provide some conceptual and numerical comparison of the various cost contributions to each random field simulation method (overhead, cost per realization, cost per evaluation). We expect ergodic properties to be important in simulating the solutions to partial differential equations with random field coefficients, and to this end, it is interesting to compare the Fourier-wavelet and various randomization methods in simulating the solution to the Darcy equation for porous media flow with the heterogeneous conductivity modeled as a homogeneous random field.

Random functions (generally referred to as random fields) provide a useful mathematical framework for representing disordered heterogeneous media in theoretical and computational studies, [52]. One example is in turbulent transport, where the velocity field $\mathbf{v}(\mathbf{x})$ representing the turbulent flow is modeled as a random field with statistics encoding important empirical features, and the temporal dynamics of the position $\mathbf{X}(t)$ of immersed particles is then governed by equations involving this random field such as

$$\begin{aligned} d\mathbf{X}(t) &= \mathbf{V}(t)\,dt, \\ m\,d\mathbf{V}(t) &= -\gamma\Big(\mathbf{V}(t)-\mathbf{v}(\mathbf{X}(t),t)\Big)\,dt+\sqrt{2k_{\mathrm{B}}T\gamma}\,d\mathbf{W}(t), \end{aligned}$$

where m is particle mass, γ is its friction coefficient, k_{B} is Boltzmann's constant, T is the absolute temperature, and $\mathbf{W}(t)$ is a random Wiener process representing molecular collisions. Another example is in transport through porous media, such as groundwater aquifers, in which the conductivity $K(\mathbf{x})$ is modeled as random field reflecting the empirical variability of the porous medium. The Darcy flow rate $\mathbf{q}(\mathbf{x})$ in response to pressure applied at the boundary is governed by the Darcy equation

$$\begin{aligned} \mathbf{q}(\mathbf{x}) &= -K(\mathbf{x})\operatorname{grad}\phi(\mathbf{x}), \\ \operatorname{div}\mathbf{q} &= 0, \end{aligned}$$

in which the random conductivity function appears as a coefficient, and the applied pressure is represented in the boundary conditions for the internal pressure head ϕ. Our concern is with the computational simulation of random fields for applications such as these.

Interesting insights into the dynamics of transport in disordered media can be achieved already through relatively simple random models for the velocity field, such as a finite superposition of Fourier modes, with each amplitude independently evolving according to an Ornstein–Uhlenbeck process. Here, efficient and accurate numerical simulations of the flow can be achieved through application of the well-developed literature on simulating stochastic ordinary differential equations. We focus instead on the question of simulating random fields which

involve challenging multiscale structures such as those relevant to porous media and turbulent flow simulations. Many questions remain open for the case of Gaussian multiscale random fields, so we confine our attention to this class. The paper [30] devoted to this study is to appear in 2005.

2. Stochastic models for flow simulation in porous media (K.K. Sabelfeld, D. Kolyukhin).

In this project, a stochastic model of a flow in incompressible porous media without the assumption of smallness of the hydraulic conductivity is constructed. The hydraulic conductivity is modeled as a divergenceless random field with a lognormal distribution by a Monte Carlo method based on the spectral representation of homogeneous Gaussian random fields described in the previous section of the present report. The Darcy law and continuity equation are solved numerically by the successive over-relaxation method which provides us with detailed statistical characteristics of the flow. The constructed numerical method is highly efficient so that we were able to outline the applicability of the spectral models derived in the first-order approximation. These results are published partly in [28] and the results of further study are to be published in [29].

3. Random walk on spherical grids for solving boundary value problems of electrostatic and elasticity potentials (K.K. Sabefeld).

Stochastic algorithms for solving high-dimensional Dirichlet problems for the Laplace equation and the system of Lamé equations are developed. The approach presented is based on the Poisson integral formula written down for each of a family of overlapping discs in 2D and spheres in 3D. The original differential boundary value problem is reformulated in the form of an equivalent system of integral equations defined on the intersection surfaces (arcs, in 2D, and caps, in 3D). A random walk algorithm can be applied then directly to the obtained system of integral equations where the random walks are living on the intersecting surfaces (arcs, in 2D, or caps, in 3D). Another version of a stochastic method is constructed as a discrete random walk for a system of linear equations approximating our system of integral equations. We develop two classes of special Monte Carlo iterative methods for solving these systems of equations which are a kind of stochastic versions of the Chebyshev iteration method and SOR method. In the case of classical potential theory, this approach improves the convergence of the well-known random walk on spheres method. What is, however, much more important is that this approach suggests a first construction of a fast convergent finite-variance Monte Carlo method for the system of Lamé equations.

Consider a homogeneous isotropic medium $G \subset \mathbf{R}^n$ with a boundary Γ whose state in the absence of body forces is governed by the boundary value problem, see, e.g., [53]:

$$\Delta \mathbf{u}(x) + \alpha \operatorname{grad} \operatorname{div} \mathbf{u}(x) = 0, \quad x \in G, \quad \mathbf{u}(y) = \mathbf{g}(y), \quad y \in \Gamma, \tag{2}$$

where $\mathbf{u}(x) = (u_1(x_1,\dots,x_n),\dots,u_n(x_1,\dots,x_n))$ is a vector of displacements, whose components are real-valued regular functions. The elastic constant $\alpha = (\lambda+\mu)/\mu$ is expressed through the Lamé constants of elasticity λ and μ.

Consider an arbitrary point x with polar coordinates (r,φ') inside a disk $K(x_0,R)$. The point y situated on the circle $S(x_0,R)$ has the coordinates (R,θ), where $\theta = \varphi' + \alpha$, and z is defined by $z = y - x$; note that α is the angle between the vectors x and y; ψ is the angle between x and z. Define also the angle φ by $\varphi = \varphi' + \psi$.

Our method is based on the following solution representation which we obtained in [53], [54]:

The solution to Equation (2) satisfies the following mean value relation, x being an arbitrary point in $K(x_0,R)$:

$$u_i(x) = \frac{R^2 - |x-x_0|^2}{2\pi R} \sum_{j=1}^{2} \int\limits_{S(x_0,R)} \frac{b_{ij}(x,y)\, u_j(y)}{|x-y|^2}\, dS_y \ , \quad i = 1,2, \tag{3}$$

where b_{ij} are functions of x,y, explicitly represented as the entries of the following matrix

$$B = \frac{\alpha}{\alpha+2} \begin{pmatrix} \frac{2}{\alpha} + 2\cos^2\varphi + \frac{|x-y|}{R}\cos(\theta+\varphi) & 2\cos\varphi\sin\varphi + \frac{|x-y|}{R}\sin(\theta+\varphi) \\ 2\cos\varphi\sin\varphi + \frac{|x-y|}{R}\sin(\theta+\varphi) & \frac{2}{\alpha} + 2\sin^2\varphi - \frac{|x-y|}{R}\cos(\theta+\varphi) \end{pmatrix} .$$

Relation (3) reads in the matrix form:

$$\mathbf{u}(x) = \int\limits_{S(x_0,R)} p(y;x)\, B\mathbf{u}(y)\, dS(y) \tag{4}$$

where $p(y;x) = [R^2 - |x-x_0|^2]/(2\pi R(|x-y|^2)$ is the kernel of the Poisson formula for the Laplace equation.

We apply this representation for two overlapping discs, γ_1 γ_2 being the inner arcs of intersection, and Γ_1 Γ_2 are the corresponding external arcs. We now can derive a system of four integral equations defined on the arcs γ_1 and γ_2. Indeed, let us introduce the notations: $v_1^{(1)}(x) = u_1(x)$ and $v_1^{(2)}(x) = u_2(x)$ for $x \in \gamma_2$, and $v_2^{(1)}(x) = u_1(x)$ and $v_2^{(2)}(x) = u_2(x)$ for $x \in \gamma_1$. Then the system (4) can be written as $\mathbf{v} = \mathbf{G}\mathbf{v} + \mathbf{F}$, or, in more detail,

$$\begin{pmatrix} v_1^{(1)} \\ v_1^{(2)} \\ v_2^{(1)} \\ v_2^{(2)} \end{pmatrix} = \begin{pmatrix} 0 & 0 & B_{11} & B_{12} \\ 0 & 0 & B_{21} & B_{22} \\ \hat{B}_{11} & \hat{B}_{12} & 0 & 0 \\ \hat{B}_{21} & \hat{B}_{22} & 0 & 0 \end{pmatrix} \begin{pmatrix} v_1^{(1)} \\ v_1^{(2)} \\ v_2^{(1)} \\ v_2^{(2)} \end{pmatrix} + \begin{pmatrix} f_1^{(1)} \\ f_1^{(2)} \\ f_2^{(1)} \\ f_2^{(2)} \end{pmatrix} \tag{5}$$

where the integral operators B_{ij}, $i,j = 1,2$, are defined, according to (3), for the points of the first disc $x \in K(x_0^{(1)})$:

$$B_{ij}v_2^{(j)}(x) = \int\limits_{\gamma_1} p(y;x)\, b_{ij}(x,y)\, v_2^{(j)}(y)\, dS(y), \quad i,j = 1,2 \ ,$$

while the integral operators $\hat{B}_{ij}$, $i,j = 1,2$, are defined for the points of the second disc $x \in K(x_0^{(2)})$:

$$\hat{B}_{ij}v_1^{(j)}(x) = \int\limits_{\gamma_2} p(y;x)\, b_{ij}(x,y)\, v_1^{(j)}(y)\, dS(y), \quad i,j = 1,2 \ .$$

The functions f_i^j are defined analogously:

$$f_i^{(j)}(x) = \sum_{k=1}^{2} \int\limits_{\Gamma_i} p(y;x)\, b_{jk}(x,y)\, g_k(y)\, dS(y), \quad i,j = 1,2 \ .$$

We have proved in [55] the following result:

The integral operator **G** *of the system (5) is a Fredholm operator with kernels continuous on* $x \in \gamma_1$ *and* $y \in \gamma_2$*, with the same type of singularities at the points of intersection of the arcs* γ_1 *and* γ_2 *as the singularities in the case of the Laplace equation. The spectral radius of* **G** *is less than* 1 *which ensures the equivalence of system (5) and problem (2).*

This scheme is extended to the case of n overlapping spheres. The numerical algorithm based on this representation is highly efficient. For illustration, we have made calculations for an elastic polymer consisting of 17 overlapping discs. The accuracy of about 0.1 % was achieved in 4.5 min on a personal computer.

4. Stochastic models for the flux and concentration footprints (K.K. Sabelfeld).

The use of footprint functions in complex flows has been questioned because of anomalous behavior reported in recent model studies. We show that the concentration footprint can be identified with Green's function of the scalar concentration equation or the transition probability of a Lagrangian formulation of the same equation and so is well behaved and bounded by 0 and 1 in both simple and complex flows. The flux footprint in contrast is not a Green function but a functional of the concentration footprint and is not guaranteed to be similarly well behaved. We show that in simple, homogeneous shear flows, the flux footprint, defined as the vertical eddy flux induced by a unit point source, is bounded by 0 and 1 but that this is not true in more general flow fields. An analysis of recent model studies also shows that the negative flux footprints reported in homogeneous plant canopy flows are an artefact of reducing a canopy with a complex source-sink distribution in the vertical to a single layer but that in canopies on hilly topography the problems are more fundamental. Finally, we compare footprint inversion with the direct mass-balance method of measuring surface exchange. We conclude first that the flux footprint is an appropriate measure of the area influencing both eddy and advective fluxes on a tower but that the concentration footprint is the correct measure when the storage term is important. Second, we deduce that there are serious obstacles to inverting flux footprints in complex terrain. The results obtained in [31], [33], [34] were generalized and published in [63]. The work is done in cooperation with Prof. Dr. T. Vesala and Dr. U. Rannik (Helsinki University, Finland), Prof. T. Foken (Universität Bayreuth), and A. Levykin (Institute of Computational Mathematics and Mathematical Geophysics, Russian Academy of Sciences, Novosibirsk).

5. A new stochastic method for the Smoluchowski equation, with applications to systems of coagulating charged particles (A. Kolodko, K.K. Sabelfeld).

We deal here with the coagulation of charged particles, and the concentration is described by the Smoluchowski equation

$$\frac{\partial n_{lz}(t,r,z)}{\partial t} = \frac{1}{2}\sum_{i+j=l}\sum_{m+k=z} K_{ijmk} n_{im} n_{jk} - n_{lz}\sum_{i=1}^{\infty}\sum_{m=-\infty}^{\infty} K_{lizm} n_{im},\ l > 2; \qquad (6)$$

$$n_l(r,0) = n_l^0(r), n_z(z,o) = n_z^0(z).$$

The kernel K_{ijmk} is given by

$$K_{ijmk} = \Gamma_{ij} K_{ij},$$

where K_{ij} is the usual coagulation coefficient which we choose as in the case of the free molecular collision regime, and Γ_{ij} is a factor which takes into account the charge on the

particle:

$$\Gamma_{i,j} = \frac{\lambda_{ij}}{exp(\lambda_{ij}) - 1} \quad \text{in the case of repulsion,}$$

$$\Gamma_{i,j} = \frac{\lambda_{ij}}{1 - exp(\lambda_{ij})} \quad \text{in the case of attraction,}$$

where

$$\lambda_{ij} = \frac{const\,|m|\,|k|}{(r_i + r_j)k_b T}, \quad k_b = 1.38 \times 10^{-16}, \quad \text{is the Bolzmann constant, and } T = 295\ K,$$

and m, k are the values of the charge (integer numbers).
It is seen from the formulation that the dimension of the problem is enormously increased, compared to the standard Smoluchowski equation, [26]. Therefore, we suggest a new method of stochastic simulation, which can be described as follows. First, we divide the set of all pairs of particles into subclasses so that in each subclass, the Neumann rejection method can be effectively applied. The sampling of the subclass is made according to the direct simulation from a discrete distribution where the Walker method is applied, see [50].
Some examples of simulations that we have made for the formation of charged aggregates of nanoparticles by combustion of aluminum droplets in air are given in [25], and some other aerosol formation applications are presented by us in [13].

References

1. F. AITSAHLIA, P. CARR, *American options: A comparison of numerical methods*, in: Numerical Methods in Finance, L.C.G. Rogers, D. Talay, Cambridge University Press, 1997, pp. 67–87.

2. P. ARTZNER, F. DELBAEN, J.M. EBER, D. HEATH, *Coherent measures of risk*, Math. Finance, **9** (1998), pp. 203–228.

3. D. BELOMESTNY, G.N. MILSTEIN, *Monte Carlo evaluation of American options using consumption processes*, working paper, 2003.

4. C. BENDER, R.J. ELLIOTT, *Arbitrage in a discrete version of the Wick-fractional Black–Scholes market*, Math. Oper. Res., **29** (2004), pp. 935–945.

5. C. BENDER, *Explicit solutions of a class of linear fractional BSDEs*, to appear in: Systems Control Lett.

6. ——, *The restriction of the fractional Itô integral to adapted integrands is injective*, to appear in: Stoch. Dyn.

7. C. BENDER, M. KOHLMANN, *Superhedging under nonconvex constraints – A BSDE approach*, WIAS Preprint no. 928, 2004.

8. C. BENDER, J.G.M. SCHOENMAKERS, *An iterative algorithm for multiple stopping: Convergence and stability*, WIAS Preprint no. 991, 2004.

9. R.C. BOSE, A. BUSH, *Orthogonal arrays of strength two and three*, Ann. Math. Statistics, **23** (1952), pp. 508–524.

10. A. BRACE, D. GATAREK, M. MUSIELA, *The market model of interest rate dynamics*, Math. Finance, **7** (1997), pp. 127–155.

11. M. BROADIE, J. DETEMPLE, *Recent advances in numerical methods for pricing derivative securities*, in: Numerical Methods in Finance, L.C.G. Rogers, D. Talay, Cambridge University Press, 1997, pp. 43–66.

12. CREDIT SUISSE FIRST BOSTON, *CreditRisk$^+$: A Credit Risk Management Framework*, available at `http://www.csfb.com/creditrisk`, 1997.

13. S. DUBCOV, E. DULCEV, A. LEVYKIN, A. ANKILOV, K.K. SABELFELD, *A study of kinetics of aerosol formation in the photolysis of tungsten hexacarbonyl under low pressure conditions*, J. Chemical Physics, in press.

14. P. EMBRECHTS, C. KLÜPPELBERG, T. MIKOSCH, *Modelling Extremal Events*, Springer, Berlin, 1997.

15. J. FRANKE, W. HÄRDLE, G. STAHL, *Measuring Risk in Complex Stochastic Systems*, Lecture Notes in Statist., **147** (2000), Springer, New York.

16. P. GAPEEV, M. REISS, *A note on optimal stopping in models with delay*, Discussion Paper of Sonderforschungsbereich 373 no. 47, Humboldt-Universität zu Berlin, 2003.

17. P. GLASSERMAN, *Monte Carlo Methods in Financial Engineering*, Springer, New York, 2003.

18. E. GOBET, M. HOFFMANN, M. REISS, *Nonparametric estimation of scalar diffusions based on low frequency data*, 2003, to appear in: Ann. Statist.

19. H. HAAF, O. REISS, J.G.M. SCHOENMAKERS, *Numerically stable computation of CreditRisk$^+$*, WIAS Preprint no. 846, 2003, Journal of Risk, **6** (2004), pp. 1–10.

20. A. HAMEL (ED.), *Risikomaße und ihre Anwendungen*, to appear as Report of Martin-Luther-Universität Halle-Wittenberg.

21. M.B. HAUGH, L. KOGAN, *Pricing American options: A duality approach*, working paper, 2001, to appear in: Oper. Res.

22. W. HÄRDLE, H. HERWARTZ, V. SPOKOINY, *Time inhomogeneous multiple volatility modelling*, Discussion Papers of Sonderforschungsbereich 373 no. 7, Humboldt-Universität zu Berlin, 2001.

23. F. JAMSHIDIAN, *LIBOR and swap market models and measures*, Finance Stoch., **1** (1997), pp. 293–330.

24. S. JASCHKE, P. MATHÉ, *Stratified sampling for risk management*, 2004, submitted.

25. V.V. KARASEV, A.A. ONISCHUK, O.G. GLOTOV, A.M. BAKLANOV, A.G. MARYASOV, V.E. ZARKO, V.N. PANFILOV, A.I. LEVYKIN, K.K. SABELFELD, *Formation of charged Al_2O_3 nanoparticles by combustion of aluminum in air*, Combustion and Flame, **138** (2004), pp. 40–54.

26. A. KOLODKO, K.K. SABELFELD, *Stochastic particle methods for Smoluchowski equation: Variance reduction and error estimations*, Monte Carlo Methods Appl., **9** (2003), pp. 315–339.

27. A. KOLODKO, J.G.M. SCHOENMAKERS, *An efficient dual Monte Carlo upper bound for Bermudan-style derivatives*, WIAS Preprint no. 877, 2003.

28. D. KOLYUKHIN, K.K. SABELFELD, *Stochastic Eulerian model for the flow simulation in porous media. Unconfined aquifers*, Monte Carlo Methods Appl., **10** (2004), pp. 345–357.

29. ——, *Direct numerical solution of the Darcy equation with random hydraulic conductivity. Mathematics and computers in simulation*, to appear in: Monte Carlo Methods Appl.

30. P. KRAMER, O. KURBANMURADOV, K.K. SABELFELD, *Extensions of multiscale Gaussian random field simulation algorithms*, to appear in: J. Comput. Phys.

31. O. KURBANMURADOV, A. LEVYKIN, U. RANNIK, K.K. SABELFELD, T. VESALA, *Stochastic Lagrangian footprint calculations over a surface with an abrupt change of roughness height*, Monte Carlo Methods Appl., **9** (2003), pp. 167–188.

32. O. KURBANMURADOV, K.K. SABELFELD, O. SMIDTS, H. VEREECKEN, *A Lagrangian stochastic model for transport in statistically homogeneous porous media*, Monte Carlo Methods Appl., **9** (2003), pp. 341–366.

33. O. KURBANMURADOV, K.K. SABELFELD, *Lagrangian stochastic models for turbulent dispersion in the atmospheric boundary layer*, Boundary-Layer Meteorology, **97** (2000), pp. 191–218.

34. O. KURBANMURADOV, U. RANNIK, K.K. SABELFELD, T. VESALA, *Estimation of mean concentration and fluxes by Lagrangian stochastic models*, Math. Comput. Simulation, **54** (2001), pp. 459–476.

35. O. KURBANMURADOV, K.K. SABELFELD, J.G.M. SCHOENMAKERS, *Lognormal approximations to LIBOR market models*, J. Computational Finance, **6** (2002), pp. 69–100.

36. P. MATHÉ, *Using orthogonal arrays to valuate* $\Delta - \Gamma$*-normal*, working paper, 2003.

37. D. MERCURIO, V. SPOKOINY, *Estimation of time dependent volatility via local change-point analysis*, WIAS Preprint no. 904, 2004.

38. G.N. MILSTEIN, O. REISS, J.G.M. SCHOENMAKERS, *A new Monte Carlo method for American options*, earlier version: WIAS Preprint no. 850, 2003, to appear in: Int. J. Theor. Appl. Finance.

39. G.N. MILSTEIN, J.G.M. SCHOENMAKERS, *Monte Carlo construction of hedging strategies against multi-asset European claims*, Stoch. Stoch. Rep., **73** (2002), pp. 125–157.

40. G.N. MILSTEIN, J.G.M. SCHOENMAKERS, V. SPOKOINY, *Forward-reverse representations for Markov chains*, working paper, 2003.

41. ——, *Transition density estimation for stochastic differential equations via forward-reverse representations*, Bernoulli, **10** (2004), pp. 281–312.

42. G.N. MILSTEIN, M.V. TRETYAKOV, *Numerical analysis of Monte Carlo finite difference evaluation of Greeks*, WIAS Preprint no. 808, 2003.

43. ——, *Simulation of a space-time bounded diffusion*, Ann. Appl. Probab., **9** (1999), pp. 732–779.

44. K.R. MILTERSEN, K. SANDMANN, D. SONDERMANN, *Closed-form solutions for term structure derivatives with lognormal interest rates*, J. Finance, **52** (1997), pp. 409–430.

45. R.B. NELSON, *An Introduction to Copulas*, Springer, New York, 1999.

46. M. REISS, *Nonparametric volatility estimation on the real line from low-frequency observations*, 2003, submitted.

47. O. REISS, *Dependent sectors and an extension to incorporate market risk*, in: CreditRisk$^+$ in the Banking Industry, M. Gundlach, F. Lehrbass, Springer, Berlin/Heidelberg, 2004.

48. ——, *Fourier inversion techniques for CreditRisk$^+$*, in: CreditRisk$^+$ in the Banking Industry, M. Gundlach, F. Lehrbass, Springer, Berlin/Heidelberg, 2004.

49. O. REISS, J.G.M. SCHOENMAKERS, M. SCHWEIZER, *From structural assumptions to a link between assets and interset rates*, Preprint no. 136 of DFG Research Center MATHEON, Technische Universität Berlin, 2004.

50. B. RIPLEY, *Stochastic Simulation*, John Wiley & Sons, New York, 1987.

51. L.C.G. ROGERS, *Monte Carlo valuation of American options*, Math. Finance, **12** (2002), pp. 271–286.

52. K.K. SABELFELD, *Monte Carlo Methods in Boundary Value Problems*, Springer, Heidelberg, New York, Berlin, 1991.

53. K.K. SABELFELD, I. SHALIMOVA, *Spherical Means for PDEs*, VSP, Utrecht, The Netherlands, 1997.

54. ——, *Random walk methods for static elasticity problems*, Monte Carlo Methods Appl., **8** (2002), pp. 171–200.

55. K.K. SABELFELD, I. SHALIMOVA, A. LEVYKIN, *Discrete random walk on large spherical grids generated by spherical means for PDEs*, Monte Carlo Methods Appl., **10** (2004), pp. 559–574.

56. J.G.M. SCHOENMAKERS, *Calibration of LIBOR models to caps and swaptions: A way around intrinsic instabilities via parsimonious structures and a collateral market criterion*, WIAS Preprint no. 740, 2002.

57. ——, *Robust Libor Modelling and Pricing of Derivatives Products*, to appear in: Chapman & Hall Fin. Math. Series.

58. J.G.M. SCHOENMAKERS, B. COFFEY, *LIBOR rate models, related derivatives and model calibration*, WIAS Preprint no. 480, 1999.

59. ——, *Stable implied calibration of a multi-factor LIBOR model via a semi-parametric correlation structure*, WIAS Preprint no. 611, 2000.

60. ——, *Systematic generation of parametric correlation structures for the LIBOR market model*, Int. J. Theor. Appl. Finance, **6** (2003), pp. 507–519.

61. D. SPIVAKOVSKAYA, A.W. HEEMINK, G.N. MILSTEIN, J.G.M. SCHOENMAKERS, *Simulation of particle concentrations in coastal waters using forward and reverse time diffusion*, tentatively accepted for: Advances in Water Resources.

62. D. TASCHE, *Capital allocation with CreditRisk*$^+$, in: CreditRisk$^+$ in the Banking Industry, F. Lehrbass, M. Gundlach, Springer, 2004.

63. T. VESALA, U. RANNIK, M. LECLERC, T. FOKEN, K.K. SABELFELD, *Flux and concentration footprints*, Agricultural and Forest Meteorology, **127** (2004), pp. 111–116.

64. T.G. ANDERSEN, L. BENZONI, J. LUND, *An empirical investigation of continuous-time equity return models*, J. Finance, **3** (2002), pp. 1239–1284.

65. R. BAILLIE, T. BOLLERSLEV, H. MIKKELSEN, *Fractionally integrated generalized autoregressive conditional heteroskedasticity*, J. Econometrics, **74** (1996), pp. 3–30.

66. T. BOLLERSLEV, *Generalised autoregressive conditional heteroskedasticity*, J. Econometrics, **31** (1986), pp. 307–327.

67. M.Y. CHENG, J. FAN, V. SPOKOINY, *Dynamic nonparametric filtering with application to volatility estimation*, in: Recent Advances and Trends in Nonparametric Statistics, M.G. Acritas, D.N. Politis, eds., Elsevier, Amsterdam, Oxford, Heidelberg, 2003, pp. 315–333.

68. R. DAHLHAUS, S.S. RAO, *Statistical inference of time-varying ARCH processes*, Preprint no. 31 of DFG Schwerpunktprogramm 1214, Universität Bremen, 2003.

69. D. DUFFIE, J. PAN, K. SINGLETON, *Transform analysis and asset pricing for affine jump diffusions*, Econometrica, **68** (2000), pp. 1343–1376.

70. R. ENGLE, *Autoregressive conditional heteroskedasticity with estimates of the variance of U.K. inflation*, Econometrica, **50** (1982), pp. 987–1008.

71. R. ENGLE, ed., *ARCH, Selected Readings*, Oxford University Press, 1995.

72. R. ENGLE, T. BOLLERSLEV, *Modelling the persistence of conditional variances*, Econometric Rev., **5** (1986), pp. 1–50, pp. 81–87.

73. J. FAN, J. GU, *Semiparametric estimation of Value at Risk*, Econom. J., **6** (2003), pp. 260–289.

74. W. HÄRDLE, H. HERWARTZ, V. SPOKOINY, *Time inhomogeneous multiple volatility modelling*, J. Financial Econom., **1** (2003), pp. 55–95.

75. A.J. MCNEIL, R. FREY, *Estimation of tail-related risk measures for heteroskedastic financial time series: An extreme value approach*, J. Empirical Finance, **7** (2000), pp. 271–300.

76. D. MERCURIO, V. SPOKOINY, *Statistical inference for time-inhomogeneous volatility models*, Ann. Statist., **32** (2004), pp. 577–602.

77. ——, *Estimation of time dependent volatility via local change-point analysis with applications to Value-at-Risk*, WIAS Preprint no. 904, 2004.

78. D. MERCURIO, C. TORRICELLI, *Estimation and arbitrage opportunities for exchange rate baskets*, Applied Econometrics, **35** (2003), pp. 1689–1698.

79. T. MIKOSCH, C. STARICA, *Is it really long memory we see in financial returns?*, in: Extremes and Integrated Risk Management, P. Embrechts, ed., Risk Books, UBS Warburg, 2000.

4.7 Research Group Thermodynamic Modeling and Analysis of Phase Transitions

4.7.1 Overview

Zum 1. September 2004 hat die offizielle Gründung der neuen Forschungsgruppe 7 stattgefunden. Dabei vereinigte sich eine Untereinheit der Forschungsgruppe 1, die sich hauptsächlich mit Analysis und Numerik partieller Differentialgleichungen beschäftigt, die im Zusammenhang mit Phasenübergängen auftreten, mit der alten Forschungsgruppe 7, deren Mitglieder hauptsächlich die thermodynamische Modellierung und Simulation von Phasenübergängen betreiben.

The new Research Group 7 was officially founded on September 1, 2004. A former subunit of Research Group 1, being mainly concerned with the analysis and numerics of PDEs associated with phase transitions, merged with the former Research Group 7, whose members mainly study thermodynamic modeling and simulations of phase transitions.

Die im Berichtszeitraum durchgeführten Untersuchungen betrafen:

1. Morphologieänderungen bei Phasenübergängen in thermomechanischen Spannungsfeldern. Die behandelten Materialien werden als Lote in mikroelektronischen Bauteilen eingesetzt. Es werden hier Phasenfeldgleichungen mit thermomechanischer Kopplung und ihre Grenzübergänge zu Evolutionsgleichungen für scharfe Phasengrenzen untersucht. Für Letztere wurden Randintegralmethoden zur Lösung etabliert und es wurden Stabilitätsfragen geklärt.

2. Berechnung von Nichtstandard-Phasendiagrammen, in denen erstmals Oberflächenenergien und deviatorische Spannungen sowie Maxima der freien Energie berücksichtigt werden. Insbesondere wird ein Vergleich mit Standard-Phasendiagrammen durchgeführt. Die Maxima werden mit kritischen Tropfen identifiziert.

During the period of this report, the conducted investigations included:

1. Morphological changes that accompany phase transitions in the presence of thermomechanical stress fields. The addressed materials are used as solders in microelectronic devices. To this end, phase-field equations with thermomechanical coupling and their sharp interface limits leading to evolution laws with sharp interfaces were studied. Boundary integral methods for the solution of the evolution laws were established, and furthermore, problems of stability of interfaces could be elucidated.

2. Calculation of non-standard phase diagrams, where surface tension and deviatoric bulk stresses as well as free-energy maxima were taken into account for the first time. Particularly, a comparison to standard phase diagrams is made. The maxima are identified with critical droplets.

3. Modellierung und Simulation der Nukleation und Evolution flüssiger Tropfen in einer kristallinen GaAs-Matrix mittels einer neuen Version der Becker-Döring-Theorie. Im Berichtszeitraum konnte ein schwerwiegender Defekt bei allen Becker-Döring-Modellen aus der Literatur, die den Bearbeitern zur Kenntnis gelangt sind, konstatiert werden.

4. Sublimationszüchtung von SiC aus der Gasphase. Im Berichtszeitraum wurde (i) die Einführung von anisotroper Wärmeleitung und (ii) die Verbesserung der Software `WIAS-HiTNIHS`, welche zurzeit Wärmetransport durch Leitung und Strahlung in einer äußerst komplexen Umgebung simuliert, bearbeitet.

5. Multiskalen-Modellierung der atomaren Kette. Diese Untersuchung betrifft grundsätzliche Fragen zum Mikro-Makro-Übergang, welcher auf der atomaren Ebene startet und in Abhängigkeit von gewissen Skalierungen bei makroskopischen Gleichungen endet. Die äußerst erfolgreiche Dissertation von Michael Herrmann, die im Dezember 2004 abgeschlossen wurde, konnte bereits mehrere subtile Fragestellungen beantworten und abschließend lösen.

6. Analysis und Einsatz von Hysterese-Operatoren. Die Motivation dieser Untersuchungen resultiert aus industriellen Anforderungen zur Simulation von piezoelektrischen Sensoren und Aktuatoren. Diese Objekte werden mittels Hysterese-Operatoren modelliert. Zurzeit wird insbesondere deren Stabilität untersucht.

3. Modeling and simulation of nucleation and evolution of liquid droplets within a crystalline GaAs solid by virtue of a new version of the Becker–Döring model. During the reporting period, a severe failure of all Becker–Döring models from the literature come to the attention of the collaborators had to be stated.

4. SiC crystal growth by sublimation from the gas phase. The activities during the period of report included (i) the introduction of anisotropic heat conduction and (ii) the improvement of the software `WIAS-HiTNIHS`, which currently simulates heat transport by conduction and radiation in a complex surrounding.

5. Multiscale modeling of the atomic chain. This study regards fundamental problems of a micro-macro transition that starts on the atomic scale and ends for certain scalings with macroscopic equations. The most successful dissertation of Michael Herrmann, that was defended in December 2004, could already answer and solve many subtle problems in this context.

6. Analysis and application of hysteresis operators. The motivation of this investigation results from industrial needs to simulate the application of piezo-electric sensors and actuators. These objects are modeled by hysteresis operators, and currently, in particular their stability is studied.

7. Dynamische Prozesse in dünnen Flüssigkeitsfilmen. Die Dynamik dünner Flüssigkeitsfilme ist von großer technologischer Bedeutung für das Design von mikroelektronischen Bauteilen, aber beispielsweise auch beim Auftragen von Hüllen (Coating), die industrielle Bauteile in einer agressiven Umgebung schützen sollen. Schlupfbedingungen, aber auch Entnetzungsvorgänge wurden im Berichtszeitraum untersucht. Es wurden vorbereitende Arbeiten zur Einführung eines neuartigen Workshops durchgeführt, der im Juli 2005 stattfinden wird. „Mathematische Probleme in der Industrie“ startet am ersten Tag mit der Formulierung von Problemen durch Vertreter der Industrie, und hat das Ziel, für diese Probleme an den darauf folgenden Tagen gemeinsam Lösungsansätze zu erarbeiten.

7. Dynamic processes of thin liquid films. The dynamics of thin liquid films is of great importance to design microelectronic devices, or for coating processes to protect industrial components in an agressive surrounding. New slip conditions and dewetting phenomena were studied in the last period. Preparatory work to establish a new kind of workshop taking place in July 2005 was done. The motto of the workshop reads “Mathematics in Industry” and it will start on the first day with representatives of industry formulating problems to be solved, and the aim is to find solution approaches together during the following days of the workshop.

8. Mechanik von dünnen Stäben und Platten. Die Untersuchungen beschäftigten sich mit der Modellierung der Deformation in dünnen Stäben und Platten als Grenzfälle der dreidimensionalen nichtlinearen Elastizitätstheorie. Es wurden elliptische Randwertprobleme gelöst.

8. Mechanics of thin rods and plates. The investigations were concerned with the modeling of deformations in these objects as limiting cases of the three-dimensional nonlinear theory of elasticity. Elliptic boundary value problems have been solved.

4.7.2 Projects

Dynamics of thin liquid films on rotating disks

Collaborators: K. Afanasiev, B. Wagner

Cooperation with: A. Münch (Humboldt-Universität zu Berlin, Heisenberg Fellow at WIAS), T. Rieckmann (Fachhochschule (FH) Köln, Fakultät für Anlagen, Energie- und Maschinensysteme)

Supported by: DFG: “Mathematical modeling and analysis of spreading polymer films”, DFG Research Center MATHEON, project C10

In this new project we develop mathematical models and algorithms for the numerical simulation of the dynamics of thin liquid films on rotating discs, typically used in so-called PET (polyethylenterephthalat) reactors.
Since PET is a commodity product with a wide range of applications, ranging from the production of technical yarns to plastic bottles, it is of great practical interest to optimize reactor design and hence PET synthesis, through the development of mathematical models that are able to predict and control the shape and thickness of the thin film.
PET is produced in polycondensation reactors that typically consist of a horizontal cylinder which is partially filled with polymer melt and contains disks rotating about the horizontal axis of the cylinder, thus picking up and spreading the melt in form of a thin film over a large area of the disks (see Figure 1). At the same time, the melt, which is fed into the cylinder from one end, slowly flows to the other end where it is removed. Therefore, the film profiles and thickness will vary from disk to disk, since the viscosity increases with the degree of polymerization.

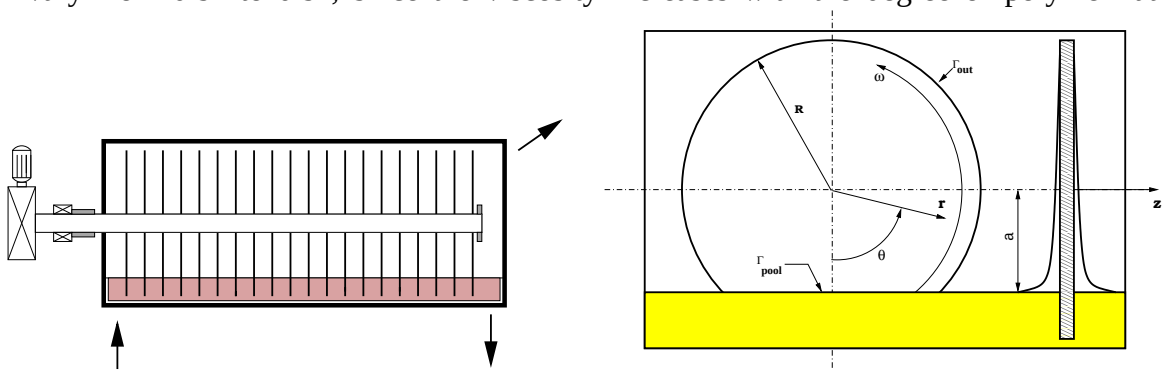

Fig. 1: Schematic of PET reactor (left). Front and side view of rotating disk (right).

For current reactor designs and operating conditions, it is typically assumed that the liquid is Newtonian. While the thickness of the film influences the reaction and output rate, they in turn do not significantly affect the film flow and thickness. Hence one can assume the chemical kinetics to decouple from the fluid dynamical part. Potential mechanisms for a coupling of the chemical kinetics to the fluid dynamics are Marangoni effects due to chemical or temperature gradients, which can be induced by the thickness-dependent evaporation of by-products, or by local release/consumption of heat by exo/endothermic reactions. However, the time scales for these effects to influence the film flow are much longer than the time required for one revolution of the disk (for typical rotation rates).

The primary problem is therefore essentially fluid-mechanical and leads to a mathematical model for the rotating-disk problem involving a coupled system of a three-dimensional mass and momentum balance (the Stokes or Navier–Stokes equations for incompressible fluids) with a free surface, where surface tension (i.e. curvature) is relevant. It is related to the classical problem of wetting a plate by pulling it out of a liquid reservoir, [1, 2]. This problem comprises two scales w.r.t. the direction normal to the plate. The small scale is the height of the thin film, merging into the reservoir via a meniscus, where the height becomes large. For such problems, surface tension plays a decisive role on how the meniscus fixes the height of the thin film. A direct three-dimensional numerical simulation of such a problem which takes into account the disparate scales is computationally very intensive. We could, however, achieve a model reduction by exploiting the two scaling regimes, making use of ideas by [3] and [4], who developed extended lubrication models from the full equations for Marangoni-driven thin film flow. We developed these methods further for the geometry of a flat, vertical, and partially submerged rotating disk and by including centrifugal forces into the model. As a result, the PDE for the film thickness, written in cylindrical coordinates, has the form:

$$\frac{\partial h}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{h^3}{3}(p_r + B sin\theta)\right) + \frac{1}{r}\frac{\partial}{\partial \theta}\left(\frac{h^3}{3}(\frac{1}{r}p_\theta + B cos\theta) + r\Omega h\right),$$

where Ω denotes the angular velocity, g gravitational acceleration, R the radius of the disk, $B = \rho g H^2/\mu U$, and the pressure p is given by

$$p = -2\left[\frac{\partial}{\partial r}\left(\frac{h_r}{N}\right) + \frac{1}{r}\frac{\partial}{\partial \theta}\left(\frac{h_\theta}{rN}\right)\right] \quad \text{with} \quad N = \left(1 + h_r^2 + \frac{h_\theta^2}{r^2}\right)^{1/2}.$$

For the boundary conditions, we require the curvature of the free surface to vanish at Γ_{out} and Γ_{pool} for $h \to \infty$, i.e.

$$p(r,\theta,t) = 0 \quad \text{for} \quad r,\theta \to \Gamma_{out} \quad \text{and} \quad r,\theta \to \Gamma_{pool}$$

and

$$p_r(r,\theta,t) = 0 \quad \text{for} \quad r,\theta \to \Gamma_{out} \quad \text{and} \quad r,\theta \to \Gamma_{pool}.$$

Furthermore, we take “natural boundary conditions” by taking the limit of the governing equation as $r \to 0$.

For a stable and efficient numerical solution of this boundary value problem for this nonlinear fourth-order PDE, we developed modifications of the Keller-box method. The algorithm is based on FEM using linear, quadratic, cubic, and mixed elements together with either direct or a numerical integration for computing the coefficients of the stiffness and/or mass matrices.

In order to test and calibrate the implementation of our numerical scheme, we first implemented our new scheme for cases of Marangoni- and gravity-driven thin film flows. For these geometrically simpler problems, our group already has accurate ADI/finite difference schemes which we used as a reference. We have also implemented the above problem for the simulation of the thin film dynamics on a rotating disk and for comparison to experimental results, performed by the group of Prof. Thomas Riekmann at the FH Cologne.

References

1. L. LANDAU, B. LEVICH, *Dragging of a liquid by a moving plate*, Acta Physicochimica U.R.S.S., **17** (1942), pp. 42–54.

2. M.S. CHRISTODOULOU, J.T. TURNER, S.D.R. WILSON, *A model for the low to moderate speed performance of the rotating disk skimmer*, J. Fluids Engrg., **476** (1990), pp. 476–480.

3. B. WAGNER, A. MÜNCH, *Numerical and asymptotic results on the linear stability of a thin film spreading down a slope of small inclination*, European J. Appl. Math., **10** (1999), pp. 297–318.

4. A. MÜNCH, *The thickness of a Marangoni-driven thin liquid film emerging from a meniscus*, SIAM J. Appl. Math., **62** (2002), pp. 2045–2063.

Numerical analysis of surface waves on permeable boundaries of poroelastic media

Collaborator: B. Albers

Cooperation with: C. Lai (European Centre for Training and Research in Earthquake Engineering, Pavia, Italy), R. Lancellotta, S. Foti (Politecnico di Torino, Italy)

In the year 2004, the work of the last years on the numerical analysis of surface waves in poroelastic media (e.g., [4], [3]) was confirmed. The theoretical research on surface waves is based on the "simple mixture model" by Wilmanski [6].
In 2004, the boundary between a porous medium and an ideal fluid has been investigated. This means that there is one additional component compared to the boundary porous medium/vacuum which has been investigated in 2003. Thus, besides the three bulk waves in the porous medium, there exists also a *P* wave in the fluid. These four waves combine into three surface waves: a leaky Rayleigh wave and both a true and a leaky Stoneley wave. Their acoustic properties (phase and group velocities, attenuations) are shown in the papers [2], [1] in dependence on two quantities: the frequency ω and the surface permeability parameter α (see figure). The variation of the second parameter, α, which controls the intensity of the in- and outflow of the fluid from the porous medium, brought to light that the true Stoneley wave exists only for very small values of this parameter, i.e. for a boundary which is almost sealed. Attenuations of both leaky waves show an interesting behavior in dependence on the frequency: for two frequencies there appear resonance effects (see figure). They seem to be not only theoretically but also experimentally observed, [5], and may be related to characteristic frequencies of the solid and the fluid, respectively.

Summary of results

The three observed surface waves possess the following attributes:

Leaky Rayleigh

– The velocity of propagation of this wave lies in the interval determined by the limits $\omega \to 0$ and $\omega \to \infty$. The high frequency limit is higher than the low frequency limit. The velocity is always smaller than c_S, i.e. slower than the *S* wave. As a function of ω, it possesses at least one inflection point.

– For low frequencies, the phase velocity for different values of the surface permeability α remains almost constant. For high frequencies, smaller values of α yield larger velocities; for the open pore case, the difference between high and low frequency limits is approximately one half of the difference for a close boundary.

– The attenuation grows linearly and unboundedly (the feature of a leaky wave), there appear singularities which depend on α and seem to be related to the characteristic frequencies $\frac{\pi}{2\rho_0^S}$ and $\frac{\pi}{2\rho_0^F}$.

Leaky Stoneley

– The phase velocity of this wave behaves similarly to the one of the leaky Rayleigh wave. However, the high frequency limit is larger for bigger values of α than for smaller ones; a maximum value appears in the region of order 100 kHz. The velocity of the leaky Stoneley wave is for each pair (ω, α) smaller than the one of the leaky Rayleigh wave.

– Also the attenuation behaves similarly to the one of the leaky Rayleigh wave. However, the singularities are more weakly dependent on α.

True Stoneley
– It exists only for small values of the surface permeability α. For different values of α, the velocity is nearly the same. It grows monotonically from the zero value for $\omega = 0$ to a finite limit which is slightly smaller (approximately 0.15 %) than the velocity c_{P2} of the $P2$ wave. The growth of the velocity of this wave in the range of low frequencies is much steeper than the one of Rayleigh waves similarly to the growth of the $P2$ velocity.
– Both the velocity and attenuation of the true Stoneley wave approach zero as $\sqrt{\omega}$ (which is not directly obvious due to the logarithmic scale of the figures).
– The attenuation of the Stoneley wave grows monotonically to a finite limit for $\omega \to \infty$. It is slightly smaller than the attenuation of $P2$ waves.

References

1. B. ALBERS, *Monochromatic surface waves at the interface between poroelastic and fluid halfspaces*, in preparation.

2. ——, *Modelling of surface waves in poroelastic saturated materials by means of a two component continuum*, WIAS Preprint no. 952, 2004, to appear in: Surface Waves in Geomechanics, Direct and Inverse Modelling for Soils and Rocks, C. Lai, K. Wilmanski, eds., CISM Courses and Lectures, Springer, Wien, New York.

3. ——, *Numerical analysis of monochromatic surface waves in a poroelastic medium*, WIAS Preprint no. 949, 2004, submitted.

4. B. ALBERS, K. WILMANSKI, *Monochromatic surface waves on impermeable boundaries in two-component poroelastic media*, submitted.

5. G. CHAO, D.M.J. SMEULDERS, M.E.H. VAN DONGEN, *Shock induced borehole waves in porous formations: Theory and experiments*, J. Acoust. Soc. Am., **116** (2004), pp. 693–702.

6. K. WILMANSKI, *Waves in porous and granular materials*, in: Kinetic and Continuum Theories of Granular and Porous Media, K. Hutter, K. Wilmanski, eds., vol. 400 of CISM Courses and Lectures, Springer, Wien, New York, 1999, pp. 131–186.

