Weierstraß-Institut
für Angewandte Analysis und Stochastik
(WIAS)

im Forschungsverbund Berlin e. V.

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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 2003 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 2003 to its colleagues, supporters, and cooperation partners. In its first part, the report informs about the progress made and the results obtained in 2003, divided into research areas, projects, and single topics. The second part gives a general account of the scientific life at WIAS.

In wissenschaftlicher Hinsicht war das Jahr 2003 wiederum erfolgreich. Die Arbeiten am *Forschungsprogramm 2001–2003* wurden weitergeführt. Es gelang dem Institut, in Zeiten knapper werdenden Geldes und wachsender Konkurrenz 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.

From a scientific point of view, the year 2003 has again been successful. Work on the *Research Program 2001–2003* has been continued. In spite of the growing shortness of money and a growing competition, WIAS 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.

Die positive Entwicklung spiegelt sich wider in der im Vergleich zum Vorjahr wiederum gesteigerten Drittmitteleinwerbung, der Anzahl der in referierten Fachzeitschriften erschienenen Publikationen und der eingeladenen Vorträge auf internationalen Tagungen.

The positive development is reflected by the again increased third-party funds that have been raised in 2003, compared to last year's funds, the number of publications that appeared in refereed journals, and the number of invited talks at international conferences.

Besonders augenfällig wird der hohe Stellenwert, den die am WIAS geleistete Arbeit in der Scientific Community hat, wiederum im Bereich der Berufungen: Im Berichtsjahr 2003 ergingen vier Rufe an Mitarbeiter des Instituts auf Professuren, davon eine ins Ausland. Ins-

The high rank of WIAS's research work in the scientific community becomes again especially clear in the field of calls: in 2003, four calls to professorships were received by WIAS collaborators, including one to a professorship abroad. Altogether, since the institute's foun-

gesamt sind nunmehr seit der Gründung des Instituts im Jahre 1992 schon 28 Rufe an Mitarbeiter/innen des Instituts auf Professuren erfolgt (davon 15 auf C4-Professuren und acht auf Professuren im Ausland), eine Bilanz, die sich bei einer Zahl von derzeit 54 etatisierten Wissenschaftlern wirklich sehen lassen kann.

dation in 1992, 28 calls have been received by collaborators of WIAS (including 15 to C4 (full) professorships and eight 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. Dabei wurden im Berichtsjahr zwei gemeinsame Berufungen mit der Technischen Universität Berlin erfolgreich abgeschlossen, nämlich die Berufung des Leiters der Forschungsgruppe „Nichtlineare Optimierung und Inverse Probleme“ auf eine C4-S-Professur für „Numerische nichtlineare Optimierung“ und die Berufung des Leiters der Forschungsgruppe „Stochastische Systeme mit Wechselwirkung“ auf eine C4-S-Professur „Vernetzte stochastische Systeme“. Insgesamt sind nunmehr fünf gemeinsame Berufungen auf C4-S-Professuren mit den Berliner Universitäten realisiert. Für eine weitere gemeinsame Berufung, nämlich die des zukünftigen Leiters der Forschungsgruppe „Partielle Differentialgleichungen und Variationsgleichungen“ auf eine C4-S-Professur für „Partielle Differentialgleichungen“ an der Humboldt-Universität zu Berlin, ist inzwischen der Ruf an den Erstplatzierten der Berufungsliste ergangen.

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. In 2003, two joint appointments with the Technical University of Berlin have been successfully completed, namely the call for the head of the research group “Nonlinear Optimization and Inverse Problems” to a C4 special professorship for “Numerical Nonlinear Optimization” and the call for the head of the research group “Interacting Random Systems” to a C4 special professorship for “Networked Stochastic Systems”. Now altogether five joint appointments to C4 special professorships with the Berlin universities have been concluded. For one further joint appointment, this one for the future head of the research group “Partial Differential Equations and Variational Equations” to a C4 special professorship “Partial Differential Equations” at Humboldt University of Berlin, meanwhile the candidate placed first in the ranked list has received the call.

Neben diesen Aktivitäten und neben der Zusammenarbeit mit den Hochschulen durch die vielfältigen von Mitarbeitern des WIAS abgehaltenen Lehrveranstaltungen, die Beteiligung an Sonderforschungsbereichen, Schwerpunktprogrammen und Graduiertenkollegs der DFG, war von zentraler Bedeutung die Kooperation im Rahmen des DFG-Forschungszentrums FZT

Besides these activities and besides the cooperation with the universities through manifold teaching activities by WIAS collaborators, the participation in DFG Collaborative Research Centers, Priority Programs, and Graduate Colleges, the cooperation in the framework of the DFG Research Center FZT 86 “Mathematics for Key Technologies” at the Technical Uni-

86 „Mathematik für Schlüsseltechnologien“ an der Technischen Universität Berlin. Das WIAS engagiert sich in erheblichem Maße finanziell und 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 12 Teilprojekten des Forschungszentrums als Teilprojektleiter beteiligt. Insgesamt acht wissenschaftliche Mitarbeiter und mehrere studentische Hilfskräfte wurden im Jahre 2003 aus Zentrumsmitteln am WIAS beschäftigt.

versity of Berlin was of central interest. WIAS is committed to the success of the Center by providing considerable financial and personal 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 12 subprojects of the Center. Altogether, eight scientific collaborators and several student assistants were employed by WIAS from Center funds in 2003.