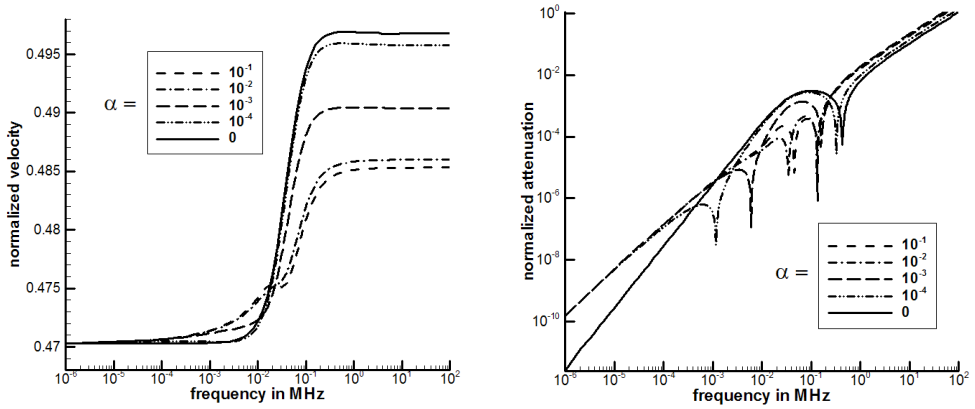

Fig. 1: Leaky Rayleigh

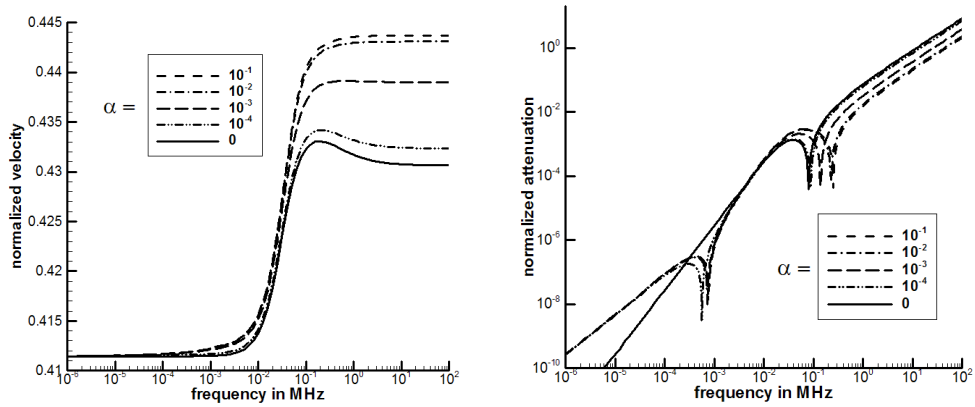

Fig. 2: Leaky Stoneley

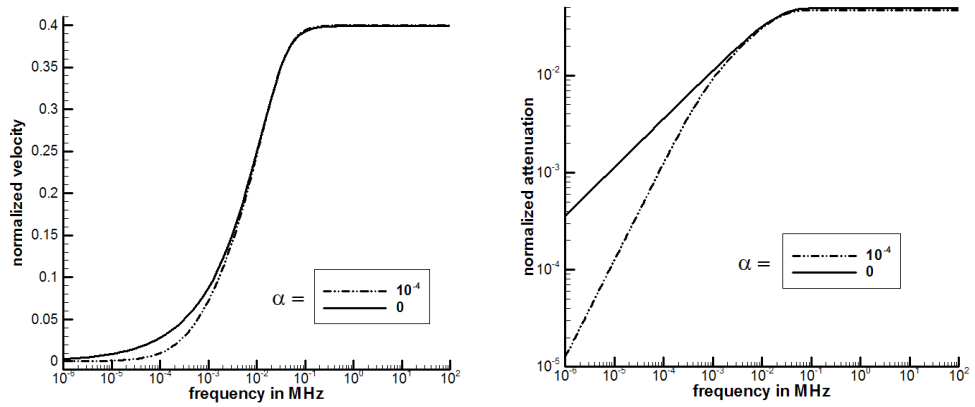

Fig. 3: Stoneley

Normalized phase velocities and attenuations of the leaky Rayleigh, leaky Stoneley, and the Stoneley wave in dependence on the frequency. Different curves correspond to different values of the surface permeability α (*in units* $\left[\frac{\mathrm{s}}{\mathrm{m}}\right]$).

A study on the Becker/Döring model

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Cooperation with: B. Niethammer (Humboldt-Universität zu Berlin), M. Jurisch, S. Eichler (Freiberger Compound Materials GmbH (FCM)), P. Rudolph, F. Kießling (Institut für Kristallzüchtung, Berlin), K. Haack (GTT-Technologies, Herzogenrath)

The Becker/Döring (BD) model describes processes where a droplet with α atoms may grow by incorporation of a single atom from the surroundings and shrink by emitting a single atom into the surroundings. Other processes, like the appearance of a droplet with $\alpha+\beta$ atoms by the reaction of a droplet with $\alpha > 1$ atoms with another droplet with $\beta > 1$ atoms, are not considered within the BD model.
The transition rates of the two processes give the number of reactions per second, and they are denoted by Γ^E_α and Γ^C_α. Their derivation for the case of precipitation of liquid droplets in GaAs is one of the objectives of this study.
We consider a distribution of droplets with $\alpha \in \{1,2,...,\nu\}$ atoms and we introduce a set of functions $Z(t,\alpha) \geq 0$, which give at any time $t \geq 0$ the number of droplets with α atoms. The number of single atoms is included here and it is given by $Z(t,1)$. The choice of the largest considered droplet with ν atoms is a subtle problem, which is not discussed here.
The evolution of $Z(t,\alpha)$ is determined by a system of ordinary differential equations that we call nowadays the BD system. For a thermodynamic system with a fixed number of atoms, it reads

$$\frac{\partial Z(t,\alpha)}{\partial t} = J_\alpha - J_{\alpha-1} \quad \text{for} \quad \alpha \in \{2,...,\nu\}, \quad \text{and} \tag{1}$$

$$\frac{\partial Z(t,1)}{\partial t} = -J_1 - \sum_{\beta=1}^{\nu} J_\beta \quad \text{with} \quad J_\alpha = \Gamma^C_\alpha Z(t,\alpha) - \Gamma^E_{\alpha+1} Z(t,\alpha+1). \tag{2}$$

Equilibrium is established for $J_\alpha = 0$, and a thermodynamic treatment provides the distribution of droplets in equilibrium by minimizing the available free energy of the system

$$\mathfrak{A} = kT \sum_{\beta=1}^{\nu} Z(t,\beta) \log\left(\frac{Z(t,\beta)}{N_D q_\beta}\right) \quad \text{with} \quad N_D = \sum_{\beta=1}^{\nu} Z(t,\beta) \quad \text{and} \quad q_\alpha = \exp\left(-\frac{\mathcal{A}_\alpha}{kT}\right). \tag{3}$$

Here, N_D denotes the total number of droplets and $\mathcal{A}_\alpha$ is the available free energy of the system containing a single droplet with α atoms.
One of the important results which were obtained during the period of this report regards the observation that the transition rates Γ^E_α and Γ^C_α are not independent from each other because we have proved the

Theorem: A sufficient condition that the BD system implies the existence of a Lyapunov function that can be identified with $\mathfrak{A}$ reading

$$\frac{\Gamma^E_{\alpha+1}}{\Gamma^C_\alpha} = \frac{N_D}{Z(t,1)} \frac{q_\alpha}{q_{\alpha+1}}. \tag{4}$$

This condition is violated in all studies of the BD system that can be found in the literature.

References

1. W. DREYER, F. DUDERSTADT, *On the Becker/Döring theory of nucleation of liquid droplets in solids*, WIAS Preprint no. 997, 2004.

2. ——, *On the modeling of semi-insulating GaAs including surface tension and bulk stresses*, WIAS Preprint no. 995, 2004.

3. W. DREYER, F. DUDERSTADT, S. QAMAR, *Diffusion in the vicinity of an evolving spherical arsenic droplet*, WIAS Preprint no. 996, 2004.

Changes of the morphology during phase transitions

Collaborators: W. Dreyer, F. Duderstadt, B. Wagner

Cooperation with: A. Münch (Humboldt-Universität zu Berlin, Heisenberg Fellow at WIAS), W.H. Müller (Technische Universität Berlin), T. Hauck (Motorola GmbH, München)

Supported by: DFG: Priority Program "Analysis, Modellbildung und Simulation von Mehrskalenproblemen" (Analysis, modeling and simulation of multiscale problems)

Under this topic, we study phase transitions that generate drastic changes of the distribution of the participating phases. In particular, we were interested in unwanted coarsening phenomena and Ostwald ripening in solder materials which are used in microelectronic devices. These phenomena are triggered by surface tension and mechanical stress deviators in the bulk. Among the investigated materials were in the past the eutectic tin/lead alloy (SnPb), which is today still the most important solder material. However, due to environmental reasons, the silver/tin (AgSn) alloy will probably substitute the SnPb alloy from next year on.
Regarding the evolution of precipitates in an eutectic SnPb alloy, we have improved the boundary integral formulation of the sharp interface limit to the phase field model.
In summary, the complete boundary integral formulation for the evolution of the precipitates is:

$$
\begin{aligned}
- \quad & \frac{1}{2}\Phi_k(\alpha,\tau) + \frac{1}{2\pi}\sum_{l=1}^{N}\int_0^{2\pi}\Phi_l(\alpha',\tau)\,\Im\left(\frac{\mathbf{s}z_{l\,\alpha'}(\alpha')}{\mathbf{s}z_l(\alpha')-\mathbf{s}z_l(\alpha)}\right)d\alpha' + \frac{1}{L_k}\sum_{l=1}^{N}\int_0^{2\pi}\Phi_l(\alpha',\tau)\,d\alpha' \\
+ \quad & \sum_{l=1}^{N} A_l \ln(\mathbf{s}z_l(\alpha)-M_l) = \mu_1|_\Gamma\,, \qquad (1)\\
& \int_0^{2\pi}\Phi_k(\alpha',\tau)\,d\alpha' = 0 \qquad k=1,\dots,N-1\,, \qquad (2)\\
& V_k^{\mathbf{sv}}(\alpha,\tau) = -\frac{1}{L_k}\sum_{l=1}^{N}\int_0^{2\pi}\Phi_{l\,\alpha'}(\alpha',\tau)\,\Re\left(\frac{\mathbf{s}z_{l\,\alpha}(\alpha)}{\mathbf{s}z_l(\alpha')-\mathbf{s}z_l(\alpha)}\right)d\alpha'\,, \qquad (3)
\end{aligned}
$$

together with $\sum_{k=1}^{N} A_k = 0$. Here, $A_k \in \mathbb{R}$, $\Phi \in \mathbb{C}$, and the complex number $M_k \in \Omega_k$ being the interior of the k-th precipitate.
This set of (integral) equations provides the normal velocity of the interfaces Γ_k for each of the interfaces $k = 1,\dots,N$, which is then used to evolve the interface (parametrized by $\mathbf{s}z_k(\alpha)$) according to

$$
\frac{\partial s_{k\alpha}}{\partial\tau} = V_{k\alpha}^{\mathbf{t}} - \theta_{k\alpha}V_k^{\mathbf{sv}} \qquad \text{and} \qquad \frac{\partial\theta_k}{\partial\tau} = \frac{V_{k\alpha}^{\mathbf{sv}} + V_k^{\mathbf{t}}\theta_{k\alpha}}{s_{k\alpha}}\,. \qquad (4)
$$

Here, $\mathbf{s}\nu_k$ and $\mathbf{s}t_k$ denote the normal and tangent vectors w.r.t. the k-th precipitate. We follow [3] for the choice of the coordinate system, where $s_{k\alpha}$ is $|\mathbf{s}z_k|$, and θ_k is the angle of the tangent vector at points on Γ_k w.r.t. the x-axis, and L_k denotes the length of the corresponding interface. The tangential component $V_k^{\mathbf{t}}$ of $d\mathbf{s}z_k/d\tau$ remains arbitrary and a special choice of the parametrization for the boundaries Γ_k will be used to simplify the numerical implementation. As it turns out, one can find a special choice for $V_k^{\mathbf{t}}$ that yields the equal arclength parametrization $s_{k\alpha} = L_k(\tau)/2\pi$ for all α, and hence the simpler ODE-PDE system

$$
\frac{\partial L_k}{\partial\tau} = -\int_0^{2\pi}\theta_{k\alpha'}\,V_k^{\mathbf{sv}}\,d\alpha' \qquad \text{and} \qquad \frac{\partial\theta_k}{\partial\tau} = \frac{2\pi}{L_k}\left(V_{k\alpha}^{\mathbf{sv}} + \theta_{k\alpha}\,V_k^{\mathbf{t}}\right)\,. \qquad (5)
$$

It turns out that there are three derivatives in the evolution equation for $\theta_{k\alpha}$. Such high derivatives will lead to numerical stiffness (the stability constraint, e.g., $\triangle t < O\left((\triangle x)^3\right)$, leads to prohibitive time stepping). However, the advantage of the above equal arclength formulation with a special choice of $V_k^{\mathbf{t}}$ is that the evolution equation for each θ_k can be written in Fourier space as

$$-\left(\frac{2\pi}{L}\right)^3 |j|^3\,\theta + \hat{N}(\alpha,\tau), \tag{6}$$

where the first term contains the high derivative and hence is the stiffest, so we treat it implicitly. In this form it is linear and diagonal in Fourier space and hence one only has to solve a diagonal system. It can be shown that the nonlinear expression $\hat{N}$ can be treated explicitly. We use a pseudospectral method (using FFT) in space, and leap-frog for the explicit and Crank–Nicholson for the implicit time integration. The integration of the L_τ ODE is done with an Adams–Bashforth integrator. Equations (1), (2), (3), and $\sum_{k=1}^{N} A_k = 0$ yield Ψ and A_k. They represent a linear system which is solved iteratively using GMRES.

Some first studies have appeared in [2] with just two precipitates. We also used this method to simulate the coarsening behavior of larger sets of precipitates and are presently deriving the sharp-interface model including mechanical effects for implementation into our code.

The change of the material and type of applications enforces several changes to the current model, which was originally designed to study the binary tin/lead alloy with two coexisting disordered phases.

For example, if eutectic SnPb is brought in contact with a copper plate, there results the ordered phase Cu_5Sn_7. An ordered phase is also present in AgSn. In both cases, the concentration variable of a binary disordered mixture is not sufficient anymore to indicate which phase is present at a local space point.

The Grinfeld instability whereupon a plane interface might become unstable if mechanical stress deviators are involved, becomes increasingly more important. We have started a study on this subject with two first objectives: (i) Establishment of a rational procedure to derive the sharp-interface equations that describe the Grinfeld instability; (ii) Examination of the influence of boundary conditions on the onset of the instability.

References

1. W. DREYER, A. MÜNCH, B. WAGNER, *On the Grinfeld instability*, to appear as WIAS Preprint.

2. W. DREYER, B. WAGNER, *Sharp-interface model for eutectic alloys. Part I: Concentration dependent surface tension*, WIAS Preprint no. 885, 2003, to appear in: Interfaces Free Bound.

3. H.J. HOU, J.S. LOWENGRUB, M.J. SHELLEY, *Removing the stiffness from interfacial flows with surface tension*, J. Comput. Phys., **114** (1994), pp. 312–338.

Micro-macro transitions via modulation theory

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Supported by: DFG: Priority Program "Analysis, Modellbildung und Simulation von Mehrskalenproblemen" (Analysis, modeling and simulation of multiscale problems)

This multi-scale study has the objective to derive the macroscopic laws of thermodynamics from microscopic models. A simple microscopic system is the atomic chain, which consists of N atoms with nonlinear interactions between nearest neighbors. This example looks innocent enough, however, it provides an extremely challenging task, and we are still far from the complete solution.
The dynamics of the chain is described by $N >> 1$ coupled ordinary differential equations of second order, which can be used to solve at any time t the positions x_α and the velocities $\dot{x}_\alpha$ of the atoms $\alpha \in \{1,..,N\}$ for given initial data. The objective is (i) to introduce a scaling parameter $\varepsilon = 1/N$ and (ii) to find admissible classes of initial data and a corresponding scaling of time and space so that in the limit $\varepsilon \to 0$, the dynamics of the chain can be described by a few partial differential equations.
Currently, the establishment of a macroscopic limit is a most contemporary issue in mathematical physics. During the period of this report, we have obtained many new partial results that exhibit the enormous difficulties of the problem.
The literature studies the scalings (i) $\bar{t} = \varepsilon^3 t$, $\bar{\alpha} = \varepsilon(\alpha + ct)$, $\bar{x} = (1/\varepsilon)x$, (ii) $\bar{t} = \varepsilon^2 t$, $\bar{\alpha} = \varepsilon(\alpha + ct)$, $\bar{x} = (1/\varepsilon)x$, where c is a constant, and considers initial data with small and smooth amplitudes. Regarding example (i), it is essential that only cold data are admissible. The resulting macroscopic equations are for (i) the Korteweg–DeVries equation and for (ii) the nonlinear Schrödinger equation. We study the hyperbolic scaling, where time, particle index, and position are scaled in the same manner: $\bar{t} = \varepsilon t$, $\bar{\alpha} = \varepsilon\alpha$, $\bar{x} = \varepsilon x$. There results formally a 4×4 system of hyperbolic conservation laws for the variables specific length r, velocity υ, wave number k, and specific entropy s:

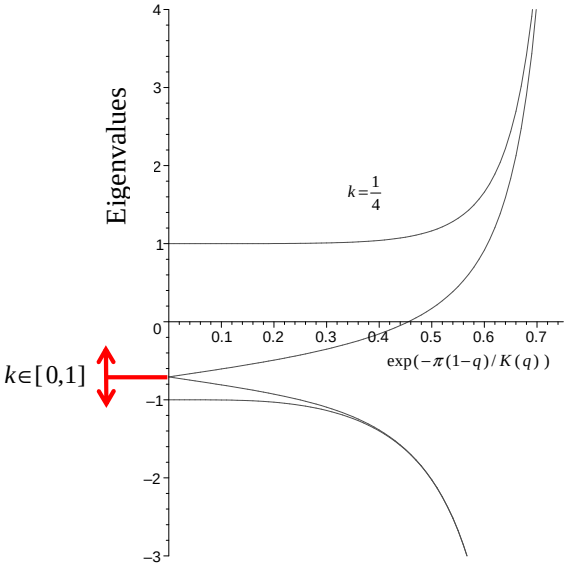
$$\frac{\partial r}{\partial \bar{t}} - \frac{\partial \upsilon}{\partial \bar{\alpha}} = 0, \quad \frac{\partial \upsilon}{\partial \bar{t}} + \frac{\partial p}{\partial \bar{\alpha}} = 0, \quad \frac{\partial k}{\partial \bar{t}} - \frac{\partial \omega}{\partial \bar{\alpha}} = 0, \quad \frac{\partial s}{\partial \bar{t}} + \frac{\partial g}{\partial \bar{\alpha}} = 0. \tag{1}$$

The four variables are related to a family of four parametric traveling wave solutions of the microscopic system. In this framework, the microscopic system gives rise to an optimization problem that yields the specific energy function $U(r,k,s)$, which is the potential for the fluxes, viz.

$$p = -\frac{\partial U}{\partial r}, \quad \omega = \frac{\partial U}{\partial s}, \quad g = -\frac{\partial U}{\partial k}. \tag{2}$$

During the last period, we have studied the justification problem, i.e. the establishment of (1) and (2) as rigorous consequences of the macroscopic limit. To this end, at least two conditions must be fulfilled: 1. The system (1) with (2) constitutes a system of evolution equations. 2. Exact traveling wave solutions are stable on the microscopic scale.
We could prove that at least for the special case that the atoms of the chain interact by means of a Toda potential, system (1) with (2) is strictly hyperbolic and genuinely nonlinear. The figure shows the four eigenvalues of the system. Stability results for traveling wave solutions are currently only available for small amplitudes. However, we have found hints that there

is an intimate relation between the stability of traveling waves and the hyperbolicity of the macroscopic system, see [1, 2] for details.
Relying on these considerations, the justification problem could be solved in the high temperature limit, i.e. for hard sphere interactions. Assuming smooth solutions of (1) and (2), a rigorous proof of the macroscopic limit could be found, see [3].



References

1. W. DREYER, M. HERRMANN, *A simplification of the stability problem for periodic traveling waves in the atomic chain*, Preprint no. 121, DFG Priority Program “Analysis, Modeling and Simulation of Multiscale Problems”, Universität Stuttgart, 2004.

2. W. DREYER, M. HERRMANN, A. MIELKE, *Micro-macro transition for the atomic chain via Whitham’s modulation equation*, Preprint no. 119, DFG Priority Program “Analysis, Modeling and Simulation of Multiscale Problems”, Universität Stuttgart, 2004, submitted.

3. M. HERRMANN, *Ein Mikro-Makro-Übergang für die nichtlineare atomare Kette mit Temperatur*, PhD thesis, Humboldt-Universität zu Berlin, 2004.

Calculation of phase diagrams including surface tension and bulk stresses

Collaborators: W. Dreyer, F. Duderstadt

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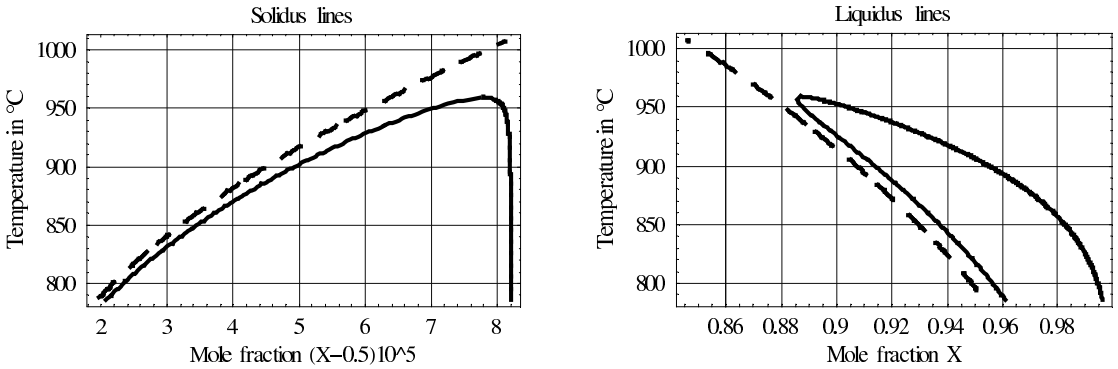
The necessary heat treatment of single crystal semi-insulating gallium arsenide (GaAs), which is deployed in micro- and optoelectronic devices, generates undesirable liquid precipitates in the solid phase. The appearance of precipitates is influenced by surface tension at the liquid/solid interface and deviatoric stresses in the solid. The central quantity for the description of the various aspects of phase transitions is the chemical potential, which can be additively decomposed into a chemical and a mechanical part. In particular, the calculation of the mechanical part of the chemical potential is of crucial importance. We determine the chemical potential in the framework of the St. Venant–Kirchhoff law, which gives an appropriate stress/strain relation for many solids in the small strain regime. We establish criteria which allow the correct replacement of the St. Venant–Kirchhoff law by the simpler Hooke law.
One important application of the model is the calculation of non-standard phase diagrams for GaAs above 786 °C, i.e. those that take into account surface tension and non-deviatoric stresses. The calculation of non-standard phase diagrams relies on the determination of the extrema of the available free energy of the considered thermodynamic system, whereas standard phase diagrams take exclusively the minima into account, [3].
We compare the results with classical phase diagrams where these phenomena are ignored.



The parameters of the phase diagram which is depicted here are the external pressure, $p_0 = 1$ bar, and the total number of moles, $N_0 = 10^{-16}$ mole. Left: solidus lines. Right: liquidus lines. Solid lines describe a liquid droplet which is embedded in a solid phase. The dashed lines show the corresponding lines of the standard phase diagram where surface tension and bulk stresses are ignored.
We observe that in the temperature range where two phases may coexist, there are two extrema for a given temperature. The parts of the solidus and liquidus lines of the non-standard phase diagram which are located near the solidus and liquidus lines, respectively, of the standard phase diagram consist of minima of the available free energy. The remaining parts of the solidus and liquidus lines correspond to maxima. The minima describe stable droplets, whereas the maxima may be related to critical droplets in the following sense: A droplet that appears by fluctuation with a radius which is smaller than the critical radius will disappear, whereas

the droplet will further grow, if it has initially a radius which is larger than the critical radius. A further difference to the standard phase diagram is a dependence of the non-standard phase diagram on the total mole number of the atoms of the system. A doubling increases the range of temperature where both phases may coexist by 5 °K.
The calculation of non-standard phase diagrams is a new subject of thermodynamics, and the results currently meet a growing interest, in particular, in the community of producers of standard phase diagrams. It is planned to transfer the model, which is up to now especially designed to describe precipitation in semi-insulating GaAs, to other materials and processes, like the formation of cementite in steel.

References

1. W. DREYER, F. DUDERSTADT, *On phase diagrams and diffusional problems in the presence of surface tension and multiaxial stresses*, in: Phasenübergänge, Workshop, June 20–26, 2004, vol. 30 of Oberwolfach Reports, Mathematisches Forschungsinstitut Oberwolfach, 2004, pp. 31–34.

2. ——, *Towards the thermodynamic modeling of nucleation and growth of liquid droplets in single crystals*, in: Free Boundary Problems. Theory and Applications. Proceedings of the International Conference, Trento, Italy, June 5–8, 2002, P. Colli, C. Verdi, A. Visintin, eds., vol. 147 of Internat. Ser. Numer. Math., Birkhäuser, Basel [u.a.], 2004, pp. 113–130.

3. ——, *On the modeling of semi-insulating GaAs including surface tension and bulk stresses*, WIAS Preprint no. 995, 2004.

4. W. DREYER, F. DUDERSTADT, S. EICHLER, M. JURISCH, *Stress analysis and bending tests for GaAs wafer*, WIAS Preprint no. 897, 2003, to appear in: Microelectronic Reliability.

Numerical simulation and optimization of SiC single crystal growth by sublimation from the gas phase

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Cooperation with: Ch. Meyer, F. Tröltzsch (Technische Universität Berlin), K. Böttcher, D. Schulz, D. Siche (Institut für Kristallzüchtung (IKZ), Berlin), P. Philip (since September 2004 Institute for Mathematics and its Applications (IMA), Minneapolis, USA)

Supported by: DFG Research Center MATHEON, project C9

Owing to numerous technical applications in electronic and optoelectronic devices, the industrial demand for high quality silicon carbide (SiC) bulk single crystals remains large. The most successful and most widely used growth technique of recent years is the sublimation growth of SiC bulk single crystals via *physical vapor transport (PVT)*, also known as the *modified Lely method*.
During PVT, a graphite crucible (see Figure 1) is placed in a low-pressure inert gas atmosphere consisting of argon. The crucible is then intensely heated, e.g., by induction heating, to temperatures up to 3000 K. Inside the crucible, polycrystalline SiC source powder sublimates, and the gaseous species diffuse through the cavity to the SiC seed. As the single-crystalline seed is kept at a temperature below that of the SiC source, the species crystallize on the seed, which thereby grows into the reactor.

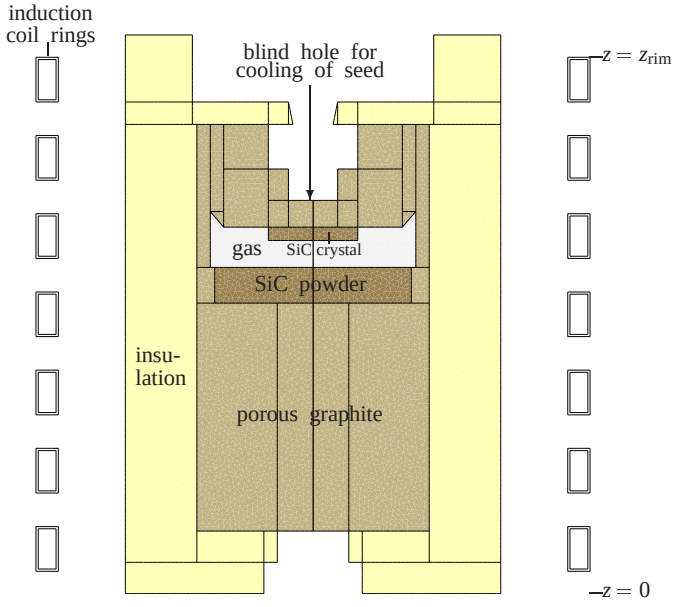

Fig. 1: Setup of growth apparatus according to [5]

The physical and mathematical modeling of the growth process leads to a highly nonlinear system of coupled partial differential equations. In addition to the kinetics of a rare gas mixture at high temperatures, one has to consider heat transport by conduction and radiation, reactive matter transport through porous and granular media, different kinds of chemical reactions and phase transitions, and the electromagnetic fields and heat sources produced by the induction heater. The main control parameters with respect to an optimization of the crystal growth process are the design of the growth apparatus, the position of the induction coil, the heating power, and the inert gas pressure.
Within the covered research period, the simulation software `WIAS-HiTNIHS` (see p. 267) has been made more flexible, such that the program can now deal with more general geometries. During runtime, the program can read descriptions of geometries from ASCII files, in which the geometry is described by a sequence of points followed by a list of polygons. Moreover, some preparations have been made to be able to use the output of a program with a GUI allowing the input of geometry description and the creation of meshes which is currently under development in the Research Group “Numerical Mathematics and Scientific Computing”.
To handle general geometries, the treatment of radiation has been generalized, such that also radiation regions with a boundary consisting of several connected components can be

considered, i.e. such that one can also deal with radiation regions surrounding some opaque objects. For two points (r,z) and (s,y) on the (r,z) boundary of the radiation region one has to determine the visibility intervals, i.e. the intervals for τ such that the points (r,τ,z) and $(s,0,y)$ (expressed in cylindrical coordinates) are mutually visible, since the ray connecting these points is not blocked by any part of the crucible. Following [1], this is done by considering the circular projection of these rays. In Figure 2, we present the circular projection of rays connected to the boundaries of the visibility intervals.

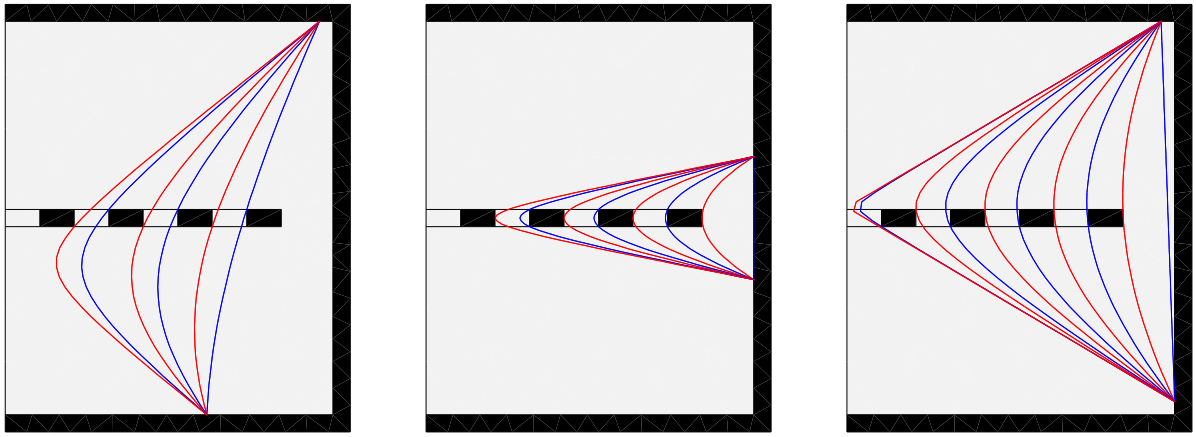

Fig. 2: Circular projections of rays corresponding to the angles being either the begin (blue lines) or the end (red lines) of visibility intervals for a radiation region surrounding four opaque objects

The handling of material parameters has been made more flexible, and `WIAS-HiTNIHS` now reads the material parameters during runtime from a material data file, see [2]. Moreover, the programming of a software with a GUI to create and edit such material data files has been started.

We have also taken into account the direction dependence of the thermal conductivity of the insulation of the crucible. Considering the coordinates (r,z), a heat flux $\vec{q}$ of the form $\vec{q} = -\kappa(T) \begin{pmatrix} \alpha_r & 0 \\ 0 & \alpha_z \end{pmatrix} \operatorname{grad} T$ is used, where T is the temperature, κ is a temperature-dependent thermal conductivity, and α_r, α_z are given positive constants. A FVM discretization for this term has been derived and implemented in `WIAS-HiTNIHS`. Some results can be found in Figure 3.

Some mathematical optimization problems connected to the SiC growth process are considered in [3], [4]. There, semilinear elliptic equations with nonlocal interface conditions are treated, modeling the diffuse-gray conductive-radiative heat transfer within the growth apparatus. Based on a minimum principle for the semilinear equation, as well as L^∞ estimates for the weak solution, the existence of an optimal solution and necessary optimality conditions have been

established. The theoretical results are illustrated by results of numerical computations.

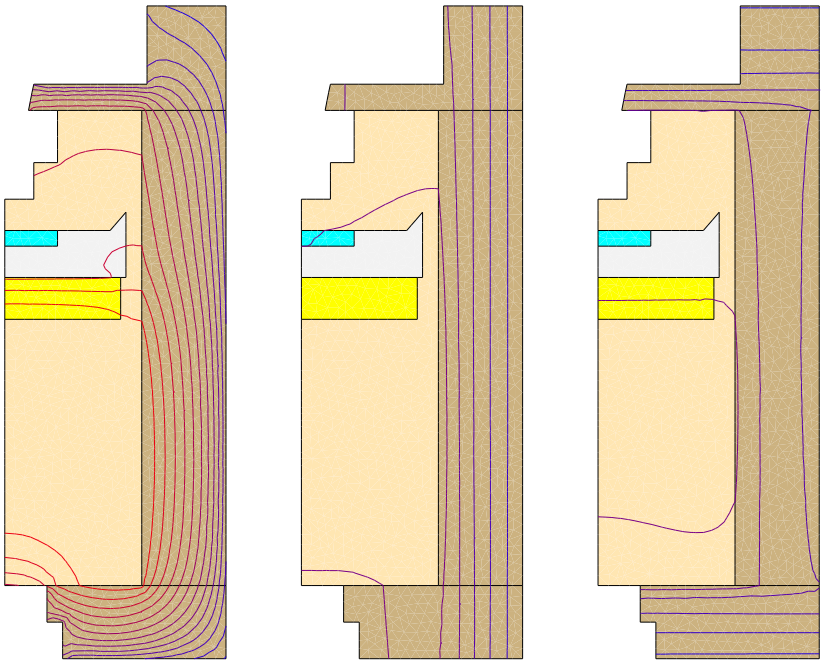

Fig. 3: Computation for isotropic and anisotropic insulations. In the left figure, we have an isotropic insulation with $\alpha_r = \alpha_z = 1$, in the middle figure, we have z-anisotropy with $\alpha_z = 1000$ for all insulation parts, and in the right figure for the upper and lower parts of the insulation, we have r anisotropy with $\alpha_r = 1000$, and for the remaining parts of the insulation, we have z anisotropy with $\alpha_z = 1000$.

References

1. F. DUPRET, P. NICODEME, Y. RYCKMANS, P. WOUTERS, M.J. CROCHET, *Global modelling of heat transfer in crystal growth furnaces*, Int. J. Heat Mass Transfer, **33**(9) (1990), pp. 1849–1871.

2. J. GEISER, O. KLEIN, P. PHILIP, *WIAS-HiTNIHS: A software tool for simulation in sublimation growth of SiC single crystals: Applications and methods*, to appear in the Proceedings of the International Congress of Nanotechnology and Nano World Expo 2004.

3. C. MEYER, P. PHILIP, F. TRÖLTZSCH, *Optimal control of a semilinear PDE with nonlocal radiation interface conditions*, WIAS Preprint no. 976, 2004, submitted.

4. C. MEYER, P. PHILIP, *Optimizing the temperature profile during sublimation growth of SiC single crystals: Control of heating power, frequency, and coil position*, WIAS Preprint no. 895, 2003, Crystal Growth & Design, **5** (2005), pp. 1145–1156.

5. M. PONS, M. ANIKIN, K. CHOUROU, J.M. DEDULLE, R. MADAR, E. BLANQUET, A. PISCH, C. BERNARD, P. GROSSE, C. FAURE, G. BASSET, Y. GRANGE, *State of the art in the modelling of SiC sublimation growth*, Materials Science and Engineering B, **61–62** (1999), pp. 18–28.

Hysteresis operators

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Phase transitions often manifest a strong hysteretic behavior due to irreversible changes in the material structure. Hysteresis operators represent a tool for modeling and efficient description of such processes, where an information on the evolution of the macroscopic state is more relevant for applications than the dynamics of each individual element in the microstructure. Within this project, the following main research directions have been pursued in 2004.

1. Mathematical modeling and control of piezoelectric actuators

A long-term cooperation with K. Kuhnen from the Saarland University at Saarbrücken is based on applications of generalized Prandtl–Ishlinskii hysteresis operators to developing fast algorithms for real-time control of piezoelectric sensors and actuators. The research in the past was focused on questions of stability of the model as well as numerical stability of the algorithms, see [10, 11]. In 2004, emphasis was put on the problem of parameter identification for the underlying hysteresis operator. As a first step, the paper [12] used the linear offline error model. The real-time identification problem was solved as a discontinuous projected dynamical system which was transformed into a continuous system involving hysteresis operators as solution operators of differential inclusions. The project will continue in 2005 with an extension of this approach to adaptive online identification methods for existing as well as refined hysteresis models.

2. Models for fatigue of elastoplastic materials

The evolution of microcracks in an elastoplastic material is generally accepted to be the cause for accumulated fatigue and damage. In order to avoid complicated considerations about the microcrack growth, the Gurson model suggests to introduce one scalar parameter related to the total relative volume of voids in the material as a measure for macroscopic fatigue. Experiments give a parameter range in which this model gives fairly reliable engineering results, see [1]. From the mathematical point of view, the Gurson model consists of an elastoplastic stress-strain law with yield surface which evolves in time as a function of the fatigue parameter which is itself in turn a function of the plastic strain. In other words, the material law can be written in the form of a rate-independent quasi-variational inequality with state-dependent constraint. While criteria for the existence of solutions to such problems were known, the problem of uniqueness and stability of solutions was completely open. A method leading to the proof of existence, uniqueness, and Lipschitz continuity of the solution mapping for a general class of quasi-variational inequalities was suggested in [3] in cooperation with M. Brokate and H. Schnabel from Munich. First estimates show that this method is applicable to the Gurson model within the relevant parameter range.

3. Nonlocal phase transition models

The system of partial differential equations proposed in [6] and [7] as a model for nonlocal phase separation, which accounts for long-range interactions between particles in a multiphase

system, has been reformulated as an abstract evolution equation of the form

$$\frac{d}{dt}u + A(\partial\Phi(u) + B(u)) \ni g$$

with a linear unbounded non-invertible operator A with non-trivial null space which stands for the diffusion term, a continuous nonlinear operator B which plays the role of the nonlocal component, and a singular convex potential Φ which represents the geometric constraints for the order parameter. The main result of the joint paper [5] with P. Colli and E. Rocca is the derivation of a sufficient condition between the null space of A and the subdifferential of Φ under which the initial-value problem is well posed. An example shows that if the condition is not fulfilled, then even a local solution may fail to exist. Another nonlocal model for phase transitions, where also the temperature evolution is taken into account, has been investigated as part of this project, and results on its well-posedness and asymptotic stability were published in [14].

4. Mechanical models for heart muscle fiber

The mechanics of the muscle fiber is particular by the fact that its material characteristics are not constant, but may vary extremely quickly as a result of electric excitations which release fast chemical reactions in the cells. In particular, in the heart, phases of active contraction, active relaxation, and passive relaxation change periodically in the normal regime. For example, during contraction, the elasticity coefficient increases by several orders of magnitude with a strong hysteresis effect. A numerical model for this behavior was proposed by a French group of engineers, biologists, and mathematicians in [4]. The model was investigated in cooperation with the research group coordinated by M. Sorine from the point of view of mathematical consistency. It was proved in [13] that the corresponding system of partial differential equations has a unique global strong solution, this solution remains bounded under bounded external excitation and, in agreement with experimental observations, tends to an equilibrium in the passive relaxation regime, that is, if no excitation is present. A simplified model where variations along the fiber are neglected shows that elasticity in this equilibrium does not vanish.

5. Outward-pointing hysteresis operators

It has been shown in [8, 9] that one can derive new uniform estimates for the solutions to some partial differential equations involving hysteresis operators, if these operators are “outward-pointing hysteresis operators” or even “strongly outward-pointing hysteresis operators”. For scalar Prandtl–Ishlinskii operators and generalizations of these operators, appropriate conditions that allow to check if these operators are pointing outwards have been formulated in [8, 9], i. e. it has been shown that a Prandtl–Ishlinskii operator is strongly pointing outwards if and only if its initial loading curve is unbounded. The work [2] in progress shows also for some class of Preisach operators that the condition of the unbounded initial loading curve is sufficient to ensure that the operator is pointing outwards. But, considering, for example, appropriate generalized play operators, one realizes that there are strongly outward-pointing Preisach operators with a bounded initial loading curve. Therefore, some further investigations will be done to complete the characterization.

References

1. H. BAASER, D. GROSS, *Crack analysis in ductile cylindrical shells using Gurson's model*, Internat. J. Solids Structures, **37** (2000), pp. 7093–7104.

2. M. BROKATE, O. KLEIN, P. KREJČÍ, in preparation.

3. M. BROKATE, P. KREJČÍ, H. SCHNABEL, *On uniqueness in evolution quasivariational inequalities* J. Convex. Anal., **11**(1) (2004), pp. 111–130.

4. D. CHAPELLE, F. CLÉMENT, F. GÉNOT, P. LE TALLEC, M. SORINE, J.M. URQUIZA, *A physiologically-based model for the active cardiac muscle*, in: FIMH 2001 (Functional Imaging and Modeling of the Heart), First International Workshop, Helsinki, Finland, November 15–16, 2001, Proceedings, T. Katila, I.E. Magnin, P. Clarysse, J. Montagnat, J. Nenonen, eds., vol. 2230 of Lecture Notes in Computer Science, Springer, 2001, pp. 128–133.

5. P. COLLI, P. KREJČÍ, E. ROCCA, J. SPREKELS, *Nonlinear evolution inclusions arising from phase change models*, WIAS Preprint no. 974, 2004.

6. H. GAJEWSKI, *On a nonlocal model of non-isothermal phase separation*, Adv. Math. Sci. Appl., **12** (2002), pp. 569–586.

7. H. GAJEWSKI, K. ZACHARIAS, *On a nonlocal phase separation model*, J. Math. Anal. Appl., **286** (2003), pp. 11–31.

8. O. KLEIN, P. KREJČÍ, *Outwards pointing hysteresis operators and asymptotic behaviour of evolution equations*, Nonlinear Anal. Real World Appl., **4** (2003), pp. 755–785.

9. ——, *Asymptotic behaviour of evolution equations involving outwards pointing hysteresis operators*, Physica B, **343** (2004), pp. 53–58.

10. P. KREJČÍ, K. KUHNEN, *Inverse control of systems with hysteresis and creep*, IEE Proc. Control Theory Appl., **148**(3) (2001), pp. 185–192.

11. ——, *Error estimates for the discrete inversion of hysteresis and creep operators*, Math. Comput. Simulation, **61** (2003), pp. 537–548.

12. ——, *Identification of linear error-models with projected dynamical systems*, Mathematical and Computer Modelling of Dynamical Systems, **10**(1) (2004), pp. 59–91.

13. P. KREJČÍ, J. SAINTE-MARIE, M. SORINE, J.M. URQUIZA, *Solutions to muscle fiber equations and their long time behaviour*, WIAS Preprint no. 973, 2004.

14. P. KREJČÍ, J. SPREKELS, *Nonlocal phase-field models for non-isothermal phase transitions and hysteresis*, Adv. Math. Sci. Appl., **14**(2) (2004), pp. 593–612.

Approximation and optimization of curved mechanical structures

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Supported by: DFG Research Center MATHEON, project C8

The work for this research project has been continued in several directions. The paper [1] concerning the optimization of rods and shells has been accepted after revision. In [2], a new reduction approximation technique has been developed to overcome the well-known "locking phenomenon" in the numerical approximation of thin curved rods. In this context, we also refer to [4].
A new type of asymptotic analysis for merely Lipschitzian curved rods has been developed in the papers [5], [6], [7].
A considerable part of the results established in this field by J. Sprekels and D. Tiba within the past years will be contained in the monograph [3].

References

1. V. ARNĂUTU, J. SPREKELS, D. TIBA, *Optimization problems for curved mechanical structures*, WIAS Preprint no. 812, 2003, to appear in: SIAM J. Control Optim.

2. ——, *A reduction approximation method for curved rods*, WIAS Preprint no. 958, 2004, to appear in: Numer. Funct. Anal. Optim.

3. P. NEITTAANMÄKI, J. SPREKELS, D. TIBA, *Optimization of Elliptic Systems. Theory and Applications*, Springer, to appear 2005.

4. J. SPREKELS, D. TIBA, *An approximation method for curved rods*, in: Nonlinear Partial Differential Equations and their Applications, N. Kenmochi, M. Otani, S. Zheng, eds., vol. 20 of Gakuto Intern. Series Math. Sci., Gakkotosho, Tokyo, 2004, pp. 305–314.

5. D. TIBA, R. VODÁK, *A general asymptotic model for Lipschitzian curved rods*, WIAS Preprint no. 942, 2004, to appear in: Adv. Math. Sci. Appl.

6. R. VODÁK, *A general asymptotic dynamic model for Lipschitzian curved rods*, WIAS Preprint no. 956, 2004, submitted.

7. ——, *Asymptotic analysis of elastic curved rods*, WIAS Preprint no. 986, 2004.

Dynamics of thin dewetting liquid films and the role of slippage

Collaborator: B. Wagner

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The occurrence and the nature of slippage of liquids on solid surfaces is vividly discussed in the literature and is of large technological interest since a sliding fluid can flow faster through, e.g., microfluidic devices. In recent years, one major focus of interest has been the process of dewetting of polymer films (typically ranging on the scale of tens to a few hundred nanometers) from hydrophobic substrates. Understanding the dynamics and morphology of this process is particularly important for the design of microelectronic devices. Theoretical progress here depends strongly on the ability to develop, analyze, and solve reduced models, such as lubrication-type models for the film dynamics, thereby addressing the presence of highly separated scales (in space as well as in time) and the high (fourth) order of the involved partial differential equations.

1. Contact line instability and sharp interface (J.R. King, A. Münch, B. Wagner).
Dewetting typically starts by the formation of holes due to spinodal decomposition or heterogeneous nucleation. As the holes grow, the displaced liquid collects in growing rims surrounding the holes. On longer time scales, the rims themselves are subject to a finger-type instability. In this project, we have derived lubrication models that account for large slip lengths. The slip length can be understood as the length below the solid/liquid interface where the velocity extrapolates to zero. We have developed numerical methods that explore the special structure of the models to yield, in combination with spatial adaptivity and parallelization, efficient codes for the dewetting process. Using linear stability analysis, we showed that, both under no-slip and full-slip boundary conditions, perturbations of the dewetting front are amplified, but the effect is greater by orders of magnitude in the full-slip case. Furthermore, the perturbations become much more asymmetrical under full-slip boundary conditions, while they develop symmetrical bulges under no-slip conditions, [3]. Additional computations that solve the lubrication model for the full three-dimensional flow confirm that these findings carry over to the nonlinear regime [2] and are in good agreement with the experimental findings, [8]. Our recent focus has been the development of multiple-scale asymptotic techniques in order to formulate simpler problems that are able to resolve the small-scale structure in the vicinity of the apparent contact line and asymptotically match the inner solution to those solving the large-scale outer problem describing the shape and dynamics of the rim. As a consequence, a further model reduction of the lubrication model to a corresponding sharp-interface model could be achieved. Here, the linear stability analysis is greatly simplified and could be investigated purely analytically, [6], [5], confirming our earlier numerical results on the linear stability of the evolving rims.

2. New slip regimes (A. Münch, B. Wagner, T.P. Witelski).
In this project, we derived lubrication models for dewetting thin films from the Navier–Stokes equations for incompressible flow, which are characterized by the orders of magnitude of the slip length. As one traverses the ranges of the slip length, the flow field will change from a

parabolic flow field to what is essentially plug flow, which implies a change from the balance of the pressure gradient with the horizontal velocity to the balance of the pressure gradient with the vertical velocity and thereby also a change of the velocity scale. For small slip lengths (at most of the order of the height of the film), we obtained the velocity scale $\mathbb{U} = \sigma\varepsilon^3/\mu$ together with the well-known dimension-reduced lubrication equation for the profile $h(x,t)$

$$\partial_t h = -\partial_x \left[\left(\tfrac{1}{3} h^3 + b h^2 \right) \partial_x \left(\partial_{xx} h - \phi(h) \right) \right], \tag{1}$$

where σ, μ, ε, ϕ denote surface tension, viscosity, capillary number, and interfacial potential, respectively. If, however, the slip length tenses much larger than the height of the film, we obtain a new lubrication model, with the velocity scale $\mathbb{U} = \sigma\varepsilon/\mu$ and the system

$$\mathrm{Re}^* \left(\partial_t f + f \partial_x f \right) = \frac{4\partial_x (h \partial_x f)}{h} + h \partial_x \left(\partial_{xx} h - \phi' \partial_x h \right) - \frac{f}{\beta_s h}, \quad \partial_t h = -\partial_x (h f), \tag{2}$$

where β_s is the slip length and $\mathrm{Re} = \rho \mathbb{U} \mathbb{H} / \mu$. This we called the "strong slip" regime. We found that the two models above are embedded in a whole family of lubrication models that can be derived for different regimes of the slip length. They are in fact distinguished limits, in the sense that they are richer in structure than the other regimes and depend explicitly on the slip length. The other regimes are limiting cases, which are the well-known no-slip regime, the intermediate regime, and the lubrication model describing retracting free foam films. The intermediate regime is obtained for the velocity scale $\mathbb{U} = \sigma\varepsilon^{2-\gamma}/\mu$, where $-1 < \gamma < 1$, for which we found the lubrication model

$$\partial_t h = -\beta_i \partial_x \left(h^2 \partial_x \left(\partial_{xx} h - \phi \right) \right) \tag{3}$$

called the "slip-dominated" lubrication model. The model for retracting free foam films is recovered by letting $\beta_s \to \infty$. For these limiting cases, we also derived solutions for the moving dewetting film through matched asymptotics, [9].
As a first application we found that the strong slip regime could capture the rim profiles of dewetting nanoscale polymer films observed in experiments by R. Konrad and K. Jacobs.

3. Rim profiles for large slippage (K. Jacobs, R. Konrad, A. Münch, B. Wagner, T.P. Witelski).
In this project, we concentrated on the rim morphology affected by slippage. Our collaborators R. Konrad and K. Jacobs have performed experiments to compare the dewetting behavior of liquid polymer films on silicon/silicon oxide wafers that have been coated with either octadecyltrichlorosilane (OTS) or dodecyltrichlorosilane (DTS). The experiments show that the dewetting rates for DTS are significantly larger than for OTS. They also compared the profile of the rim that forms as the film dewets and found that it develops a spatially decaying oscillatory structure on the side facing the undisturbed film if an OTS-coated wafer is used, but is monotonically decaying for DTS. For this situation, only the solid/liquid friction coefficient can be different, suggesting that slippage plays a role in this transition. For the first time, we showed that this transition is in fact captured by a lubrication model that can be derived from the Navier–Stokes equations with a Navier-slip boundary condition at the liquid/solid interface, and accounts for large slip lengths; it is the strong slip model (2) introduced above.
For this model, an approximate description of the portion of the profile of the dewetting rim that connects to the undistributed uniform film $h = 1$ for $x \to \infty$ was developed to find the evolution of the film near the flat state. The dominant contributions could be derived to obey the ODE

$-\dot{s}^2\beta\,\mathrm{Re}\partial_\xi\varphi = 4\dot{s}\beta\partial_\xi^2\varphi + \partial_\xi^3\varphi - \dot{s}\varphi$ for the perturbation φ about the flat state. Here, $\xi = x - s(t)$ and $s(t)$ denotes the position of the contact line. The normal mode solutions $\varphi(\xi) = e^{\omega\xi}$ of this ODE, which decay for $\xi \to \infty$, are spatially oscillating due to a pair of complex conjugate ω, if the discriminant corresponding to the dispersion relation for ω,

$$D = \frac{4\dot{s}^4\beta^3}{3^3}(\mathrm{Re} - 4\beta)\,\mathrm{Re}^2 + \frac{8\beta^2\dot{s}^2}{3}\mathrm{Re} - \frac{4^4\beta^3\dot{s}^2}{3^3} + 1, \tag{4}$$

is positive. Hence, the rim passes over into a damped capillary wave. But if it is negative, the complex conjugate ω is replaced by two real modes, which allows the solution $\varphi(\xi)$ to decay monotonically for $\xi \to \infty$. In our case, the Re number is extremely small and can be neglected, so that the transition from complex conjugate to real decaying modes occurs when $\beta > \beta_{th}(\dot{s}) = (3/4)/(4\dot{s}^2)^{1/3}$. This threshold is shown in Figure 1. We also found the transition from complex conjugate to real decaying modes can also be found from the full Stokes equation. In Figure 1, we also show the corresponding threshold that was numerically obtained from the normal mode solution of the linearized Stokes problem.

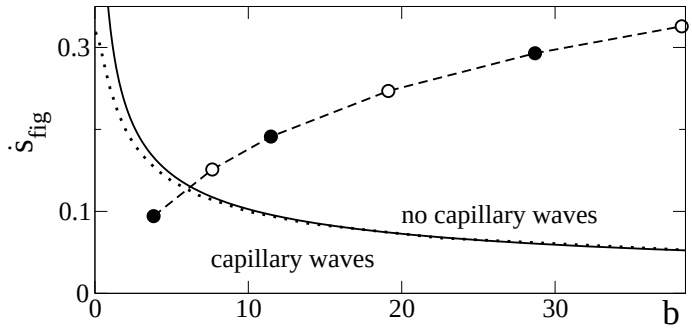

Fig. 1: Transition curves in $(b, \dot{s}_{\mathrm{fig}})$ parameter space for profiles with to without capillary waves, calculated from the lubrication model (solid line) and Stokes model (dotted line). The dashed line shows the contact-line speed for different slip lengths, calculated from the lubrication model.

One observes that as b is increased, the dewetting rate increases, and for slip lengths larger than the threshold, the dashed line in Figure 1 leaves the region where capillary waves are expected. Inspection of the profile in a semilog plot of the profiles in Figure 2 showed a second maximum for the smallest b, indicating that we have the oscillatory structure of a wave.

These findings compared very well with the experimental results where on OTS-covered substrates, the rim of the dewetting PS film exhibits an oscillatory shape, whereas on DTS-covered surfaces, at the same temperature, no oscillation is observed, [7].

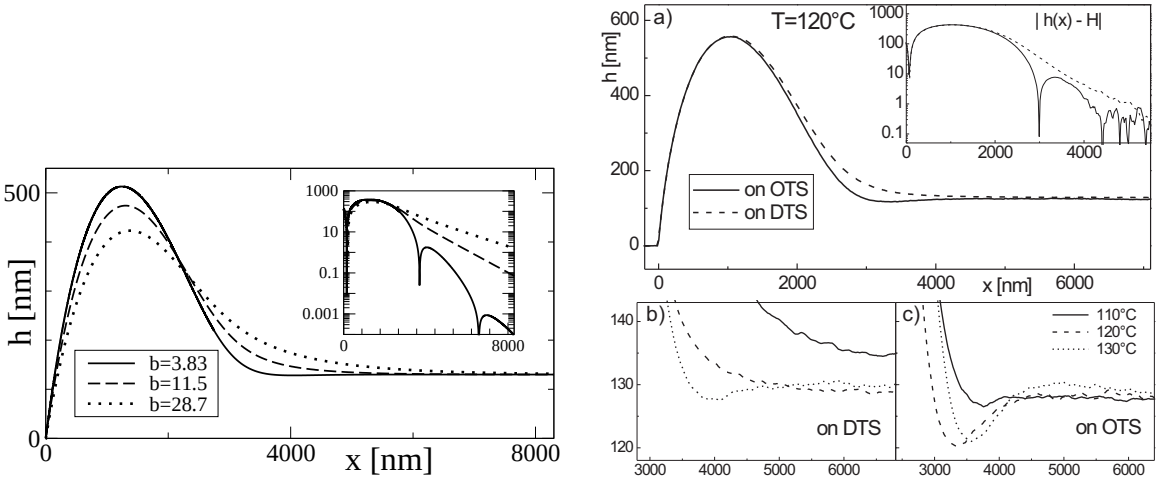

Fig. 2: *Left*: Rim profiles for different slip lengths b non-dimensionalized with H =130 nm. The inset shows a semilog plot of $\max(|h(x)-H|, 10^{-5})$.
Right: Rim profiles of 130 nm PS films on DTS- and OTS-covered Si wafers a) at constant temperature (the inset depicts a semilog plot of $|h(x)-H|$), b) and c) at three different temperatures on DTS and OTS surfaces, respectively. Profiles are shown with the three-phase contact line shifted into the origin.

4. Lubrication models for viscoelastic liquids (R. Blossey, A. Münch, M. Rauscher, B. Wagner).

In the range where the polymer chain length begins to be comparable with the film thickness, the dynamics of the thin films becomes non-Newtonian, leading to novel dynamical signatures. In order to describe such effects, various different models have been postulated in an ad hoc or, at best, a phenomenological manner, leading to controversies about the interpretation of experimental results.

Given the success of the lubrication approximation for the dynamics of thin films of Newtonian character, we were prompted to look at this issue for the case of non-Newtonian liquids and addressed the question of the derivation of thin-film equations based on the lubrication approximation for viscoelastic fluids, [10]. We introduced a general model class of viscoelastic fluids which was the basis for our derivation. Subsequently, we demonstrated how to derive thin-film equations for the non-Newtonian liquid, stressing the underlying physical assumptions. For the situations we have in mind, we assumed the liquid to be incompressible with mass density ρ. With this, the equation of mass conservation reduces to $\nabla \cdot \vec{u} = 0$, with the velocity field $\vec{u} = (u_x, u_y, u_z)$. The equation of momentum conservation is $\rho \frac{\mathrm{d}\vec{u}}{\mathrm{d}t} = -\nabla p_R + \nabla \cdot \tau$, with the reduced pressure $p_R = p + V$. The hydrostatic pressure is p, the pressure induced by external fields such as gravity or van der Waals-type dispersion forces V, and the deviatoric (traceless) part of the stress tensor is τ (which is symmetric). With $= \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial}{\partial t} + \vec{u}\cdot\nabla$, we denote the materials (or total) derivative and with $\nabla = (\partial_x, \partial_y, \partial_z)$ the gradient operator.

Starting with the co-rotational Jeffreys model, we found that in order to obtain a closed-form lubrication model, only the linear versions

$$\tau_{iz} + \lambda_1 \frac{\partial \tau_{iz}}{\partial t} = \partial_z u_i + \lambda_2 \frac{\partial \partial_z u_i}{\partial t}, \tag{5}$$

with $i = x, y$, respectively, are in general allowed. For this we found for the lubrication

approximation the following system

$$\frac{\partial h}{\partial t}+\lambda_2\left[\frac{\partial^2 h}{\partial t^2}+\nabla_{||}\cdot\left(\frac{\partial h}{\partial t}\,\vec{u}_{||_{|z=h}}\right)\right]=\nabla_{||}\cdot\left\{\left[\left(1+\lambda_1\frac{\partial}{\partial t}\right)\frac{h^3}{3}+\left(1+\lambda_2\frac{\partial}{\partial t}\right)b\,h^2\right]\nabla_{||}\,p_R\right\}$$
$$-\nabla_{||}\cdot\left[\left(\frac{h^2}{2}\lambda_1+b\,h\,\lambda_2\right)\frac{\partial h}{\partial t}\nabla_{||}p_R\right] \quad (6)$$

with $\vec{u}_{||_{|z=h}}$ given by

$$u_i \;=\; -b\,h\,\partial_i p_R \;+\; \left(\frac{z^2}{2}-hz\right)\frac{\lambda_1}{\lambda_2}\partial_i p_R \;+\; \int_{-\infty}^{t}\frac{\mathrm{e}^{-\frac{t-t'}{\lambda_2}}}{\lambda_2}\left[\left(\frac{z^2}{2}-hz\right)\left(1-\frac{\lambda_1}{\lambda_2}\right)\partial_i p_R\right]dt'. \quad (7)$$

The reduced pressure is independent of z and we can use p_R at the film surface $p_R = V_{|z=h}-\frac{\sigma}{2}\nabla_{||}^2 h$. We found that this system collapses to a single equation when $\lambda_2\to 0$ and this limit corresponds to the simplest Maxwell model. In the case $\lambda_1=\lambda_2$, we recovered the lubrication model for Newtonian fluid, [10].
We presently discuss how the models we obtained relate to the phenomenological models discussed in the literature so far.

References

1. A. MÜNCH, *Dewetting rates of thin liquid films*, WIAS Preprint no. 992, 2004, to appear in: J. Phys.: Condensed Matter.
2. ——, *Fingering instability in dewetting films induced by slippage*, Preprint no. 151 of DFG Research Center MATHEON, Technische Universität Berlin, 2004.
3. A. MÜNCH, B. WAGNER, *Contact-line instability of dewetting thin films*, WIAS Preprint no. 924, 2004, to appear in: Physica D.
4. K. JACOBS, R. SEEMANN, G. SCHATZ, S. HERMINGHAUS, *Growth of holes in liquid films with partial slippage*, Langmuir, **14** (1998), pp. 4961–4963.
5. J.C. FLITTON, J.R. KING, *Surface-tension-driven dewetting of Newtonian and power-law fluids*, J. Engrg. Math, **50** (2004), pp. 241–266.
6. J. KING, A. MÜNCH, B. WAGNER, *Stability of a dewetting ridge*, in preparation.
7. R. KONRAD, K. JACOBS, A. MÜNCH, B. WAGNER, T.P. WITELSKI, *New slip regimes and the shape of dewetting thin liquid films*, WIAS Preprint no. 993, 2004, submitted.
8. R. SEEMANN, S. HERMINGHAUS, K. JACOBS, *Gaining control of pattern formation of dewetting films*, J. Phys.: Condensed Matter, **13** (1998), pp. 4925–4938.
9. A. MÜNCH, B. WAGNER, T.P. WITELSKI, *Lubrication models for small to large slip lengths*, in preparation.
10. R. BLOSSEY, A. MÜNCH, M. RAUSCHER, B. WAGNER, *Thin-film equations for viscoelastic liquids*, in preparation.
11. C. REDON, J.B. BRZOSKA, F. BROCHARD-WYART, *Dewetting and slippage of microscopic polymer films*, Macromolecules, **27** (1994), pp. 468-471.

Thermodynamic foundations for modeling saturated poroelastic bodies

Collaborator: K. Wilmański

The modeling of thermoporoelastic materials which has been the subject of research for eight years has been completed in 2004. In particular, the following problems were solved

– The general form of the energy balance equation for thermoporoelastic materials: It has been shown, for instance, that the so-called simple mixture model yields in the Lagrangian description the following form of relation between the entropy flux **H** and the heat flux **Q**, [3], [4],

$$\mathbf{H} = \frac{1}{T}\left(\mathbf{Q} - \rho^F \psi^F \acute{\mathbf{X}}^F\right), \quad \acute{\mathbf{X}}^F = \mathbf{F}^{S-1}\left(\acute{\mathbf{x}}^F - \acute{\mathbf{x}}^S\right),$$

where T is the absolute temperature, ψ^F denotes the Helmholtz free energy of the fluid, $\mathbf{F}^S$ is the deformation gradient of the skeleton, and $\acute{\mathbf{x}}^F, \acute{\mathbf{x}}^S$ are velocities of components. This has also been proved in the case of a generalized model with a nonlinear dependence on the diffusion velocity $\acute{\mathbf{X}}^F$.

– It has been shown that the classical linear Biot model with added mass effects follows as a nonobjective approximation of a nonlinear model in which the following definition of the objective relative acceleration has been introduced, [4], [5],

$$\mathbf{a}_r = \frac{\partial}{\partial t}\left(\acute{\mathbf{x}}^F - \acute{\mathbf{x}}^S\right) - (1-\mathfrak{z})\,\acute{\mathbf{X}}^F \cdot \mathrm{Grad}\,\acute{\mathbf{x}}^F - \mathfrak{z}\acute{\mathbf{X}}^F \cdot \mathrm{Grad}\,\acute{\mathbf{x}}^S,$$

where $\mathfrak{z}$ is a material parameter. In the same work, it has been shown that the added mass effect cannot be related to tortuosity in spite of frequent claims in the literature.

– As the result of the micro-macro analysis [6], the balance equation for porosity has been corrected for an equilibrium contribution

$$\frac{\partial (n - n_E)}{\partial t} + \mathrm{Div}\left(\Phi_0 \acute{\mathbf{X}}^F\right) = -\frac{n - n_E}{\tau},$$

where n_E denotes the equilibrium porosity, and n_E, Φ_0, τ are constitutive quantities, the latter being the relaxation time of porosity. In particular, in the linear Biot model ($\tau \to \infty$), this equation yields the relation for porosity [6]

$$n = n_E + n_0 \frac{\Phi}{n_0}\left(\varepsilon - \mathrm{tr}\mathbf{e}^S\right), \quad n_E = n_0\left(1 + \delta \mathrm{tr}\mathbf{e}^S\right), \quad \varepsilon = \frac{\rho_0^F - \rho^F}{\rho_0^F},$$

where δ is the material constant. This relation checks with results of micro-macro transitions.

The model described above has been investigated in application to the description of linear and nonlinear waves. It has been shown ([4], [7], [1]) that linear acoustic waves correspond qualitatively with waves following from Biot's model. Quantitative discrepancies may be as large as 30 % and in some cases (e.g., attenuation), they indicate that the new model

is physically better justified and in some cases (e.g., dependence of speeds on coupling of stresses), they are better within Biot's model. The new model yields also important results for surface waves (e.g., [2]). The analysis of nonlinear waves has been performed for the model in which material parameters are dependent on porosity, [8], [9]. It has been shown that for some physically justified cases, the P1 wave may yield the creation of strong discontinuities which have been attributed to the liquefaction. This conclusion is confirmed by comparison with theoretical results of Osinow within a one-component hypoplastic model and with experiments on Karlsruhe sands.

References

1. B. ALBERS, K. WILMANSKI, *On modeling acoustic waves in saturated poroelastic media*, to appear in: J. Engrg. Mech.

2. ——, *Monochromatic surface waves on impermeable boundaries in two-component poroelastic media*, to appear in: Contin. Mech. Thermodyn.

3. K. WILMANSKI, *Thermodynamics of simple two-component thermo-poroelastic media*, in: Recent Trends and Applications of Mathematics to Mechanics, S. Rionero, G. Romano, eds., Springer, Milano, 2005.

4. ——, *Tortuosity and objective relative accelerations in the theory of porous media*, to appear in: Proc. Roy. Soc. London, Ser. A.

5. ——, *Objective relative accelerations in theories of porous materials*, in: Thermodynamische Materialtheorien, Workshop, December 12–18, 2004, vol. **55** of Oberwolfach Reports, Mathematisches Forschungsinstitut Oberwolfach, 2004, pp. 36–37.

6. ——, *On microstructural tests for poroelastic materials and corresponding Gassmann-type relations*, Géotechnique, **54** (2004), pp. 593–603.

7. ——, *Linear sound waves in poroelastic materials: Simple mixtures vs. Biot's model*, to appear in: Trends in Applications of Mathematics to Mechanics, K. Hutter, Y. Wang, eds., Shaker-Verlag.

8. ——, *Critical time for acoustic waves in weakly nonlinear poroelastic materials*, to appear in: Contin. Mech. Thermodyn.

9. ——, *Threshold to liquefaction in granular materials as a formation of strong wave discontinuities in poroelastic media*, to appear in: Biot Centennial Conference, Oklahoma 2005, A. Cheng, ed.

4.8 Projects interconnecting research groups

4.8.1 Projects

Calculation of electronic band structure of InAsSb multi quantum wells

Collaborators: U. Bandelow (FG 1), M. Baro (FG 1), Th. Koprucki (FG 3)

Cooperation with: J. Tomm and F. Weik (both Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie (MBI), Berlin), M. Grau (Walter-Schottky-Institut, Technische Universität München)

Supported by: MBI, DFG: Research Center MATHEON, project D4; Priority Program "Analysis, Modellbildung und Simulation von Mehrskalenproblemen" (Analysis, Modeling and Simulation of Multiscale Problems)

Indium-arsenide-antimonide (InAsSb) heterostructures, having the lowest band gap of all III-V semiconductors, are of great interest in the recent development of infrared optoelectronic devices like lasers and photodetectors. The aim of the project is the calculation of the electronic band structure of InAsSb multi-quantum-well (MQW) lasers.
The MQW structures we investigate are grown at the Walter Schottky Institute and are potential candidates for the optically active region of infrared LEDs. The structures consist of a stack of 10-nm-thick strained $InAs_xSb_{1-x}$ quantum wells sandwiched between 20 nm or 40 nm $Al_{0.15}In_{0.85}As_{0.78}Sb_{0.22}$ barriers. The arsenic content of the well material varies between the samples, which leads to a different strain for each sample. The investigation of the influence of the strain on the bandgap is a central point of the investigations.
Characterization and measurements of the structures are carried out at the Max Born Institute (MBI).
The most economical description of the energy bands in semiconductors is the multiband k·p method. According to this method the quantum-confined states $F_{\mu l}(z;\mathbf{k}_\parallel)$ and the corresponding subband dispersions $E_l(\mathbf{k}_\parallel)$ are solutions of the respective eigenvalue problem

$$H_{\mu\nu}\left(\mathbf{k}_\parallel, k_\perp = -i\frac{\partial}{\partial z};\ldots\right) F_{\nu l}(z;\mathbf{k}_\parallel) = E_l(\mathbf{k}_\parallel) F_{\mu l}(z;\mathbf{k}_\parallel) \tag{1}$$

where z denotes the growth direction. For consistently modeling the mixing of conduction and valence bands in our low-gap material we use eight-band k·p Hamiltonians $H_{\mu\nu}$. The structure of the corresponding Hamiltonians can be found in [2], their spectral properties are studied in [3]. The `WIAS-QW` software package (see [1]) uses an eight-band k·p model and is successfully applied to the simulation of the InAsSb/AlInAsSb nanostructures described above. Moreover, the results are compared with the measured values of MBI.
Our simulation parameters are obtained from Vurgaftman et al. [4] by means of the ternary and quaternary interpolation schemes described there. The bandgap E_g and the spin-split-

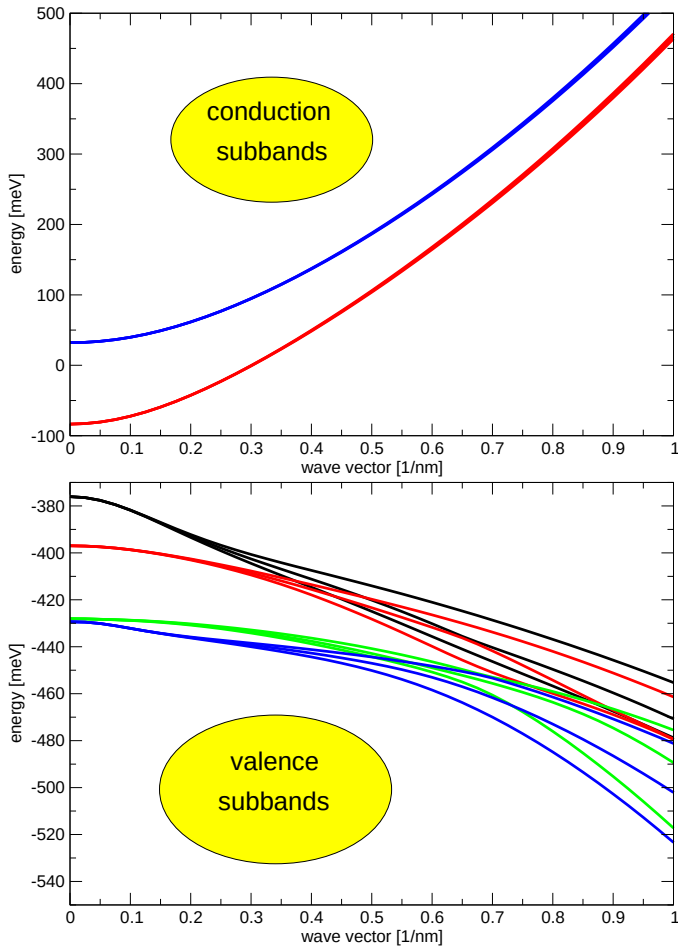

Fig. 1: Subband structure $E_n(|\mathbf{k}_{\|}|)$ for three different directions of $\mathbf{k}_{\|}$ of our selected sample

off energy are obtained by quadratic interpolation, whereas the remaining material parameters are derived by linear interpolation. For the calculations, the in-plane strain is determined by the formula $(a_0 - a)/a$, where $a_0 = 0.6096\,\mathrm{nm}$ is the lattice constant of the GaSb substrate, and a is the lattice constant of the corresponding layer material. The calculated strain values agree with the measured values. The calculated bandgap varies linearly with the strain, with a slope of about 84 meV, which compares well with the experimental findings obtained by MBI, [5].

As an example, we plot the subband structure of one sample in Figure 1. It exhibits a strong nonparabolicity, especially for the valence subbands. For the latter, also strong warping (angular dependence) is detected, which is also a result of the band-band interaction, which involves electrons, heavy holes, light holes, and spin-split-off holes.

For further illustration, we plot the local density distributions within the MQW structures for our selected sample in Figure 1. For these illustrations, we assume charge neutrality with sheet densities given by $N = P = 10^{11}/cm^2$. We observe very good confinement of the electrons as well as of the holes within the quantum wells. That is, their difference (which is the net charge density) remains small and not much screening takes place. As can also be seen by the density distribution in Figure 2, the quantum wells are well isolated from each other by the barriers, such that calculations with single quantum wells yield the same results as calculations on the full MQW structure.

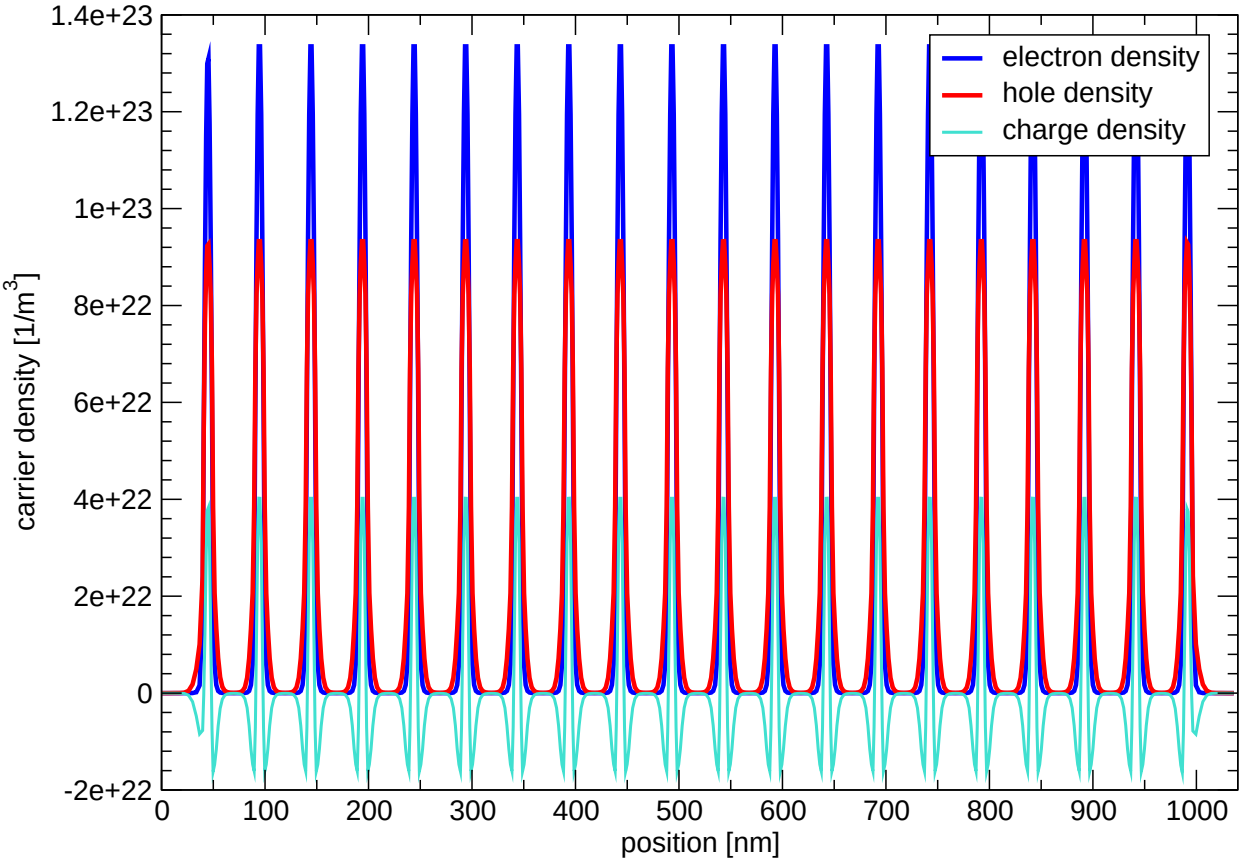

Fig. 2: Local carrier density distribution in the MQW region of a selected sample with 20 quantum wells for a sheet density $N = P = 10^{11}/cm^2$. Blue: electron density n, red: hole density p, cyan: charge density $n - p$.

References

1. http://www.wias-berlin.de/software/qw/.

2. P. ENDERS, A. BÄRWOLFF, M. WOERNER, D. SUISKY, *kp theory of energy bands, wave functions, and optical selection rules in strained tetrahedral semiconductors*, Phys. Rev. B, **51**(23) (1995), pp. 16695–16704.

3. U. BANDELOW, H.-CHR. KAISER, TH. KOPRUCKI, J. REHBERG, *Spectral properties of k·p Schrödinger operators in one space dimension*, Numer. Funct. Anal. Optim., **21**(3&4) (2000), pp. 379–409.

4. I. VURGAFTMAN, J.R. MEYER, L.R. RAM-MOHAN, *Band parameters for III/V compound semiconductors and their alloys*, J. Appl. Phys., **89** (2001), pp. 5815–5875.

5. TH. KOPRUCKI, M. BARO, U. BANDELOW, T.Q. TIEN, F. WEIK, J.W. TOMM, M. GRAU, M.-CHR. AMANN, *Electronic structure and optoelectronic properties of strained InAsSb/GaSb multi quantum-wells*, WIAS Preprint no. 1028, 2005.

Modeling, analysis and simulation of mode-locked semiconductor lasers

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Cooperation with: B. Hüttl, R. Kaiser, (Fraunhofer-Institut für Nachrichtentechnik, Heinrich-Hertz-Institut (HHI), Berlin)

Supported by: Terabit Optics Berlin (project B4)

Mode-locked semiconductor lasers have attracted considerable research interest for many years, for their high speed potential as well as the possible generation of intense pulses. Together with our partners, we are aiming at an optical data transmission at rates of 40 GHz. A typical device under consideration is sketched in Figure 1.

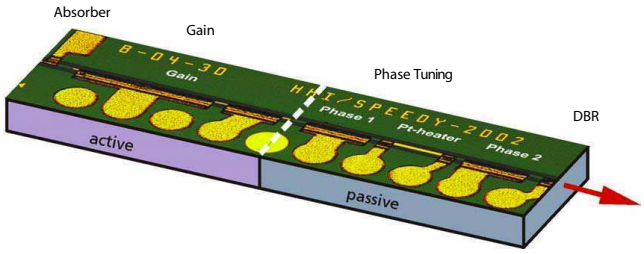

Fig. 1: Monolithic multisection DBR laser as fabricated at HHI Berlin. It consists of a reversely biased saturable absorber section, a forward biased gain section, a passive phase tuning section, and a passive distributed Bragg reflector (DBR) section and is designed for emission of pulse trains with 40 GHz repetition frequency.

In a mode-locked laser, a spatio-temporal structure develops across the entire device, which has to be properly accounted for. An adequate description is given by the traveling wave equations (TWE)

$$\left(-\frac{i}{v_g}\frac{\partial}{\partial t} \mp i\frac{\partial}{\partial z} + \beta\right) E_{\pm} + \kappa E_{\mp} = 0 \tag{1}$$

for the slowly varying amplitudes $E_+(z,t)$ and $E_-(z,t)$ of the forward and back traveling waves, respectively. The boundary conditions are $E_-(L,t) = r_L E_+(L,t)$ and $E_+(0,t) = r_0 E_-(0,t)$ at the facets of the laser. β is a function of the locally distributed carrier density $n(z,t)$, which itself is governed by

$$\partial_t n = J(z,t) - R(n) - v_g \, \Re e[E^*(g + 2\mathcal{D})E]. \tag{2}$$

Especially in the absorber and the gain section, the model for β is

$$\beta = -i\frac{\alpha}{2} + (i + \alpha_H)\frac{g}{2} + i\mathcal{D} \qquad \text{(active sections)}, \tag{3}$$

where the gain g also depends on n. $\mathcal{D}$ is a dispersion operator defined by

$$\mathcal{D}E^{\pm} \stackrel{def}{=} \frac{\bar{g}}{2}(E^{\pm} - p^{\pm}) \qquad \text{and} \tag{4}$$

$$-i\partial_t p^{\pm} = -i\bar{\gamma}(E^{\pm} - p^{\pm}) + \bar{\omega}p^{\pm}. \tag{5}$$

More details can be found in [1]. The above distributed time-domain model will be in the following shortly referred to as the TWE model. In practise, we use this TWE model for numerical simulation (LDSL) and quantitative comparison with the experiment.

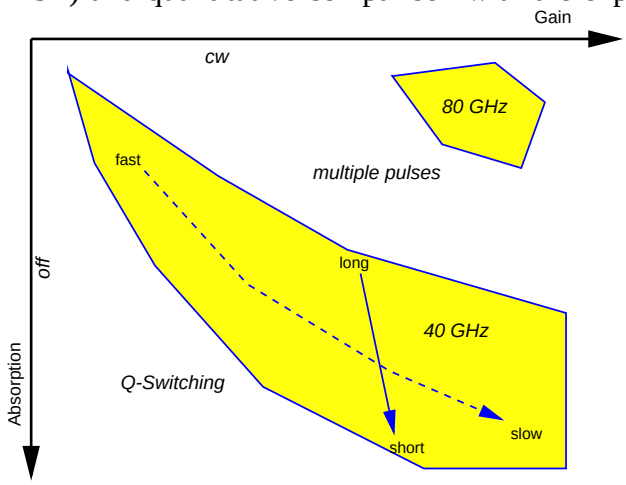

Fig. 2: Typical simulation results obtained with `LDSL-tool` on mode-locked lasers. Stable mode locking occurs in the shaded areas where also the repetition frequencies are given. Outside these areas, mode locking becomes unstable: Supermodulation by slower Q-switching as well as multiple pulses can appear.

Typical simulation results are schematically drawn in Figure 2. As indicated there, other effects occur outside the mode-locking areas which hinder applications. These effects influence smoothly the mode-locking behavior already within the shaded areas, resulting in an increasing *amplitude noise*, if one approaches the boundaries. Above the 40-GHz area, we discovered a region where a two-pulse (instead of one) scenario appears.

To our surprise, we observed the stabilization of the two pulses when we decreased the absorption even more and increased the gain slightly, thereby approaching the upper right area in Figure 2 called *80 GHz*. In this situation the two pulses keep the maximum distance in the resonator and counter-propagate through it. This is indicated by the completely correlated output pulses at the two end facets, drawn in the upper Figure 3, with a repetition frequency of 80 GHz. The latter is twice the roundtrip frequency, such that we can call it *harmonic mode locking*. The surprising thing is that there is no specific geometrical construction as, e.g., a ring resonator or a colliding pulse scheme which would support this type of mode locking: The pulses meet simply somewhere in the phase tuning section without specifically gaining from that. The harmonic mode locking appears to be self-starting and is stable over a finite range of parameters. So far, this was our first observation from numerical simulations with the TWE model. Later in 2004, this phenomenon has, indeed, been measured at the HHI with autocorrelation techniques. The measured autocorrelation trace is depicted in the lower Figure 3 and displays a periodic signal with a repetition frequency of 80 GHz, which corresponds to our prediction.

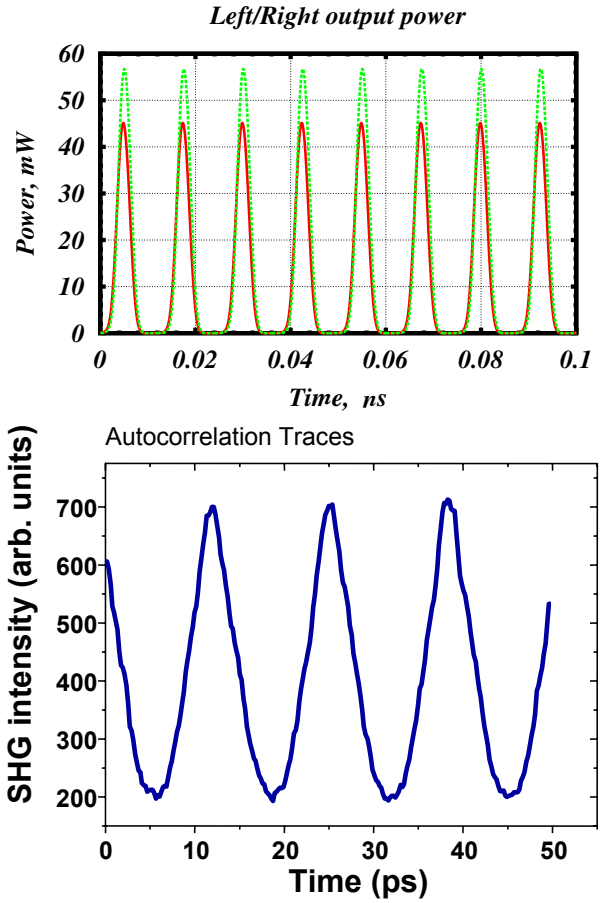

Fig. 3: 80-GHz mode locking. Upper: Time trace of output power at both facets of the harmonic mode-locked laser, prediction by simulation. Lower: Measured autocorellation trace.

Even more, the harmonic mode locking has been measured in the same region of parameters as predicted by the theory, cf. shaded “80 GHz” areas in Figure 2 and in Figure 4.

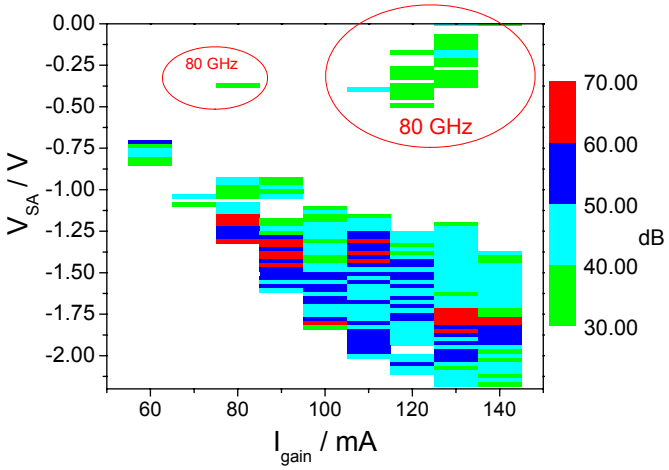

Fig. 4: Mode-locking areas incl. 80 GHz harmonic mode locking, measured at HHI

For a qualitative analysis, we use in addition lumped differential-delay models [2], similar to the Lang–Kobayashi treatment of lasers with external feedback. When deriving these models, we do not use the approximations of small gain and loss per cavity round trip and weak

saturation. Therefore, our models are capable of describing mode locking in the parameter range of semiconductor lasers. In the first, ring cavity model, the equations governing the time evolution of the electric field amplitude $a(t)$ at the entrance of the gain section, saturable gain $g(t)$, and saturable loss $q(t)$ take the form of delay differential equations, [2, 3],

$$\gamma^{-1}\partial_t a(t) + a(t) = \sqrt{\xi} e^{(1-i\alpha_{H2})g(t-T)/2-(1-i\alpha_{H1})q(t-T)/2+i\phi} a(t-T), \tag{6}$$

$$\partial_t q(t) = -q_0 - \frac{q(t)}{\tau_1} - s\left(1-e^{-q(t)}\right)|A(t)|^2, \tag{7}$$

$$\partial_t g(t) = g_0 - \frac{g(t)}{\tau_2} - e^{-q(t)}\left(e^{g(t)}-1\right)|A(t)|^2. \tag{8}$$

The second, linear cavity model, assumes that both gain and saturable absorber sections are thin as compared to the pulse width. In the case when the absorber section is situated close to one of the two cavity mirrors, this model takes the form:

$$\gamma^{-1}\partial_t a(t) + a(t) = \sqrt{\xi_1\xi_2} e^{(1-i\alpha_{H2})[g(t-T)+g(t-T+\tau)]/2-(1-i\alpha_{H1})q(t-T)+i\phi} a(t-T), \tag{9}$$

$$\partial_t q(t) = -q_0 - \frac{q(t)}{\tau_1} - s\left(1-e^{-q(t)}\right)\left(1+\xi_1 e^{-q(t)}\right)|a(t)|^2, \tag{10}$$

$$\partial_t g(t) = g_0 - \frac{g(t)}{\tau_2} - \xi_1\left(e^{g(t)}-1\right)e^{g(t-\tau)-2q(t-\tau)}|a(t-\tau)|^2 - \left(e^{g(t)}-1\right)|a(t)|^2. \tag{11}$$

As a result, this simplified model covers qualitatively all prominent effects which we have calculated with the TWE model. The results of an analytic consideration are shown in Figure 5.

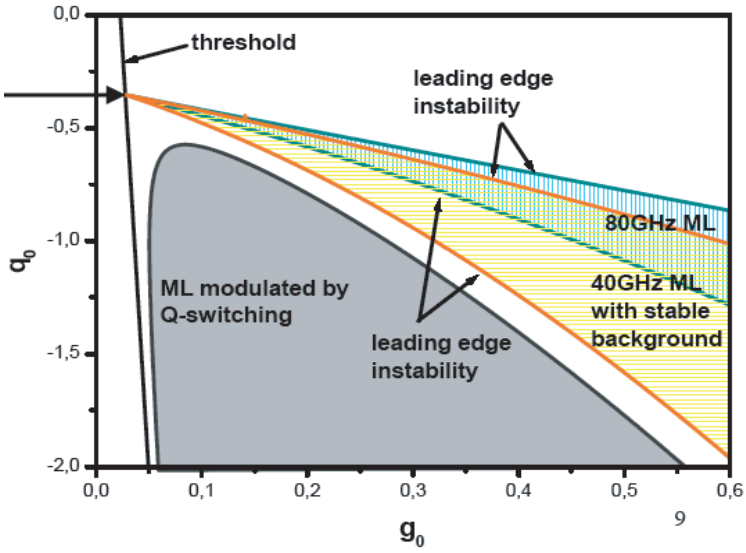

Fig. 5: Results of an analytical stability analysis with delay differential model

References

1. U. BANDELOW, M. RADZIUNAS, J. SIEBER, M. WOLFRUM, *Impact of gain dispersion on the spatio-temporal dynamics of multisection lasers*, IEEE J. Quantum Electronics, **37**(2) (2001), pp. 183–188.

2. A.G. VLADIMIROV, D. TURAEV, G. KOZYREFF *Delay differential equations for mode-locked semiconductor lasers*, Opt. Lett., **29** (2004), pp. 1221–1223.

3. A.G. VLADIMIROV, D. TURAEV, *A new model for a mode-locked semiconductor laser*, to appear in: Radiophys. and Quantum Electronics, 2004.

A descent method for the free energy of multicomponent systems

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Cooperation with: J. Beuthan, O. Minet (Charité, Institut für Medizinische Physik und Lasermedizin, Berlin)

Supported by: BMBF-Verbundprojekt: „Anwendung eines nichtlokalen Phasenseparationsmodells zur Bildbewertung in der Rheumadiagnostik" (Joint Project: Application of a nonlocal phase separation model to optical diagnosis of rheumatic diseases)

To describe phase-separation processes, we consider a closed system with interacting particles of type $i \in \{0,1,\dots,m\}$ occupying a spatial Lipschitz domain $\Omega \subset \mathbb{R}^n$. We assume that the particles jump around on a given microscopically scaled lattice following a stochastic exchange process. Exactly one particle sits on each lattice site (exclusion principle). Two particles of type i and ℓ change their sites x and y with a certain probability $p_{i\ell}(x,y)$ due to *diffusion* and *interaction*. The *hydrodynamical limit* (see [2]) leads to a system of $m+1$ *conservation laws:*

$$u_i' + \nabla \cdot j_i = 0 \text{ in } (0,T)\times\Omega, \quad \nu \cdot j_i = 0 \text{ on } (0,T)\times\partial\Omega, \quad u_i(0) = u_{0i} \text{ in } \Omega, \tag{1}$$

with *mass densities* $u_0,\dots,u_m$, their *initial values* $u_{00},\dots,u_{0m}$, and *current densities* $j_0,\dots,j_m$. Due to the exclusion principle, we can assume $\sum_{i=0}^m u_i = 1$, $\sum_{i=0}^m u_{0i} = 1$, and $\sum_{i=0}^m j_i = 0$. Hence, we can describe the state of the system by $u = (u_1,\dots,u_m)$ and $u_0 = 1 - \sum_{i=1}^m u_i$.