Neben der wissenschaftlichen Arbeit war jedoch das zentrale Ereignis des Jahres 2003 die Anfang Juli erfolgte Evaluierung des Instituts durch den Senat der Leibniz-Gemeinschaft, die einen erheblichen Aufwand in der Vorbereitung erforderte. Das Ergebnis der Evaluierung war außerordentlich positiv. Zentrales Statement des Bewertungsberichts der Evaluierungskommission war:

The central event in 2003, in addition to the scientific work, however, was the institute’s evaluation, early in July, by the Leibniz Association’s Senate, that required a considerable amount of preparatory work. The evaluation’s result was exceptionally positive. 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 Gesamteindruck 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 mit seiner forschungsstrategischen Ausrichtung „einzigartig positioniert“ zu sein (national und international).

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 “singularly positioned” (nationally and internationally) for the strategic orientation of its research work.

Die Mitarbeiter des Instituts sehen sich in dieser äußerst positiven Einschätzung darin bestätigt, in den vergangenen Jahren hervorragende Arbeit geleistet zu haben. Gleichzeitig ist dies ein Ansporn für das gesamte WIAS, den beschrittenen Weg konsequent fortzusetzen.

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 zunehmenden Mittelknappheit in allen Bereichen immer schwieriger. Bisher hat sich das WIAS erfolgreich dem wissenschaftlichen Wettbewerb um die Fördermittel gestellt und die erfolgten Kürzungen durch vermehrte Anstrengungen in der Drittmitteleinwerbung weitgehend kompensieren können. Allerdings gibt es hierfür eine Grenze: Eine hinreichende Grundausstattung ist unerlässlich, damit das Institut auch weiterhin erfolgreich im wissenschaftlichen Wettbewerb bestehen kann.

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.

WIAS's collaborators find themselves confirmed by this utterly positive estimation to have done a very good job in the last years. At the same time, this is an encouragement for the whole institute to follow persistently the chosen path.

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 growing shortness of funds in all areas. Thus far, WIAS has successfully taken up the challenge of the scientific competition for additional funds from support programs and has been able to compensate for the financial cuts by an intensified effort in the raising of third-party funds. But there is a limit to this: A sufficient basic equipment is imperative for the institute to remain successful in the scientific competition.

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 start to cooperate with us.

Berlin, im April 2003 / in April 2003

J. Sprekels

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 over 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 2, FG 3 und FG 4)
- Simulation and control of chemical plants (in FG 2, 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 1)
- Problems of Optimal Shape Design (in FG 1)

3.1.3 Phasenübergänge / Phase transitions

- Wärmebehandlung und Schweißverfahren bei Stählen (Modellierung und Simulation; in FG 1)
- Heat treatment and welding processes for steels (modeling and simulation, in FG 1)
- 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 1 und FG 7)

- Stochastic modeling of phase transitions and spin glasses (in FG 5)
- Growth processes of SiC and GaAs single crystals (in FG 1 and 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 1 und FG 4)
- 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 (`WIAS-TeSCA`, `ClusCorr98`®, `DiPoG`, `COG`, `LDSL-tool`, `pdelib` und andere, siehe S. 255; in FG 1, FG 2, FG 3, FG 4 und FG 6)

- 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 1 and FG 4)
- 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 (`WIAS-TeSCA`, `ClusCorr98`®, `DiPoG`, `COG`, `LDSL-tool`, `pdelib` and others, see page 255; in FG 1, FG 2, FG 3, FG 4, and FG 6)

3.2 Organisatorische Struktur / Organizational Structure

Zur Erfüllung seiner wissenschaftlichen Aufgabenstellung war das WIAS im Berichtsjahr 2003 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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FORSCHUNGSGRUPPE/ RESEARCH GROUP 4
Nichtlineare Optimierung und Inverse Probleme / Nonlinear Optimization and Inverse Problems
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FORSCHUNGSGRUPPE/ RESEARCH GROUP 5
Stochastische Systeme mit Wechselwirkung / Interacting Random Systems
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FORSCHUNGSGRUPPE/ RESEARCH GROUP 6
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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. Die betrachteten Gleichungen modellieren komplexe Phänomene und Prozesse insbesondere aus Physik, Chemie, Materialwissenschaften und Technik und bilden die Grundlage zu deren numerischer Simulation.
Die Forschungsschwerpunkte der Forschungsgruppe lagen im Jahr 2003 auf den Gebieten

- Stoff-, Ladungs- und Energietransport in heterogenen Halbleiterstrukturen,
- Modellierung optoelektronischer Bauelemente unter Einbeziehung von Quantisierungseffekten,
- Phasenfeldmodelle, Züchtungssimulation und Hysterese-Phänomene bei Phasenübergängen.