Equilibrium distributions $u^* = (u_1^*,\dots,u_m^*) : \Omega \to \mathbb{R}^m$ of the multicomponent system, and more generally, steady states of the evolution system can be supposed to be *local minimizers* of the *free energy functional* F under the constraint of mass conservation:

$$F(u^*) = \min\big\{F(u) : \textstyle\int_\Omega (u_i - u_{0i})\,dx = 0 \text{ for } i \in \{1,\dots,m\}\big\},$$

or solutions (u^*,μ^*) of the Euler–Lagrange equations including Lagrange multipliers $\mu^* \in \mathbb{R}^m$:

$$DF(u^*) = \textstyle\sum_{i=1}^m \mu_i^* g_i, \quad \langle g_i, u\rangle = \int_\Omega u_i\,dx, \quad \langle g_i, u^* - u_0\rangle = 0, \quad i \in \{1,\dots,m\}. \tag{2}$$

In many applications, one is originally interested in u^*. However, F is in general not convex, so it seems to be difficult to solve (2) directly. One can try to construct u^* as steady state of the evolution system (1): In view of the fact that the Lagrange multipliers μ_i^* should be constant, one assumes their antigradients to be driving forces towards equilibrium. This leads to the evolution system (1) with current densities $j_i = -\sum_{\ell=1}^m a_{i\ell}(u)\nabla\mu_\ell$ and positively semidefinite mobility matrix $(a_{i\ell})$ (see [2], [3]). Evidently, F is a Lyapunov function of (1), and the authors have developed a dissipative discretization scheme with respect to space and time. However, from the practical point of view that approach becomes questionable if meta-stable states occur. Hence, we want to establish a descent method to solve (2) directly (see [1]):

To formulate our problem, we use standard spaces $H = L^2(\Omega;\mathbb{R}^m)$ and $V = L^\infty(\Omega;\mathbb{R}^m)$. We consider the decomposition of $H = H_0 + H_1$ into the closed subspace $H_0 = \{u \in H : \int_\Omega u\,dx = 0\}$ and the m-dimensional subspace $H_1 \subset V$ of constants. Let $J \in \mathcal{L}(H;H^*)$ be the duality map between H and H^*. Then the annihilator $H_0^0 = J[H_1]$ is the m-dimensional subspace of elements $f = \sum_{i=1}^m \mu_i g_i$ where $\mu \in \mathbb{R}^m$ and $g_1,\dots,g_m \in J[V]$ are given by $\langle g_i, u\rangle = \int_\Omega u_i\,dx$, $u \in H$.

We split the *free energy functional* $F : H \longrightarrow \mathbb{R} \cup \{+\infty\}$ into a sum $F = \Phi + \Psi$ of a *chemical* part $\Phi : H \to \mathbb{R} \cup \{+\infty\}$ and a *nonlocal interaction* part $\Psi : H \longrightarrow \mathbb{R}$ as follows:

We introduce a lower semicontinuous and strongly convex functional $\Phi : H \longrightarrow \mathbb{R} \cup \{+\infty\}$ by

$$\Phi(u) = \begin{cases} \int_\Omega \varphi(u)\,dx & \text{if } u \in \operatorname{dom}(\Phi), \\ +\infty & \text{otherwise,} \end{cases} \qquad \varphi(z) = \begin{cases} \sum_{i=0}^m z_i \log(z_i) & \text{if } z \in \operatorname{dom}(\varphi), \\ +\infty & \text{otherwise,} \end{cases} \tag{3}$$

where $\operatorname{dom}(\Phi) = \{u \in H : 0 \le u_0, u_1, \dots, u_m \le 1\}$ and $\operatorname{dom}(\varphi) = \{z \in \mathbb{R}^m : 0 \le z_0, z_1, \dots, z_m \le 1\}$. Additionally, we fix $l \in J[V]$ and $d \in \mathbb{R}$ and define a quadratic functional $\Psi : H \longrightarrow \mathbb{R}$ by

$$\Psi(u) = \tfrac{1}{2}\langle Tu, u\rangle + \langle l, u\rangle + d, \quad u \in H, \tag{4}$$

where $T \in \mathcal{L}(H; H^*)$ is a self-adjoint and completely continuous operator such that $T|V$ is a completely continuous operator in $\mathcal{L}(V; J[V])$. Then we can find constants α, $\beta > 0$ such that

$$\big\langle \partial\Phi(u) - \partial\Phi(v), u - v\big\rangle \ge \alpha \|u - v\|_H^2, \quad \|D\Psi(u) - D\Psi(v)\|_{H^*} \le \beta \|u - v\|_H, \quad u, v \in \operatorname{dom}(\Phi).$$

If we specify $\bar{u} \in \operatorname{int}\operatorname{dom}(\varphi)$ and the set $K = \big\{u \in \operatorname{dom}(\Phi) : \int_\Omega (u - \bar{u})\,dx = 0\big\}$ of mass constraints, then the functional $F : H \to \mathbb{R} \cup \{+\infty\}$ is bounded from below, and there exists a solution $u^* \in K$ of the constrained minimum problem $F(u^*) = \min\big\{F(u) : u \in K\big\}$.

In view of the above assumptions on monotonicity, continuity, and compactness, we can find convex subsets $C \subset K$ and $M \subset H_0^0$ which are closed in V and $J[V]$, respectively, such that for all initial values $u_0 \in K$, we can define iteration sequences $(u_k) \subset K$ and $(v_k, f_k) \in C \times M$ by

$$u_{k+1} = \tau v_k + (1 - \tau)u_k, \quad f_k \in \partial\Phi(v_k) + D\Psi(u_k), \quad k \in \mathbb{N}. \tag{5}$$

Here, the relaxation parameter $\tau \in (0, 1]$ satisfies $\alpha > \beta\tau$ which ensures the decay and the convergence of $(F(u_k))$ due to the descent property

$$\|u_k - u_{k+1}\|_H^2 \le \tfrac{2\tau}{\alpha - \beta\tau}\big(F(u_k) - F(u_{k+1})\big), \quad k \in \mathbb{N}.$$

Moreover, using analyticity properties of φ, we can apply a Łojasiewicz–Simon-type inequality to prove that the sequence $(u_k, f_k) \subset K \times M$ defined by (5) converges to a solution $(u^*, f^*) \in C \times M$ of the Euler–Lagrange equation (see (2))

$$f^* = \textstyle\sum_{i=1}^m \mu_i^* g_i \in \partial\Phi(u^*) + D\Psi(u^*),$$

in the sense of $\lim_{k\to\infty} F(u_k) = F(u^*)$, $\lim_{k\to\infty} \|u_k - u^*\|_V = 0$, and $\lim_{k\to\infty} \|f_k - f^*\|_{J[V]} = 0$.

To apply our descent method to image processing, we describe the nonlocal interaction by means of inverse operators corresponding to second-order elliptic operators with appropriate regularity properties. To do so, for $r > 0$ we consider the family of elliptic operators $E_r \in \mathcal{L}\big(H^1(\Omega); H^1(\Omega)^*\big)$ (including Neumann boundary conditions) given by

$$\big\langle E_r v, h\big\rangle = \int_\Omega \big(r^2 \nabla v \cdot \nabla h + vh\big)\,dx, \quad v, h \in H^1(\Omega).$$

We want to emphasize that the inverse $E_r^{-1} \in \mathcal{L}\big(H^1(\Omega)^*; H^1(\Omega)\big)$ is completely continuous from $L^2(\Omega)$ into $L^2(\Omega)$ as well as from $L^\infty(\Omega)$ into $L^\infty(\Omega)$.

To control the qualitative behavior of nonlocal interaction, we prescribe *effective ranges* ρ, $r > 0$ and *intensities* $\sigma_{i\ell}$, $s_{i\ell} \in \mathbb{R}$ of interaction forces between particles of type i and $\ell \in \{0, 1, \dots, m\}$,

respectively. Clearly, both matrices $(\sigma_{i\ell})$ and $(s_{i\ell})$ are assumed to be symmetric. The cases $\sigma_{i\ell} > 0$ and $\sigma_{i\ell} < 0$ represent repulsive and attractive interaction, respectively. The nontrivial choice of $(s_{i\ell})$ enables us to get final states close to the corresponding initial values $u_0 \in K$ if we define the quadratic functional $\Psi : H \longrightarrow \mathbb{R}$ according to (4):

$$\Psi(u) = \tfrac{1}{2} \sum_{i=0}^{m} \sum_{\ell=0}^{m} \int_\Omega \left(u_i \sigma_{i\ell} E_\rho^{-1} u_\ell + (u_i - u_{0i}) s_{i\ell} E_r^{-1} (u_\ell - u_{0\ell}) \right) dx, \quad u \in H.$$

In our joint BMBF project, we use the above nonlocal image segmentation method to analyze medical images regarding the scattering light distribution of the near-infrared spectral range on rheumatoid finger joints. Rheumatoid arthritis is the most common inflammatory arthropathy; it often affects the small joints, especially the finger joints. Inflammation of joints caused by rheumatic diseases starts with an inflammatory process of capsule synovial structures. Later, granulation tissue develops in the synovialis and destroys the cartilage and even the bone structure. Figures 1 and 2 show two examples of healthy and rheumatoid finger joints and the corresponding results of image segmentation with respect to three components (bone, cartilage, and synovial fluid):

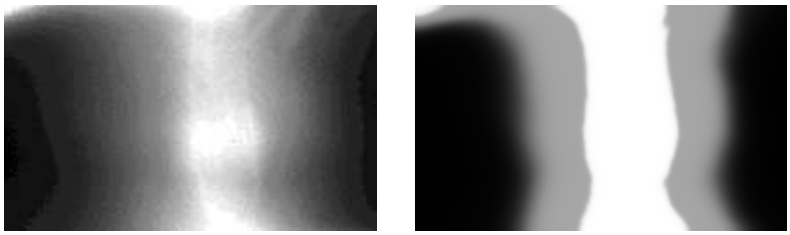

Fig. 1: Healthy finger joint

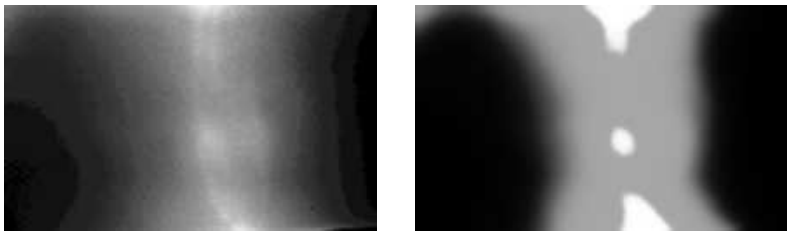

Fig. 2: Rheumatoid finger joint

References

1. H. GAJEWSKI, J.A. GRIEPENTROG, *A descent method for the free energy of multicomponent systems*, WIAS Preprint no. 980, 2004.

2. G. GIACOMIN, J.L. LEBOWITZ, R. MARRA, *Macroscopic evolution of particle systems with short- and long-range interactions*, Nonlinearity, **13** (2000), pp. 2143–2162.

3. J.A. GRIEPENTROG, *On the unique solvability of a phase separation problem for multicomponent systems*, Banach Center Publ., **66** (2004), pp. 153–164.

Optoelectronical sensors

Collaborators: H. Gajewski (FG 1), R. Nürnberg (FG 1), G. Schmidt (FG 4)

Cooperation with: CiS Institut für Mikrosensorik gGmbH, Erfurt; Silicon Sensor International AG, Berlin

The project is concerned with the mathematical modeling and numerical simulation of optoelectronical semiconductor sensors for microsystem technology. Optical sensors and radiation detectors play an important role in robot engineering, material science, and many other areas of modern technology. And semiconductor structures are ideally suited for converting incoming information such as light, X-rays, or particle radiation into an electrical signal.

A simultaneous mathematical modeling of light diffusion and absorption as well as charge generation and transport is needed for both the physical understanding and the optimization of optical semiconductor detectors. An adequate model consists of Maxwell equations for the optical processes and drift-diffusion and heat flow equations for the electronical processes. These equations are coupled via optical, avalanche, and thermal source terms.

The aim of the project was to extend and further develop the simulation program `WIAS-TeSCA` with regard to new requirements in the development of these devices. This included the analytical foundation, implementation, and testing of efficient solution algorithms for the coupled system of equations. The results will be evaluated with the help of real-life optical sensors, namely position sensors and avalanche photodiodes, taken from the manufacturing line of our project partners.

The main focus of the project was on the integration of a module to calculate light diffusion in structured optical films into the device simulation tool `WIAS-TeSCA`. The interaction between light rays and charge transport is modeled with the generation rates in the corresponding partial differential equations. This optical charge generation is described with the ansatz

$$G_{opt}(x,y) = \frac{\lambda}{hc} \cdot \eta \cdot \alpha \cdot I(x,y),$$

where λ is the wavelength of incoming light, η is the quantum efficiency, α is the absorption constant. The intensity I of the electromagnetic field depends on the optical and geometric characteristics of the structure and on properties of the incoming light, such as spectral distribution, polarization, coherence, and contact angle. Since the wavelength is comparable with the dimensions of relevant sensors, diffraction effects come into play. Hence, geometrical optics approaches are no longer sufficient and the light intensity has to be obtained as a solution of the time-harmonic Maxwell equation. Under assumptions of constant permeability μ and of the invariance of the structure in z direction, but oblique incidence of the plane electromagnetic waves $e^{i(\alpha x-\beta y+\gamma z)+i\omega t}$, that are valid here, this equation can be reduced to a system of two-dimensional Helmholtz equations. More precisely, the z components of the electromagnetic field have the form $E_z(x,y)e^{i\gamma z}$, $H_z(x,y)e^{i\gamma z}$ and the functions E_z, H_z satisfy the Helmholtz equations

$$(\Delta + k_\gamma^2) E_z = (\Delta + k_\gamma^2) H_z = 0$$

in each part of the cross section of the structure, in which the refractive index ε_{opt} is continuous. The coefficient k_γ is given by $k_\gamma^2 = k_0^2 \varepsilon_{opt} - \gamma^2$. At material interfaces Λ_j, where the refractive

index is discontinuous, one has to impose the transmission conditions

$$\left[E_z\right]_{\Lambda_j} = \left[H_z\right]_{\Lambda_j} = 0\,,$$
$$\left[\frac{\gamma}{k_\gamma^2}\partial_t H_z + \frac{\omega\varepsilon_{opt}}{k_\gamma^2}\partial_n E_z\right]_{\Lambda_j} = \left[\frac{\gamma}{k_\gamma^2}\partial_t E_z - \frac{\omega\mu}{k_\gamma^2}\partial_n H_z\right]_{\Lambda_j} = 0\,,$$

where ∂_n and ∂_t denote the normal and tangential derivative. Here $\left[v\right]_{\Lambda_j}$ denotes the jump of the function v across the interface Λ_j. Additionally, the solution E_z, H_z has to satisfy radiation conditions at infinity, which ensure finite energy. The mathematical treatment of this so-called conical diffraction is given in [4] and [5]. Due to the periodicity, the system of equations can be solved in a bounded periodic cell, capturing the details of the sensor's structure, such as optical grids and microlenses. The radiation conditions as well as the incoming light are modeled with the help of nonlocal boundary conditions.

To solve the Helmholtz equations, we make use of the program `DiPoG` which was developed at WIAS to simulate and optimize periodic diffraction gratings, [6], and was enlarged for this application. The program is based on the Finite Element Method and the forward solver calculates the efficiency of gratings under conical incidence of plane electromagnetic waves. In order to integrate this module into the program `WIAS-TeSCA`, we, in particular, implemented an efficient method to model thick layers inside the optical structure, different routines to postprocess the calculated field distributions and an effective exchange of the field and intensity distributions, inside the semiconductor structure.

For the project partner CiS, we have successfully simulated a position sensor. In this case, there are several optical layers on the CiS photodiode, two of which have a chrome strip and can be moved against each other. As the structure's dimensions are within a few μm, the light diffusion in the optical grid is determined by diffraction effects. The computed entities are the characteristics of the photodiode, the photocurrent with fixed voltage depending on the lateral translations of the structured layers with respect to each other.

When the sensor is used in practice, the incoming light is not monochromatic and its angle varies depending on the used optics. That is why a whole bundle of rays that sufficiently describes the spectral distribution and the angle variation has to be used in the optical simulation. Solving the Helmholtz equation, the spatial and temporal coherence cannot be accounted for by simply using correction coefficients. Hence, the computational expense increases considerably. In relevant test examples (a Gaussian spectral distribution with a half band width of 40 *nm* and an angle variation of $\pm 1^\circ$), computational costs for a "mean" characteristic curve are similar to the costs for 100 single ones, in order to obtain practically usable and stable results. Note that in order to compute a single characteristic curve, the optical equations had to be solved about 30 times.

The above-mentioned demands illustrate why we have focused on making our simulation software highly efficient. In particular, this covers the appropriate choice of grids for the structured optical layers as well as the effective organization of variations in the geometry (lateral translations), in the wavelength and in the angle of incidence.

The following figures show the dependence of the displacement characteristics on the wavelength and the angle of the incoming light.

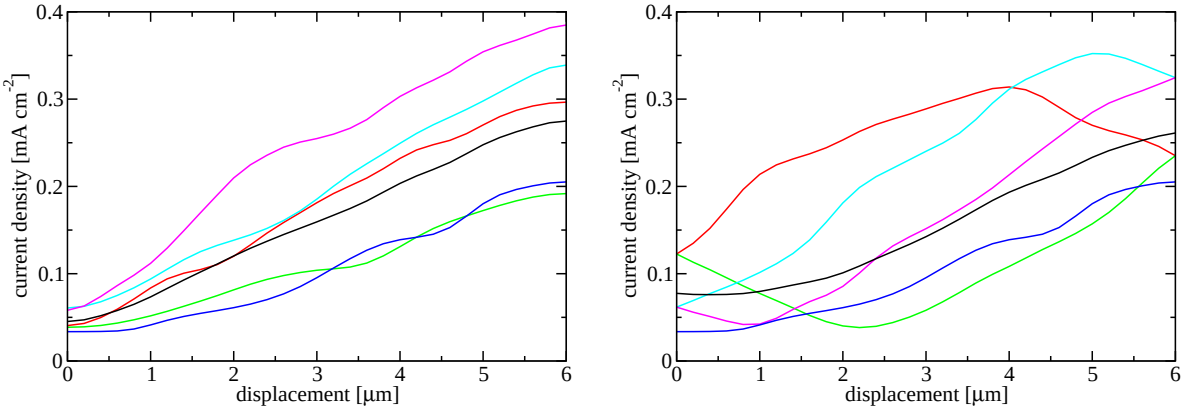

Fig. 1: Current-displacement characteristics of the position sensor for a variation (a) of wavelength and (b) of incidence angle of incoming light

The characteristics for spatially and temporally scattered light enabled us to predict the effect of varying the layer structure and of coating the chrome strips. In this coating example, the modulation depth increased by approximately 25 %.

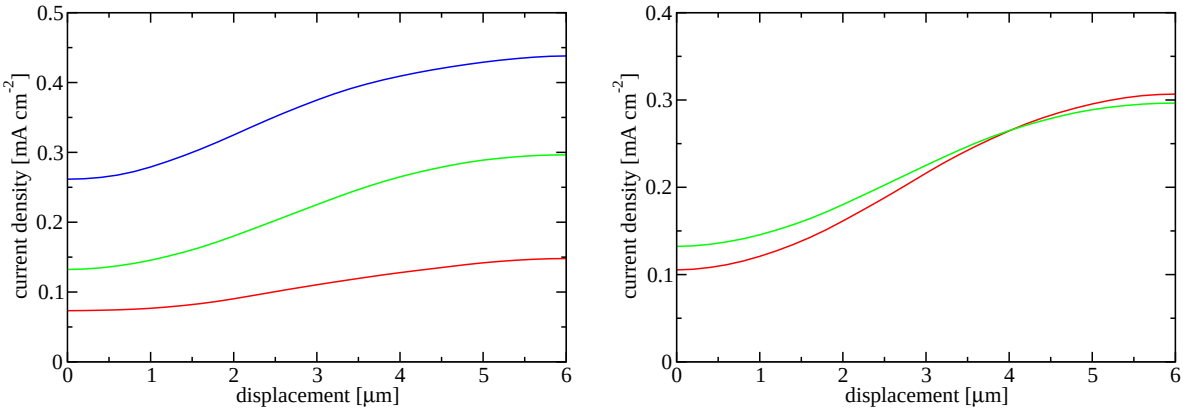

Fig. 2: Current-displacement characteristics of the position sensor using scattered light (a) for different strip and gap widths and (b) for the effect of coating

The main focus for the project partner Silicon Sensor International AG was the modeling and simulation of impact ionization in semiconductor sensors and their interaction with charge transport and thermal processes. Test structures for avalanche photodiodes were modeled in cooperation with the industry partner. The impact ionization models implemented in the package `WIAS-TeSCA` were extended and advanced in accordance with the ideas in [7, 8, 9]. During the investigation of the static and dynamic behavior of special optical sensors, which are able to count single photons by the help of avalanche generation, careful attention was paid to local thermal effects.

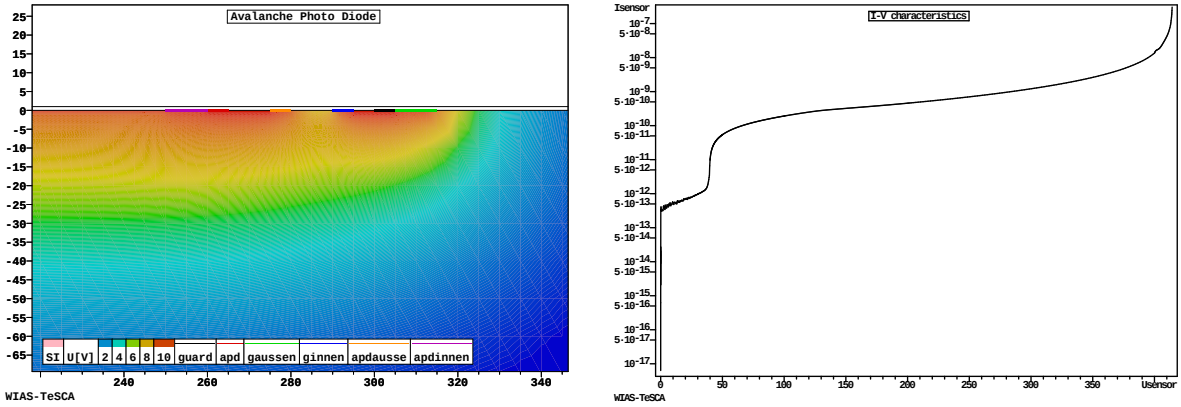

Fig. 3: WIAS-TeSCA simulation of an avalanche photodiode (APD):
(a) 2D electrostatic potential distribution; (b) current-voltage characteristics

During the course of the project both project partners received a program installation that they could use in order to run simulations independently. In addition, CiS purchased a user license for the program package WIAS-TeSCA / DiPoG.

References

1. G. ALBINUS, H. GAJEWSKI, R. HÜNLICH, *Thermodynamic design of energy models of semiconductor devices*, Nonlinearity, **15** (2002), pp. 367–383.

2. H. GAJEWSKI, I.V. SKRYPNIK, *On unique solvability of nonlocal drift-diffusion-type problems*, Nonlinear Anal., **56** (2004), pp. 803–830.

3. H. GAJEWSKI ET AL., WIAS-TeSCA. http://www.wias-berlin.de/software/tesca, 2004.

4. J. ELSCHNER, R. HINDER, F. PENZEL, G. SCHMIDT, *Existence, uniqueness and regularity for solutions of the conical diffraction problem*, Math. Models Methods Appl. Sci., **10**(3) (2000), pp. 317–341.

5. J. ELSCHNER, R. HINDER, G. SCHMIDT, *Finite element solution of conical diffraction problems*, Adv. Comput. Math., **16**(2–3) (2002), pp. 139–156.

6. G. SCHMIDT, *Benutzer-Handbuch Dipog-1.4*, WIAS Technical Report no. 8, 2004.

7. G. WACHUTKA, *Rigorous thermodynamic treatment of heat generation and conduction in semiconductor device modeling*, IEEE Trans. CAD, **9** (1990), pp. 1141–1149.

8. J.W. SLOTBOOM ET AL., *Non-local impact ionization in silicon devices*, Technical Digest, Electron Devices Meeting, 1991, pp. 127–130.

9. A. SCHENK, *Advanced Physical Models for Silicon Device Simulation*, Springer, Wien, 1998.

Optimal regularity for elliptic operators with nonsmooth data

Collaborators: J. Elschner (FG 4), H.-Chr. Kaiser (FG 1), J. Rehberg (FG 1), G. Schmidt (FG 4)

The reported work continues efforts to prove existence, uniqueness, and regularity results for elliptic and parabolic equations and systems which describe phenomena in physics, chemistry, and biology (see Annual Research Reports 2000, p. 19 et sqq., 2002, p. 39 et sqq., and 2003, p. 178 et sqq.).

In view of the applications which we have in mind, one is nearly always confronted with nonsmooth domains, discontinuous coefficients and/or mixed boundary conditions. In particular, in simulation of the current flow in real semiconductor devices——a project area of WIAS——the latter is unavoidable, or the model is meaningless, [18]. As is well known, the usual regularity properties which hold in case of smooth constellations then break down. So, one has to look for suitable substitutes. It turns out that for the successful treatment of such equations it is of great use to have optimal regularity results for the corresponding elliptic operators $-\nabla\cdot\mu\nabla$ between $W_\Gamma^{1,q}$ and $W_\Gamma^{-1,q}$ (with homogeneous Dirichlet boundary conditions on $\partial\Omega\setminus\Gamma$) at hand where q is larger than the space dimension. In [12], Gröger proved that q may be taken always larger than 2 under very general conditions on the domain, the coefficients, and the Neumann boundary part. This result is very useful in many spatially two-dimensional applications, see [2, 4, 9, 11, 14]. One cannot expect $q>3$ in this general setting (see [17] and the Example below). But the necessity grows to study not only two-dimensional problems (mostly as cuts of the original three-dimensional ones) but the three-dimensional models themselves; this means that one needs $q>3$. This is true in semiconductor device modeling (see [10], [15]) but also in many other application areas. Thus, we intend to define a class of three-dimensional domains Ω, (possibly discontinuous) coefficient functions μ, and Neumann boundary parts Γ such that

$$\nabla\cdot\mu\nabla : W_\Gamma^{1,q}(\Omega)\mapsto W_\Gamma^{-1,q}(\Omega) \tag{1}$$

is a topological isomorphism for a $q>3$ (and, hence, by interpolation and duality, for all $\tilde q\in[q',q]$). Let us emphasize that our principal aim is to generate a setting where many situations of practical relevance, subject to research at the Weierstrass Institute and elsewhere, are included.

For some nonsmooth situations one has this already at hand: the pure Dirichlet and Neumann Laplacian on Lipschitz domains was considered in [13] and [19], respectively. Concerning mixed boundary conditions, M. Dauge proved in [3] the following result:

Proposition 1. Let Ω be a convex polyhedron and Γ be the Neumann boundary part of $\partial\Omega$. If $\overline{\Gamma}\cap(\partial\Omega\setminus\Gamma)$ is a connected curve which consists of finitely many line segments, then

$$-\Delta : W_\Gamma^{1,q}(\Omega)\longmapsto W_\Gamma^{-1,q}(\Omega) \tag{2}$$

is a topological isomorphism for some $q>3$.

Let us emphasize that in particular the suppositions are fulfilled if Ω is the unit cube and Γ is one half of its ground plate.

While in the afore-mentioned cases, the coefficients are constant, we proved in a joint paper [16] with V. Maz'ya the following result:

Theorem 1. Let Ω be a Lipschitzian polyhedron which splits up into finitely many subpolyhedra. Let μ be a coefficient function on Ω which takes its values in the set of real, symmetric, positive definite 3×3 matrices and is constant on any subpolyhedron.

For any edge E and $\mathbf{x} \in E$ take an orthogonal transformation O_E which transforms this edge into a line which is parallel to the z-axis. Consider the resulting transformed coefficient matrix function $\mu_{E,\mathbf{x}}$ under the mapping $\mathbf{y} \mapsto O_E\mathbf{y} - O_E\mathbf{x}$. Denote by $\hat{\mu}$ the upper left 2×2 matrix function, restricted to the intersection of the x-y plane with $O_E(\Omega - \mathbf{x})$. By passing to polar coordinates (r,θ), multiplying by r^2, and taking the Mellin transform with respect to r, one obtains from the corresponding two-dimensional boundary value problem the following one-dimensional problem with parameter λ on an interval of angles

$$\Pi(\lambda)\tilde{u} \stackrel{\text{def}}{=} -\partial_\theta(b_2\partial_\theta\tilde{u}) - \lambda\partial_\theta(b_1\tilde{u}) - \lambda b_1\partial_\theta\tilde{u} - \lambda^2 b_0\tilde{u} = \tilde{g}\,, \tag{3}$$

supplemented by transmission conditions (see [16] for details).
If for every edge E, the possible λs, satisfying (3) with right-hand side zero and the transmission conditions, have real parts not contained in the interval $]0,1/3]$, then there is a $q > 3$ such that

$$-\nabla\cdot\mu\nabla : W_0^{1,q}(\Omega) \longmapsto W^{-1,q}$$

is a topological isomorphism.
Unfortunately, for each edge the set of occurring λs is identical with the set of zeros of a transcendental equation which is not at all easy to discuss in general. Nevertheless, we succeeded in proving the following result which covers completely the case of polygonal, layered structures:

Theorem 2 (to be published in [7]). Assume that the following conditions are fulfilled: Ω is a three-dimensional Lipschitzian polyhedron. There are hyperplanes $\mathcal{H}_1 \ldots \mathcal{H}_n$ in R^3 intersecting (within $\overline{\Omega}$) with each other at most in a vertex of the polyhedron such that the coefficient function μ is a constant real symmetric positive definite 3×3 matrix on each of the connected components of $\Omega \setminus \cup_{l=1}^n \mathcal{H}_l$. Moreover, for every edge on the boundary, induced by a hetero-interface $\mathcal{H}_l$, the angles between the outer boundary plane and the hetero-interface do not exceed π and at most one of them may equal π. Then the operator $-\nabla\cdot\mu\nabla$ provides a topological isomorphism between $W_0^{1,q}(\Omega)$ and $W^{-1,q}(\Omega)$ for all $q \in [2,4]$.
In the case of nonsmooth interfaces, q exceeds 2 only arbitrarily little, as the following instructive counterexample by J. Elschner shows.

Example (to be published in [7]). Consider the following coefficient function ρ on R^2:

$$\rho(x,y) = \begin{pmatrix} 1 & 0 \\ 0 & t^2 \end{pmatrix} \quad \text{if } x,y > 0 \qquad \text{and} \qquad \begin{pmatrix} t & 0 \\ 0 & t \end{pmatrix} \quad \text{elsewhere on } R^2$$

(t positive) and, correspondingly, the following elliptic problem on R^2:

$$\nabla\cdot\rho\nabla w = 0, \quad w \in W_{loc}^{1,2}(R^2). \tag{4}$$

Following again [16], one evaluates the λs with the smallest positive real part as

$$\lambda = \frac{8\pi^2}{4\pi^2 + \ln^2 t} \pm i\frac{4\pi\ln t}{4\pi^2 + \ln^2 t}. \tag{5}$$

If $t \mapsto \infty$, then the real part of λ converges to 0. This provides a local solution of (4) which behaves like $(x^2+y^2)^{\lambda/2}$ in a neighborhood of $0 \in R^2$. Tending with t to ∞, these solutions lack any common (local) integrability of order larger than 2 for their first-order derivatives.

Clearly, the example is not restricted to two dimensions, namely, one can add arbitrarily many dimensions by extending the solution constantly in these directions——at least in a neighborhood of zero.
However, in case of an inner C^1 interface, we proved the following result which generalizes the linear regularity result of [1].

Theorem 3 (to be published in [8]). Let Ω be a Lipschitz domain and $\Omega_\circ \subset \Omega$ be a C^1 domain which does not touch the boundary of Ω. Suppose that the coefficient function μ is uniformly continuous on $\Omega \setminus \bar{\Omega}_\circ$ and on $\Omega_\circ$. Then there is a $q > 3$ such that

$$-\nabla \cdot \mu \nabla : W_0^{1,q} \longmapsto W^{-1,q}$$

is a topological isomorphism.
Further, from Proposition 1 one may conclude by localization techniques and perturbation arguments the following

Theorem 4 (to be published in [8]). Let $Q \subset R^3$ denote the unit cube and Υ one half of its ground plate. Assume that the coefficient function μ is uniformly continuous. For any $\mathbf{x} \in \bar{\Gamma} \cap (\partial\Omega \setminus \Gamma)$ there is an open neighborhood $\mathcal{U}_\mathbf{x}$ in R^3 and a homeomorphism $\Psi_\mathbf{x}$ from $\mathcal{U}_\mathbf{x}$ onto an open set $\mathcal{V}_\mathbf{x}$ which satisfy $\Psi(\mathcal{U}_\mathbf{x} \cap (\Omega \cup \Gamma) = Q \cup \Upsilon$ and $\Psi(\mathbf{x}) = 0$. Moreover, every $\Psi_\mathbf{x}$ and its inverse are continuously differentiable and the derivative is uniformly continuous on $\mathcal{U}_\mathbf{x}$. Then there is a $q > 3$ such that $-\nabla \cdot \mu \nabla$ is a topological isomorphism between $W_\Gamma^{1,q}$ and $W_\Gamma^{-1,q}$.
Finally, one can define a global setting which includes all the above-mentioned situations in a certain sense as its local constituents, see [8].

References

1. L.A. CAFFARELLI, I. PERAL, *On $W^{1,p}$ estimates for elliptic equations in divergence form*, Comm. Pure Appl. Math., **51** (1998), pp. 1–21.

2. L. CONSIGLIERI, M.M.C. MUNIZ, *Existence of solutions for a free boundary problem in the thermoelectrical modelling of an aluminium electrolytic cell*, Eur. J. Appl. Math., **14** (2003), pp. 201–216.

3. M. DAUGE, *Neumann and mixed problems on curvilinear polyhedra*, Integral Equations Operator Theory, **15** (1992), pp. 227–261.

4. P. DEGOND, S. GÉNIEYS, A. JÜNGEL, *A steady-state system in non-equilibrium thermodynamics including thermal and electrical effects*, Math. Methods Appl. Sci., **21** (1998), pp. 1399–1413.

5. J. ELSCHNER, G. SCHMIDT, *Diffraction in periodic structures and optimal design of binary gratings. I. Direct problems and gradient formulas*, Math. Methods Appl. Sci., **21** (1998), pp. 1297–1342.

6. J. ELSCHNER, R. HINDER, F. PENZEL, G. SCHMIDT, *Existence, uniqueness and regularity for solutions of the conical diffraction problem*, Math. Models Methods Appl. Sci., **10** (2000), pp. 317–341,

7. J. ELSCHNER, H.-CHR. KAISER, J. REHBERG, G. SCHMIDT, *$W^{1,q}$ regularity results for elliptic transmission problems on heterogeneous polyhedra*, in preparation.

8. ——, *Optimal regularity for elliptic operators occurring in real-world problems*, in preparation.

9. P. FABRIE, T. GALLOUËT, *Modeling wells in porous media flow*, Math. Models Methods Appl. Sci., **10** (2000), pp. 673–709.

10. H. GAJEWSKI, H.-CHR. KAISER, H. LANGMACH, R. NÜRNBERG, R.H. RICHTER, *Mathematical modeling and numerical simulation of semiconductor detectors*, in: Mathematics—Key Technology for the Future. Joint Projects Between Universities and Industry, W. Jäger, H.J. Krebs, eds., Springer-Verlag, Berlin, Heidelberg, 2003, pp. 355–364.

11. A. GLITZKY, R. HÜNLICH, *Global estimates and asymptotics for electro-reaction-diffusion systems in heterostructures*, Appl. Anal., **66** (1997), pp. 205–226.

12. K. GRÖGER, *A $W^{1,p}$-estimate for solutions to mixed boundary value problems for second order elliptic differential equations*, Math. Ann., **283** (1989), pp. 679–687.

13. D. JERISON, C.E. KENIG, *The inhomogeneous Dirichlet problem in Lipschitz domains*, J. Funct. Anal., **130** (1995), pp. 161–219.

14. A. JÜNGEL, *Regularity and uniqueness of solutions to a parabolic system in nonequilibrium thermodynamics*, Nonlinear Anal. TMA, **41** (2000), pp. 669–688.

15. G. LUTZ, R.H. RICHTER, L. STRÜDER, *DEPMOS-Arrays for X-ray imaging*, in: XRAY Optics, Instruments and Missions III, J. Trümper, B. Aschenbach, eds., Proceedings of SPIE, **4012** (2000), pp. 249–256.

16. V. MAZ'YA, J. ELSCHNER, J. REHBERG, G. SCHMIDT, *Solutions for quasilinear nonsmooth evolution systems in L^p*, Arch. Ration. Mech. Anal., **171** (2004), pp. 219–262.

17. N.G. Meyers, *An L^p-estimate for the gradient of solutions of second order elliptic divergence equations*, Ann. Scuola Norm. Sup. Pisa Cl. Sci., **17** (1963), pp. 189–206.

18. S. SELBERHERR, *Analysis and simulation of semiconductor devices*, Springer-Verlag, Wien, New York, 1984.

19. D. ZANGER, *The inhomogeneous Neumann problem in Lipschitz domains*, Comm. Partial Differential Equations, **25** (2000), pp. 1771–1808.

5 Scientific-technical Services

5.1 Bibliothek / Library

Die Bibliothek des WIAS ist eine wissenschaftliche Spezialbibliothek und sammelt ihr Material hauptsächlich auf den Gebieten der Angewandten Analysis und Stochastik. Der Literaturbestand der Bibliothek umfasst ca. 70 000 Medieneinheiten (Bücher, Preprints, Reports und gebundene Zeitschriftenbände) und 73 laufende Zeitschriften. Neben dem elektronischen Zugriff auf die meisten abonnierten Zeitschriften besteht elektronischer Zugriff auf über 1000 Zeitschriften der Verlage Kluwer und Springer auf der Grundlage von Verträgen des Friedrich-Althoff-Konsortiums mit den Verlagen. Den wissenschaftlichen Zielen und den aktuellen Projekten des Instituts wird durch die Berücksichtigung benachbarter Gebiete der Natur- und Ingenieurwissenschaften entsprochen:

- Numerische Mathematik und Wissenschaftliches Rechnen,
- Mikro-, Nano- and Optoelektronik, Phasenübergänge,
- Strömungs- und Transportprobleme,
- Stochastik in Naturwissenschaften und Finanzmathematik.

The library of WIAS is a specialized scientific library which collects material mainly in the areas of applied analysis and stochastics. The stock of the library's literature encompasses 70 000 media units (books, preprints, reports, and bound volumes of journals), approximately, and 73 current journals. Besides the electronic access to most subscribed journals, electronic access exists to more than 1000 journals of the publishers Kluwer and Springer, based upon agreements between the Friedrich-Althoff-Konsortium and the publishers. According to the scientific objectives and actual projects of the institute, neighboring areas of science and engineering are also taken into account:

- Numerical Mathematics and Scientific Computing;
- Micro-, Nano- and Optoelectronics, Phase Transitions;
- Flow and Transport Problems;
- Stochastics in Natural Sciences and Financial Mathematics.

Die Bibliothek ist montags bis freitags von 9 Uhr bis 16 Uhr geöffnet. Im Lesesaal steht den Lesern ein herkömmlicher Zettelkatalog zur Verfügung, um die benötigte Literatur zu suchen. Zusätzlich wird ein elektronischer Katalog aufgebaut, der jetzt ungefähr den Bestand enthält, der in den letzten zwölf Jahren erworben wurde. Zur Vorbereitung der elektronischen Ausleihe und der elektronischen Verwaltung der Nutzerkonten werden die älteren Teile des Bestandes schrittweise hinzugefügt.

The opening hours of the library are from Monday through Friday from 9 a.m. to 4 p.m. In the reading room the readers are provided with a conventional card catalogue to search for the literature they need for their purposes. An electronic catalogue is being built up which covers now the part of the stock obtained during the last twelve years, approximately. For preparing electronic lending, including the electronic administration of readers' accounts, the older parts of the stock are added step by step.

Neben den gedruckten Bänden hat man im Lesesaal auch Zugriff auf zahlreiche elektronische Zeitschriften und Datenbanken. Das meiste von diesem elektronischen Material können die Mitarbeiter auch über ihre Workstations lesen.

Die Bibliothek des WIAS ist Mitglied im „Arbeitskreis Bibliotheken und Informationseinrichtungen der Leibniz-Gemeinschaft“ und in der „Arbeitsgemeinschaft deutscher Spezialbibliotheken“. Die Bibliothek vertritt das WIAS im „Friedrich-Althoff-Konsortium“, einer Organisation wissenschaftlicher Bibliotheken in Berlin und Brandenburg.

Apart from printed volumes of the stock of the library’s literature, the reading room provides access to various e-journals and databases. Most of this electronic material can also be read by the WIAS collaborators on their workstations.

The WIAS library is a member of the “Arbeitskreis Bibliotheken und Informationseinrichtungen der Leibniz-Gemeinschaft” (working group of libraries and information institutions of the Leibniz Association) and of the “Arbeitsgemeinschaft deutscher Spezialbibliotheken” (study group of German specialized libraries). It represents WIAS in the “Friedrich-Althoff-Konsortium” which is an organization of scientific libraries in Berlin and Brandenburg.

Statistische Informationen über das Jahr 2004 / Statistical information about the year 2004

Erwerbungen:	Acquisitions:
104 Bücher	104 books
287 gebundene Zeitschriftenbände	287 bound volumes of journals
775 Preprints und Reports	775 preprints and reports
45 Loseblattsammlungen	45 loose-leaf collections
Entleihungen und Verlängerungen aus der Bibliothek des WIAS:	Lent and renewed from the WIAS library:
8980 Bücher	8980 books
Aus anderen Bibliotheken beschaffte Literatur:	Literature provided from other libraries:
588 Bücher	588 books
415 Artikel	415 articles

5.2 Fachinformation / Science Information

Die Fachinformation des WIAS bietet unterschiedliche Recherchemöglichkeiten in bibliographischen Informations-Datenbanken und in Volltext-Datenbanken für alle Mitarbeiter des WIAS an:

- Die für die Mathematik wichtigsten Datenbanken „Zentralblatt MATH/Database“ und „MathSci“ (Mathematical Reviews),
- Zugangsmöglichkeiten zu natur- und ingenieurwissenschaftlichen Online-Datenbanken,
- Neben die bibliographischen Nachweis-Datenbanken treten zunehmend Volltext-Datenbanken im WWW, die mitunter (in ihren Anfangszeiten) noch frei zugänglich, meist aber lizenzpflichtig sind (Beispiel: Zeitschriftenartikel).

  Von der Fachinformation werden auf dem WIAS-Server in der Kollektion „Scientific-information“ (http://www.wias-berlin.de/main/services/scientific-information/index.html.de) u. a. Links zu den im WWW angebotenen elektronischen Versionen mathematischer Zeitschriften gesetzt (soweit diese für das WIAS relevant sind).
- Zusätzlich werden Offline-Recherchemöglichkeiten (kostenpflichtige CD-ROM-Datenbanken) an speziellen Recherche-PCs (u. a. in der Bibliothek) angeboten.

The Science Information (SI) offers the following facilities for data-recall from different bibliographic databases and from full-text databases

- Access to the mathematical databases “Zentralblatt MATH/Database” and “MathSci” (Mathematical Reviews);
- Online data-recall from databases for natural sciences and engineering;
- Licenced access to full-text databases on the Web for articles in scientific journals.

  The WIAS server provides links to electronic versions of mathematical journals relevant for the research at WIAS (see http://www.wias-berlin.de/main/services/scientific-information/index.html.en).
- Offline data-recall from CD-ROM databases on special PCs (e.g., in the library).

Die Nutzungsmöglichkeiten sind aufgabenorientiert variabel gestaltet, z. B. ist die

- institutsoffene Nutzung von „Zbl. MATH“ über das WWW und von „MathSciNet“ (Math. Rev. on the Web) für alle Rechnerplattformen realisiert, so dass von jedem Arbeitsplatz zugegriffen werden kann. Dagegen erfolgt die

The facilities for data retrieval are flexibly realized, depending on the respective tasks.

- The access to the data-recall facility within the databases “Zentralblatt MATH” and “MathSciNet” is possible from any workstation in WIAS.

- Durchführung von Recherchen in den nichtmathematischen Datenbanken zentral in der Fachinformation. Den Nutzungsschwerpunkt bildet die Datenbank INSPEC des IEE über den Host STN/FIZ Karlsruhe.

- The data-recall facility within other databases (e.g., INSPEC) requires a professional approach. Therefore, this service can be realized only via SI.

Außer dem Datenbank-Retrieval gab es die folgenden Aktivitäten der Fachinformation:

Further activities of the SI

- Auf dem WIAS-Server werden die im Institut erstellten Preprints, Reports und Technical Reports in den derzeit üblichen Formaten bereitgestellt: http://www.wias-berlin.de/main/publications/wias-publ/index.cgi.de. Ihre Abstracts (bibliographische Beschreibung plus Summary) werden metasprachlich mit dem Dublin Core indiziert. Damit wird erreicht, dass diese Web-Dokumente des WIAS weltweit recherchierbar sind, z. B. mit MPRESS (**M**ath. **Pre**print **S**earch **S**ystem).

- Supply of the WIAS Preprints, Reports, and Technical Reports Series on the WIAS server http://www.wias-berlin.de/main/publications/wias-publ/index.cgi.en. The abstracts of these publications are indexed metalinguistically by means of the Dublin Core. This way, these WIAS web documents can be retrieved worldwide, e.g., by MPRESS (**M**ath. **Pre**print **S**earch **S**ystem).

- Die Datenbanken von ISI/Thomsson Scientific *Science Citation Index* WoS (Web of Science), *Current Contents Connect* und *Journal Citation Reports* sind jetzt im WIAS institutsweit nutzbar.

- ISI/Thomsson Scientific's data bases *Science Citation Index* WoS (Web of Science), *Current Contents Connect*, and *Journal Citation Reports* can now be used from all workplaces at WIAS.

- Das WIAS ist Mitglied des Math-Net und dort mit einer standardisierten „Secondary Homepage" präsent: http://www.wias-berlin.de/math-net/index.html.de.

- WIAS is a member of Math-Net and is represented there by a standardized "Secondary Homepage": http://www.wias-berlin.de/math-net/index.html.en.

5.3 Rechentechnik / Computer Department

Die Gruppe Rechentechnik besteht aus fünf Mitarbeitern. Zwei Mitarbeiter sind für die technische Betreuung der Rechner und deren Verkabelung sowie für die Betreuung der Windows-Software zuständig. Außerdem betreuen sie die Klima- und Belüftungstechnik, die Multimediatechnik, die Telefonanlage des Instituts und betreuen und organisieren die von externen Firmen durchgeführten Installationsarbeiten. Zwei Mitarbeiter kümmern sich um die Softwarebetreuung der Unix/Linux-Rechner sowie um das Management des gesamten Rechnersystems einschließlich der Ankopplung des hausinternen Netzes an das Weitverkehrsnetz. Ein Mitarbeiter unterstützt Anwendergruppen bei der Anwendung der installierten Software (z. B. Bibliotheksrecherche und mathematische Spezialsoftware) und betreut die Internet-Informationsdienste.

Folgende Projekte bestimmten die Entwicklung der Rechentechnik des WIAS im Jahr 2004:

1. LAN

Die Erweiterung des LAN wurde abgeschlossen. Dadurch sind die Anschlussmöglichkeiten in den Arbeitszimmern wesentlich verbessert worden. Das Backbone wurde fast vollständig auf Gigabit-Ethernet umgestellt. Dazu wurden zentrale Switches Marconi ESR-6000 und ESR-5000 installiert und in Betrieb genommen.

2. Fileserver

Der im Vorjahr installierte Fileserver hat sich voll bewährt. Seine Kapazität wurde auf ca. 6 TByte erweitert.

The Computer Department consists of five collaborators. Two of them are in charge of the computers and their cabling as well as of the Windows software support. They also look after the air-conditioning, the ventilating system, the multimedia systems, and the telephone system of the institute and organize and supervise installation work done by external firms. Two collaborators are in charge of the software support for the Unix/Linux computers and of the management of the entire computer system including the coupling of the WIAS internal network to the wide area network. One collaborator gives support to groups of users in the application of the existing software (e.g., data-recall facilities and specialized mathematical software). He is also in charge of the internet information services.

The following projects have determined the development of the Computer Department in the year 2004:

1. LAN

The extension of the LAN was finished. The number of connectors for computers in the offices was essentially increased. We changed the backbone to Gigabit Ethernet. Marconi ESR-5000 and ESR-6000 Enterprise Switch Routers were installed and put in operation.

2. File server

The file server installed in 2003 has proved its worth. Its capacity has been increased to about 6 TByte.

3. Blade-Server

Die Intelbasis wurde durch den Einsatz eines Blade-Servers von HP um 15 Xeon-basierte Systeme erweitert. Diese werden sowohl als Managementrechner als auch als Anwendungsrechner im Windows- und Linux-Umfeld eingesetzt. Als Managementsoftware wird Altiris für die Verwaltung und Pflege der Systemsoftware genutzt.

4. Windows

Es wurde ein Windows-Cluster als ADS-Server sowie als Fileserver im Windowsbereich installiert und in Betrieb genommen. Außerdem wurde eine Citrix-Farm in Betrieb genommen, die auch den Unix/Linux-Nutzern ermöglicht, Windows-Software an ihrem Arbeitsplatz zu nutzen.

5. Unix/Linux

Es wurde begonnen, an den Arbeitsplätzen Linux-basierte Workstations einzusetzen.

6. Vortragsraum

Der Vortragsraum wurde mit einer modernen schwerhörigengerechten Audioanlage ausgestattet. Außerdem wurden die Möglichkeiten für Multimediapräsentationen erweitert.

3. Blade server

The server environment based on Intel processors has been expanded by 15 computers contained in a HP Blade Server System. These computers are used as management systems as well as as application servers based on Windows or Linux. Altiris is used as management software for the deployment and support of system software.

4. Windows

A Windows cluster has been installed and used as ADS and Windows file server. Furthermore, a Citrix farm was installed and used as application server giving all Unix/Linux users the possibility to use Windows applications at their workplace.

5. Unix/Linux

We began to use Linux-based workstations as scientists' workplace computers.

6. Lecture room

A modern acoustic system was installed, which can be used by people with defective hearing. The possibilities for multimedia presentations were extended.

6 Publications, Scientific Life[1]

6.1 Publications

6.1.1 Monographs

G.N. MILSTEIN, M.V. TRETYAKOV, *Stochastic Numerics for Mathematical Physics*, vol. XX of Scientific Computation, Springer, Berlin/Heidelberg, 2004.

K.K. SABELFELD, ed., *Selection of Papers Presented at the IV IMACS Seminar on Monte Carlo Methods, Berlin, September, 15–19, 2003*, vol. 10 of Monte Carlo Methods Appl., VSP, Utrecht, Boston, 2004.

Monographs (to appear)

P. NEITTAANMÄKI, D. TIBA, J. SPREKELS, *Optimization of Elliptic Systems. Theory and Applications*, Springer.

I. MÜLLER, W. WEISS, *Entropy and Energy. A Universal Competition. Interaction of Mechanics and Mathematics*, Springer.

C. LAI, K. WILMANSKI, eds., *Surface Waves in Geomechanics: Direct and Inverse Modelling for Soils and Rocks*, CISM Courses and Lectures, Springer, Wien [u.a.].

6.1.2 Articles in Refereed Journals

E. BÄNSCH, *Uniaxial, extensional flows in liquid bridges*, J. Fluid Mech., 521 (2004), pp. 353–379.

E. BÄNSCH, P. AZERAD, *Quasi-stability of the primary flow in a cone and plate viscometer*, J. Math. Fluid Mech., 6 (2004), pp. 253–271.

A. BAMBERGER, E. BÄNSCH, K.G. SIEBERT, *Experimental and numerical investigation of edge tones*, ZAMM Z. Angew. Math. Mech., 84 (2004), pp. 632–646.

E. BÄNSCH, F. HAUSSER, O. LAKKIS, B. LI, A. VOIGT, *Finite element method for epitaxial growth with attachment-detachment kinetics*, J. Comput. Phys., 194 (2004), pp. 409–434.

E. BÄNSCH, P. MORIN, R.H. NOCHETTO, *Surface diffusion of graphs: Variational formulation, error analysis, and simulation*, SIAM J. Numer. Anal., 42 (2004), pp. 733–799.

E. BÄNSCH, P. MORIN, R.H. NOCHETTO, *Finite element method for surface diffusion. Free boundary problems*, Internat. Ser. Numer. Math., 147 (2004), pp. 53–63.

E. BÄNSCH, D. DAVIS, H. LANGMACH, W. MILLER, U. REHSE, G. REINHARD, M. UHLE, *Axisymmetric and 3D calculations of melt flow during VCz growth*, J. Crystal Growth, 266 (2004), pp. 60–66.

[1] In the sequel the collaborators of WIAS are underlined.

M. BARO, H.-CHR. KAISER, H. NEIDHARDT, J. REHBERG, *Dissipative Schrödinger-Poisson systems,* J. Math. Phys., 45 (2004), pp. 21–43.

——, *A quantum transmitting Schrödinger-Poisson system*, Rev. Math. Phys., 16 (2004), pp. 281–330.

C. BENDER, R.J. ELLIOTT, *Arbitrage in a discrete version of the Wick-fractional Black-Scholes market,* Math. Oper. Res., 29 (2004), pp. 935–945.

M. BIRKNER, *A condition for weak disorder for directed polymers in random environment*, Electron. Comm. Probab., 9 (2004), pp. 22–25.

E. BAAKE, M. BAAKE, A. BOVIER, M. KLEIN, *An asymptotic maximum principle for essentially linear evolution models,* J. Math. Biol., DOI: 10.1007/s00285-004-0281-7 (2004).

A. BOVIER, M. ECKHOFF, V. GAYRARD, M. KLEIN, *Metastability in reversible diffusion processes I. Sharp asymptotics for capacities and exit times,* J. Eur. Math. Soc. (JEMS), 6 (2004), pp. 399–424.

A. BOVIER, I. KURKOVA, *Derrida's generalized random energy models. 1. Models with finitely many hierarchies*, Ann. Inst. H. Poincare Probab. Statist., 40 (2004), pp. 439–480.

——, *Derrida's generalized random energy models. 2. Models with continuous hierarchies*, Ann. Inst. H. Poincare Probab. Statist., 40 (2004), pp. 481–495.

A. BOVIER, I. MEROLA, E. PRESUTTI, M. ZAHRADNÍK, *On the Gibbs phase rule in the Pirogov–Sinai regime,* J. Statist. Phys., 114 (2004), pp. 1235–1267.

J. ČERNÝ, *Critical path analysis for continuum percolation,* Ann. Inst. H. Poincaré Probab. Statist., 40 (2004), pp. 661–675.

W. DREYER, S. QAMAR, *Kinetic flux-vector splitting schemes for the hyperbolic heat conduction,* J. Comput. Phys., 198 (2004), pp. 403–423.

W. DREYER, M. HERRMANN, M. KUNIK, *Kinetic solutions of the Boltzmann–Peierls equation and its moment systems*, Contin. Mech. Thermodyn., 16 (2004), pp. 453–469.

J. ELSCHNER, M. YAMAMOTO, *Uniqueness results for an inverse periodic transmission problem*, Inverse Problems, 20 (2004), pp. 1841–1852.

V. MAZ'YA, J. ELSCHNER, J. REHBERG, G. SCHMIDT, *Solutions for quasilinear nonsmooth evolution systems in L^p*, Arch. Ration. Mech. Anal., 171 (2004), pp. 219–262.

K. FLEISCHMANN, A.M. ETHERIDGE, *Compact interface property for symbiotic branching,* Stochastic Process. Appl., 114 (2004), pp. 127–160.

K. FLEISCHMANN, C. MUELLER, *Super-Brownian motion with extra birth at one point*, SIAM J. Math. Anal., 36 (2004), pp. 740–772.

K. FLEISCHMANN, A. STURM, *A super-stable motion with infinite mean branching*, Ann. Inst. H. Poincare Probab. Statist., 40 (2004), pp. 513–537.

K. FLEISCHMANN, J. SWART, *Trimmed trees and embedded particle systems*, Ann. Probab., 32 (2004), pp. 2179–2221.

M. EFENDIEV, J. FUHRMANN, S. ZELIK, *The long-time behaviour of the thermoconvective flow in a porous medium*, Math. Methods Appl. Sci., 27 (2004), pp. 907–930.

H. GAJEWSKI, I.V. SKRYPNIK, *On unique solvability of nonlocal drift-diffusion-type problems*, Nonlinear Anal., 56 (2004), pp. 803–830.

——, *To the uniqueness problem for nonlinear parabolic equations*, Discrete Contin. Dyn. Syst., 10 (2004), pp. 315–336.

O. SCHENK, K. GÄRTNER, *Solving unsymmetric sparse systems of linear equations with PARDISO*, Future Generation Computer Systems, 20 (2004), pp. 475–487.

N. BERGLUND, B. GENTZ, *On the noise-induced passage through an unstable periodic orbit I: Two-level model*, J. Statist. Phys., 114 (2004), pp. 1577–1618.

A. GLITZKY, *Electro-reaction-diffusion systems with nonlocal constraints*, Math. Nachr., 277 (2004), pp. 14–46.

A. GLITZKY, W. MERZ, *Single dopant diffusion in semiconductor technology*, Math. Methods Appl. Sci., 27 (2004), pp. 133–154.

A. GLITZKY, R. HÜNLICH, *Stationary solutions of two-dimensional heterogeneous energy models with multiple species*, Banach Center Publ., 66 (2004), pp. 135–151.

J. GRIEPENTROG, *On the unique solvability of a nonlocal phase separation problem for multicomponent systems*, Banach Center Publ., 66 (2004), pp. 153–164.

R. HENRION, W. RÖMISCH, *Hölder and Lipschitz stability of solution sets in programs with probabilistic constraints*, Math. Program., 100 (2004), pp. 589–611.

P. BOSCH, A. JOURANI, R. HENRION, *Sufficient conditions for error bounds and applications*, Appl. Math. Optim., 50 (2004), pp. 161–181.

D. HÖMBERG, *A mathematical model for induction hardening including mechanical effects*, Nonlinear Anal. Real World Appl., 5 (2004), pp. 55–90.

A. HUTT, *Effects of nonlocal feedback on traveling fronts in neural fields subject to transmission delay*, Phys. Rev. E (3), 70 (2004), pp. 052902–1–052902–4.

O. KLEIN, *Asymptotic behaviour for a phase-field model with hysteresis in one-dimensional thermo-visco-plasticity*, Appl. Math., 49 (2004), pp. 309–341.

O. KLEIN, P. PHILIP, J. SPREKELS, *Modeling and simulation of sublimation growth of SiC bulk single crystals*, Interfaces Free Bound., 6 (2004), pp. 295–314.

A. KOLODKO, J.G.M. SCHOENMAKERS, *Upper bounds for Bermudan style derivatives*, Monte Carlo Methods Appl., 10 (2004), pp. 331–343.

D. KOLYUKHIN, K.K. SABELFELD, *Stochastic Eulerian model for the flow simulation in porous media. Unconfined aquifers*, Monte Carlo Methods Appl., 10 (2004), pp. 345–357.

P. KREJČÍ, M. BROKATE, H. SCHNABEL, *On uniqueness in evolution quasivariational inequalities*, J. Convex Anal., 11 (2004), pp. 111–130.

P. KREJČÍ, K. KUHNEN, *Identification of linear error-models with projected dynamical systems*, Math. Comput. Model. Dyn. Syst., 10 (2004), pp. 59–91.

P. KREJČÍ, J. SPREKELS, *Nonlocal phase-field models for non-isothermal phase transitions and hysteresis*, Adv. Math. Sci. Appl., 14 (2004), pp. 593–612.

P. MATHÉ, *Numerical integration using V-uniformly ergodic Markov chains*, J. Appl. Probab., 41 (2004), pp. 1104–1112.

——, *Saturation of regularization methods for linear ill-posed problems in Hilbert spaces*, SIAM J. Numer. Anal., 42 (2004), pp. 968–973.

P. MATHÉ, G. WEI, *Quasi-Monte Carlo integration over* $\mathbb{R}^d$, Math. Comp., 73 (2004), pp. 827–841.

T. ICHINOSE, H. NEIDHARDT, V.A. ZAGREBNOV, *Trotter–Kato product formula and fractional powers of self-adjoint generators*, J. Funct. Anal., 207 (2004), pp. 33–57.

J. POLZEHL, S. ZWANZIG, *On a symmetrized simulation extrapolation estimator in linear errors-in-variables models*, Comput. Statist. Data Anal., 47 (2004), pp. 675–688.

D.I. RACHINSKII, *On a bifurcation of stable large-amplitude cycles for equations with hysteresis*, Autom. Remote Control, 65 (2004), pp. 1915–1937.

A.M. KRASNOSEL'SKII, D.I. RACHINSKII, *Remark on the Hopf bifurcation theorem*, Math. Nachr., 272 (2004), pp. 95–103.

——, *Solution branching at infinity for equations with degeneration of multiplicity two*, Dokl. Math., 69 (2004), pp. 79–83.

A.M. KRASNOSEL'SKII, A.V. POKROVSKII, D.I. RACHINSKII, *On guaranteed estimates of convergence rate for one class of iteration procedures*, Autom. Remote Control, 65 (2004), pp. 1635–1640.

S. BAUER, J. KREISSL, M. RADZIUNAS, H.-J. WÜNSCHE, F. HENNEBERGER, J. SIEBER, M. SARTORIUS, O. BROX, *Nonlinear dynamics of semiconductor lasers with active optical feedback*, Phys. Rev. E (3), 69 (2004), pp. 016206–1–016206–10.

N. NEFEDOV, M. RADZIUNAS, K.R. SCHNEIDER, *Analytic-numerical investigation of delayed exchange of stabilities in singularly perturbed parabolic problems*, Comput. Math. Math. Phys., 44 (2004), pp. 1213–1220.

J. SIEBER, M. RADZIUNAS, K.R. SCHNEIDER, *Dynamics of multisection semiconductor lasers*, Math. Model. Anal., 9 (2004), pp. 51–66.

M. REISS, *Estimating the delay time in affine stochastic delay differential equations*, Internat. J. Wavelets, Multiresolution and Information Processing, 2 (2004), pp. 525–544.

A. COHEN, M. HOFFMANN, M. REISS, *Adaptive wavelet Galerkin methods for linear inverse problems*, SIAM J. Numer. Anal., 42 (2004), pp. 1479–1501.

E. GOBET, M. HOFFMANN, M. REISS, *Nonparametric estimation for scalar diffusions based on low-frequency data*, Ann. Statist., 32 (2004), pp. 2223–2253.

H. HAAF, O. REISS, J.G.M. SCHOENMAKERS, *Numerically stable computation of CreditRisk+*, J. Risk, 6 (2004), pp. 1–10.

G.N. MILSTEIN, O. REISS, J.G.M. SCHOENMAKERS, *A new Monte Carlo method for American options*, Int. J. Theor. Appl. Finance, 7 (2004), pp. 591–614.

K.K. SABELFELD, I. SHALIMOVA, A. LEVYKIN, *Discrete random walk on large spherical grids generated by spherical means for PDEs*, Monte Carlo Methods Appl., 10 (2004), pp. 559–574.

A.A. ONISCHUK, V.V. KARASEV, O.G. GLOTOV, A.M. BAKLANOV, A.G. MARYASOV, V.E. ZARKO, A.I. LEVYKIN, K.K. SABELFELD, *Formation of charged aggregates of Al_20_3 nanoparticles by combustion of aluminum droplets in air*, Combustion and Flames, 138 (2004), pp. 40–54.

T. VESALA, U. RANNIK, M. LECLERC, T. FOKEN, K.K. SABELFELD, *Flux and concentration footprints*, Agricultural and Forest Meteorology, 127 (2004), pp. 111–116.

G. HEBERMEHL, J. SCHEFTER, R. SCHLUNDT, TH. TISCHLER, H. ZSCHEILE, W. HEINRICH, *Simulation of microwave circuits and laser structures including PML by means of FIT*, Advances in Radio Sciences, Kleinheubacher Berichte 2003, 2 (2004), pp. 107–112.

F. LANZARA, V. MAZ'YA, G. SCHMIDT, *Numerical solution of the Lippmann–Schwinger equation by approximate approximations*, J. Fourier Anal. Appl., 6 (2004), pp. 645–660.

J. SIEBER, L. RECKE, K.R. SCHNEIDER, *Dynamics of multisection semiconductor lasers*, J. Math. Sci. (N. Y.), 124 (2004), pp. 5298–5309. Translated from Sovremennaya Matematika. Fundamental'nye Napravleniya (Contemporary Mathematics. Fundamental Directions), Vol. 2, Differential and Functional Differential Equations. Part 2, 2003.

K.R. SCHNEIDER, S. YANCHUK, L. RECKE, *Dynamics of two mutually coupled semiconductor lasers: Instantaneous coupling limit*, Phys. Rev. E (3), 69 (2004), pp. 056221–1–056221–12.

D. SPIVAKOVSKAYA, A.W. HEEMINK, J.G.M. SCHOENMAKERS, G.N. MILSTEIN, *Stochastic modeling of transport in coastal waters using forward and reverse time diffusion*, Computational Methods in Water Resources, (2004), pp. 1813–1824.

G.N. MILSTEIN, J.G.M. SCHOENMAKERS, V. SPOKOINY, *Transition density estimation for stochastic differential equations via forward-reverse representations*, Bernoulli, 10 (2004), pp. 281–312.

A. GOLDENSHLUGER, V. SPOKOINY, *On the shape-from-moments problem and recovering edges from noisy Radon data*, Probab. Theory Related Fields, 128 (2004), pp. 123–140.

V. SPOKOINY, D. MERCURIO, *Statistical inference for time-inhomogeneous volatility models*, Ann. Statist., 32 (2004), pp. 577–602.

D. TIBA, C. ZALINESCU, *On the necessity of some constraint qualification conditions in convex programming*, J. Convex Anal., 11 (2004), pp. 95–110.

V. TRONCIU, *Investigation of self-pulsation and excitability of tandem blue lasers*, AIUB Journal of Science and Engineering AJSF, 3 (2004), pp. 7–10.

S.V. GONCHENKO, D.V. TURAEV, L.P. SHILNIKOV, *Infinitely many elliptic periodic orbits in four-dimensional symplectic diffeomorphisms with a homoclinic tangency*, Proc. Steklov Inst. Math., 244 (2004), pp. 106–131.

A.G. VLADIMIROV, D.V. TURAEV, G. KOZYREFF, *Delay differential equations for mode-locked semiconductor lasers*, Opt. Lett., 29 (2004), pp. 1221–1223.

R. VODÁK, *Behaviour of weak solutions of compressible Navier-Stokes equations for isothermal fluids with a nonlinear stress sensor*, J. Evol. Equ., 4 (2004), pp. 213–247.

——, *On a decay rate for a Landau–Ginzburg system with viscosity for martensitic phase transitions in shape memory alloys*, Adv. Math. Sci. Appl., 14 (2004), pp. 295–305.

C. LECOT, W. WAGNER, *A quasi-Monte Carlo scheme for Smoluchowski's coagulation equation*, Math. Comp., 73 (2004), pp. 1953–1966.

K. WILMANSKI, *On microstructural tests for poroelastic materials and corresponding Gassman-type relations*, Géotechnique, 54 (2004), pp. 593–603.

B. FIEDLER, C. ROCHA, M. WOLFRUM, *Heteroclinic orbits between rotating waves of semilinear parabolic equations on the circle*, J. Differential Equations, 201 (2004), pp. 99–138.

S. YANCHUK, A. STEFANSKI, J. WOJEWODA, T. KAPITANIAK, *Simple estimation of synchronization threshold in ensembles of diffusively coupled chaotic systems*, Phys. Rev. E (3), 70 (2004), pp. 026217–1–026217–11.

Articles in Refereed Journals (to appear)

A. MÜNCH, *Dewetting rates of thin liquid films*, J. Phys.: Condensed Matter.

B. ALBERS, K. WILMANSKI, *On modeling acoustic waves in saturated poroelastic media*, J. Engrg. Mech.

M. BARO, N.B. ABDALLAH, P. DEGOND, A.E. AYYADI, *A 1D coupled Schrödinger drift-diffusion model including collisions*, J. Comput. Phys.

M. BARO, H. NEIDHARDT, J. REHBERG, *Current coupling of drift-diffusion models and dissipative Schrödinger–Poisson systems: Dissipative hybrid models*, SIAM J. Math. Anal.

D. BELOMESTNY, *Reconstruction of the general distribution from the distribution of some statistics*, Theory Probab. Appl.

C. BENDER, *Explicit solution of a class of linear fractional BSDEs*, Systems Control Lett.

M. BIRKNER, J.L. MIMBELA, A. WAKOLBINGER, *Comparison results and steady states for the Fujita equation with fractional Laplacian*, Ann. Inst. H. Poincare Anal. Non Lineaire.

A. BOVIER, V. GAYRARD, M. KLEIN, *Metastability in reversible diffusion processes II. Precise asymptotics for small eigenvalues*, J. Eur. Math. Soc. (JEMS).

J. ČERNÝ, G. BEN AROUS, *Bouchaud's model exhibits two different aging regimes in dimension one*, Ann. Appl. Probab.

G. BEN AROUS, J. ČERNÝ, T. MOUNTFORD, *Aging in two-dimensional Bouchaud's model*, Probab. Theory Related Fields.

A. DEMIRCAN, U. BANDELOW, *Supercontinuum generation by the modulation instability*, Optics Communications.

W. DREYER, S. QAMAR, *Second order accurate explicit finite volume schemes for the solution of Boltzmann–Peierls equation*, ZAMM Z. Angew. Math. Mech.

W. DREYER, F. DUDERSTADT, S. EICHLER, M. JURISCH, *Stress analysis and bending tests for GaAs wafer*, Microelectronic Reliability.

W. DREYER, B. WAGNER, *Sharp-interface model for eutectic alloys. Part I: Concentration dependent surface tension*, Interfaces Free Bound.

J. ELSCHNER, M. YAMAMOTO, *Uniqueness in determining polygonal sound-hard obstacles*, Appl. Anal.

G. BRUCKNER, J. ELSCHNER, *The numerical solution of an inverse periodic transmission problem*, Math. Methods Appl. Sci.

K. EPPLER, H. HARBRECHT, *2nd order shape optimization using wavelet BEM*, Optim. Methods Softw.

——, *Exterior electromagnetic shaping using wavelet BEM*, Math. Methods Appl. Sci.

——, *Fast wavelet BEM for 3D electromagnetic shaping*, Math. Methods Appl. Sci.

——, *A regularized Newton method in electrical impedance tomography using shape Hessian information*, Control Cybernet.

D. DAWSON, K. FLEISCHMANN, J. XIONG, *Uniqueness for cyclically symbiotic branching diffusions*, Statist. Probab. Lett.

K. FLEISCHMANN, V. VATUTIN, *Multi-scale clustering for a non-Markovian spatial branching process*, J. Theoret. Probab.

H. GAJEWSKI, K. GÄRTNER, *On a nonlocal model of image segmentation*, Z. Angew. Math. Phys.

H. GAJEWSKI, J. GRIEPENTROG, *A descent method for the free energy of multicomponent systems*, Discrete Contin. Dyn. Syst.

J. GEISER, *Discretisation methods with analytical solutions for a convection-diffusion-dispersion-reaction equation and applications in 2D and 3D for waste-scenarios*, Numer. Methods Partial Differential Equations.

A. GLITZKY, R. HÜNLICH, *Global existence result for pair diffusion models*, SIAM J. Math. Anal.

R. HENRION, J. OUTRATA, *Calmness of constraint systems with applications*, Math. Program.

A. HUTT, *Stability and bifurcations in neural fields with axonal delay and general connectivity*, SIAM J. Appl. Math.

F. ATAY, A. HUTT, *Stability and bifurcations in neural fields with finite propagation speed and general connectivity*, SIAM J. Appl. Math.

H.-CHR. KAISER, H. NEIDHARDT, J. REHBERG, *Classical solutions of quasilinear parabolic systems on two dimensional domains*, NoDEA Nonlinear Differential Equations Appl.

D. KOLYUKHIN, K.K. SABELFELD, *Direct numerical solution of the Darcy equation with random hydraulic conductivity*, Math. Comput. Simulation.

R. KRAHL, E. BÄNSCH, *Numerical investigation of the non-isothermal contact angle*, Microgravity – Science and Technology.

H.-J. MUCHA, H.-G. BARTEL, J. DOLATA, *Techniques of rearrangements in binary trees (dendrograms) and applications*, MATCH Commun. Math. Comput. Chem.

S. ALBEVERIO, J.F. BRASCHE, M.M. MALAMUD, H. NEIDHARDT, *Inverse spectral theory for symmetric operators with several gaps: Scalar-type Weyl functions*, J. Funct. Anal.

P. PHILIP, O. KLEIN, *Transient conductive-radiative heat transfer: Discrete existence and uniqueness for a finite volume scheme*, Math. Models Methods Appl. Sci.

M. BROKATE, D.I. RACHINSKII, *Global stability of Armstrong–Frederick models with periodic uniaxial inputs*, NoDEA Nonlinear Differential Equations Appl.

——, *On global stability of the scalar Claboche models*, Nonlinear Anal. Real World Appl.

A.M. KRASNOSEL'SKII, D.I. RACHINSKII, *On a number of unbounded solution branches near the asymptotic bifurcation point*, Funct. Anal. Appl.

D.I. RACHINSKII, K.R. SCHNEIDER, *Dynamic Hopf bifurcations generated by nonlinear terms*, J. Differential Equations.

N. NEFEDOV, M. RADZIUNAS, K.R. SCHNEIDER, A. VASIL'EVA, *Change of the type of contrast structures in parabolic Neumann problems*, Comput. Math. Math. Phys.

M. REISS, *Adaptive estimation for affine stochastic delay differential equations*, Bernoulli.

A. DALALYAN, M. REISS, *Asymptotic statistical equivalence for ergodic diffusions*, Probab. Theory Related Fields.

S. DUBCOV, E. DULCEV, A. LEVYKIN, A. ANKILOV, K.K. SABELFELD, *A study of kinetics of aerosol formation in the photolysis of volfram hexacarbonil under low pressure conditions*, J. Chem. Phys.

P. KRAMER, O. KURBANMURADOV, K.K. SABELFELD, *Extensions of multiscale Gaussian random field simulation algorithms*, J. Comput. Phys.

K.R. SCHNEIDER, L. KALACHEV, *Global behavior and asymptotic reduction of a chemical kinetics system with continua of equilibria*, J. Math. Chem.

K.R. SCHNEIDER, B. LANI-WAYDA, *Delayed loss of stability in nonautonomous differential equations with retarded argument*, SIAM J. Math. Anal.

J.G.M. SCHOENMAKERS, E. VAN DEN BERG, A.W. HEEMINK, H.X. LIN, *Probability density estimation in stochastic environmental models using reverse representations*.

A. SAMAROV, V. SPOKOINY, C. VIAL, *Component identification and estimation in nonlinear high-dimensional regression models by structural adaptation*, J. Amer. Statist. Assoc.

V. ARNĂUTU, J. SPREKELS, D. TIBA, *Optimization problems for curved mechanical structures*, SIAM J. Control Optim.

H. STEPHAN, *Probleme pentu clasa a VIII-a (Challenges for year eight – in Romanian)*, Recreatii Matematice, Anul VI.

D. TIBA, R. VODÁK, *A general asymptotic model for Lipschitzian curved rods*, Adv. Math. Sci. Appl.

A.G. VLADIMIROV, D.V. TURAEV, *A new model for a mode-locked semiconductor laser*, Quantum Electronics and Radiophysics.

B.A. WAGNER, *The modified porous medium equation: Self-similar solutions and the dipole problem*, J. Engrg. Math.

A. BARBERO, V. PALUMBERI, B.A. WAGNER, R. SADER, M. GROTE, I. MARTIN, *Experimental and mathematical study of the influence of growth factors and the kinetics of adult human articular chondrocytes*, J. Cellular Physiology.

A. MÜNCH, B.A. WAGNER, *Contact-line instability for dewetting thin films*, Phys. D.

K. WILMANSKI, *Critical time for acoustic waves in weakly nonlinear poroelastic materials*, Contin. Mech. Thermodyn.

——, *Tortuosity and objective relative accelerations in the theory of porous materials*, Proc. R. Soc. Lond. Ser. A Math. Phys. Eng. Sci.

M. WOLFRUM, J. HÄRTERICH, *Describing a class of global attractors via symbol sequences*, Discrete Contin. Dyn. Syst.

S. YANCHUK, *Properties of stationary states of delay equations with large delay and applications to laser dynamics*, Math. Methods Appl. Sci.

6.1.3 Contributions to Collected Editions

E. BÄNSCH, P. MORIN, R.H. NOCHETTO, *Finite element methods for surface diffusion*, in: Free Boundary Problems. Theory and Applications. Proceedings of the International Conference, Trento, Italy, June 5–8, 2002, P. Colli, C. Verdi, A. Visintin, eds., vol. 147 of Internat. Ser. Numer. Math., Birkhäuser, Basel [u.a.], 2004, pp. 53–63.

A. BOVIER, *Metastability and ageing in stochastic dynamics*, in: Dynamics and Randomness II, Proceedings of the II. Workshop on dynamics and randomness, Santiago de Chile, Chile, December 9–13, 2002, A. Maas, S. Martinez, J.S. Martin, eds., vol. 10 of Nonlinear Phenomena and Complex Systems, Kluwer Acad. Publishers, Dordrecht, 2004, pp. 17–80.

W. DREYER, F. DUDERSTADT, *On phase diagrams and diffusional problems in the presence of surface tension and multiaxial stresses*, in: Phasenübergänge, Workshop, June 20–26, 2004, vol. 30 of Oberwolfach Reports, Mathematisches Forschungsinstitut Oberwolfach, 2004, pp. 31–34.

——, *Towards the thermodynamic modeling of nucleation and growth of liquid droplets in single crystals*, in: Free Boundary Problems. Theory and Applications. Proceedings of the International Conference, Trento, Italy, June 5–8, 2002, P. Colli, C. Verdi, A. Visintin, eds., vol. 147 of Internat. Ser. Numer. Math., Birkhäuser, Basel [u.a.], 2004, pp. 113–130.

R. HENRION, *Perturbation analysis of chance-constrained programs under variation of all constraint data*, in: Dynamic Stochastic Optimization, IFIP Workshop on Dynamic Stochastic Optimization, Laxenburg, Austria, March 11–14, 2002, K. Marti, ed., vol. 532 of Lecture Notes in Economics and Mathematical Systems, Springer, Heidelberg, 2004, pp. 257–274.

D. HÖMBERG, S. VOLKWEIN, W. WEISS, *Optimal control strategies for the surface hardening of steel*, in: Proceedings of the 2nd International Conference on Thermal Process Modelling and Computer Simulation, Nancy, France, March 31 – April 2, 2003, S. Denis, P. Archambault, J.-M. Bergheau, R. Fortunier, eds., vol. 120 of J. Physique IV, EDP Sciences, 2004, pp. 325–335.

O. KLEIN, P. KREJČÍ, *Asymptotic behaviour of evolution equations involving outwards pointing hysteresis operators*, in: Proceedings of the Fourth International Symposium on Hysteresis and Micromagnetic Modeling, Salamanca, Spain, 28–30 May 2003, L. Lopez-Dias, L. Torres, O. Alejos, eds., vol. 343 of Physica B: Condensed Matter, Elsevier B.V., 2004, pp. 53–58.

R. KRAHL, M. ADAMOV, M.L. AVILÉS, E. BÄNSCH, *A model for two phase flow with evaporation*, in: Two-Phase Flow Modelling and Experimentation 2004, Proceedings of the Second International Symposium on Two-Phase Flow Modelling and Experimentation, Pisa, Italy, 22-25 September, 2004, G.P. Celata, P.D. Marco, A. Mariani, R.K. Shah, eds., Edizioni ETS, Pisa, 2004, pp. IV–2381–IV–2388.

H.J. MUCHA, *Automatic validation of hierarchical clustering*, in: COMPSTAT 2004 — Proceedings in Computational Statistics, 16th Symposium Held in Prague, Czech Republic, 2004, J. Antoch, ed., Physica, Heidelberg, 2004, pp. 1535–1542.

H.J. MUCHA, H.G. BARTEL, *ClusCorr98 — Adaptive clustering, multivariate visualization, and validation of results*, in: Innovations in Classification, Data Science, and Information Systems, D. Baier, K.D. Wernecke, eds., Springer, Berlin, 2004, pp. 46–53.

H.J. MUCHA, H.G. BARTEL, B. PAZ, M. FIELDER, C. HÖPKEN, S. PÀNCZÈL, *Mathematisch-statistische Untersuchungen zur Provenienz römischer Gläser aus Dakien (Apulum, Porolissum)*, in: Archäometrie und Denkmalpflege — Kurzberichte 2004, U. Schüssler, E. Pernicka, eds., 2004, pp. 68–70.

J. DOLATA, H.J. MUCHA, H.G. BARTEL, *Eine Anwendung der hierarchischen Clusteranalyse: "Unbekannt1" als Provenienz einer bekannten obergermanischen Heeresziegelei?*, in: Archäometrie und Denkmalpflege — Kurzberichte 2004, U. Schüssler, E. Pernicka, eds., 2004, pp. 28–30.

B. PAZ, C. SWART, H.G. BARTEL, H.J. MUCHA, M. FIEDLER, C. HÖPKEN, *Analytische Untersuchung römischer Gläser aus Dakien mit der ICP*, in: Archäometrie und Denkmalpflege — Kurzberichte 2004, U. Schüssler, E. Pernicka, eds., 2004, pp. 65–67.

U. SIMON, H.J. MUCHA, R. BRÜGGEMANN, *Model-based cluster analysis applied to flow cytometry data*, in: Innovations in Classification, Data Science, and Information Systems, D. Baier, K.D. Wernecke, eds., Springer, Berlin, 2004, pp. 69–76.

C. SWART, B. PAZ, J. DOLATA, G. SCHNEIDER, J. SIMON, H.G. BARTEL, H.J. MUCHA, *Analyse römischer Ziegel mit ICP-MS/-OES: Methodenvergleich zwischen RFA und ICP*, in: Archäometrie und Denkmalpflege — Kurzberichte 2004, U. Schüssler, E. Pernicka, eds., 2004, pp. 25–27.

N. KORNEYEV, M. RADZIUNAS, H.-J. WÜNSCHE, F. HENNEBERGER, *Mutually injecting semiconductor lasers: Simulations for short and zero delay*, in: Proceedings of SPIE: Semiconductor Lasers and Laser Dynamics Conference "Photonics Europe", Strasbourg, France, April 26–30, 2004, vol. 5452, SPIE, Washington, 2004, pp. 63–70.

O. REISS, *Dependent sectors and an extension to incorporate market risk*, in: CreditRisk+ in the Banking Industry, M. Gundlach, F. Lehrbaß, eds., vol. XII, Springer Finance, 2004, pp. 203–218.

——, *Fourier inversion techniques for CreditRisk+*, in: CreditRisk+ in the Banking Industry, M. Gundlach, F. Lehrbaß, eds., vol. XII, Springer Finance, 2004, pp. 107–124.

H. HAAF, O. REISS, J.G.M. SCHOENMAKERS, *Numerically stable computation of Credit Risk+*, in: CreditRisk+ in the Banking Industry, M. Gundlach, F. Lehrbass, eds., vol. XII, Springer, Berlin Heidelberg, 2004, pp. 67–76.

G. HEBERMEHL, F.-K. HÜBNER, R. SCHLUNDT, TH. TISCHLER, H. ZSCHEILE, W. HEINRICH, *Eigen mode computation of microwave and laser structures including PML*, in: Scientific Computing in Electrical Engineering, W.H.A. Schilders, S.H.M.J. Houben, E.J.W. ter Maten, eds., Mathematics in Industry, Springer, 2004, pp. 196–205.

D. SPIVAKOVSKAYA, A.W. HEEMINK, J.G.M. SCHOENMAKERS, G.N. MILSTEIN, *Stochastic modeling of transport in coastal waters using forward and reverse time diffusion*, in: Computational Methods in Water Resources, XVth International Conference on Computational Methods in Water Resources (CMWR XV), Chapel Hill, USA, June 13–17, 2004, C.T. Miller, M.W. Farthing, W.G. Gray, G.F. Pinder, eds., 2004, pp. 1813–1824.

H. SI, K. GÄRTNER, *An algorithm for three-dimensional constrained Delaunay tetrahedralizations*, in: Proceedings of the Forth International Conference on Engineering Computational Technology, B. Toppings, C.M. Soares, eds., Civil-Comp Press, Stirling, 2004, p. 16. ISBN 0-948749-97-0 CD-ROM.

J. SPREKELS, D. TIBA, *An approximation method for curved rods*, in: Nonlinear Partial Differential Equations and their Applications, N. Kenmochi, M. Otani, S. Zheng, eds., vol. 20 of Gakuto Intern. Ser. Math. Sci. Appl., Gakkotosho, Tokyo, 2004, pp. 305–314.

V. TRONCIU, R.A. ABRAM, M. YAMADA, *Dynamics of blue InGaN laser. Self pulsation and excitability*, in: The International Conference "40 years of TUM", Chisinau, Moldova, 2004, pp. 112–113.

W. WAGNER, *Stochastic models and Monte Carlo algorithms for Boltzmann type equations*, in: Monte Carlo and Quasi-Monte Carlo Methods 2002, H. Niederreiter, ed., Springer, New York, 2004, pp. 129–153.

K. WILMANSKI, *Objective relative accelerations in theories of porous materials*, in: Thermodynamische Materialtheorien, Workshop, December 12–18, 2004, vol. 55 of Oberwolfach Reports, Mathematisches Forschungsinstitut Oberwolfach, 2004, pp. 36–37.

S. YANCHUK, K.R. SCHNEIDER, L. RECKE, *Dynamics of two F2F coupled lasers: Instantaneous coupling limit*, in: Proceeding of SPIE: Semiconductor Lasers and Laser Dynamics Conference "Photonics Europe", Strasbourg, France, April 26–30, 2004, vol. 5452, SPIE, Washington, USA, 2004, pp. 51–62.

Contributions to Collected Editions (to appear)

B. ALBERS, *Modelling of surface waves in poroelastic saturated materials by means of a two component continuum*, in: Surface Waves in Geomechanics: Direct and Inverse Modelling for Soils and Rocks, C. Lai, K. Wilmanski, eds., CISM Courses and Lectures, Springer, Wien [u.a.].

——, *Numerical analysis of monochromatic surface waves in a poroelastic medium*, in: Trends in the Application of Mathematics to Mechanics. Proceedings of the XIVth International Symposium on Trends in Applications of Mathematics to Mechanics (STAMM'2004), Seeheim, Germany, 22–28 August 2004, K. Hutter, Y. Wang, eds., Shaker, Aachen.

U. BANDELOW, H. GAJEWSKI, R. HÜNLICH, *Fabry–Perot lasers: Thermodynamics-based modeling*, in: Optoelectronic Devices — Advanced Simulation and Analysis, J. Piprek, ed., Springer Series in Physics & Astronomy, Springer, New York.

K. EPPLER, H. HARBRECHT, *Second order Lagrange multiplier approximation for constrained shape optimization problems*, in: Control and Boundary Analysis, IFIP TC 7 Conference on System Modeling and Optimization, Sophia Antipolis, France, July 21–25, 2003, J. Zolésio, J. Cagnol, eds., Taylor & Francis.

J. GEISER, *WIAS-HiTNIHS: Software-tool for simulation in crystal growth for SiC single crystal: Application and methods*, in: Proceeding of the International Congress of Nanotechnology, San Francisco, USA, November 1–3, 2004.

M. ANTHONISSEN, D. HÖMBERG, W. WEISS, *Real-time control of surface hardening*, in: Proceedings of the 13-th European Conference on Mathematics for Industry (ECMI 2004), Eindhoven, The Netherlands, June 21–25, 2004.

A. KOLODKO, J.G.M. SCHOENMAKERS, *Iterative construction of the optimal Bermudan stopping time*, in: Proc. IASTED Financial Engineering and Applications.

H.J. MUCHA, *Automatic validation of hierarchical cluster analysis with application in dialectometry*, in: Proceedings of the 28th Annual Conference of GfKl, Springer.

H.J. MUCHA, H.G. BARTEL, *Model-based cluster analysis of Roman bricks and tiles from Worms and Rheinzabern*, in: Proceedings of the 28th Annual Conference of GfKl, Springer.

M. BROKATE, D.I. RACHINSKII, O. RASSKAZOV, A.V. POKROVSKII, *Differential equations with hysteresis in examples*, in: The Science of Hysteresis, I. Meyergoyz, G. Bertotti, eds., Elsevier Science, San Diego, USA.

M. RADZIUNAS, H.-J. WÜNSCHE, *Multisection lasers: Longitudinal modes and their dynamics*, in: Optoelectronic Devices — Advanced Simulation and Analysis, J. Piprek, ed., Springer Series in Physics & Astronomy, Springer, New York.

J. REHBERG, *Quasilinear parabolic equations in L^p*, in: Proceedings of the Workshop "Nonlinear Elliptic and Parabolic Problems: A Special Tribute to the Work of Herbert Amann", Zurich, Switzerland, June 28–30, 2004.

O. REISS, *CreditRisk+: Numerische Methoden, Risikobeiträge und Verallgemeinerungen*, in: Risikomaße und ihre Anwendungen, Report der Martin-Luther-Universität Halle, A. Hamel, ed.

D. TIBA, J. SPREKELS, *Optimal design of mechanical structures*, in: Proceedings, Conference "Control Theory of Partial Differential Equations", Georgetown University, May 30 – June 1, 2003, Lecture Notes in Pure and Applied Mathematics, Marcel Dekker.

I. MÜLLER, W. WEISS, *Entropy and energy — A universal competition*, in: Trends in Applications of Mathematics to Mechanics. Proceedings of the XIVth International Symposium on Trends in Applications of Mathematics to Mechanics (STAMM'2004), Seeheim, Germany, 22–28 August 2004, K. Hutter, Y. Wang, eds., Shaker, Aachen.

K. WILMANSKI, *Elastic modeling of surface waves in single and multicomponent systems*, in: Surface Waves in Geomechanics: Direct and Inverse Modelling for Soils and Rocks, C. Lai, K. Wilmanski, eds., CISM Courses and Lectures, Springer, Wien [u.a.].

——, *Linear sound waves in poroelastic materials: Simple mixtures vs. Biot's model*, in: Trends in Applications of Mathematics to Mechanics. Proceedings of the XIVth International Symposium on Trends in Applications of Mathematics to Mechanics (STAMM'2004), Seeheim, Germany, 22–28 August 2004, K. Hutter, Y. Wang, eds., Shaker, Aachen.

——, *Thermodynamics of simple two-component thermo-poroelastic media*, in: Trends and Applications of Mathematics to Mechanics, STAMM'2002, G. Romano, S. Rionero, eds., Springer, Berlin [u.a.].

6.2 Preprints, Reports

6.2.1 WIAS Preprints Series

Preprints 2004[2] [3]

M. BROKATE, A. POKROVSKII, D. RACHNINSKII, *Asymptotic stability of continual sets of periodic solutions to systems with hysteresis*, Preprint no. 902, WIAS, Berlin, 2004.

M. ERMAKOV, *Minimax and Bayes estimation in deconvolution problem*, Preprint no. 982, WIAS, Berlin, 2004.

——, *On moderate deviation probabilities of empirical bootstrap measure*, Preprint no. 983, WIAS, Berlin, 2004.

S.V. GONCHENKO, K.R. SCHNEIDER, D. TURAEV, *Quasiperiodic regimes in multisection semiconductor lasers*, Preprint no. 967, WIAS, Berlin, 2004.

S.V. GONCHENKO, L. SHILNIKOV, D. TURAEV, *Homoclinic tangencies of arbitrarily high orders in conservative and dissipative two-dimensional maps*, Preprint no. 968, WIAS, Berlin, 2004.

Y. INGSTER, I. SUSLINA, *On estimation and detection of smooth high-dimensional function*, Preprint no. 960, WIAS, Berlin, 2004.

T.G. KURTZ, J. XIONG, *A stochastic evolution equation arising from the fluctuation of a class of interacting particle systems*, Preprint no. 933, WIAS, Berlin, 2004.

Z. LI, H. WANG, J. XIONG, *Conditional excursion representation for a class of interacting superprocesses*, Preprint no. 935, WIAS, Berlin, 2004.

——, *Conditional log-Laplace functionals of immigration superprocesses with dependent spatial motion*, Preprint no. 900, WIAS, Berlin, 2004.

C. MEYER, P. PHILIP, F. TRÖLTZSCH, *Optimal control of a semilinear PDE with nonlocal radiation interface conditions*, Preprint no. 976, WIAS, Berlin, 2004.

A. MÜNCH, *Dewetting rates of thin liquid films*, Preprint no. 992, WIAS, Berlin, 2004.

A. MÜNCH, P.L. EVANS, *Marangoni-driven liquid films rising out af a meniscus onto a nearly horizontal substrate*, Preprint no. 941, WIAS, Berlin, 2004.

V. TRONCIU, M. YAMADA, R. ABRAM, T. KAWAKAMI, S. ITO, T. OHNO, M. TANEYA, *Self-pulsation and excitability of blue-violet InGaN lasers*, Preprint no. 940, WIAS, Berlin, 2004.

V. VATUTIN, J. XIONG, *Some limit theorems for a particle system of single point catalytic branching random walks*, Preprint no. 919, WIAS, Berlin, 2004.

[2] http://www.wias-berlin.de/publications/preprints/index-2004.html

[3] Preprints that have been written by guests during their stay at WIAS have been listed in front of those written by the collaborators of WIAS.

J. XIONG, *Long-term behavior for superprocesses over a stochastic flow*, Preprint no. 906, WIAS, Berlin, 2004.

J. XIONG, Z. YANG, *Optimal investment strategy under saving/borrowing rates spread with partial information*, Preprint no. 908, WIAS, Berlin, 2004.

B. ALBERS, *Modelling of surface waves in poroelastic saturated materials by means of a two component continuum – Lecture notes*, Preprint no. 952, WIAS, Berlin, 2004.

——, *Numerical analysis of monochromatic surface waves in a poroelastic medium*, Preprint no. 949, WIAS, Berlin, 2004.

U. BANDELOW, H. GAJEWSKI, R. HÜNLICH, *Thermodynamics-based modeling edge-emitting quantum well lasers*, Preprint no. 971, WIAS, Berlin, 2004.

E. BÄNSCH, P. MORIN, R.H. NOCHETTO, *A finite element method for surface diffusion: The parametric case*, Preprint no. 910, WIAS, Berlin, 2004.

M. BARO, N.B. ABDALLAH, P. DEGOND, A.E. AYYADI, *A 1D coupled Schrödinger drift-diffusion model including collisions*, Preprint no. 923, WIAS, Berlin, 2004.

M. BARO, H. NEIDHARDT, J. REHBERG, *Current coupling of drift-diffusion models and dissipative Schrödinger–Poisson systems: Dissipative hybrid models*, Preprint no. 946, WIAS, Berlin, 2004.

D. BELOMESTNY, G.N. MILSTEIN, *Monte Carlo evaluation of American options using consumption processes*, Preprint no. 930, WIAS, Berlin, 2004.