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. The equations under study model complex phenomena and processes particularly from physics, chemistry, materials science, and technology and form the basis for their numerical simulation.

In 2003, the group's research work focused on the areas

- Materials, charge, and energy transport in heterogeneous semiconductor structures;
- Modeling of opto-electronical components including quantization effects;
- Phase-field models, growth simulation, and hysteresis phenomena in phase transitions.

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. Das zentrale Forschungsthema der Gruppe war die

- Nichtlineare Dynamik von Mehrsektions-Halbleiterlasern.

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

The mathematical modeling of scientific and technological processes requires the efficient numerical solution of systems of nonlinear or-

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.

dinary 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 Arbeiten dieser Forschungsgruppe befassten sich mit der theoretischen Analyse, Entwicklung und Implementierung numerischer Methoden für große Probleme der Optimierung und Inversen Modellierung. Die Themenschwerpunkte lagen in den Bereichen

- Modellierung und optimales Design diffraktiver Strukturen der Mikrooptik,
- Nichtlineare und stochastische Optimierung in der Verfahrenstechnik,
- Inverse Probleme der Elektromagnetik und Optik.

This research group was occupied with the theoretical analysis, development, and implementation of numerical methods for large problems originating from the fields of optimization and inverse modeling. The main areas of research were

- Modeling and optimal design of diffractive structures in micro-optics;
- Nonlinear and stochastic optimization in process engineering;
- Inverse problems of electromagnetics and optics.

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

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

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

- 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. 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 research group worked on problems from Applied Stochastics and Financial Mathematics. 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 Kontinuumsmechanik / Research Group Continuum Mechanics

Die Arbeiten dieser Forschungsgruppe befassten sich im Berichtszeitraum mit speziellen kontinuumsmechanischen und thermodynamischen Fragestellungen, die bei konkreten Anwendungsproblemen aus Naturwissenschaften und Technik auftreten. Die Arbeitsschwerpunkte lagen dabei in den Bereichen

- Wellenausbreitung und Massenaustausch in porösen Medien,
- Mikro-Makro-Übergänge.

The research group concentrated its work in the year under review on specific problems of continuum mechanics and thermodynamics that appeared in concrete applications in sciences and technology. The main areas of research were

- Wave propagation and mass exchange in porous media;
- Micro-macro transitions.

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 ar-

The *Administration* attends to the administrative and organizational tasks thus enabling the institute to fulfil its mission. WIAS has legally joined forces with seven more 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 administra-

beitsteilig von der *Gemeinsamen Verwaltung des FVB* und den *Institutsverwaltungen* erbracht. Dem *Geschäftsführer* des FVB obliegt die Führung der Verwaltungsgeschäfte.

tive 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 mikro- und optoelektronischen Bauelementen sowie von Phasenumwandlungen fortgesetzt. Ihre analytischen Arbeiten reichen von grundlegenden Untersuchungen zur Existenz, Einzigkeit und dem qualitativen Verhalten von Lösungen der Modellgleichungen über die Begründung, Implementierung und praktische Erprobung von Näherungsverfahren bis zur Installation von Lösungsalgorithmen bei Kooperationspartnern.

According to the WIAS research program the research group has continued its work in mathematical modeling and analysis of micro- and optoelectronic devices and phase transitions. The analytical work covers basic investigations on existence, uniqueness, and qualitative behavior of solutions to the model equations, foundation, implementation, and practical testing of approximative procedures up to the implemention of solution algorithms for cooperation partners.

Die Forschungsgruppe ist am DFG-Forschungszentrum „Mathematik für Schlüsseltechnologien“ mit folgenden Projekten beteiligt:

The research group takes part in the DFG Research Center “Mathematics for Key Technologies” with the projects:

- Formoptimierung und Kontrolle gekrümmter mechanischer Strukturen,
- Optimale Steuerung der Sublimations-Züchtung von SiC-Einkristallen,
- Quantenmechanische und makroskopische Modelle optoelektronischer Bauelemente.