D. BELOMESTNY, V. SPOKOINY, *Local likelihood modelling via stagewise aggregation*, Preprint no. 1000, WIAS, Berlin, 2004.

C. BENDER, M. KOHLMANN, *Optimal superhedging under nonconvex constraints – A BSDE approach*, Preprint no. 928, WIAS, Berlin, 2004.

C. BENDER, J. SCHOENMAKERS, *An iterative algorithm for multiple stopping: Convergence and stability*, Preprint no. 991, WIAS, Berlin, 2004.

M. BIRKNER, J. BLATH, M. CAPALDO, A. ETHERIDGE, M. MÖHLE, J. SCHWEINSBERG, A. WAKOLBINGER, *Alpha-stable branching and beta-coalescents*, Preprint no. 979, WIAS, Berlin, 2004.

A. BOVIER, F. DEN HOLLANDER, F.R. NARDI, *Sharp asymptotics for Kawasaki dynamics on a finite box with open boundary*, Preprint no. 920, WIAS, Berlin, 2004.

A. BOVIER, I. KURKOVA, *Much ado about Derrida's GREM*, Preprint no. 981, WIAS, Berlin, 2004.

——, *Poisson convergence in the restricted k-partioning problems*, Preprint no. 964, WIAS, Berlin, 2004.

A. BOVIER, J. CERNY, O. HRYNIV, *The opinion game: Stock price evolution from microscopic market modelling*, Preprint no. 903, WIAS, Berlin, 2004.

A. BOVIER, A. FAGGIONATO, *Spectral characterisation of ageing: The REM-like trap model*, Preprint no. 927, WIAS, Berlin, 2004.

J. CERNY, *The behaviour of aging functions in one-dimensional Bouchaud's trap model*, Preprint no. 961, WIAS, Berlin, 2004.

D. DAVIS, F. SMITH, *Flow solution properties in full-zone thermocapillary liquid bridges*, Preprint no. 936, WIAS, Berlin, 2004.

W. DREYER, F. DUDERSTADT, *On the Becker/Döring theory of nucleation of liquid droplets in solids*, Preprint no. 997, WIAS, Berlin, 2004.

——, *On the modelling of semi-insulating GaAs including surface tension and bulk stresses*, Preprint no. 995, WIAS, Berlin, 2004.

W. DREYER, F. DUDERSTADT, S. QAMAR, *Diffusion in the vicinity of an evolving spherical arsenic droplet*, Preprint no. 996, WIAS, Berlin, 2004.

J. ELSCHNER, M. YAMAMOTO, *Uniqueness results for an inverse periodic transmission problem*, Preprint no. 932, WIAS, Berlin, 2004.

K. EPPLER, H. HARBRECHT, *Efficient treatments of stationary free boundary problems*, Preprint no. 965, WIAS, Berlin, 2004.

——, *A regularized Newton method in electrical impedance tomography using shape Hessian information*, Preprint no. 943, WIAS, Berlin, 2004.

——, *Shape optimization for 3D electrical impedance tomography*, Preprint no. 963, WIAS, Berlin, 2004.

A. FAGGIONATO, H. SCHULZ-BALDES, D. SPEHNER, *Mott law as lower bound for a random walk in a random environment*, Preprint no. 955, WIAS, Berlin, 2004.

K. FLEISCHMANN, J. XIONG, *Large deviation principle for the single point catalytic super-Brownian motion*, Preprint no. 937, WIAS, Berlin, 2004.

K. FLEISCHMANN, V. VAKHTEL, *Large scale localization of a spatial version of Neveu's branching process*, Preprint no. 951, WIAS, Berlin, 2004.

R. EYMARD, J. FUHRMANN, K. GÄRTNER, *A finite volume scheme for nonlinear parabolic equations derived from one-dimensional local Dirichlet problems*, Preprint no. 966, WIAS, Berlin, 2004.

H. GAJEWSKI, I.V. SKRYPNIK, *Existence and uniqueness results for reaction-diffusion processes of electrically charged species*, Preprint no. 938, WIAS, Berlin, 2004.

H. GAJEWSKI, J. GRIEPENTROG, *A descent method for the free energy of multicomponent systems*, Preprint no. 980, WIAS, Berlin, 2004.

N. BERGLUND, B. GENTZ, *Universality of residence-time distributions in non-adiabatic stochastic resonance*, Preprint no. 957, WIAS, Berlin, 2004.

J. GRIEPENTROG, *On the unique solvability of a nonlocal phase separation problem for multicomponent systems*, Preprint no. 898, WIAS, Berlin, 2004.

J. BUKSZAR, R. HENRION, M. HUJTER, T. SZANTAI, *Polyhedral inclusion-exclusion*, Preprint no. 913, WIAS, Berlin, 2004.

R. HENRION, J. OUTRATA, *Calmness of constraint systems with applications*, Preprint no. 929, WIAS, Berlin, 2004.

D. HÖMBERG, A. KHLUDNEV, *A thermoelastic contact problem with a phase transition*, Preprint no. 914, WIAS, Berlin, 2004.

A. HUTT, *Effects of nonlocal feedback on traveling fronts in neural fields subject to transmission delay*, Preprint no. 953, WIAS, Berlin, 2004.

A. HUTT, F.M. ATAY, *Analysis of nonlocal neural fields for both general and gamma-distributed connectivities*, Preprint no. 969, WIAS, Berlin, 2004.

A. HUTT, M. SCHRAUF, *Detection of transient generalized and mutual phase synchronization by clustering and application by single brain signals*, Preprint no. 925, WIAS, Berlin, 2004.

A. KOLODKO, J. SCHOENMAKERS, *Iterative construction of the optimal Bermudan stopping time*, Preprint no. 926, WIAS, Berlin, 2004.

D. KOLYUKHIN, K.K. SABELFELD, *Stochastic Eulerian model for the flow simulation in porous media. Unconfined aquifers*, Preprint no. 912, WIAS, Berlin, 2004.

R. KRAHL, E. BÄNSCH, *Computational comparison between the Taylor–Hood and the conforming Crouzeix–Raviart element*, Preprint no. 989, WIAS, Berlin, 2004.

——, *Numerical investigation of the non-isothermal contact angle*, Preprint no. 972, WIAS, Berlin, 2004.

R. KRAHL, M. ADAMOV, M.L. AVILES, E. BÄNSCH, *A model for two phase flow with evaporation*, Preprint no. 899, WIAS, Berlin, 2004.

P. KREJČÍ, J. SANTE-MARIE, M. SORINE, J.M. URQUIZA, *Solutions to muscle fiber equations and their long time behaviour*, Preprint no. 973, WIAS, Berlin, 2004.

P. COLLI, P. KREJČÍ, E. ROCCA, J. SPREKELS, *Nonlinear evolution inclusions arising from phase change models*, Preprint no. 974, WIAS, Berlin, 2004.

P. MATHÉ, *Degree of ill-posedness of statistical inverse problems*, Preprint no. 959, WIAS, Berlin, 2004.

D. MERCURIO, V. SPOKOINY, *Estimation of time dependent volatility via local change point analysis*, Preprint no. 904, WIAS, Berlin, 2004.

J. POLZEHL, S. ZWANZIG, *SIMEX and TLS: An equivalence result*, Preprint no. 999, WIAS, Berlin, 2004.

J. POLZEHL, V. SPOKOINY, *Spatially adaptive regression estimation: Propagation-separation approach*, Preprint no. 998, WIAS, Berlin, 2004.

——, *Varying coefficient GARCH versus local constant volatility modeling. Comparison of the predictive power*, Preprint no. 977, WIAS, Berlin, 2004.

J. POLZEHL, V. SPOKOINY, C. STARICA, *When did the 2001 recession really start?*, Preprint no. 934, WIAS, Berlin, 2004.

M. BROKATE, D. RACHINSKII, *Hopf bifurcations and simple structures of periodic solution sets in systems with the Preisach nonlinearity*, Preprint no. 921, WIAS, Berlin, 2004.

D. RACHINSKII, A. VLADIMIROV, *Q-switching instability in a mode-locked semiconductor laser*, Preprint no. 975, WIAS, Berlin, 2004.

M. RADZIUNAS, *Numerical bifurcation analysis of traveling wave model of multisection semiconductor lasers*, Preprint no. 985, WIAS, Berlin, 2004.

N.N. NEFEDOV, M. RADZIUNAS, K.R. SCHNEIDER, A.B. VASIL'EVA, *Change of the type of contrast structures in parabolic Neumann problems*, Preprint no. 984, WIAS, Berlin, 2004.

M. RADZIUNAS, H.J. WÜNSCHE, *Longitudinal modes of multisection semiconductor lasers and their dynamics*, Preprint no. 939, WIAS, Berlin, 2004.

M. REISS, *Nonparametric volatility estimation on the real line from low-frequency data*, Preprint no. 911, WIAS, Berlin, 2004.

D. BETHMANN, M. REISS, *A simple method to study the transitional dynamics in endogenous growth models*, Preprint no. 917, WIAS, Berlin, 2004.

A. DALALYAN, M. REISS, *Asymptotic statistical equivalence for ergodic diffusions*, Preprint no. 916, WIAS, Berlin, 2004.

M. HOFFMANN, M. REISS, *Nonlinear estimation for linear inverse problems with error in the operator*, Preprint no. 990, WIAS, Berlin, 2004.

K.K. SABELFELD, I. SHALIMOVA, A. LEVYKIN, *Discrete random walk on large spherical grids generated by spherical means for PDEs*, Preprint no. 970, WIAS, Berlin, 2004.

G. HEBERMEHL, J. SCHEFTER, R. SCHLUNDT, TH. TISCHLER, H. ZSCHEILE, W. HEINRICH, *Simulation of microwave and semiconductor laser structures including PML: Computation of the eigenmode problem, the boundary value problem, and the scattering matrix*, Preprint no. 987, WIAS, Berlin, 2004.

——, *Simulation of microwave circuits and laser structures including PML by means of FIT*, Preprint no. 905, WIAS, Berlin, 2004.

A. GRIN, K.R. SCHNEIDER, *On some classes of limit cycles of planar dynamical systems*, Preprint no. 931, WIAS, Berlin, 2004.

K.R. SCHNEIDER, E. SHCHETININA, V. SOBOLEV, *Integral manifolds for slow-fast differential systems loosing their attractivity in time*, Preprint no. 948, WIAS, Berlin, 2004.

E. SHCHETININA, *On existence of a bounded solution in a problem with a control parameter*, Preprint no. 918, WIAS, Berlin, 2004.

A. GOLDENSHLUGER, V. SPOKOINY, *Recovering edges of an image from noisy tomographic data*, Preprint no. 909, WIAS, Berlin, 2004.

V. ARNAUTU, J. SPREKELS, D. TIBA, *A reduction approximation method for curved rods*, Preprint no. 958, WIAS, Berlin, 2004.

H. STEPHAN, *A dimension-reduced description of general Brownian motion by non-autonomous diffusion-like equations*, Preprint no. 994, WIAS, Berlin, 2004.

——, *Lyapunov functions for positive linear evolution problems*, Preprint no. 978, WIAS, Berlin, 2004.

D. TIBA, R. VODÁK, *A general asymptotic model for Lipschitzian curved rods*, Preprint no. 942, WIAS, Berlin, 2004.

A. VLADIMIROV, D. TURAEV, *Passive mode-locking with slow saturable absorber: A delay differential model*, Preprint no. 947, WIAS, Berlin, 2004.

R. VODÁK, *Asymptotic analysis of elastic curved rods*, Preprint no. 986, WIAS, Berlin, 2004.

——, *A general asymptotic dynamic model for Lipschitzian curved rods*, Preprint no. 956, WIAS, Berlin, 2004.

A. BARBERO, V. PALUMBERI, B. WAGNER, R. SADER, M. GROTE, I. MARTIN, *Experimental and mathematical study of the influence of growth factors and the kinetics of adult human articular chondrocytes*, Preprint no. 988, WIAS, Berlin, 2004.

R. KONRAD, K. JACOBS, A. MÜNCH, B. WAGNER, T. WITELSKI, *New slip regimes and the shape of dewetting thin liquid films*, Preprint no. 993, WIAS, Berlin, 2004.

B. WAGNER, A. MÜNCH, *Galerkin approximation for Rayleigh–Benard convection*, Preprint no. 907, WIAS, Berlin, 2004.

A. MÜNCH, B. WAGNER, *Contact-line instability of dewetting thin films*, Preprint no. 924, WIAS, Berlin, 2004.

W. WAGNER, *Monte Carlo methods and numerical solutions*, Preprint no. 954, WIAS, Berlin, 2004.

O. MUSCATO, W. WAGNER, *Time step truncation in direct simulation Monte Carlo for semiconductors*, Preprint no. 915, WIAS, Berlin, 2004.

K. WILMANSKI, *Elastic modelling of surface waves in single and multicomponent systems – Lecture notes*, Preprint no. 945, WIAS, Berlin, 2004.

——, *Linear sound waves in poroelastic materials: Simple mixture vs. Biot's model*, Preprint no. 950, WIAS, Berlin, 2004.

——, *Thermodynamics of simple two-component thermo-poroelastic media*, Preprint no. 901, WIAS, Berlin, 2004.

——, *Tortuosity and objective relative acceleration in the theory of porous materials*, Preprint no. 922, WIAS, Berlin, 2004.

S. YANCHUK, *Properties of stationary states of delay equations with large delay and applications to laser dynamics*, Preprint no. 944, WIAS, Berlin, 2004.

S. YANCHUK, M. WOLFRUM, *Instabilities of stationary states in lasers with long-delay optical feedback*, Preprint no. 962, WIAS, Berlin, 2004.

6.2.2 Preprints/Reports in other Institutions

W. DREYER, M. HERRMANN, *A simplification of the stability problem for periodic traveling waves in the atomic chain*, Preprint no. 121, DFG Priority Program "Analysis, Modeling and Simulation of Multiscale Problems", Stuttgart, 2004.

W. DREYER, M. HERRMANN, A. MIELKE, *Micro-macro transition for the atomic chain via Whitham's modulation equation*, Preprint no. 119, DFG Priority Program "Analysis, Modeling and Simulation of Multiscale Problems", Stuttgart, 2004.

W. DREYER, B. WAGNER, *Sharp-interface model for eutectic alloys, Part I: Concentration dependent surface tension*, Preprint no. 120, DFG Priority Program "Analysis, Modeling and Simulation of Multiscale Problems", Stuttgart, 2004.

J. ELSCHNER, M. YAMAMOTO, *Uniqueness in determining polygonal sound-hard obstacles*, Preprint no. 6, University of Tokyo, Graduate School of Mathematical Sciences, 2004.

O. SCHENK, K. GÄRTNER, *On fast factorization pivoting methods for sparse symmetric indefinite systems*, Technical Report no. CS-2004-004, Universität Basel, 2004.

A. HUTT, T.D. FRANK, *Stability, critical fluctuations and* $1/f^{\alpha}$ *-activity of neural fields involving transmission delays*, Preprint no. 140, DFG Research Center MATHEON, Technische Universität Berlin, 2004.

A. ZISOWSKY, A. ARNOLD, M. EHRHARDT, TH. KOPRUCKI, *Discrete transparent boundary conditions for time-dependent systems of Schrödinger equations*, Preprint no. 155, DFG Priority Program "Analysis, Modeling and Simulation of Multiscale Problems", Stuttgart, 2004.

M. LICHTNER, M. RADZIUNAS, *Well posedness and smooth dependence for a semilinear hyperbolic system with nonsmooth data*, Preprint no. 174, DFG Research Center MATHEON, Technische Universität Berlin, Berlin, 2004.

W. WAGNER, *Explosion phenomena in stochastic coagulation-fragmentation models*, NI04006-IGS, Isaac Newton Institute for Mathematical Sciences, Cambridge, 2004.

6.3 Membership in Editorial Boards

E. BÄNSCH, Editor, Electronic FBP News (http://fbp.Imc.fc.pt/index.html).

A. BOVIER, Editorial Board, Markov Processes and Related Fields, Polymat, Moscow, Russia.

K. FLEISCHMANN, Editorial Board, Annals of Probability, Institute of Mathematical Statistics, Beachwood, Ohio, USA.

H. GAJEWSKI, Advisory Board, Mathematische Nachrichten, Wiley-VCH Verlag GmbH, Berlin.

——, Editorial Board, Teubner-Texte zur Mathematik, B.G. Teubner Verlagsgesellschaft mbH, Leipzig.

——, Editorial Board, Zeitschrift für Angewandte Mathematik und Mechanik (ZAMM), Wiley-VCH Verlag GmbH, Berlin.

R. HENRION, Editorial Board, Journal of Chemometrics, Wiley, New York, USA.

P. KREJČI, Editor, Applications of Mathematics, Czech Academy of Sciences, Prague, Czech Republic.

P. MATHÉ, Editorial Board, Monte Carlo Methods and Applications, VSP, Zeist, The Netherlands.

J. POLZEHL, Editorial Board, Computational Statistics, Physica Verlag, Heidelberg.

——, Editorial Board, Journal of Multivariate Analysis, Elsevier, Amsterdam, The Netherlands.

K.K. SABELFELD, Editor, Monte Carlo Methods and Applications, VSP, Zeist, The Netherlands.

——, Senior Editor, Mathematics and Computers in Simulation, Elsevier, Amsterdam.

V. SPOKOINY, Editorial Board, Statistics and Decisions, Oldenbourg Wissenschaftsverlag, München.

——, Editorial Board, Annals of Statistics, IMS, Beachwood, USA.

J. SPREKELS, Editorial Board, Applications of Mathematics, Academy of Science of the Czech Republic, Prague.

——, Editor, Advances in Mathematical Sciences and Applications, Gakkōtosho, Tokyo, Japan.

W. WAGNER, Editorial Board, Monte Carlo Methods and Applications, VSP, Zeist, The Netherlands.

6.4 Talks, Posters, and Contributions to Exhibitions

6.4.1 Scientific Talks

B. ALBERS, *Poröse Medien in Geotechnik und Bauwesen — Auftreten, Modellierung, Anwendungen*, Technische Universtät Graz, Institut für Allgemeine Mechanik, Austria, January 29.

——, *Surface waves on an impermeable boundary of a poroelastic medium*, XXI International Congress of Theoretical and Applied Mechanics (21st ICTAM 2004), August 15–21, Polish Academy of Sciences, Institute of Fundamental Technological Research, Warsaw, Poland, August 17.

——, *Porous and granular materials, transport of pollutants, surface waves in multi-component systems*, Marie-Curie Forum at the XXI International Congress of Theoretical and Applied Mechanics (21st ICTAM 2004), August 15–21, Polish Academy of Sciences, Institute of Fundamental Technological Research, Warsaw, Poland, August 19.

——, *Numerical analysis of monochromatic surface waves in a poroelastic medium*, 2004 Symposium on Trends in Applications of Mathematics to Mechanics (STAMM2004), August 22–28, Technische Universität Darmstadt, Institut für Mechanik, Seeheim-Jugenheim, August 26.

——, *Modeling of surface waves in poroelastic saturated materials by means of a two component continuum*, Advanced School "Surface Waves in Geomechanics. Direct and Inverse Modeling for Soils and Rocks", 4 talks, International Centre for Mechanical Sciences, Udine, Italy, September 6–10.

U. BANDELOW, *Modellierung und Simulation von Pulsquellen*, Status Seminar of the Terabit-Optics-Berlin Project, Technische Universität Berlin, May 3.

——, *Time-domain modeling of ps-OEIC*, Joint International Workshops OPTIMIST, EPIC and COST288, June 2–4, Athens, Greece, June 3.

——, *Modeling of 40 GHz mode-locked semiconductor lasers*, European Semiconductor Laser Workshop (ESLW'04), September 2–4, Chalmers University of Technology, Department of Microtechnology and Nanoscience, Särö, Sweden, September 4.

——, *40 GHz mode-locked semiconductor lasers: Theory, simulation and experiments*, Annual Meeting 2004 of the Optical Society of America (OSA) "Frontiers in Optics", October 10–14, Rochester, USA, October 11.

——, *Modellierung und Simulation von Pulsquellen*, Status Seminar of the Terabit-Optics-Berlin Project, Technische Universität Berlin, November 2.

U. BANDELOW, A. DEMIRCAN, M. KESTING, *Pulse propagation in nonlinear optical fibers*, Meeting within the Terabit-Optics-Berlin Project, Fraunhofer-Institut für Nachrichtentechnik, Heinrich-Hertz-Institut, Berlin, April 28.

U. BANDELOW, M. RADZIUNAS, *Time domain simulation of 40 GHz mode-locked semiconductor lasers*, WIAS Mini-Symposium on Mode-locked Semiconductor Lasers, March 22–23, Berlin, March 22.

E. BÄNSCH, *Finite element methods for curvature driven problems*, Technische Universität Chemnitz, Mathematisches Institut, January 7.

——, *Finite element methods for surface diffusion*, Mini-Workshop "Multiscale Modeling in Epitaxial Growth", January 18–24, Mathematisches Forschungsinstitut Oberwolfach, January 19.

——, *Uniaxial, extensional flows in liquid bridges*, 7th Drop Tower Days and Catapult Inauguration, September 12–15, Universität Bremen, Zentrum für angewandte Raumfahrttechnologie und Mikrogravitation (ZARM), September 14.

M. BARO, *Quantum-classical coupling including collisions*, Second Annual Meeting of the HYKE Network "Around Hyperbolic and Kinetic Equations 2" (A-HYKE-2), April 14–17, Ecole Normale Supérieure, Institut Henri Poincaré, Paris, France, April 16.

——, *Quantum and coupled quantum-classical models for semiconductor devices*, Colloquium of the Institute of Mathematics, Technische Universität Clausthal-Zellerfeld, May 12.

——, *On a coupled Schrödinger drift-diffusion model*, Fourth Workshop "Multiscale Problems in Quantum Mechanics and Averaging Techniques" (DFG Priority Program "Analysis, Modeling and Simulation of Multiscale Problems"), November 4–5, Technische Universität München, November 5.

D. BELOMESTNY, *Evaluation of American options for generalized Black–Scholes model using consumption processes*, DYNSTOCH Workshop 2004 "Statistical Methods for Dynamical Stochastic Models", June 3–5, University of Copenhagen, H.C. Ørsted Institute, Denmark, June 5.

——, *Local modelling via stagewise aggregation*, Workshop on Mathematical Statistics IV, December 13–17, Luminy, France, December 13.

C. BENDER, *Integration bezüglich einer fraktionalen Brown'schen Bewegung*, Oberseminar Stochastik, Martin-Luther-Universität Halle-Wittenberg, Institut für Optimierung und Stochastik, Halle, May 27.

——, *Arbitrage in a discrete version of the Wick-fractional Black–Scholes market*, 3rd World Congress of the Bachelier Finance Society, July 21–24, Chicago, USA, July 24.

——, *Superhedging under constraints — A BSDE approach*, Workshop on New Techniques in Applied Stochastics, August 16–18, Helsinki University of Technology, Finland, August 16.

——, *Eine stabile Methode zur Strategieverbesserung bei Bermuda-Optionen*, Universität Ulm, Abteilung für Stochastik, October 22.

——, *Mathematik in der Finanzökonomie*, Universität Konstanz, Fachbereich für Mathematik und Statistik, October 25.

M. BIRKNER, *Ein (größen)verzerrter Blick auf gerichtete Polymere, verzweigende Populationen und zufällige Umgebungen*, Friedrich-Alexander-Universität Erlangen-Nürnberg, Mathematisches Institut, February 5.

——, *Continuous-mass stable branching and its resampling counterpart*, BRG Workshop, February 23–24, EURANDOM, Eindhoven, The Netherlands, February 24.

——, *Critical binary branching random walks with state-dependent branching rate*, Winter School of the Graduate College "Stochastic Processes and Probabilistic Analysis", March 15–19, Mathematical Research and Conference Center, Bedlewo, Poland, March 17.

——, *Spatial critically branching particle systems with state-dependent branching rate*, Karlsruher Stochastik-Tage 2004, March 23–26, Universität Karlsruhe, March 23.

——, *Spatial critically branching particle systems with state-dependent branching rate*, Durham Symposium: Mathematical Genetics, July 5–15, London Mathematical Society, Durham, UK, July 8.

——, *Stochastic models for spatially extended populations*, Universität Bielefeld, Fakultät für Mathematik, July 22.

——, *Continuous-mass stable branching and its resampling counterpart*, BIRS Workshop "Stochastic Processes in Evolutionary and Disease Genetics", August 7–15, Banff International Research Station, Alberta, Canada, August 9.

A. BOVIER, *Metastability in stochastic dynamics*, University of Cambridge, Statistical Laboratory, Centre for Mathematical Sciences, UK, March 2.

——, *Metastability and ageing*, Centre des Etudes de Saclay, CES, Paris, France, March 9.

——, *Nucleation in local Kawasaki dynamics*, Workshop "Phasenübergänge", June 21–25, Mathematisches Forschungsinstitut Oberwolfach, June 25.

——, *Metastability and potential theory*, World Congress of the Bernoulli Society, July 26–30, University of Barcelona, Mathematical Institute, Barcelona, Spain, July 27.

——, *Order book dynamics and interacting particle systems*, Workshop on Volatility of Financial Markets: Theoretical Models, Forecasting, and Trading, October 18–29, University of Leiden, The Netherlands, October 25.

——, *Extremes and Gibbs states on Gaussian processes on the hypercube with hierarchical covariance structure*, Technion—Israel Institute of Technology, William Davidson Faculty of Industrial Engineering and Management, Haifa, Israel, December 28.

J. ČERNÝ, *Aging in Bouchaud's trap model on Z^d*, International Conference on Equilibrium and Dynamics of Spin Glasses, April 18–23, Centro Stefano Franscini, Monte Verità, Ascona, Switzerland, April 22.

——, *Stock price evolution from microscopic market modelling*, Tandem Workshop "Stochastik-Numerik", DFG Research Center MATHEON, Humboldt-Universität zu Berlin, Berlin, June 11.

——, *Stock price evolution from microscopic market modelling*, BRG Workshop "Stochastic processes from physics and biology", November 26–27, The Erwin Schrödinger International Institute for Mathematical Physics (ESI), Vienna, Austria, November 27.

W. DREYER, *Phase diagrams with surface tension and bulk stresses*, Freiberger Compound Materials GmbH, January 6.

——, *On the Grinfeld instability*, Workshop “Modelling of Phase Transitions and Interface Dynamics across the Length Scales”, January 28–30, Universität Karlsruhe, Fachbereich für Informatik, January 30.

——, *Phase diagrams with surface tension and bulk stresses*, GTT-Technologies, Herzogenrath, March 22.

——, *On phase diagrams and diffusional problems in the presence of surface tensions and multiaxial stresses*, Workshop “Phasenübergänge”, June 20–26, Mathematisches Forschungsinstitut Oberwolfach, June 24.

——, *The atomic chain with temperature. Part I: Hyperbolic scaling and thermodynamic limit*, 7th Hirschegg Workshop on Conservation Laws, August 29 – September 4, Hirschegg, August 30.

——, *On the Becker Döring system and related items in the presence of surface tension and multiaxial stresses*, INdAM Workshop “Dissipative Models in Phase Transitions”, September 5–11, Cortona, Italy, September 9.

F. DUDERSTADT, *Nichtstandard-Phasendiagramme elastisch verzerrter Festkörper mit flüssigen Ausscheidungen*, Working group meeting “Werkstoffverhalten bei hoher Temperatur”, Deutsche Gesellschaft für Materialkunde e.V., September 27–28, Universität Bayreuth, Fachbereich Metalle, September 28.

J. ELSCHNER, *Recent progress in inverse periodic diffraction problems*, Workshop “Mathematical Analyses and Numerical Methods for Applied Inverse Problems”, January 19–21, University of Tokyo, Japan, January 20.

——, *Direct and inverse problems for the periodic Helmholtz equation I*, University of Tokyo, Department of Mathematical Sciences, Japan, February 12.

——, *Direct and inverse problems for the periodic Helmholtz equation II*, University of Tokyo, Department of Mathematical Sciences, Japan, February 13.

——, *Inverse scattering for diffraction gratings*, European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2004), June 24–28, Jyväskylä, Finland, June 26.

——, *Inverse scattering of plane waves from periodic surfaces*, Chemnitzer Minisymposium 2004 zu Inversen Problemen, Universität Chemnitz, September 23.

G. ENCHÉRY, *Sedimentary basin simulations in oil exploration*, Project Meeting of DFG SPP 1135 on the topic of “Deep reaching fluid flow in the North-East German Basin”, WIAS, Berlin, October 29.

K. EPPLER, *Potential methods for elliptic shape optimization problems*, Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria, January 19.

——, *About two- and tridimensional exterior electromagnetic shaping of liquid metals*, IFIP Workshop “Boundary Control and Optimization”, February 26–28, Scuola Normale Superiore, Pisa, Italy, February 28.

——, *About two- and tridimensional exterior electromagnetic shaping of liquid metals*, European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2004), June 24–28, Jyväskylä, Finland, June 26.

——, *Free boundary computations by second order shape optimization methods*, IFIP Conference on Free and Moving Boundaries, Simulation and Control, December 2–4, Houston, USA, December 4.

V. ESSAOULOVA, *Adaptive wavelet thresholding by AWS*, Annual Meeting of DFG SPP 1114, September 21–23, Schloss Etelsen, Langwedel-Etelsen, September 22.

A. FAGGIONATO, *Mott law from random walk in random environment*, BRG Workshop, February 23–24, EURANDOM, Eindhoven, The Netherlands, February 24.

——, *Spectral characterization of aging: the REM-like trap model*, International Conference on Equilibrium and Dynamics of Spin Glasses, April 18–23, Centro Stefano Franscini, Monte Verità, Ascona, Switzerland, April 21.

——, *Spectral characterization of ageing: The REM-like trap model*, EURANDOM, Eindhoven, The Netherlands, June 8.

——, *Mott law as lower bound for a random walk in a random environment*, Workshop "Large Scale Stochastic Dynamics", August 30 – September 3, Mathematisches Forschungsinstitut Oberwolfach, September 1.

J. FUHRMANN, *A detailed numerical model for Direct Methanol Fuel Cells*, The 13-th European Conference on Mathematics for Industry (ECMI 2004), Mini-Symposium "Batteries and Fuel Cells", June 21–24, Eindhoven University of Technology, The Netherlands, June 22.

——, *A detailed numerical model for Direct Methanol Fuel Cells*, September 8, Laboratoire de Mathématiques, Université Paris Sud, Orsay, France, September 8.

——, *Thermal convection in the North-East German Basin*, Project Meeting of DFG SPP 1135 on the topic of "Deep reaching fluid flow in the North-East German Basin", WIAS, Berlin, October 29.

H. GAJEWSKI, *Über Diffusionsgleichungen mit nichtlokalem Driftterm*, Universität Stuttgart, Institut für Angewandte Analysis und Numerische Simulation, January 29.

——, *Über Diffusionsgleichungen mit nichtlokalem Driftterm*, Albert-Ludwigs-Universität Freiburg, Institut für Angewandte Mathematik, January 30.

——, *Zur Numerik des Ladungsträgertransports in Halbleiterbauelementen*, Technische Universität München, Institut für Technische Elektrophysik, February 5.

——, *Existence and uniqueness results for reaction-diffusion processes of electrically charged species*, Nonlinear Elliptic and Parabolic Problems: A Special Tribute to the Work of Herbert Amann, June 28–30, Universität Zürich, Institut für Mathematik, Switzerland, June 28.

K. GÄRTNER, *PARDISO: The current state and algorithmic goals for the future*, PARA'04 Workshop on State-of-the-Art in Scientific Computing, Mini-Symposium "Sparse direct linear solvers", June 20–2, Technical University of Denmark, Lyngby, Copenhagen, Denmark, June 22.

——, *Dissipative discretization schemes for drift-diffusion and phase separation models with applications*, International Workshop "Advances in Modeling and Simulation of Semiconductor Devices (AMaSiS'04)", July 14–16, WIAS, Berlin, July 15.

J. GEISER, *Discretization methods for parabolic equations based on finite volume and related methods and applications in fluid- and gas-mechanics*, Graduate College "Nichtlineare Differential-Gleichungen", Universität Freiburg, Institut für Angewandte Mathematik, October 28.

——, *WIAS-HiTNIHS: Software tool for simulation in crystal growth for SiC single crystal: Application and methods*, The International Congress of Nanotechnology and Nano World Expo, November 7–10, San Francisco, USA, November 8.

——, *Simulations in crystal growth for SiC single crystal: Numerical methods and applications*, Center for Applied Scientific Computing, Lawrence-Livermoore National Lab, Livermore, USA, November 11.

——, *Discretization and optimization methods for a parabolic equation and application on simulation in crystal growth*, Seminar "Parabolic Differential Equations", Technical University of Athens, Institute of Mathematics, Greece, November 30.

——, *Mixed discretization methods for convection-diffusion-reaction equations with analytical test functions*, SIAM Conference on Analysis of Partial Differential Equations (PD04), December 6–8, Houston, USA, December 7.

B. GENTZ, *Stochastic slow-fast systems*, International School "Does noise simplify or complicate the dynamics of nonlinear systems?", 5 talks, University of Turin, Italy, April 13–17.

——, *Universality of residence-time distributions in non-adiabatic stochastic resonance*, BRG Workshop "Stochastic processes from physics and biology", November 26–27, The Erwin Schrödinger International Institute for Mathematical Physics (ESI), Vienna, Austria, November 26.

J. GRIEPENTROG, *A decent method for the free energy of multicomponent systems*, Nonlinear Elliptic and Parabolic Problems: A Special Tribute to the Work of Herbert Amann, June 28–30, Universität Zürich, Institut für Mathematik, Switzerland, June 29.

R. HENRION, *Selected aspects of structure, stability and numerics in chance-constrained optimization problems*, Workshop on Optimization of Stochastic Systems, Stevens Institute of Technology, Hoboken, USA, April 30.

——, *Optimization problems with probabilistic constraints*, 10th International Conference on Stochastic Programming, October 8–15, University of Arizona, Tucson, USA, October 9.

——, *(Sub-)Differentiability and Lipschitz properties of singular normal distributions*, 10th International Conference on Stochastic Programming, October 8–15, University of Arizona, Tucson, USA, October 15.

——, *Sur des applications multivôques du type 'calme'*, Séminaire de l'Equipe ACSIOM (Analyse, Calcul Scientifique Industriel et Optimisation de Montpellier), Université Montpellier, France, November 16.

——, *Caractérisation de la propriété 'calme' pour des systèmes de contraintes*, Séminaire du Laboratoire d'Analyse non linéaire et Géométrie, Université d'Avignon, France, November 25.

——, *Some results on stability, structure and numerics in programs with probabilistic constraints*, Universität Zürich, Wirtschaftswissenschaftliche Fakultät, Switzerland, December 20.

R. HENRION, J. OUTRATA, *Calmness of constraint systems with applications*, French-German-Spanish Conference on Optimization, September 20–24, University of Avignon, France, September 21.

M. HERRMANN, *The atomic chain with temperature. Part II: The macroscopic system*, 7th Hirschegg Workshop on Conservation Laws, August 29 – September 4, Hirschegg, September 30.

D. HÖMBERG, *Widerstandsschweißen und Oberflächenhärtung von Stahl — Modellierung, Analysis und optimale Steuerung*, Colloquium of Sfb 393, Technische Universität Chemnitz, Institut für Mathematik, February 13.

——, *Thermoelastische Phasenübergänge in Stahl*, Humboldt-Universität zu Berlin, Institut für Mathematik, May 13.

——, *Simulation und Optimierung der Lasermaterialbearbeitung*, Seminar des Forschungsschwerpunktes Photonik, Technische Universität Berlin, Optisches Institut, June 18.

——, *Modelling, simulation and control issues in laser-induced thermotherapy*, 13-th European Conference on Mathematics for Industry (ECMI 2004), June 21–25, Eindhoven University of Technology, Eindhoven, The Netherlands, June 22.

——, *On a thermomechanical model of phase transitions in steel*, INdAM Workshop "Dissipative Models in Phase Transitions", September 5–11, Cortona, Italy, September 10.

——, *On a thermomechanical model of surface heat treatments*, University of Tokyo, Department of Mathematical Sciences, Japan, October 14.

——, *The induction hardening of steel — Modelling, analysis and optimal design of inductor coils*, University of Kyoto, Department of Mathematics, Japan, October 21.

——, *Modellierung, Analysis und optimale Steuerung der Lasermaterialbearbeitung*, Kolloquium der Angewandten Mathematik, Universität Münster, December 3.

A. HUTT, *Pattern formation in neural fields subject to propagation delay*, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, February 3.

——, *Detection of mutual phase synchronization in chaotic data and brain signals*, Spring Meeting of Deutsche Physikalische Gesellschaft (DPG), March 8–12, Regensburg, March 9.

——, *Pattern formation in neural fields subject to transmission delay*, April 22–24, Universidad Complutense de Madrid, Instituto Pluridisciplinar, Spain, April 23.

——, *Mutual phase synchronization in single data sets*, Max-Planck-Institut für Hirnforschung, Frankfurt am Main, July 21.

H.-CHR. KAISER, *Convexity of trace functionals and Schrödinger operators*, GAMM Annual Meeting 2004, March 21–27, Technische Universität Dresden, March 23.

——, *Convexity and differentiability of trace functionals*, Fourth Workshop "Multiscale Problems in Quantum Mechanics and Averaging Techniques" (DFG Priority Program "Analysis, Modeling and Simulation of Multiscale Problems"), November 4–5, Technische Universität München, November 5.

O. KLEIN, *Optimierung des Temperaturfeldes bei der Sublimationszüchtung von SiC Einkristallen*, DGKK Arbeitskreis Angewandte Simulation in der Kristallzüchtung, February 5–6, Deutsche Gesellschaft für Kristallwachstum und Kristallzüchtung e.V., Volkach, February 5.

——, *Long-time behaviour of solutions to equations involving outwards pointing hysteresis operators*, International Workshop on Hysteresis & Multi-Scale Asymptotics (HAMSA 2004), March 17–21, University College Cork, Ireland, March 19.

——, *Asymptotic behaviour for a phase-field model with hysteresis in thermo-visco-plasticity*, INdAM Workshop "Dissipative Models in Phase Transitions", September 5–11, Cortona, Italy, September 9.

TH. KOPRUCKI, *Electronic states in semiconductor nanostructures and upscaling to semiclassical models*, Fifth Colloquium of the DFG Priority Program "Analysis, Modeling and Simulation of Multiscale Problems", May 20–21, Physikzentrum, Bad Honnef, May 20.

R. KRAHL, *A model for two phase flow with evaporation*, Workshop on Evaporation, Universität Bremen, Zentrum für angewandte Raumfahrttechnologie und Mikrogravitation (ZARM), February 9.

——, *Reorientierung einer Flüssigkeitsoberfläche bei plötzlicher Reduzierung der Schwerkraft*, Workshop Graduiertenkolleg 827 "Transportvorgänge an bewegten Phasengrenzflächen", April 30 – May 1, Berlin-Schmöckwitz, May 1.

——, *Numerische Untersuchung der Reorientierung von Flüssigkeitsoberflächen bei plötzlicher Reduzierung der Schwerkraft*, Universität Bremen, Zentrum für angewandte Raumfahrttechnik und Mikrogravitation (ZARM), May 12.

——, *Numerical investigation of the conforming Crouzeix–Raviart element for Navier–Stokes equations*, Second European Finite Element Fair, June 4–5, Humboldt-Universität zu Berlin, June 5.

——, *Numerical investigation of the non-isothermal contact angle*, 7th Drop Tower Days and Catapult Inauguration, September 12–15, Universität Bremen, Zentrum für angewandte Raumfahrttechnologie und Mikrogravitation (ZARM), September 13.

——, *A model for two phase flow with evaporation*, 3rd International Symposium on Two-Phase Flow Modelling and Experimentation, September 22–25, Università di Pisa, Facolta di Ingegneria, Pisa, Italy, September 24.

P. KREJČÍ, *Thermodynamic consistency of easily invertible non-symmetric hysteresis models*, International Workshop on Hysteresis & Multi-Scale Asymptotics (HAMSA 2004), March 17–21, University College Cork, Ireland, March 20.

——, *Good news and bad news about evolution inclusions with non-invertible operators*, Workshop "Evolution Problems in memory of Brunello Terreni" (EP 2004), March 26–27, Rapallo, Italy, March 26.

——, *The mathematics of hysteresis — A partial survey of recent work*, 1st General Assembly of the European Geosciences Union (EGU 2004), April 25–30, European Geosciences Union, Nice, France, April 27.

——, *Inéquations quasivariationelles d'évolution et problème d'unicité*, Séminaires 2004 (SOSSO2), Institut National de Recherche en Informatique et Automatique (INRIA), Rocquencourt, France, June 24.

——, *Contrôle d'actuateurs hystérétiques en temps réel*, Séminaires 2004 (SOSSO2), Institut National de Recherche en Informatique et Automatique (INRIA), Rocquencourt, France, June 27.

——, *Representation and thermodynamic consistency of non-symmetric invertible hysteresis models*, 2004 Symposium on Trends in Applications of Mathematics to Mechanics (STAMM2004), August 22–28, Technische Universität Darmstadt, Institut für Mechanik, Seeheim-Jugenheim, August 24.

——, *Existence and non-existence of solutions to evolution inclusion with non-invertible operators*, INdAM Workshop "Dissipative Models in Phase Transitions", September 5–11, Cortona, Italy, September 6.

P. MATHÉ, *Statistically ill-posed problems under general source conditions*, MCM 2004 "Modern Computational Methods in Applied Mathematics", June 14–19, Mathematical Research and Conference Center Bedlewo, Poznan, Poland, June 15.

——, *Stratified sampling for risk management*, Dagstuhl Seminar on Algorithms and Complexity for Continuous Problems, September 26 – October 1, Conference and Research Center for Computer Science, Dagstuhl, October 1.

——, *Parameter choice principles under general source conditions*, Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria, November 17.

——, *Adaptive regularization of some inverse statistical problems*, Workshop on Mathematical Statistics IV, December 13–17, Luminy, France, December 14.

D. MERCURIO, *Estimation of time dependent volatility via local change point analysis*, DYNSTOCH Workshop 2004 "Statistical Methods for Dynamical Stochastic Models", June 3–5, University of Copenhagen, H.C. Ørsted Institute, Denmark, June 4.

H.J. MUCHA, *Automatic validation of hierarchical cluster analysis with application in dialectometry*, 28th Annual Meeting of Gesellschaft für Klassifikation (GfKl), March 9–11, Universität Dortmund, March 10.

——, *Model-based cluster analysis of Roman bricks and tiles from Worms and Rheinzabern*, 28th Annual Meeting of Gesellschaft für Klassifikation (GfKl), March 9–11, Universität Dortmund, March 11.

——, *Techniques of rearrangements in binary trees (dendrograms) and applications*, 6th HDT Workshop "Partial Order in Environmental Sciences and Chemistry", April 14–16, Universität Bayreuth, April 15.

——, *Automatische Validierung hierarchischer Clusteranalysen*, 3rd SPSS Academic Convention, June 16–17, Weimar, June 17.

——, *Automatic validation of hierarchical clustering*, COMPSTAT 2004, 16th Symposium of IASC, August 23–27, Prague, Czech Republic, August 26.

——, *Mathematisch-statistische Untersuchungen zur Provenienz römischer Gläser aus Dakien (Apulum, Porolissum)*, Annual Meeting Archäometrie und Denkmalpflege 2004, October 6–9, Curt-Engelhorn-Zentrum für Archäometrie, Mannheim, October 7.

H. NEIDHARDT, *Hybrid models for semiconductors and dissipative Schrödinger-Poisson systems*, Academy of Sciences of the Czech Republic, Nuclear Physics Institute, Prague, February 17.

——, *Hybrid models for semiconductors*, Workshop "Advances in Mathematical Semiconductor Modelling: Devices and Circuits", March 2–6, Chinese-German Centre for Science Promotion, Beijing, China, March 4.

——, *A model for resonant tunneling diodes*, Seminar in Statistical Physics & Condensed Matter, July 2, Centre de Physique Théorique, Marseille, France, June 2.

——, *Convexity of trace functionals and Schrödinger operators*, Johannes Gutenberg-Universität Mainz, Mathematisches Institut, September 12.

——, *Hybrid models for semiconductors*, QMath9, September 12–16, Giens, France, September 12.

——, *Zeno product formula*, 4th Workshop "Operator Theory in Krein Spaces and Applications", December 17–19, Technische Universität Berlin, December 19.

J. POLZEHL, *Structural adaptive smoothing methods*, Georg-August-Universität Göttingen, Institut für Mathematische Stochastik, January 14.

——, *Adaptive estimation for a varying coefficient GARCH model*, Karlsruher Stochastik-Tage 2004, March 23–26, Universität Karlsruhe, March 23.

——, *On a nonstationary structural adaptive approach to volatility estimation*, University of Gothenburg, Centre for Finance, Sweden, May 5.

——, *Smoothing by adaptive weights: An overview*, Chalmers University of Technology, Department of Mathematical Statistics, Gothenburg, Sweden, May 11.

——, *Structural adaptive smoothing methods and possible applications in imaging*, Charité Berlin, NeuroImaging Center, Berlin, July 1.

——, *Structural adaptive smoothing methods*, Tandem-Workshop on Non-linear Optimization at the Crossover of Discrete Geometry and Numerical Analysis, July 15–16, Technische Universität Berlin, Institut für Mathematik, July 15.

——, *Structural adaptive smoothing methods*, 6th World Congress of the Bernoulli Society and the Institute of Mathematical Statistics, July 26–31, Universitat de Barcelona, Institut de Matemàtica, Spain, July 27.

——, *Local likelihood modeling by structural adaptive smoothing*, University of Minnesota, School of Statistics, Minneapolis, USA, September 9.

——, *Structural adaptive smoothing methods for imaging problems*, Annual Conference of Deutsche Mathematiker-Vereinigung (DMV), September 13–17, Heidelberg, September 14.

——, *Structural adaptive smoothing methods for imaging problems*, German-Israeli Binational Workshop, October 20–22, Ollendorff Minerva Center for Vision and Image Sciences, Technion, Haifa, Israel, October 21.

——, *Spatially adaptive smoothing: A propagation-separation approach*, Workshop on New Inference Concepts for Analysing Complex Data, November 14–19, Mathematisches Forschungszentrum Oberwolfach, November 15.

D.I. RACHINSKII, *Bifurcations in systems with hysteresis*, 1st General Assembly of the European Geosciences Union (EGU 2004), April 26–30, European Geosciences Union, Nice, France, April 27.

——, *Fading memory of some models with ratchetting*, University College Cork, Department of Applied Mathematics, Ireland, September 20.

——, *Nonlocal results on Hopf bifurcations*, University College Cork, Department of Applied Mathematics, Ireland, October 7.

M. RADZIUNAS, *Simulation and analysis of 40 GHz monolithic mode-locked lasers*, Joint International Workshop OPTIMIST, EPIC and COST288, October 17–20, Università "La Sapienza", Rome, Italy, October 20.

——, *Forced locking in multimode semiconductor lasers*, WIAS Workshop "Synchronization and High-dimensional Chaos in Coupled Systems", November 15–16, Berlin, November 16.

A. RATHSFELD, *Simulation und Optimierung diffraktiver Strukturen für die Mikrooptik*, Seminar des Forschungsschwerpunktes Photonik, Technische Universität Berlin, Optisches Institut, October 22.

J. REHBERG, *The two-dimensional van Roosbroeck system has solutions in L^p*, Workshop "Advances in Mathematical Semiconductor Modelling: Devices and Circuits", March 2–6, Chinese-German Centre for Science Promotion, Beijing, China, March 5.

——, *Quasilinear parabolic equations in L^p*, Nonlinear Elliptic and Parabolic Problems: A Special Tribute to the Work of Herbert Amann, June 28–30, Universität Zürich, Institut für Mathematik, Switzerland, June 29.

——, *Elliptische und parabolische Probleme mit unglatten Daten*, Technische Universität Darmstadt, Fachbereich Mathematik, December 14.

M. REISS, *Asymptotic statistical equivalence for ergodic diffusions*, Université Paris VI "Pierre et Marie Curie", Laboratoire de Probabilités et Modèles Aléatoires, France, March 11.

——, *Asymptotic statistical equivalence for ergodic diffusions*, Karlsruher Stochastik-Tage 2004, March 23–26, Universität Karlsruhe, March 25.

——, *Nonparametric estimation for diffusion processes on the real line from low-frequency observations*, Université Paris VI "Pierre et Marie Curie", Institut Henri Poincaré, France, March 29.

——, *Stochastische Optimierung ökonomischer Modelle unter Zeitverzögerungseffekten*, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, April 23.

——, *Asymptotic equivalence in nonparametric statistics*, Uppsala University, Department of Mathematics, Sweden, June 2.

——, *Estimating the delay length in affine SDDEs*, DYNSTOCH Workshop 2004 "Statistical Methods for Dynamical Stochastic Models", June 3–5, University of Copenhagen, H.C. Ørsted Institute, Denmark, June 4.

——, *Nichtparametrische Schätzung der Lévy-Charakteristik aus Optionsdaten*, Universität Heidelberg, Institut für Mathematik, November 10.

——, *Statistik für Diffusionsprozesse*, 3 talks, Universität Heidelberg, Institut für Mathematik, November 11.

——, *Nonlinear estimation for inverse problems with error in the operator*, Workshop on New Inference Concepts for Analysing Complex Data, November 14–19, Mathematisches Forschungszentrum Oberwolfach, November 19.

——, *Statistik für Diffusionsprozesse*, 3 talks, Universität Heidelberg, Institut für Mathematik, November 25.

——, *An ill-posed problem arising in the calibration of Lévy models*, Workshop on Mathematical Statistics IV, December 13–17, Luminy, France, December 13.

K.K. SABELFELD, *New random walk method for solving boundary value problems with divergent Neumann series*, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, January 22.

——, *Random iterative procedures for integral equations*, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, January 23.

——, *Random iteration methods for boundary integral equations*, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, April 8.

——, *Discrete random walk on boundary for solving PDEs*, MC^{2}QMC 2004, June 7–10, Juan-les-Pins, France, June 8.

——, *Iterative Markov chain technique for solving a system of elliptic equations*, MC^{2}QMC 2004, June 7–10, Juan-les-Pins, France, June 8.

——, *Stochastic Eulerian model for the flow simulation in porous media. Unconfined aquifers*, MC^{2}QMC 2004, June 7–10, Juan-les-Pins, France, June 10.

——, *Eulerian–Lagrangian model of transport in a porous layer*, The International Conference on Computational Mathematics (ICCM 2004), June 21–25, Novosibirsk, Russia, June 22.

——, *A random walk on fixed spheres and ellipsoids for boundary value problems*, International Conference on Computational Mathematics, June 21–25, Novosibirsk, Russia, June 24.

——, *Simulation of oil prices using potential random fields*, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, August 12.

G. SCHMIDT, *Numerical solution of the Lippmann–Schwinger equation*, 5th International Conference on Functional Analysis and Approximation Theory (FAAT 2004), June 16–23, Acquafredda di Maratea, Italy, June 22.

——, *Electromagnetic scattering by crossed anisotropic gratings*, The University of Liverpool, Department of Mathematical Sciences, UK, September 22.

K.R. SCHNEIDER, *Invariante Mannigfaltigkeiten für zufällige dynamische Systeme mit schnellen und langsamen Variablen*, Workshop GAMM-Fachausschuss „Dynamik und Regelungstheorie“ und VDI/VDE-GMA-Ausschuss 1.40 „Theoretische Verfahren der Regelungstechnik“, Universität Kassel, Regelungstechnik und Systemdynamik, March 8.

——, *Systeme mit schnellen und langsamen Variablen unter zufälligen Einwirkungen*, Colloquium „Singularly Disturbed Systems and Complex Dynamics“, June 16, Moscow State University, Faculty of Physics, Russia, June 16.

——, *Invariant manifolds for random dynamical systems with two time scales*, Moscow State University, Faculty of Physics, Russia, September 16.

J.G.M. SCHOENMAKERS, *New Monte Carlo Methods for American and Bermudan style derivatives*, Delft University of Technology, Faculty of Information Technology and Systems Numerical Analysis Group, The Netherlands, January 30.

——, *Numerically stable computation of CreditRisk+*, Karlsruher Stochastik-Tage 2004, March 23–26, Universität Karlsruhe, March 25.

——, *Interactive construction of the optimal Bermudan stopping time*, Eidgenössische Technische Hochschule Zürich, Institut für Mathematik, Switzerland, May 6.

——, *Transition density estimation for stochastic differential equations via forward-reverse representations*, Tandem-Workshop Stochastik-Numerik, June 11, Humboldt-Universität zu Berlin, June 11.

——, *Iterative construction of the optimal Bermudan stopping time*, 2nd IASTED International Conference on Financial Engineering and Applications (FEA 2004), November 8–10, Cambridge, USA, November 8.

——, *Interest rate modelling — Practical calibration and implementation techniques*, Incisive Media Events, Hong Kong, China, December 8.

N. SCURTU, *Numerical aspects of instationary incompressible non-Newtonian fluid flow*, Brandenburgische Technische Universität Cottbus, Lehrstuhl Aerodynamik und Strömungslehre, May 26.

E. SHCHETININA, *Integral manifolds for slow-fast differential systems loosing their attractivity in time*, Seminar on Applied Analysis, April 20, Humboldt-Universität zu Berlin, April 20.

——, *Integral manifolds for slow-fast differential systems without dichotomy*, International Workshop on Nonlinear Modelling and Control, June 21–26, Nayanova University, Samara, Russia, June 24.

H. SI, *An algorithm for 3D constrained Delaunay triangulations*, The Fourth International Conference on Engineering Computational Technology, September 7–9, Instituto Superior Técnico, Universidade Técnica de Lisboa, Portugal, September 9.

V. SPOKOINY, *Varying coefficient GARCH modeling in financial engineering*, Workshop "Statistics in Finance", January 10–17, Mathematisches Forschungszentrum Oberwolfach, January 12.

——, *Local likelihood modeling by adaptive weights smoothing*, Tampere University of Technology, Institute of Mathematics, Finland, May 4.

——, *Local likelihood modeling by adaptive weights smoothing*, Eidgenössische Technische Hochschule Zürich, Forschungsinstitut für Mathematik, Switzerland, June 3.

——, *Pointwise adaptive estimation via local change point analysis with applications to Value-at-Risk*, Université Paris VI "Pierre et Marie Curie", Laboratoire de Probabilités et Modèles Aléatoires, France, June 7.

——, *Varying coefficient GARCH versus local constant modelling*, 24th International Symposium of Forecasting, July 4–6, Sydney, Australia, July 5.

——, *When did the 2001 recession really start and really end?*, Conference on Threshold Models and New Developments in Time Series, July 12–14, The University of Hong Kong, China, July 14.

——, *Local likelihood modeling by adaptive weights smoothing*, National University of Singapore, Department of Statistics and Applied Probability, July 15.

——, *Component identification and estimation in nonlinear high-dimensional regression model*, The 6th ICSA International Conference, July 21–23, National University of Singapore, Faculty of Science, July 21.

——, *Varying coefficient GARCH versus local constant modelling*, The 6th ICSA International Conference, July 21–23, National University of Singapore, Faculty of Science, July 23.

——, *Adaptive estimation using propagation-separation approach*, Workshop on Mathematical Statistics IV, December 13–17, Luminy, France, December 13.

J. SPREKELS, *Phasenfeld-Modelle und Hysteresis-Operatoren*, Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria, March 3.

——, *Modeling and analysis of curved mechanical structures*, Università di Pavia, Dipartimento di Matematica, Italy, September 2.

——, *On nonlocal phase-field models*, Seminar MOX, Politecnico di Milano, Dipartimento di Matematica, Italy, September 3.

——, *Mathematical modeling of Direct Methanol Fuel Cells*, BMBF/BMWA Workshop "New Links between Basic Research and Applied Energy R&D – The Computational Approach", November 8–9, WIAS, Berlin, November 8.

——, *On nonlocal phase-field models*, Workshop "Thermodynamische Materialtheorien", December 12–15, Mathematisches Forschungsinstitut Oberwolfach, December 14.

H. STEPHAN, *Parameter reduction for diffusion problems*, International Conference Crimean Autumn Mathematical School-Symposium (KROMSH-2004), Spectral and Evolution Problems, September 18–29, Laspi-Batiliman, Crimea, Ukraine, September 26.

D. TIBA, *New results in shape optimization*, Fourth European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2004), July 24–28, Jyväskylä, Finland, July 27.

——, *Shape optimization of curved mechanical structures*, The 13-th Conference on Mathematics for Industry (ECMI 2004), June 21–25, Eindhoven University of Technology, The Netherlands, June 24.

——, *Lectures on shape optimization with applications in mechanics*, series of lectures at the 14th Jyväskylä Summer School, University of Jyväskylä, Finland, July 29 – August 8.

——, *New results in optimal design*, 7ème Colloque Franco-Roumain de Mathématiques Appliquées, August 30 – September 3, Bucharest, Romania, August 31.

——, *Shape optimization problems*, 10 talks, Central China Normal University, The Center for Optimal Control and Discrete Mathematics, Wuhan, October 16 – November 17.

A.G. VLADIMIROV, *DDE-based modelling of passively mode-locked 40 GHz semiconductor lasers*, WIAS Mini-Symposium on Mode-locked Semiconductor Lasers, March 22–23, Berlin, March 22.

A.G. VLADIMIROV, D. TURAEV, G. KOZYREV, *Delay differential equations for a passively mode-locked laser*, EPS-QEOD Europhoton Conference on Solid State and Fiber Coherent Light Sources, August 29 – September 3, European Physical Society, Lausanne, Switzerland, August 31.

R. VODÁK, *A general asymptotic model for Lipschitzian curved rods*, 6th International Summer School on Evolution Equations (EVEQ 2004), July 12–16, Charles University, Faculty of Mathematics and Physics, Prague, Czech Republic, July 15.

——, *On a decay rate for 2-D viscous compressible Navier–Stokes equations*, Joint EMS Mathematical Weekend, September 3–5, Prague, Czech Republic, September 4.

B. WAGNER, *Sharp interface model for eutectic alloys*, University of Basel, Department of Mathematics, Switzerland, February 13.

W. WAGNER, *Stochastic models and Monte Carlo algorithms for the Boltzmann equation*, Kolloquium Fachbereich Mathematik, Universität Darmstadt, January 21.

——, *Modelling nanoparticle dynamics: Coagulation, sintering, particle inception and surface growth*, MC^{2}QMC 2004, June 7–10, Juan-les-Pins, France, June 7.

——, *Numerical simulation of coagulation dynamics using quasi-random numbers*, MC^{2}QMC 2004, June 7–10, Juan-les-Pins, France, June 7.

——, *Monte Carlo methods and numerical solutions*, 24th International Symposium on Rarefied Gas Dynamics, July 11–16, Bari, Italy, July 12.

——, *Stochastic numerics for the Boltzmann equation*, 6th International Workshop on Mathematical Aspects of Fluid and Plasma Dynamics, September 19–23, Kyoto University, Japan, September 19.

——, *Monte Carlo methods for nonlinear kinetic equations*, Keio University, Department of Mathematics, Yokohama, Japan, October 1.

——, *Monte Carlo methods for nonlinear kinetic equations*, Kyoto University, Department of Mathematics, Japan, October 8.

W. WEISS, *Simulation and optimization of the laser surface hardening of steel*, 13-th European Conference on Mathematics for Industry (ECMI 2004), June 21–25, Eindhoven University of Technology, The Netherlands, June 22.

——, *Simulation and optimization of laser surface hardening*, Meeting "Topics in Continuum Mechanics and Thermodynamics", September 26 – October 1, Schmalkalden, September 27.

K. WILMANSKI, *Large deformations of poroelastic materials — Thermodynamical modeling and applications*, Polish Academy of Sciences, Department of Mechanics of Materials and Biomechanics, Warsaw, March 8.

——, *Liquefaction of granular media — Experiment and model*, Polish Academy of Sciences, Department of Mechanics and Physics of Fluids, Warsaw, March 10.

——, *Micro-macro transitions in modeling of granular media*, Polish Academy of Sciences, Department of Theory of Continuous Media, Warsaw, March 12.

——, *Critical time for acoustic waves in weakly nonlinear poroelastic materials*, XXI International Congress of Theoretical and Applied Mechanics (21st ICTAM 2004), August 15–21, Polish Academy of Sciences, Institute of Fundamental Technological Research, Warsaw, Poland, August 17.

——, *Linear sound waves in poroelastic materials: Simple mixtures vs. Biot's model*, 2004 Symposium on Trends in Applications of Mathematics to Mechanics (STAMM2004), August 22–28, Technische Universität Darmstadt, Institut für Mechanik, Seeheim-Jugenheim, August 26.

——, *Elastic modeling of surface waves in single and multicomponent systems*, Advanced School "Surface Waves in Geomechanics. Direct and Inverse Modeling for Soils and Rocks", 6 talks, International Centre for Mechanical Sciences, Udine, Italy, September 6–10.

——, *Threshold of liquefaction due to weakly nonlinear acoustic waves in a poroelastic medium*, Meeting "Topics in Continuum Mechanics and Thermodynamics", September 26 – October 1, Schmalkalden, September 28.

——, *Objective relative accelerations in theories of porous media*, Workshop "Thermodynamische Materialtheorien", December 12–15, Mathematisches Forschungsinstitut Oberwolfach, December 14.

K. WILMANSKI, H. ZORSKI, *On the mathematical structure of phenomenological thermodynamics*, 2004 Symposium on Trends in Applications of Mathematics to Mechanics (STAMM2004), August 22–28, Technische Universität Darmstadt, Institut für Mechanik, Seeheim-Jugenheim, August 24.

S. YANCHUK, *Dynamics of two F2F coupled lasers: Instantaneous coupling limit*, SPIE Photonics Europe 2004 Conference "Semiconductor Lasers and Laser Dynamics", April 27–30, Strasbourg, France, April 28.

——, *Singularly perturbed delay-differential equations. What do they have in common with ODEs and maps?*, Seminar "Nonlinear Oscillations", National Academy of Sciences of Ukraine, Institute of Mathematics, Kiev, July 12.

——, *Intermittent synchronization in a system of coupled lasers*, WIAS Workshop "Synchronization and High-dimensional Chaos in Coupled Systems", November 15–16, Berlin, November 15.

——, *Pattern formation in systems with large delay*, Seminar "Synchronization and Chaos", National Academy of Sciences of Ukraine, Institute of Mathematics, Kiev, December 28.

6.4.2 Talks for a More General Public

B. GENTZ, *Ein Kartentrick – und die Mathematik dahinter*, Marie-Curie-Gymnasium, Ludwigsfelde, November 4.

A. HUTT, *Lineare Algebra und Gehirnforschung*, 9. Berliner Tag der Mathematik (9th Berlin Day of Mathematics), Freie Universität Berlin, May 15.

——, *Was hat Mathematik mit Gehirnforschung zu tun?*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2004, Berlin, June 12.

J. REHBERG, *Wozu braucht man irrationale Zahlen und wie gelangt man zu ihnen?*, 9. Berliner Tag der Mathematik (9th Berlin Day of Mathematics), Freie Universität Berlin, May 15.

G. REINHARDT, *Textverschlüsselung und (etwas) Zahlentheorie*, 9. Berliner Tag der Mathematik (9th Berlin Day of Mathematics), Freie Universität Berlin, May 15.

J. SPREKELS, *Mathematik – Schlüsseltechnologie des 21. Jahrhunderts*, Bühring-Oberschule (2. Gymnasium), Berlin-Weißensee, September 21.

M. WOLFRUM, *Das Chaos im Sonnensystem*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2004, Berlin, June 12.

6.4.3 Posters

M. BARO, *A quantum transmitting Schrödinger-Poisson system*, Workshop "Resonances — From Physics to Mathematics and back", Dresden, January 26–30.

W. DREYER, M. HERRMANN, J. SPREKELS, *Micro-macro transitions in the atomic chain*, Evaluation Colloquium of the DFG Priority Program "Analysis, Modeling and Simulation of Multiscale Problems", Bad Honnef, May 20–21.

G. ENCHÉRY, J. FUHRMANN, *Verification of thermohaline simulations*, DFG SPP 1135 Rundgespräch, Schloß Eringerfeld, December 1–3.

V. ESSAOULOVA, *Adaptive methods in volatility estimation and wavelet shrinkage*, Workshop on Multivariate Time Series Analysis, Heidelberg, February 25–28.

J. FUHRMANN, H.-CHR. KAISER, TH. KOPRUCKI, G. SCHMIDT, *Electronic states in semiconductor nanostructures and upscaling to semi-classical models*, Evaluation Colloquium of the DFG Priority Program "Analysis, Modeling and Simulation of Multiscale Problems", Bad Honnef, May 20–21.

H. GAJEWSKI, R. HÜNLICH, H.-CHR. KAISER, M. BARO, *Quantum mechanical and macroscopic models for optoelectronic devices*, DFG Research Center MATHEON, Technische Universität Berlin, July 19.

H.-CHR. KAISER, *Density functional theory for multi-excitons in quantum boxes*, "Molecular Simulation: Algorithmic and Mathematical Aspects", Institut Henri Poincaré, Paris, France, December 1–3.

P.H. THIESEN, A. ROBERS, K. KESORE, H.J. MUCHA, B. NIEMEYER, *Adsorption of malodours air in food industry — Adsorption- and desorption properties of modified clay minerals*, 12. Wolfgang-Ostwald-Kolloquium, Kiel, June 25–26.

B. WAGNER, A. MÜNCH, *The role of slippage in dewetting thin films*, Workshop "Pattern Formation through Instabilities in Thin Liquid Films: From Fundamental Aspects to Applications", Dresden, September 21–28.

A. MÜNCH, B. WAGNER, *The role of slippage in dewetting thin films*, Workshop of the DFG Priority Program "Nano- & Microfluidics: Bridging the Gap between Molecular Motion and Continuum Flow", Bad Honnef, November 15–17.

6.5 Visits to other Institutions[4]

E. BÄNSCH, Mathematisches Forschungsinstitut Oberwolfach, program "Research in Pairs", Oberwolfach-Walke, March 1–20.

C. BENDER, Helsinki University of Technology, Institute of Mathematics, Finland, August 10–27.

M. BIRKNER, Johann Wolfgang Goethe-Universität Frankfurt, Fachbereich Mathematik, January 19–23.

——, Friedrich-Alexander-Universität Erlangen-Nürnberg, Mathematisches Institut, February 2–6.

——, University of Oxford, Department of Mathematics, UK, October 4–21.

——, The Erwin Schrödinger International Institute for Mathematical Physics (ESI), Vienna, Austria, November 1 – December 23.

A. BOVIER, University of Cambridge, Statistical Laboratory, Centre for Mathematical Sciences, UK, March 1–5.

——, Centre des Etudes de Saclay, CEA, Paris, France, March 8–11.

——, University of Cambridge, Statistical Laboratory, Centre for Mathematical Sciences, UK, August 2–6.

——, Technion — Israel Institute of Technology, William Davidson Faculty of Industrial Engineering and Management, Haifa, Israel, December 22, 2004 – January 9, 2005.

J. ČERNÝ, École Polytechnique Fédérale de Lausanne, Département de Mathématiques, Switzerland, August 9–13.

J. ELSCHNER, University of Tokyo, Department of Mathematical Sciences, Japan, January 13 – February 13.

K. EPPLER, Christian-Albrechts-Universität zu Kiel, Institut für Informatik, March 15–19.

——, Christian-Albrechts-Universität zu Kiel, Institut für Informatik, November 22–26.

A. FAGGIONATO, EURANDOM, Eindhoven, The Netherlands, June 7–17.

J. FUHRMANN, Université de Marne-la-Vallée, Département de Mathématiques, Champs-sur-Marne, France, September 8–11.

R. HENRION, Stevens Institute of Technology, Department of Mathematical Sciences, Hoboken, USA, April 20 – May 5.

——, Université d'Avignon, Département de Mathématiques, France, November 8 – December 3.

[4]Only stays of more than three days are listed.

D. HÖMBERG, University of Tokyo, Department of Mathematical Sciences, Japan, October 11–22.

D. KOLYUKHIN, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, November 29 – December 25.

P. KREJČÍ, Institut National de la Recherche en Informatique et Automatique (INRIA), Rocquencourt, France, May 3–28.

P. MATHÉ, Austrian Academy of Sciences, Johann Radon Institute for Computational and Applied Mathematics, Linz, November 7–19.

H. NEIDHARDT, Academy of Sciences of the Czech Republic, Nuclear Physics Institute, Prague, February 16–20.

——, Centre Physique Théorique, Marseille, France, June 28 – July 4.

J. POLZEHL, Chalmers University of Technology, Department of Mathematical Statistics, Gothenburg, Sweden, May 3–12.

——, University of Minnesota, School of Statistics, Minneapolis, USA, September 1–10.

D.I. RACHINSKII, University College Cork, Department of Applied Mathematics, Ireland, September 15–21.

——, University College Cork, Department of Mathematics, Ireland, October 6–9.

——, University College Cork, Department of Applied Mathematics, Ireland, October 27–30.

J. REHBERG, Université Paul Sabatier – Toulouse, France, May 26 – June 2.

M. REISS, Université Paris VI “Pierre et Marie Curie”, Laboratoire de Probabilités et Modèles Aléatoires, France, March 1–31.

K.K. SABELFELD, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, March 29 – May 8.

——, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, July 22 – August 22.

——, Florida State University, Department of Computer Science, Tallahassee, USA, August 23–30.

——, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, December 7, 2004 – January 14, 2005.

G. SCHMIDT, The University of Liverpool, Department of Mathematical Sciences, UK, September 20–24.

K.R. SCHNEIDER, Moscow State University, Department of Physics, Russia, June 15–20.

V. SPOKOINY, University of Technology, Institute of Mathematics, Tampere, Finland, May 2–7.

——, University of Western Australia, Department of Mathematics, Perth, Australia, June 26 – July 3.

——, National University of Singapore, Department of Statistics and Applied Probability, July 9–24.

J. SPREKELS, Università di Pavia, Dipartimento di Matematica, and Politecnico di Milano, Dipartimento di Matematica, Italy, August 31 – September 4.

D. TIBA, University of Jyväskylä, Finland, July 29 – August 8.

——, Central China Normal University, The Center for Optimal Control and Discrete Mathematics, Wuhan, October 16 – November 17.

A.G. VLADIMIROV, Université Libre de Bruxelles, Theoretical Nonlinear Optics, Belgium, May 18–30.

——, Université Libre de Bruxelles, Theoretical Nonlinear Optics, Belgium, November 21 – December 4.

W. WAGNER, Kyoto University, Department of Aeronautics and Astronautics, Graduate School of Engineering, Japan, September 16 – October 15.

6.6 Academic Teaching[1]

E. BÄNSCH, *Adaptive Finite-Elemente-Verfahren* (seminar), Freie Universität Berlin, 2 SWS, winter semester 2003/2004.

——, *Numerik für partielle Differentialgleichungen* (seminar), Freie Universität Berlin, 2 SWS, winter semester 2003/2004.

——, *Einführung in die Numerische Mathematik (Numerik I)* (lecture), Freie Universität Berlin, 4 SWS, summer semester 2004.

——, *Einführung in die Numerische Mathematik (Numerik I)* (exercises), Freie Universität Berlin, 2 SWS, summer semester 2004.

E. BÄNSCH, H. GAJEWSKI, J. SPREKELS, F. TRÖLTZSCH, R. KLEIN, C. SCHÜTTE, P. DEUFLHARD, R. KORNHUBER, *Numerische Mathematik/Scientific Computing* (senior seminar), Freie Universität Berlin, 2 SWS, winter semester 2003/2004.

——, *Numerische Mathematik/Scientific Computing* (senior seminar), Freie Universität Berlin, 2 SWS, summer semester 2004.

C. BENDER, *Integraltransformationen und partielle Differentialgleichungen für Ingenieure* (lecture), Technische Universität Berlin, 2 SWS, summer semester 2004.

A. BOVIER, *Mathematische Physik I* (lecture), Technische Universität Berlin, 4 SWS, winter semester 2003/2004.

——, *Mathematische Physik II* (lecture), Technische Universität Berlin, 4 SWS, summer semester 2004.

——, *Mathematische Physik III* (lecture), Technische Universität Berlin, 4 SWS, winter semester 2004/2005.

A. BOVIER, B. GENTZ, H. FÖLLMER, P. IMKELLER, U. KÜCHLER, J.-D. DEUSCHEL, J. GÄRTNER, M. SCHEUTZOW, *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), WIAS, 2 SWS, winter semester 2003/2004.

——, *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), Technische Universität Berlin, 2 SWS, summer semester 2004.

——, *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2004/2005.

W. DREYER, W.H. MÜLLER, *Grundlagen der Kontinuumsmechanik* (lecture), Technische Universität Berlin, 4 SWS, winter semester 2003/2004.

——, *Nichtlineare Kontinuumsmechanik* (lecture), Technische Universität Berlin, 4 SWS, summer semester 2004.

——, *Grundlagen der Kontinuumsmechanik* (lecture), Technische Universität Berlin, Institut für Mechanik, 4 SWS, winter semester 2004/2005.

[1] SWS = semester periods per week

K. EPPLER, *Lineare Algebra für Ingenieure* (lecture), Technische Universität Berlin, 2 SWS, winter semester 2003/2004.

——, *Differentialgleichungen für Ingenieure* (lecture), Technische Universität Berlin, 2 SWS, summer semester 2004.

G. BÄRWOLFF, J. FUHRMANN, M. SCHERFNER, G. PENN-KARRAS, *Analysis II für Ingenieure* (lecture), Technische Universität Berlin, 4 SWS, summer semester 2004.

D. FERUS, J. FUHRMANN, J. RAMBAU, M. STEINBACH, *Analysis I für Ingenieure* (lecture), Technische Universität Berlin, 4 SWS, winter semester 2003/2004.

B. GENTZ, *Zufällige Störungen schnell-langsamer Systeme* (lecture), Technische Universität Berlin, 2 SWS, winter semester 2004/2005.

A. GLITZKY, *Optimale Steuerung bei parabolischen Differentialgleichungen* (lecture), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2003/2004.

——, *Monotone dynamische Systeme* (lecture), Humboldt-Universität zu Berlin, 2 SWS, summer semester 2004.

——, *Mathematische Modellierung von Reaktions-Diffusionsprozessen und nichtlokalen Wechselwirkungen* (lecture), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2004/2005.

R. HENRION, *Lösungsstabilität in stochastischen Optimierungsproblemen* (lecture), Martin-Luther-Universität Halle-Wittenberg, 2 SWS, winter semester 2003/2004.

——, *Optimierungsprobleme mit Zufallsparametern* (lecture), Martin-Luther-Universität Halle-Wittenberg, 4 SWS, winter semester 2003/2004.

——, *Risikotheorie* (lecture), Martin-Luther-Universität Halle-Wittenberg, 2 SWS, winter semester 2003/2004.

——, *Stochastische Optimierung I* (lecture), Humboldt-Universität zu Berlin, 2 SWS, summer semester 2004.

R. HENRION, W. RÖMISCH, M. STEINBACH, *Numerik stochastischer Modelle* (seminar), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2003/2004.

——, *Numerik stochastischer Modelle* (seminar), Humboldt-Universität zu Berlin, 2 SWS, summer semester 2004.

——, *Numerik stochastischer Modelle* (seminar), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2004/2005.

D. HÖMBERG, *Nichtlineare Optimierung* (lecture), Technische Universität Berlin, 4 SWS, winter semester 2003/2004.

——, *Optimalsteuerung bei partiellen Differentialgleichungen* (lecture), Technische Universität Berlin, 4 SWS, summer semester 2004.

——, *Analysis I für Ingenieure* (lecture), Technische Universität Berlin, 4 SWS, winter semester 2004/2005.

O. KLEIN, *Mathematik für Chemiker I* (lecture), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2003/2004.

——, *Mathematik für Chemiker II* (lecture), Humboldt-Universität zu Berlin, 2 SWS, summer semester 2004.

M. REISS, *Stochastische Differentialgleichungen* (lecture), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2003/2004.

K.R. SCHNEIDER, *Qualitative Theorie gewöhnlicher Differentialgleichungen* (lecture), Humboldt-Universität zu Berlin, 2 SWS, summer semester 2004.

K.R. SCHNEIDER, B. FIEDLER, *Nichtlineare Dynamik* (senior seminar), WIAS, Freie Universität Berlin, 2 SWS, winter semester 2003/2004.

K.R. SCHNEIDER, L. RECKE, H.J. WÜNSCHE, *Mathematische Modelle der Photonik* (seminar), WIAS, Humboldt-Universität zu Berlin, 2 SWS, winter semester 2003/2004.

——, *Mathematische Modelle der Photonik* (seminar), WIAS, Humboldt-Universität zu Berlin, 2 SWS, summer semester 2004.

K.R. SCHNEIDER, B. FIEDLER, M. WOLFRUM, *Nichtlineare Dynamik* (senior seminar), WIAS, Freie Universität Berlin, 2 SWS, summer semester 2004.

V. SPOKOINY, *Nichtparametrische stochastische Verfahren und ihre Anwendungen* (seminar), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2003/2004.

V. SPOKOINY, W. HÄRDLE, *Mathematische Statistik* (research seminar), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2003/2004.

——, *Mathematische Statistik* (research seminar), Humboldt-Universität zu Berlin, 2 SWS, summer semester 2004.

——, *Mathematische Statistik* (research seminar), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2004/2005.

V. SPOKOINY, J.G.M. SCHOENMAKERS, *Statistische Verfahren mit Anwendungen auf Finanzmärkte* (seminar), Humboldt-Universität zu Berlin, 2 SWS, summer semester 2004.

——, *Statistische Verfahren mit Anwendungen auf Finanzmärkte* (seminar), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2004/2005.

J. SPREKELS, *Inkorrekt gestellte Probleme* (lecture), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2003/2004.

——, *Analysis I* (lecture), Humboldt-Universität zu Berlin, 4 SWS, summer semester 2004.

——, *Analysis II* (lecture), Humboldt-Universität zu Berlin, 4 SWS, winter semester 2004/2005.

H. GAJEWSKI, J. SPREKELS, F. TRÖLTZSCH, R. KLEIN, C. SCHÜTTE, P. DEUFLHARD, R. KORNHUBER, *Numerische Mathematik/Scientific Computing* (senior seminar), Freie Universität Berlin, 2 SWS, winter semester 2004/2005.

H. STEPHAN, *Arithmetische und rekursive Folgen* (lecture), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2003/2004.

——, *Konvexität und Ungleichungen* (lecture), Humboldt-Universität zu Berlin, 2 SWS, summer semester 2004.

——, *Einführung in die lineare Algebra* (lecture), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2004/2005.

W. WEISS, *Kinetische Theorie* (lecture), Technische Universität Berlin, 2 SWS, winter semester 2003/2004.

W. WEISS, *Mathematische Hilfsmittel der Thermo- und Fluiddynamik* (lecture), Technische Universität Berlin, 4 SWS, summer semester 2004.

——, *Kinetische Theorie* (lecture), Technische Universität Berlin, 4 SWS, winter semester 2004/2005.

K. WILMANSKI, *Dynamik von mehrkomponentigen Körpern* (lecture), Technische Universität Berlin, 2 SWS, winter semester 2003/2004.

——, *Mechanische Wellen* (lecture), Technische Universität Berlin, 2 SWS, summer semester 2004.

——, *Dynamik von mehrkomponentigen Körpern* (lecture), Technische Universität Berlin, 2 SWS, winter semester 2004/2005.

K. WILMANSKI, I. MÜLLER, P. STREHLOW, W. WEISS, *Thermodynamisches Seminar* (seminar), WIAS, Technische Universität Berlin, 2 SWS, summer semester 2004.

——, *Thermodynamisches Seminar* (seminar), WIAS, Technische Universität Berlin, 2 SWS, winter semester 2004/2005.

M. WOLFRUM, J. HÄRTERICH, *Nichtlineare Dynamik* (senior seminar), WIAS, Freie Universität Berlin, 2 SWS, winter semester 2004/2005.

K.R. SCHNEIDER, L. RECKE, H.J. WÜNSCHE, M. WOLFRUM, *Mathematische Modelle der Photonik* (seminar), WIAS, Humboldt-Universität zu Berlin, 2 SWS, winter semester 2004/2005.

6.7 Calls, Awards and Distinctions, Habilitations, Ph.D. Theses

Calls

E. BÄNSCH, C4 professorship, March 10, Universität Erlangen, Institut für Angewandte Mathematik.

D.I. RACHINSKII, C3 professorship, November 30, University College Cork, Department of Applied Mathematics, Ireland.

Awards and Distinctions

P. MATHÉ, *Prize for Achievement in Information-Based Complexity, Columbia University, New York, USA*, October 1.

D.I. RACHINSKII, *Heisenberg Fellowship of the Deutsche Forschungsgemeinschaft (German Research Foundation)*, October 26.

V. SPOKOINY, *Fellow of the Institute of Mathematical Statistics, Beachwood, USA.*

J. SPREKELS, *member of the International Scientific Board of the Institute of Mathematics "Simion Stoilow" of the Romanian Academy, Bucharest.*

D. TIBA, *Honorary Medal of the University of Jyväskylä, Finland*, August 6.

Ph.D. Theses

I. MATTHEIS, *Stochastische gewichtete Partikelverfahren für die räumlich homogene Boltzmann-Gleichung*, Humboldt-Universität zu Berlin, supervisor: Priv.-Doz. Dr. W. Wagner, January 7.

M. HERRMANN, *Ein Mikro-Makro-Übergang für die nichtlineare atomare Kette mit Temperatur*, Humboldt-Universität zu Berlin, supervisor: Priv.-Doz. Dr. W. Dreyer, December 20.

D. MERCURIO, *Adaptive estimation for financial time series*, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, supervisor: Prof. Dr. V. Spokoiny, June 21.

E. SHCHETININA, *Integral manifolds of nonautonomous slow-fast systems without dichtomy*, Humboldt-Universität zu Berlin, supervisor: Priv.-Doz. Dr. K.R. Schneider, July 20.

R. VODÁK, *Existence of a solution to Navier–Stokes equations for isothermal compressible fluids and its qualitative properties (in Czech)*, Palacký University, Olomouc, Czech Republic, supervisor: Prof. Dr. I. Straskraba, May 12.

6.8 Conferences, Colloquiums, and Workshops

6.8.1 WIAS Conferences, Colloquiums, and Workshops

INTERNATIONAL MINI-SYMPOSIUM ON MODE-LOCKED SEMICONDUCTOR LASERS
Berlin, March 22–23
Organized by: WIAS (FG 1, 2) and Fraunhofer-Institut für Nachrichtentechnik Heinrich-Hertz-Institut (HHI), Berlin

The International Mini-symposium on Mode-locked Semiconductor Lasers has been organized by U. Bandelow (FG 1), R. Kaiser and B. Hüttl (HHI). It is in some sense a continuation of the workshops on laser dynamics held three times at WIAS up to now, but with a special focus on mode-locked lasers. The latter topic is of major interest in the project Terabit Optics Berlin, especially for the project partners from HHI. A very similar kind of devices is a research topic at the Technical University of Denmark (DTU), Kgs. Lyngby, where four workshop guests came from. The modeling and simulation of such devices challenges many groups in the world—there were respective contributions from WIAS, DTU, and the University of the Balearic Islands, Mallorca/Spain.
The aim of this mini-symposium was to discuss problems in modeling such semiconductor lasers as well as in understanding measured and calculated effects, therefore discussions in a productive atmosphere took more time than the talks themselves. Talks on modeling and simulation have been given by U. Bandelow, A. Vladimirov (WIAS), and J. Mulet (Mallorca) on the first day at WIAS. On the second day at HHI, K. Yvind and D. Larsson (DTU) talked about design and performance of specific mode-locked lasers, followed by talks of C. Kindel and M. Kroh (HHI) on their devices and measurements. The number of participants was limited to 20 persons which were present.

KOLLOQUIUM "SIMULATION KOMPLEXER PROZESSE" (SIMULATION OF COMPLEX PROCESSES)
Berlin, March 23
Organized by: WIAS (FG 3)

A festive colloquium on the occasion of the 65th birthday of Prof. Dr. Friedrich Grund has been organized on March 23, 2004, by the research group "Numerical Mathematics and Scientific Computing". The talks given focused on the simulation of large electric networks and chemical process simulation, the main areas Prof. Grund contributed to. Review lectures outlined the analysis and implementation of numerical methods for the solution of high-dimensional systems of linear, nonlinear, and differential–algebraic equations on workstations and parallel computers. A further topic of the colloquium has been the simulation of microwave circuits.

MINI-WORKSHOP "HOMOCLINIC DYNAMICS"
Berlin, April 6
Organized by: WIAS (FG 2)
Sponsored by: Alexander von Humboldt Foundation, WIAS

The mini-workshop "Homoclinic Dynamics" was devoted to the richness of global behavior in dynamical systems possessing degenerate homoclinic orbits. Such orbits are characterized by

a non-transversal intersecting of stable and unstable manifolds. Homoclinic orbits exhibiting homoclinic tangencies form a special class of degenerate homoclinic orbits where bifurcations lead to unpredictable behavior. In the three talks given: "Global bifurcations connected with the disappearing of a periodic orbit" (L.P. Shilnikov), "Homoclinic tangencies in a periodically figure eight of a saddle" (S.V. Gonchenko), and "On the richness of Hamiltonian dynamics" (D. Turaev), the variety of bifurcation scenarios has been described which is connected with the arising of global bifurcations of degenerate homoclinic orbits. All lectures have been delivered by outstanding representatives of the famous Nizhny Novgorod school headed by the Humboldt-Price laureate Prof. L.P. Shilnikov. 12 participants attended the mini-workshop.

FESTIVE COLLOQUIUM IN THE FRAMEWORK OF THE SENIOR SEMINAR "NONLINEAR DYNAMICS"
Berlin, April 27
Organized by: WIAS (FG 2)

This colloquium was organized in order to honor the outstanding achievements of PD Dr. Klaus Schneider in his scientific vita, who has been one of the organizers of the Senior Seminar "Nonlinear Dynamics" for more than one decade.
The four invited speakers were selected among former PhD students, coworkers, and cooperation partners. In their talks, they presented a broad range of mathematical fields, related to the work of Klaus Schneider, including singular perturbed systems, invariant manifolds, delayed loss of stability, and applications in optoelectronics. 39 participants attended the colloquium.

INTERNATIONAL WORKSHOP "ADVANCES IN MODELING AND SIMULATION OF SEMICONDUCTOR DEVICES (AMASIS'04)"
Berlin, July 14–16
Organized by: WIAS (FG 1)
Sponsored by: WIAS, DFG

The workshop brought together applied mathematicians and scientists from semiconductor physics and gave them the opportunity to exchange experience in the field of modeling and simulation of micro-, nano-, and optoelectronic semiconductor devices. Based on financial support of the DFG it was possible to invite experts from Europe and the USA which made the workshop an event of high scientific significance. Sixty-one participants attended the workshop, a lot of high-quality lectures (twenty invited lectures and seven contributed talks) were given. The main topics were

- Physical modeling of micro-, nano-, and optoelectronic devices and their technology;
- Design of efficient simulation software;
- Presentation of simulation results of state-of-the-art devices;
- Analytical and numerical investigation of relevant model equations;
- Qualitative properties of systems of partial differential equations arising in related application areas.

Some of the contributions will be published in the Journal of Applied Mathematics and Mechanics (ZAMM), issue November 2005. Further details concerning the workhop can be found at AMaSiS'04 http://www.wias-berlin.de/workshops/amasis04.

MINI-WORKSHOP "NEW DIRECTIONS OF RESEARCH FOR ROBOTICS IN FLEXIBLE MANUFACTORING PROCESSES"
Berlin, September 27–28
Organized by: WIAS (FG 4)
Sponsored by: DFG Research Center MATHEON, WIAS

The degree of automation is increasing in many branches of industry. Moreover, there is a strong demand to reduce the cycle time in production lines. Hence, more and more robots have to work simultaneously on one component part. This poses a number of new questions in process optimization.
The aim of this workshop was to discuss these problems with an emphasis on applications in the automotive industry as well as on typical SME applications.
The main topics were the coupling of process modeling, e.g., glueing or laser treatments, and robot path planning, the issue of cooperative robots as well as the problem of uncertainties in the process data. The mini-workshop has been attended by ten participants, seven talks were given, among them three by industry representatives.

WORKSHOP "SYNCHRONIZATION AND HIGH-DIMENSIONAL CHAOS IN COUPLED SYSTEMS"
Berlin, November 15–16
Organized by: WIAS (FG 2), Humboldt-Universität zu Berlin
Sponsored by: DFG Research Center MATHEON, WIAS

Synchronization and high-dimensional chaos plays an important role in several fields of application, such as biology, neuroscience, optoelectronics, and communication technology. The 15 lectures given in this workshop were related to the mathematical issues connected with this field as well as to concrete problems from various applied sciences. The workshop was important for WIAS to establish and to intensify the contact to many international experts in this field. With 53 participants from 10 countries, the workshop got an unexpected high resonance.

6.8.2 Non-WIAS Conferences, Colloquiums, and Workshops co-organized by WIAS and / or having taken place at WIAS

PRESENTATION OF THE SCILAB CONSORTIUM
Berlin, April 29
Organized by: French Embassy in Berlin
Sponsored by: French Embassy in Berlin

The Counsellor for Science and Technology of the French Embassy in Germany, Prof. M. Berveiller, and the Director of WIAS, Prof. J. Sprekels greeted the participants. Then representatives of INRIA, the SCILAB Consortium, and German-French cooperation programs introduced their institutions and their projects. The presentation ended with a discussion about possible contributions of the participants to the development of SCILAB.

VIth Workshop MATHEMATICA
Berlin, October 15
Organized by: mathemas (Kiel), WIAS
Sponsored by: WOLFRAM RESEARCH (UK), mathemas (Kiel), WIAS

The workshop on the computer algebra MATHEMATICA offered an established stage for an interdisciplinary exchange of information between producers and users of this software.
For example, problem solutions for nonlinear optimization, analysis and application of special integrals, advanced graphics methods (Bump Mapping) and for scientific publishing were treated in an international framework.
The invited main lecture, held by Prof. Paul Abbott (Perth/Australia), was titled “The Ins & Outs of Mathematica: Approaches to problem solving using Mathematica”.
Twenty-five participants from all over Germany took part in the workshop, where scientists from universities and non-university research institutes were brought together with industrial partners.

TELI International Science and Technology Congress “Innovation for People”
Berlin, October 17–20
Organized by: TELI (Journalistenvereinigung für technisch-wissenschaftliche Publizistik)
Sponsored by: TELI and others

Latest news from German research have been presented to journalists from all over Europe. On October 20, 35 participants of the Congress came to WIAS. 11 talks were given on the topic “Innovation Made in Germany”, e.g., by representatives of Siemens AG, Merck KGaA, Degussa AG, and Novartis Pharma GmbH. The hosting institute has been introduced by its director J. Sprekels during a 45 minutes presentation.

BMBF/BMWA/IEA Workshop “New Links Between Basic Research and Applied Energy R&D — The Computational Approach”
Berlin, November 8–9
Organized by: Project Management Organization Jülich of BMBF and BMWA, WIAS
Sponsored by: BMWA

This workshop was planned jointly by the two German ministries responsible for research and economy and took place within the framework of the IEA’s Ad Hoc Group on Science and Energy Technologies (AHGSET). Focusing on the technical “pull” from engineers and the scientific “push” from applied mathematicians, it offered a forum for mathematicians and energy researchers to demonstrate the role that applied mathematics can play in energy science. Taking the examples of fusion power, fuel cells, combustion, daylighting, and recovery of oil and gas, participants discussed opportunities and new paths for enhanced cooperation to reinforce links between mathematics and energy engineering. WIAS research has been introduced in a 30 minutes presentation “Mathematical modelling of direct methanol fuel cells” given by J. Sprekels.

6.9 Visiting Scientists[2]

6.9.1 Guests

V.A. ADAMYAN, I.I. Mechnikov Odessa National University, Department of Theoretical Physics, Ukraine, February 25 – March 12.

H. AMANN, Universität Zürich, Institut für Mathematik, Switzerland, November 15–26.

V. ARNĂUTU, University "Al.I. Cuza", Department of Mathematics, Iaşi, Romania, November 15 – December 15.

N. BEN ABDALLAH, Université Paul Sabatier, Laboratoire de Mathématiques pour l'Industrie et la Physique, Toulouse, France, November 29 – December 3.

N. BERGLUND, CNRS-Centre de Physique Théorique, Marseille, and Université de Toulon et du Var, Physique Mathématique, France, February 20–29.

——, July 12 – August 31.

——, October 21 – November 1.

——, December 14, 2004 – January 2, 2005.

J. BLATH, University of Oxford, Department of Mathematics, UK, August 27 – October 1.

J.C.R. BLOCH, DFG-Forschungszentrum MATHEON, Berlin, January 1 – November 14.

R. BLOSSEY, Interdisciplinary Research Center (IRI), Villeneuve, France, May 3–7.

E. BURMAN, Ecole Polytechnique Fédérale de Lausanne, Faculté de Mathématiques, Switzerland, February 19–22.

C. BUTUCEA, Université Paris VI "Pierre et Marie Curie", Laboratoire de Probabilités et Modèles Aléatoires, France, April 12–30.

V. BUTUZOV, Moscow State University, Department of Physics, Russia, April 2–29.

K. CHEŁMINSKI, Cardinal St. Wyszynski University, Faculty for Mathematics and Sciences, Warsaw, Poland, June 7 – July 4.

L.A. CHERKAS, Belarussian State University of Informatics and Radioelectronics, Minsk, May 11–21.

A. DALALYAN, Université Paris VI "Pierre et Marie Curie", Laboratoire de Probabilités et Modèles Aléatoires, France, April 13–26.

E. DARRIGRAND, Université de Rennes 1, Institut de Recherche Mathématiques de Rennes, France, August 2–21.

J. DORIGNAC, Max-Planck-Institut für Physik komplexer Systeme, Dresden, May 4–31.

[2]Only stays of more than three days are listed.

M.A. EFENDIEV, Universität Stuttgart, Mathematisches Institut A, March 9–16.

——, June 22–29.

——, August 10–17.

——, August 18–25.

——, September 5–11.

——, December 15–22.

A.E. AYYADI, Johannes Gutenberg-Universität Mainz, Fachbereich Mathematik und Informatik, March 14–19.

G. ENCHÉRY, Institut Français du Pétrole, Rueil-Malmaison, France, June 12–18.

R. EYMARD, Université de Marne-la-Vallée, Département de Mathématiques, Champs-sur-Marne, France, June 12–18.

S. FLACH, Max-Planck-Institut für Physik komplexer Systeme, Dresden, March 17–20.

S. FOREST, Ecole des Mines de Paris, Centre des Matériaux, France, February 15–28.

T. FRANK, Universität Münster, Institut für theoretische Physik, February 16–27.

A. GARCIA, San José State University, Department of Physics, USA, October 14 – November 13.

A. GOLDENSHLUGER, University of Haifa, Department of Statistics, Israel, August 29 – September 14.

S. GONCHENKO, Institute for Applied Mathematics and Cybernetics, Nizhny Novgorod, Russia, April 1–11.

I. GRAMA, Université de Bretagne Sud, Laboratoire SABRES, Vannes, France, February 1–29.

M. HOFFMANN, Université de Marne-la-Vallée, Laboratoire d'Analyse et de Mathématiques Appliquées, Champs-sur-Marne, France, September 13–22.

W. HORN, California State University, Department of Mathematics, Northridge, USA, June 30 – July 16.

——, December 11–24.

A. HRYN, State University of Grodno, Algebra, Geometry and Mathematics Teaching Methods, Belarus, May 11–21.

Y. INGSTER, Electrotechnical University (LETI), Department of Mathematics II, St. Petersburg, Russia, July 1 – August 31.

D. IOFFE, University of Cambridge, Statistical Laboratory, Centre for Mathematical Sciences, UK, June 15–20.

D. IOFFE, Technion — Israel Institute of Technology, William Davidson Faculty of Industrial Engineering and Management, Haifa, Israel, August 26–29.

A. JUDITSKY, Université Joseph Fourier Grenoble I, Laboratoire de Modélisation et Calcul, France, August 19 – September 7.

T. KAPITANIAK, Technical University of Łodz, Poland, November 14–20.

J.R. KING, University of Nottingham, School of Mathematical Sciences, UK, August 9–12.

D. KLEINHANS, Universität Münster, Institut für theoretische Physik, September 6–10.

A. KLENKE, Friedrich-Alexander-Universität Erlangen-Nürnberg, Mathematisches Institut, March 1–12.

P. KORDULOVÁ, Silesian University of Opava, Czech Republic, December 6–13.

A. KRASNOSEL'SKII, Institute for Information Transmission Problems, Moscow, Russia, November 1–14.

B. KRAUSKOPF, University of Bristol, Department of Engineering Mathematics, UK, November 13–24.

O. KURBANMURADOV, Turkmen State University, Physics and Mathematics Research Center, Ashkhabat, October 1 – November 30.

I. KURKOVA, Université Paris VI "Pierre et Marie Curie", Laboratoire de Probabilités et Modèles Aléatoires, France, March 21 – April 4.

——, November 15–25.

O. LEPSKI, Université de Provence, Centre de Mathématiques et d'Informatique, Marseille, France, October 9–17.

A. LEVYKIN, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, February 29 – March 29.

A. LINKE, DFG-Forschungszentrum MATHEON, Berlin, January 1 – December 31.

O. LYKOVA, National Academy of Sciences of Ukraine, Institute of Mathematics, Kiev, November 21–28.

G.N. MILSTEIN, Ural State University, Department of Mathematics, Ekaterinburg, Russia, November 15, 2004 – April 15, 2005.

A. MIRANVILLE, Université de Poitiers, Laboratoire d'Applications des Mathématiques, Chasseneuil Futuroscope, France, February 8–20.

P. MÖRTERS, University of Bath, Department of Mathematical Sciences, UK, June 14 – July 12.

O. MUSCATO, University of Catania, Department of Mathematics and Informatics, Italy, February 25–28.

N.N. NEFEDOV, Moscow State University, Faculty of Physics, Russia, April 2–30.

C. NEGULESCU, Université Paul Sabatier, Laboratoire de Mathématiques pour l'Industrie et la Physique, Toulouse, France, December 16–22.

M. NIZETTE, Université Libre de Bruxelles, Optique Non-linéaire Théorique, Belgium, September 13–24.

K. PAKDAMAN, Épidémiologie et Sciences de l'Information, Paris, France, August 15–20.

A. PINKUS, Technion —Israel Institute of Technology, Department of Mathematics, Haifa, September 12–19.

M. RAUSCHER, Max-Planck-Institut für Metallforschung, Stuttgart, May 3–7.

E. ROCCA, Università degli Studi di Milano, Dipartimento di Matematica, Italy, November 3 – December 3.

O. SCHENK, Universität Basel, Fachbereich Informatik, Switzerland, October 12–18.

S. SCHWABIK, Academy of Sciences of the Czech Republic, Mathematical Institute, Prague, December 13–18.

A. SEEGER, Université d'Avignon, Département de Mathématiques, France, February 23 – March 12.

I. SHALIMOVA, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, January 31 – March 31.

——, August 28 – September 28.

J. SIEBER, University of Bristol, Department of Engineering Mathematics, UK, December 4–12.

M. ŠILHAVÝ, Università di Pisa, Dipartimento di Matematica, Italy, January 14–18.

I.V. SKRYPNIK, National Academy of Sciences of Ukraine, Institute of Applied Mathematics and Mechanics, Donetsk, Ukraine, November 18 – December 16.

J. SOKOŁOWSKI, Université de Nancy I, Laboratoire de Mathématiques, Vandœuvre-lès-Nancy, France, April 4–10.

S. SPERLICH, Universidad Carlos III de Madrid, Departamento de Estadística y Econometría, Spain, December 15, 2004 – January 22, 2005.

C. STARICA, Chalmers University of Technology, Department of Mathematical Statistics, Gothenburg, Sweden, February 8–29.

——, November 6–14.

U. STEFANELLI, Istituto di Matematica Applicata e Tecnologie Informatiche (IMATI) — CNR, Pavia, Italy, September 27 – October 22.

A. STEFANSKI, Technical University of Łodz, Poland, November 14–20.

J. SWART, Universität Erlangen-Nürnberg, Mathematisches Institut, July 25 – August 22.

C. TAMAGNINI, Università degli Studi di Perugia, Dipartimento di Ingegneria Civile e Ambientale, Italy, November 10 – December 12.

M. TLIDI, Université Libre de Bruxelles, Optique Non-linéaire Théorique, Belgium, April 16–25.

——, June 30 – July 12.

F. TONINELLI, EURANDOM, Eindhoven, The Netherlands, January 20–31.

D. TURAEV, Ben-Gurion University of the Negev, Department of Mathematics, Beer-Sheva, Israel, March 30 – April 15.

——, August 4–11.

——, August 12–25.

M. TVRDY, Academy of Sciences of the Czech Republic, Mathematical Institute, Prague, December 13–18.

S. VAN BELLEGEM, Université Catholique de Louvain, Institut de Statistique, Louvain-la-Neuve, Belgium, March 22–27.

A.A. VLADIMIROV, Russian Academy of Sciences, Institute for Information Transmission Problems, Moscow, January 25 – February 25.

P. VOGT, University of Bath, Department of Mathematical Sciences, UK, December 14–18.

T. WITELSKI, Duke University, Mathematics Department, Durham, USA, July 1–31.

M. YAMAMOTO, University of Tokyo, Department of Mathematical Sciences, Japan, March 15–28.

——, September 11 – October 3.

M. ZAHRADNÍK, Charles University, Faculty of Mathematics and Physics, Prague, Czech Republic, December 2–17.

S.V. ZELIK, Russian Academy of Sciences, Institute for Information Transmission Problems (at that time: Universität Stuttgart, Institut für Angewandte Analysis und Numerische Simulation), Moscow, August 11–18.

——, August 19–25.

S. ZHENG, Fudan University, Institute of Mathematics, Shanghai, China, June 3–30.

6.9.2 Scholarship Holders

A. MÜNCH, Humboldt-Universität zu Berlin, Institut für Mathematik, Heisenberg Fellowship of the Deutsche Forschungsgemeinschaft (German Research Foundation), November 1, 2003 – October 31, 2006.

L. SHILNIKOV, Institute for Applied Mathematics and Cybernetics, Nizhny Novgorod, Russia, Humboldt Research Award, January 25 – February 22, 2004.

——, Humboldt Research Award, March 25 – April 23, 2004.

J. XIONG, University of Tennessee, Department of Mathematics, Knoxville, USA, Humboldt Research Fellowship, July 1, 2003 – June 30, 2004.

6.9.3 Doctoral Candidates and Post-docs supervised by WIAS Collaborators

M. ADAMOV, Technische Universität Berlin, Graduate College 827 “Transport Phenomena with Moving Boundaries”, doctoral candidate, June 1, 2004 – June 30, 2005.

M. AN DER HEIDEN, Technische Universität Berlin, Graduate College “Stochastic Processes and Probabilistic Analysis”, doctoral candidate, since May 1.

A. DEPPERSCHMIDT, Technische Universität Berlin, doctoral candidate, since January 1.

A. KLIMOVSKI, Technische Universität Berlin, Graduate College “Stochastic Processes and Probabilistic Analysis”, doctoral candidate, since June 1.

6.10 Guest Talks

V.A. ADAMYAN, I.I. Mechnikov Odessa National University, Department of Theoretical Physics, Ukraine, *Modeling of electronic structure of nanowires*, March 10.

H. AMANN, Universität Zürich, Institut für Mathematik, Switzerland, *Über das Perona-Malik-Paradoxon*, November 17.

V. ARNĂUTU, University "Al.I. Cuza", Department of Mathematics, Iaşi, Romania, *Some aspects concerning the linear age-dependent population dynamics*, December 7.

A. BALANOV, Lancaster University, Department of Physics, UK, *Delayed feedback control of chaotic and stochastic oscillations*, October 21.

E. BARTH, Universität Lübeck, Institut für Neuro- und Bioinformatik, *Mathematische Probleme des künstlichen Sehens aus der Perspektive spezifischer Anwendungen*, November 22.

N. BEN ABDALLAH, Université Paul Sabatier, Laboratoire de Mathématiques pour l'Industrie et la Physique, Toulouse, France, *Strong confinement limit for the three dimensional Schrödinger equation*, December 1.

S. BERRES, Universität Stuttgart, Institut für Angewandte Analysis und Numerische Simulation, *On strongly degenerate parabolic-hyperbolic systems modeling polydisperse sedimentation*, October 27.

M. BESTEHORN, Brandenburgische Technische Universität Cottbus, Institut für Physik und Chemie, *3D large scale convection in thin liquid films*, February 25.

J.C.R. BLOCH, DFG-Forschungszentrum MATHEON, Berlin, *Branch continuation and bifurcations of coupled reaction-diffusion equations*, July 8.

R. BLOSSEY, Interdisciplinary Research Center (IRI), Villeneuve, France, *On the integro-differential equations of nonlocal electronics*, May 5.

M. BÖHM, TFH Berlin/ITWM Kaiserslautern, *Online -Inspektion von metallischen Oberflächen*, December 6.

J.-P. BOUCHAUD, Centre d'Etudes de Saclay & Capital Fund Management, Paris, France, *Fluctuations and response in financial markets: The subtle nature of "random" price changes*, May 19.

G. BRAMANN, H.-J. WÜNSCHE, Fraunhofer-Institut für Nachrichtentechnik Berlin, Heinrich-Hertz-Institut, and Humboldt-Universität zu Berlin, Fachbereich Physik, *Signal competition in ultra-long semiconductor amplifiers. Theory and experiment*, February 5.

E. BURMAN, Ecole Polytechnique Fédérale de Lausanne, Faculté de Mathématiques, Switzerland, *Edge stabilization: An interior penalty method for the incompressible Navier–Stokes equation*, February 19.

K. CHEŁMINSKI, Cardinal St. Wyszynski University, Faculty for Mathematics and Sciences, Warsaw, Poland, *Elasto-plastische Cosserat-Materialien — Modellierung und mathematische Analyse*, June 17.

L.A. CHERKAS, Belarussian State University of Informatics and Radioelectronics, Minsk, *Limit cycles of polynomial vector fields*, May 18.

M. CLEMENS, Helmut-Schmidt-Universität Hamburg, FB Elektrotechnik, *Simulation elektromagnetischer Felder mit diskreten Feldformulierungen: Theoretische Modelle und praktische Anwendungen*, September 20.

F. COURTY, Technische Universität Berlin, Institut für Mathematik, *Application of optimization to PDE: From optimal shape to optimal meshes*, December 14.

E. DARRIGRAND, Université de Rennes 1, Institut de Recherche Mathématiques de Rennes, France, *Fast multipole method and microlocal discretization for solving integral equations in electromagnetism*, August 10.

J. DORIGNAC, Max-Planck-Institut für Physik komplexer Systeme, Dresden, *Isochronism and bifurcation of band edge modes in Hamiltonian lattices*, April 7.

K. ECKER, Freie Universität Berlin, *Local monotone quantities for some nonlinear diffusion equations*, November 10.

M.A. EFENDIEV, Universität Stuttgart, Mathematisches Institut A, *Longtime behaviour of solutions of a nonlinear reaction-diffusion system arising in modeling of biofilms*, March 11.

——, *Mapping properties of nonlinear operators related to pseudodifferential ones and its applications*, August 12.

——, *How to avoid multivaluedness of semigroups: Theory and applications*, December 16.

A. EL AYYADI, Johannes Gutenberg-Universität Mainz, Fachbereich Mathematik und Informatik, *Hybrid models for semiconductor device simulations*, March 17.

G. ENCHÉRY, Institut Français du Pétrole, Rueil-Malmaison, France, *Numerical approximation of a two-phase flow problem in a porous medium with space discontinuous capillary forces*, June 17.

A. ERDMANN, Fraunhofer-Institut für Integrierte Systeme und Bauelementetechnologie Erlangen, *Simulation photolithographischer Prozesse — Grundlagen, Anwendungspotential und Herausforderungen*, August 23.

H. ERZGRÄBER, Free University of Amsterdam, Department of Physics and Astronomy, The Netherlands, *Compound laser modes in delay coupled semiconductor lasers*, November 18.

R. EYMARD, Université de Marne-la-Vallée, Département de Mathématiques, Champs-sur-Marne, France, *Convergence of a finite volume scheme for the transient Navier–Stokes equations*, June 17.

S. FLACH, Max-Planck-Institut für Physik komplexer Systeme, Dresden, *Broken space-time symmetries and rectification phenomena induced by AC fields*, March 19.

D. GERTEISEN, Fraunhofer-Institut für Solare Energiesysteme, Freiburg, *Modelistic AC impedance study on porous electrodes of proton exchange membrane fuel cells using an agglomerate model*, November 23.

W. GOVAERTS, Rijksuniversiteit Gent, Department of Applied Mathematics and Computer Science, Belgium, *Numerical methods for periodic orbits and their bifurcations*, May 6.

H. GROSS, Carl Zeiss AG Oberkochen, *Inverse Probleme in der klassischen Optik*, October 25.

M. GROTE, University of Basel, Department of Mathematics, Switzerland, *Nonreflecting boundary conditions for multiple scattering problems*, July 1.

K.-H. HASLER, Ferdinand-Braun-Institut für Höchstfrequenztechnik, Berlin, *Simulation of long monolithic mode-locked lasers with LDSL: First results*, January 29.

M. HERRMANN, Humboldt-Universität zu Berlin, Institut für Mathematik, *Modulated traveling waves in atomic chains*, October 26.

CH. HILGERS, Rheinisch-Westfälische Technische Hochschule Aachen, Geologie – Endogene Dynamik, *The role of fluids during deformation — Inferences from veins*, April 22.

B. HÜTTL, Fraunhofer-Institut für Nachrichtentechnik Berlin, Heinrich-Hertz-Institut, *Mode-locked semiconductor laser: New experimental results*, June 10.

——, *Recent improvements on 40 GHz mode-locked lasers*, December 9.

D. IOFFE, University of Cambridge, Statistical Laboratory, Centre for Mathematical Sciences, UK, *On the birth of a critical droplet*, June 16.

L. KALACHEV, University of Montana, Department of Mathematical Sciences, Missoula, USA, *Singularly perturbed parabolic equations with alternating boundary layer type solutions*, March 29.

C. KINDEL, Fraunhofer-Institut für Nachrichtentechnik Berlin, Heinrich-Hertz-Institut, *Mode-locked semiconductor laser: New experimental results*, June 17.

J.R. KING, University of Nottingham, School of Mathematical Sciences, UK, *Wetting and dewetting of power-low fluids*, August 11.

B. KLEEMANN, Carl Zeiss AG Oberkochen, *Periodische Helmholtz-Solver in der elektromagnetischen Optik*, October 25.

R. KLEIN, Potsdam-Institut für Klimafolgenforschung (PIK), *Mathematische Modellierung im Kontext der Klimafolgenforschung*, July 5.

A. KLENKE, Universität Mainz, Fachbereich Mathematik und Informatik, *Multifraktales Spektrum Brownscher Intersektionslokalzeiten*, March 3.

C. KOHLER, Universität Stuttgart, Institut für Theoretische und Angewandte Physik, *Atomistic simulation of dislocation pinning in precipitation hardened materials*, November 26.

P. KORDULOVÁ, Silesian University of Opava, Czech Republic, *Quasilinear hyperbolic equations with hysteresis operators*, December 10.

A. KRASNOSEL'SKII, Institute for Information Transmission Problems, Moscow, Russia, *On existence of large subharmonics*, November 11.

B. KRAUSKOPF, University of Bristol, Department of Engineering Mathematics, UK, *Saddle-node Hopf bifurcation with global reinjection*, November 23.

J.Y. LEE, University of Pittsburgh, USA, *Modeling diblock copolymer/nanoparticle composites*, July 2.

A. LINKE, DFG-Forschungszentrum MATHEON, Berlin, *Algebraische Mehrgitter-Methoden und (symmetrische) Sattelpunktprobleme*, July 8.

M. LIPINSKI, Ruhr-Universität Bochum, Fakultät für Mathematik, *Two a posteriori error estimators for a saddle-point formulation of the Poisson equation with Dirichlet boundary conditions*, June 24.

M. LÖWE, Universität Münster, Institut für Mathematische Statistik, *The voter model with antivoter bounds*, February 4.

T. MAGATH, Technische Universität Hamburg-Harburg, Arbeitsbereich Hochfrequenztechnik, *Quasioptische Strahlformung mittels rechnergenerierter Hologramme*, March 22.

A. MIRANVILLE, Université de Poitiers, Laboratoire d'Applications des Mathématiques, Chasseneuil Futuroscope, France, *Hyperbolic perturbations of phase field systems with logarithmic potentials*, February 11.

M. MÖHLE, Eberhard-Karls-Universität Tübingen and Universität Köln, Mathematisches Institut, *Coalescent trees with simultaneous multiple collisions of ancestral lineages*, February 11.

N.F. MOROZOV, St. Petersburg State University, Russia, *The solid mechanics method in nanotechnology*, April 14.

P. NEČESAL, University of West Bohemia, Centre for Applied Mathematics, Pilsen, Czech Republic, *The Fučik spectrum for spatial differential operators*, September 24.

C. NEGULESCU, Université Paul Sabatier, Toulouse, France, *The WKB approximation for the modeling of quantum ballistic transport in nanoscale MOSFETs*, December 22.

M. NIZETTE, Université Libre de Bruxelles, Optique Non-linéaire Théorique, Belgium, *Stability of square oscillations in delayed-feedback electro-optical systems*, September 16.

O. OMEL'CHENKO, National Academy of Sciences of Ukraine, Institute of Mathematics, Kiev, *Periodic contrast structures in singularly perturbed parabolic equations*, November 9.

I. OMELCHENKO MATSKIV, Y. MAISTRENKO, National Academy of Sciences of Ukraine, Institute of Mathematics, Kiev, *Stability of synchronized states in coupled map systems with different coupling structures*, September 23.

A. PINKUS, Technion — Israel Institute of Technology, Department of Mathematics, Haifa, *Mathematics and life of C. Müntz*, September 16.

V.V. PUKHNACHOV, Novosibirsk State University, Russia, *Hierarchy of models in the convection theory*, April 7.

M. RAUSCHER, Max-Planck-Institut für Metallforschung, Stuttgart, *Continuum modelling of anisotropic etching of silicon in KOH*, May 5.

L. RECKE, Humboldt-Universität zu Berlin, *Über lokale Existenz, Eindeutigkeit und Regularität bei quasilinearen parabolischen Randanfangswertaufgaben mit nichtglatten Daten*, October 20.

A. RENDALL, Max-Planck-Institut für Gravitationsphysik, Golm, *Das Einstein-Vlasov-System*, April 21.

A. REUSKEN, Rheinisch-Westfälische Technische Hochschule Aachen, Lehrstuhl für Numerische Mathematik, *Schnelle iterative Löser für diskrete Stokes-Gleichungen*, December 9.

E. ROCCA, Università degli Studi di Milano, Dipartimento di Matematica, Italy, *Existence of a global attractor for some singular phase transitions systems*, November 24.

M. ROEGER, Technical University of Eindhoven, The Netherlands, *Mathematical analysis of a model describing tissue degradation by bacteria*, October 27.

A. SCHEEL, University of Minnesota, Institute for Mathematics and its Applications, Minneapolis, USA, *Coarsening fronts*, December 21.

H. SCHURZ, South Illinois University, Department of Mathematics, Carbondale, USA, *Some topics in stability of stochastic systems*, June 3.

S. SCHWABIK, Academy of Sciences of the Czech Republic, Prague, *Recent possibilities of integrating Banach space-valued functions*, December 15.

A. SEEGER, Université d'Avignon, Département de Mathématiques, France, *An approximation result in the space of convex cones: Applications to nonlinear analysis and mathematical economics*, March 11.

L. SHILNIKOV, Institute for Applied Mathematics and Cybernetics, Nizhny Novgorod, Russia, *Bifurcations and the Lorenz model*, February 12.

J. SIEBER, University of Bristol, Department of Engineering Mathematics, UK, *Delay compensation in the coupling in hybrid experimental/numerical systems*, December 7.

M. ŠILHAVÝ, Università di Pisa, Dipartimento di Matematica, Italy, *Fluxes of mechanical quantities across fractal boundaries*, January 16.

I.V. SKRYPNIK, National Academy of Sciences of Ukraine, Institute of Applied Mathematics and Mechanics, Donetsk, Ukraine, *Behavior and existence of positive solutions to nonlinear elliptic equations in exterior domains*, November 24.

J. SOKOŁOWSKI, Université de Nancy I, Laboratoire de Mathématiques, Vandœuvre-lès-Nancy, France, *Optical tomography, using shape optimization*, April 6.

U. STEFANELLI, Istituto di Matematica Applicata e Tecnologie Informatiche (IMATI) — CNR, Pavia, Italy, *Microscopic movements and phase transition models*, October 22.

C. TAMAGNINI, Università degli Studi di Perugia, Dipartimento di Ingegneria Civile e Ambientale, Italy, *Plasticity of soils: Stress-dilatancy based modelling of granular materials*, November 24.

F. THEIL, Warwick Mathematics Institute, UK, *Crystallization in two dimensions*, November 23.

U. THIELE, Max-Planck-Institut für Physik komplexer Systeme, Dresden, *Thin liquid films on a slightly inclined heated plate: From Cahn–Hillard to Kuramoto–Sivashinsky behaviour*, December 1.

J. TIMMER, Albert-Ludwigs-Universität Freiburg, Zentrum für Datenanalyse und Modellbildung, *Data-based modeling of the dynamics of a cellular signaling pathway*, November 1.

M. TLIDI, Université Libre de Bruxelles, Optique Non-linéaire Théorique, Belgium, *Localized structure formation in cavity nonlinear optics*, April 22.

——, *Dissipative vegetation structures in arid ecosystems*, July 8.

F. TONINELLI, EURANDOM, Eindhoven, The Netherlands, *The Kac limit for finite-range spin glasses*, January 28.

V. TRONCIU, Technical University of Moldova, Department of Physics, Chisinau, Moldova, *Dynamics of blue InGaN lasers with different saturable absorber designs*, May 27.

D. TURAEV, Ben-Gurion University of the Negev, Department of Mathematics, Beer-Sheva, Israel, *On maps close to identity*, July 6.

M. TVRDY, Academy of Sciences of the Czech Republic, Mathematical Institute, Prague, *The method of lower and upper functions in singular periodic problems for second order nonlinear differential equations*, December 14.

O. USHAKOV, Humboldt-Universität zu Berlin, Institut für Physik, *Impact of external noise on self-pulsating lasers*, June 24.

J.J.L. VELAZQUEZ, Universidad Complutense de Madrid, Departamento de Matemática Aplicada, Spain, *Singular solutions of the Keller–Segel model*, January 28.

A.A. VLADIMIROV, Russian Academy of Sciences, Institute for Information Transmission Problems, Moscow, *Hysteresis methods in queuing theory*, February 4.

S. VÖLLINGER, Albert-Ludwigs-Universität Freiburg, Institut für Mathematische Stochastik, *Geometrie der Schrödingergleichung und stochastischer Massentransport*, April 28.

H. WENZEL, Ferdinand-Braun-Institut für Höchstfrequenztechnik, Berlin, *High power DFB laser: Modelling and experiments*, November 25.

H. WILKE, K.A. CLIFFE, Max-Born- Institut für Nichtlineare Optik und Kurzzeitspektroskopie, Institut für Kristallzüchtung, *A modular software concept for the Institute of Crystal Growth*, May 27.

T. WITELSKI, Duke University, Mathematics Department, Durham, USA, *Dynamics for a critical-case unstable generalized thin film equation*, July 7.

J. XIONG, University of Tennessee, Knoxville, USA, *A degenerate stochastic partial differential equation for superprocesses with singular interaction*, February 18.

Y. YAGI, Osaka University, Institute of Scientific and Industrial Research, Japan, *Exponential attractors and pattern formation for chemotaxis-growth system*, June 25.

M. YAMAMOTO, University of Tokyo, Department of Mathematical Sciences, Japan, *Stability in determining a semilinear term in a reaction-diffusion equation*, March 25.

——, *Inverse problems for hyperbolic equations from a geometrical optics viewpoint*, September 30.

S.V. ZELIK, Russian Academy of Sciences, Institute for Information Transmission Problems (at that time: Universität Stuttgart, Institut für Angewandte Analysis und Numerische Simulation), Moscow, *Sinai–Buinimovich space-time chaos in reaction-diffusion systems in R^n*, August 17.

S. ZHENG, Fudan University, Institute of Mathematics, Shanghai, China, *On the Cahn–Hilliard equations with dynamic boundary conditions*, June 23.

C. ZIEGLER, Fraunhofer-Institut für Solare Energiesysteme, Freiburg, *Investigation of the dynamics of the proton exchange membrane fuel cell*, November 23.

6.11 Membership in Organizing Committees of non-WIAS Meetings

E. BÄNSCH, member of the Local Organizing Committee, *The Second European Finite Element Fair*, Humboldt-Universität zu Berlin, June 4–5.

A. BOVIER, member of the Organizing Committee, *BRG Workshop (Dutch-German Research Group)*, EURANDOM, Eindhoven, The Netherlands, February 23–24.

——, co-organizer, *International Conference on Equilibrium and Dynamics of Spin Glasses*, Centro Stefano Franscini, Monte Verità, Ascona, Switzerland, April 18–22.

P. KREJČÍ, member of the Scientific Committee, *International Workshop on Hysteresis & Multi-Scale Asymptotics (HAMSA 2004)*, University College Cork, Ireland, March 17–21.

——, member of the Scientific Committee and co-organizer, *Sixth International Summer School on Evolution Equations (EVEQ 2004)*, Charles University, Faculty of Mathematics and Physics, Prague, Czech Republic, July 12–16.

K.K. SABELFELD, member of the Program Committee, *The International Conference on Computational Mathematics (ICCM 2004)*, Novosibirsk, Russia, June 21–25.

V. SPOKOINY, member of the Organizing Committee, *Workshop on New Inference Concepts for Analysing Complex Data*, Mathematisches Forschungszentrum Oberwolfach, November 14–20.

J. SPREKELS, organizer, *INdAM Workshop "Disipative Models in Phase Transitions"*, Cortona, Italy, September 5–11.

——, member of the Organizing Committee, *First Indo-German Conference on PDE, Scientific Computing and Optimization in Applications*, Universität Trier, Fachbereich Mathematik, September 8–10.

——, member of the Scientific Committee, *INTERPHASE 2004, Numerical Methods for Free Boundary Problems*, Dipartimento di Matematica "G. Castelnuovo", Università di Roma "La Sapienza", Italy, September 13–16.

D. TIBA, organizer of a mini-symposium, *7ème Colloque Franco-Roumain de Mathématiques Appliquées*, Bucharest, Romania, August 30 – September 3.

W. WAGNER, member of the Organizing Committee, *The Sixth International Workshop on Mathematical Aspects of Fluid and Plasma Dynamics*, Kyoto University, Japan, September 19–23.

K. WILMANSKI, organizer, chair, *Marie-Curie Forum* at the *XXI International Congress of Theoretical and Applied Mechanics (21st ICTAM 2004)*, Polish Academy of Sciences, Institute of Fundamental Technological Research, Warsaw, Poland, August 15–21.

——, co-organizer, chair, *XXI International Congress of Theoretical and Applied Mechanics (21st ICTAM 2004)*, Polish Academy of Sciences, Institute of Fundamental Technological Reseach, Warsaw, Poland, August 15–21.

6.12 Software

AWS (contact: J. Polzehl, phone: +49 30/20372-481)
AWS is an **A**daptive **W**eights **S**moothing package. A reference implementation of the adaptive weights smoothing procedures (AWS) is available in form of a contributed package of the R-Project for Statistical Computing (http://www.r-project.org/). The package includes functions for local polynomial structural adaptive smoothing in regression models with additive errors and for local constant structural adaptive smoothing in exponential family models, the latter including binary response, Poisson regression, exponential regression, and volatility models. The special case of a grid design allows for efficient reconstruction of non-smooth images in 2D and 3D.
The package can be obtained from http://CRAN.R-project.org/.
An extension of this package currently allows for multivariate models and contains functions for the analysis of fMRI and dMRI data.

BOP (contact: J. Borchardt, phone: +49 30/20372-485)
The simulator BOP (**B**lock **O**rientend **P**rocess simulator) is a software package for large-scale process simulation. It allows to solve dynamic as well as steady-state problems. Due to an equation-based approach, a wide range of processes as they occur in chemical process industries or other process engineering environments can be simulated.
The modeling language of BOP is a high-level language which supports a hierarchically unit-oriented description of the process model and enables a simulation concept that is based on a divide-and-conquer strategy. Exploiting this hierarchical modeling structure, the generated system of coupled differential and algebraic equations (DAEs) is partitioned into blocks, which can be treated almost concurrently. The used numerical methods are especially adopted for solving large-scale problems on parallel computers. They include backward differentiation formulae (BDF), block-structured Newton-type methods, and sparse matrix techniques.
BOP is implemented under UNIX on parallel computers with shared memory (Cray J90, SGI Origin2000, Compaq AlphaServer) but can also be run on different single processor machines as well as under Windows XP on PCs. So far it has been successfully used for the simulation of several real-life processes in heat-integrated distillation, sewage sludge combustion or gas turbine simulation, for example.
Detailed information: http://www.wias-berlin.de/software/BOP

ClusCorr98® (contact: H.-J. Mucha, phone: +49 30/20372-573)
The statistical software ClusCorr98® is an interactive statistical computing environment. It uses the Excel spreadsheet environment and its database connectivity. The programming language is Visual Basic for Applications (VBA). Tu run a macro inside Excel is quite an easy task. ClusCorr98® performs exploratory data analysis mainly by using adaptive methods of cluster analysis, classification, and multivariate visualization. The main focus here is on simple stable models accompanied by appropriate multivariate (graphical) methods like principal components analysis. Usually, the performance and stability of these methods can be improved by using them in a local and adaptive local fashion. Another highlight is the automatic validation technique of cluster analysis results performed by a general built-in validation tool for all hierarchical clustering methods that are available in the statistical software ClusCorr98®. This validation via resampling techniques is based on the adjusted Rand index. By doing so,

both the appropriate number of clusters can be validated and the stability of each cluster can be assessed. Furthermore, one can compare the performance of different cluster analysis methods. Please find further information under http://www.wias-berlin.de/software/ClusCorr98 and http://www.wias-berlin.de/people/mucha/Clustering.

DiPoG (contact: G. Schmidt, phone: +49 30/20372-456)
The program package `DiPoG` (**D**irect and **i**nverse **P**roblems for **o**ptical **G**ratings) provides simulation and optimization of periodic diffractive structures with multilayer stacks.
The direct solver computes the field distributions and efficiencies of given gratings for TE and TM polarization as well as under conical mounting for arbitrary polygonal surface profiles. The inverse solver deals with the optimal design of binary gratings, realizing given optical functions, for example, far-field patterns, efficiency, or phase profiles. The algorithms are based on coupled generalized finite/boundary elements and gradient-type optimization methods.
For detailed information please see also http://www.wias-berlin.de/software/DIPOG.

gltools (contact: J. Fuhrmann, phone: +49 30/20372-560)
`gltools` has been designed with the needs of numerical analysts in mind. Thus, unlike many other packages available, it can be used to enhance existing codes with interactive or non-interactive graphical output. It enhances the OpenGL API with the following additional functionality:

– multiple independent windows;
– basic interactive handling through mouse and keyboard;
– interactive three-dimensional rendering volume;
– character output;
– high-quality frame dump in encapsulated postscript format;
– MPEG video recording of window contents;
– piecewise linear function rendering on two- and three-dimensional simplex meshes (landscape view of plane sections, isolevel surfaces, isolines) with an
– universal, callback-based mesh interface.

Please find further information under http://www.wias-berlin.de/software/gltools.

LDSL-tool (contact: M. Radziunas, phone: +49 30/20372-441)
`LDSL-tool` (**L**ongitudinal **D**ynamics in **S**emiconductor **L**asers) is a tool for the simulation and analysis of the nonlinear longitudinal dynamics in multi-section semiconductor lasers. This software is used to investigate and to design lasers which exhibit various nonlinear effects such as self-pulsations, chaos, hysteresis, mode switching, excitability, and synchronization to an external signal frequency.
`LDSL-tool` combines models of different complexity, ranging from partial differential equation (PDE) to ordinary differential equation (ODE) systems. A mode analysis of the PDE system, a comparison of the different models, and a numerical bifurcation analysis of PDE systems are also possible.
Detailed information: http://www.wias-berlin.de/software/ldsl

pdelib (contact: J. Fuhrmann, phone: +49 30/20372-560)
`pdelib` is a collection of software components which are useful to create simulators based on partial differential equations. The main idea of the package is modularity, based on a pattern-oriented bottom-up design. Among others, it provides libraries for

– iterative solvers;
– sparse matrix structures with preconditioners and direct solver interfaces;
– simplex grid handling;
– graphical output using `gltools` and OpenGL;
– user interface based on the scripting language Lua.

Further, based on the finite volume implicit Euler method, a solver for systems of nonlinear reaction-diffusion-convection equations in heterogeneous one-, two-, and three-dimensional domains has been implemented which is part of the package.
For more information please see also http://www.wias-berlin.de/software/pdelib.

WIAS-HiTNIHS (contact: O. Klein, phone: +49 30/20372-533)
The WIAS-**Hi**gh **T**emperature **N**umerical **I**nduction **H**eating **S**imulator constitutes a transient simulation tool for the temperature evolution in axisymmetric technical systems that are subject to intense heating by induction. The simulator accounts for heat transfer by radiation through cavities, and it allows for changes in the material parameters due to the rising temperature and for some kinds of anisotropy within the thermal conductivity.
The simulator is designed to deal with complicated axisymmetric setups having a polygonal 2D projection. The software is based on the WIAS program package `pdelib` for the numerical solution of partial differential equations.
`WIAS-HiTNIHS` has been and is further developed within the project *"Numerical simulation and optimization of SiC single crystal growth by sublimation from the gas phase"* (see p. 161) supported by BMBF (until 2003) and DFG (since 2002).
Please find further information under http://www.wias-berlin.de/software/hitnihs.

WIAS-SHarP (contact: D. Hömberg, phone: +49 30/20372-491)
Based on `pdelib`, `WIAS-SHarP` (**S**urface **Har**dening **P**rogram) is a software for the simulation of electron and laser beam surface hardening. It contains a data bank with material parameters for 20 important steels as well as routines to describe the phase transition kinetics during one heat treatment cycle. Moreover, it allows for an easy implementation of different radiation flux profiles. To facilitate its usage, a Java-based GUI has been developed.
For more information see http://www.wias-berlin.de/software/sharp.

WIAS-TeSCA (contact: R. Nürnberg, phone: +49 30/20372-570)
`WIAS-TeSCA` is a **T**wo- and thre**e**-dimensional **S**emi-**C**onductor **A**nalysis package. It serves to simulate numerically the charge carrier transport in semiconductor devices based upon the drift-diffusion model. This van Roosbroeck system is augmented by a vast variety of additional physical phenomena playing a role in the operation of specialized semiconductor devices, as, e.g., the influence of magnetic fields, optical radiation, temperature, or the kinetics of deep (trapped) impurities.
The strategy of `WIAS-TeSCA` for solving the resulting highly nonlinear system of partial differential equations is oriented towards the Lyapunov structure of the system which describes

the currents of electrons and holes within the device. Thus, efficient numerical procedures, for both the stationary and the transient simulation, have been implemented, the spatial structure of which is a finite volume method. The underlying finite element discretization allows the simulation of arbitrarily shaped two-dimensional device structures.
`WIAS-TeSCA` has been successfully used in the research and development of semiconductor devices such as transistors, diodes, sensors, detectors, and lasers.
The semiconductor device simulation package `WIAS-TeSCA` operates in a UNIX environment and is available for a variety of configurations as, e.g., SUN, COMPAQ, HP, SGI, but also for Linux PC.
For more information please look up http://www.wias-berlin.de/software/tesca.

WIAS-QW (contact: U. Bandelow, phone: +49 30/20372-471)
`WIAS-QW` is a numerical code for the simulation of strained multi-quantum-well structures. Based upon multiband kp models it allows to treat band mixing effects, confinement effects, crystal symmetry, and the influence of mechanical strain.
In particular, `WIAS-QW` calculates the

– subband dispersion;
– eigenfunctions;
– transition matrix elements;
– miniband effects in multi-quantum-well structures.

In dependence on the sheet carrier densities and the temperature, `WIAS-QW` calculates the

– optical response function;
– gain spectrum;
– radiative recombination rate;
– carrier density distributions.

Furthermore, the calculations can be done selfconsistently, comprising pure kp calculations, but also calculations which include the Hartree–Coulomb potential, obtained from Poisson's equation, as well as density-dependent exchange-correlation potentials, which account for the bandgap-shift—one of the most prominent many-particle effects.
Please find further information under http://www.wias-berlin.de/software/qw.

6.13 Grants

Bundesministerium für Bildung und Forschung (Federal Ministry of Education and Research), Bonn

- **Mathematik für Innovation in Industrie und Dienstleistungen (Mathematics for innovations in industry and services)**

  "Anwendung eines nichtlokalen Phasenseparationsmodells zur Bildbewertung in der Rheumadiagnostik" (Application of a nonlocal phase separation model to optical diagnosis of rheumatic diseases, FG 1)

- **Technische Anwendungen der Nichtlinearen Dynamik (Technical applications in nonlinear dynamics)**

  "Hochfrequente Selbstpulsationen in Mehrsektions-Halbleiterlasern: Analysis, Simulation und Optimierung" (High frequency self-pulsations in multi-section semiconductor lasers: Analysis, simulations, and optimization, FG 2)

- **COMPERE** (BMBF-DLR: Treibstoffverhalten in Tanks von Raumtransportsystemen — Comportement des Ergols dans les Réservoirs, FG 3)

Deutsche Forschungsgemeinschaft (German Research Foundation), Bonn

- **DFG-Forschungszentrum** MATHEON **"Mathematik für Schlüsseltechnologien" (DFG Research Center** MATHEON **"Mathematics for Key Technologies")**, Technische Universität Berlin

  A3: "Image and signal processing in medicine and biosciences" (FG 6)

  C1: "Coupled systems of reaction-diffusion equations and application to the numerical solution of direct methanol fuel cell (DMFC) problems" (FG 3)

  C2: "Efficient simulation of flows in semiconductor melts" (FG 3)

  C7: "Mean-risk models for electricity portfolio management and stochastic programming" (FG 4)

  C8: "Shape optimization and control of curved mechanical structures" (FG 1)

  C9: "Optimal control of sublimation growth of SiC bulk single crystals" (FG 1)

  C10: "Modelling, asymptotic analysis and numerical simulation of thin liquid films" (FG 7)

  C11: "Modeling and optimization of phase transitions in steel" (FG 3, 4)

  D3: "Global singular perturbations" (FG 2)

  D4: "Quantum mechanical and macroscopic models for optoelectronic devices" (FG 1)

  D8: "Nonlinear dynamical effects in integrated optoelectronic structures" (FG 1, 2)

  E1: "Microscopic modelling of complex financial assets" (FG 5)

  E5: "Statistical and numerical methods in modeling of financial derivatives and valuation of portfolio risk" (FG 6)

- Collaborative Research Centre (Sfb) 555, Humboldt-Universität zu Berlin,
  "Komplexe Nichtlineare Prozesse. Analyse — Simulation — Steuerung — Optimierung" (Complex non-linear processes. Analysis — simulation — control — optimization)

  "Analytische und numerische Untersuchungen zur raum-zeitlichen Strukturbildung in Halbleiterlasern" (Analytical and numerical investigations on the spatio-temporal formation of structures in semiconductor lasers, FG 1, 2)

- Priority Program: "Analysis, Modellbildung und Simulation von Mehrskalenproblemen" (Analysis, modeling and simulation of multiscale problems)

  "Mehrskalenmethoden zur Beschreibung elektronischer Zustände in Halbleiter-Nanostrukturen" (Multiscale methods for the description of electronic states in semiconductor nanostructures, FG 1, 3, 4)

  "Mehrskalenmodellierung thermomechanischer Körper" (Multiscale models of thermomechanical bodies, FG 1, 7)

  "Mikro-Makro-Übergänge in der atomaren Kette für verschiedene Skalierungen" (Micro-macro transitions in the atomic chain for various scalings, FG 1, 7)

- Priority Program: "Mathematische Methoden der Zeitreihenanalyse und digitalen Bildverarbeitung" (Mathematical methods for time series analysis and digital image processing)

  "Structure adaptive smoothing procedures with applications in imaging and functional MRI" (FG 6)

- Priority Program "Dynamik sedimentärer Systeme unter wechselnden Spannungsregimen am Beispiel des zentraleuropäischen Beckens" (Dynamics of sedimentary systems under varying stress regimes: The example of the Central European Basin)

  "Deep reaching fluid-flow in the Central European Basin System" (FG 3)

- **Normalverfahren (Individual Grants)**

  "Spektralparameterabhängige Randwertprobleme und Hybridmodelle der Halbleitersimulation" (Boundary value problems depending on the spectral parameter and hybrid models in semiconductor simulation, FG 1)

  "Energiemodelle für heterogene Halbleiterstrukturen" (Energy models for heterogeneous semiconductor structures, FG 1)

  "Einfluss räumlicher Fluktuationen auf das Gelationsverhalten von Koagulationsprozessen" (Influence of spatial fluctuations on the gelation behavior of coagulation processes, FG 5)

  "Hydrodynamische Fluktuationen von Verzweigungsmodellen in katalytischen Medien mit unendlicher Erwartung" (Hydrodynamic fluctuations of branching models in catalytic media with infinite expectations, FG 5)

  "Models for phase transition with thermo-mechanical interaction" (FG 7)

  "Mathematical modeling and analysis of spreading polymer films" (FG 7)

- Graduate College, Technische Universität Berlin
  "Stochastische Prozesse und Probabilistische Analysis" (Stochastic processes and probabilistic analysis, FG 5, 6)

- Graduate College, Technische Universität Berlin
  "Transportvorgänge an bewegten Phasengrenzflächen" (Transport phenomena with moving boundaries)

  Project 2: "Numerische Verfahren und Simulation für die Fallfilmverdampfung" (Numerical methods and simulation of thin film instabilities including evaporation effects, FG 3)

- Cooperation project "Singulär gestörte Systeme und Stabilitätswechsel" (Singularly perturbed systems and exchange of stability) of German and Russian scientists in the framework of the *Memorandum of Understanding* between DFG and RFFI (FG 2)

- In 2004, WIAS hosted two scientists with a Heisenberg fellowship (FG 2, 7).

- A part of the WIAS guest program was supported by DFG grants.

Alexander von Humboldt-Stiftung (Alexander von Humboldt Foundation)

- 1 Humboldt Laureate (FG 2) and 1 scholarship holder (FG 5), see page 256

Deutscher Akademischer Austauschdienst (German Academic Exchange Service), Bonn

- PROCOPE (FG 1)

International Projects

- **NATO Linkage Grant:** "Stochastic and computational models of transport in porous media" (FG 6)

- **ESF** (European Science Foundation) Programme "Phase transitions and fluctuation phenomena for random dynamics in spatially extended systems (RDSES)" (FG 5)

- The head of Research Group 5 is a member of the Bilateral Research Group "Mathematics of random spatial models from physics and biology" (DFG/NWO (Netherlands Organization for Scientific Research)), project: "Equilibrium and ageing in glassy systems".

Verbundforschungsvorhaben (research network project): "Terabit Optics Berlin", project B4: "Modellierung und Simulation von Pulsquellen" (Modeling and simulation of pulse sources)

- "Simulation der Pulsausbreitung in nichtlinearen optischen Fasern" (Simulation of pulse propagation in nonlinear optical fibers, FG 1)

- "Modeling and simulation of mode-locked semiconductor lasers" (FG 2)

Mission-oriented research

- ALSTOM (Switzerland) Ltd., Baden: "Prozesssimulation bei industriellen Gasturbinen" (Process simulation for industrial gas turbines, FG 3)

- autronic-MELCHERS GmbH, Karlsruhe: “3D Delaunay grid generation using TetGen” (FG 3)
- Bankgesellschaft Berlin: “Implementation of the LIBOR market model, calibration and pricing of derivative products” (FG 6)
- Carl Zeiss, Oberkochen: Verbundprojekt/Collaborative project HYBROS (Grundlegende Untersuchungen zu Design und Realisierung neuartiger hybrider Optik-Systeme — basic research into design and implementation of novel hybrid optics systems, FG 4)
- Intel Corp. Hillsboro, Oregon, USA: “Optimization of the sparse direct solver PARDISO for use in the Intel Math Kernel Library” (FG 3)
- Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie, Berlin: “Berechnung der elektronischen Bandstruktur von InAsSb-Quantenwells” (Calculation of the electronic band structure of InAsSb multiquantum wells, FG 1)
- Reuters Financial Software Paris: Consulting contract (FG 6)
- Rücker GmbH, Weingarten: “Bahnplanung für Industrieroboter und Menschmodelle” (Path planning for robots and human models, FG 4)
- Science & Tec, Lisieux, France: “Assistance à la mise en place d’une méthodologie de la mesure du comportement des matériaux sous irridation dans le réacteur RJH” (FG 5)
- Volkswagen AG, Wolfsburg: “Modellierung und Parameteridentifikation für Kostenparameter von Fabriken” (Modeling and parameter identification for cost parameters of factories, FG 4)

HP Integrity for Research Program

- Donation of an Itanium-based Integrity server by Hewlett-Packard Company

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