- Shape optimization and control of curved mechanical structures;
- Optimal control of sublimation growth of SiC bulk single crystals;
- Quantum mechanical and macroscopic models for optoelectronic devices.

Durch Drittmittel werden auch weitere Arbeiten der Forschungsgruppe finanziert. Dazu gehören die im Rahmen des BMBF-Programms „Neue Mathematische Methoden in Industrie und Dienstleistungen“ geförderten Projekte:

Moreover, further research work of the group has been funded from external sources:
The following projects have been supported by the BMBF Program “New Mathematical Methods in Industry and Services”.

- Optische Sensoren,
- Numerische Simulation und Optimierung der Züchtung von SiC-Einkristallen durch Sublimation aus der Gasphase.

- Optical sensors;
- Numerical simulation and optimization of SiC single crystal growth by sublimation from the gas phase.

Die DFG unterstützte die Forschungsprojekte:

- Multiskalenmodellierung thermomechanischer Körper,
- Enveloppenfunktionsapproximation für elektronische Zustände in Halbleiter-Nanostrukturen,
- Hysterese-Operatoren in Phasenfeld-Gleichungen,
- Kopplung von van Roosbroeck- und Schrödinger-Poisson-Systemen mit Ladungsträgeraustausch,
- Physikalische Modellierung und numerische Simulation von Strom- und Wärmetransport bei hoher Trägerinjektion und hohen Temperaturen,
- Analytische und numerische Untersuchungen zur Strukturbildung in Halbleitern.

Von der Industrie finanziert wurde das Projekt:

- `WIAS-TeSCA`-Simulationen von Laserdioden.

Vom Projekt Terabit Optics Berlin wurde das Thema

- Simulation der Pulsausbreitung in nichtlinearen optischen Fasern

finanziert.

The DFG has sponsored the research projects

- Multi-scale modeling of thermomechanical bodies;
- Envelope function approximation for electronic states in semiconductor nanostructures;
- Hysteresis operators in phase-field equations;
- Coupling between van Roosbroeck and Schrödinger-Poisson systems including exchange of carriers;
- Physical modeling and numerical simulation of current and heat transport at high carrier injection and high temperatures;
- Analytical and numerical investigations on structure formation in semiconductors.

The project

- `WIAS-TeSCA` simulations of laser diodes

has been supported by industrial funds.

The project Terabit Optics Berlin has funded the theme

- Simulation of pulse propagation in nonlinear optical fibers.

4.1.2 Projects

Simulation of pulse propagation in nonlinear optical fibers

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

Cooperation with: Fraunhofer-Institut für Nachrichtentechnik, Heinrich-Hertz-Institut (HHI), Berlin

Supported by: Terabit Optics Berlin (project B4)

Wave propagation in dispersive nonlinear media has become a topic of intense research activities, in part stimulated by its potential application to optical fiber communication systems. Propagation of optical pulses in monomode optical fibers is mainly influenced by the group velocity dispersion and the refractive index nonlinearity. The propagation of sub-picosecond optical pulses is governed by a generalized nonlinear Schrödinger equation (NLSE) (1), which can be derived from the underlying Maxwell equations within the slowly varying envelope approximation (see [1]). This means that the pulse envelope $A(z,t)$ modulating the underlying carrier wave $\exp[i(k_0 z - \omega_0 t)]$ is assumed to be slowly varying in time and space. The pulse width has to be much longer than the carrier oscillation period and the spectral content of the field has to be narrower than the carrier frequency ω_0 itself. This is satisfied for optical pulses with widths down to 10 fs.
The general form of the NLSE for the complex envelope $A(z,\tau)$ of a pulse is given by

$$\begin{aligned}\frac{\partial A}{\partial z} &= -\frac{i}{2}\beta_2\frac{\partial^2 A}{\partial \tau^2} + \frac{1}{6}\beta_3\frac{\partial^3 A}{\partial \tau^3} + \frac{i}{24}\beta_4\frac{\partial^4 A}{\partial \tau^4} - \frac{1}{2}\alpha A \\ &\quad + i\gamma|A|^2 A - a_1\frac{\partial}{\partial \tau}\left(|A|^2 A\right) - i a_2 A\frac{\partial}{\partial \tau}\left(|A|^2\right), \end{aligned} \tag{1}$$

where the initial value problem $A(0,\tau) = f(\tau)$ along z within a retarded time frame $\tau = t - z/v_g$ has to be solved. The linear terms on the right-hand side of Eq. (1) are the group velocity dispersion (GVD), namely second-order (SOD), third-order (TOD) and fourth-order dispersion (FOD) and the attenuation term corresponding to the fiber loss α. The main contribution to the group velocity dispersion is represented by the parameter β_2, which leads in general to a broadening of the pulse shape. TOD and FOD are higher-order effects originating from the wavelength dependence of the group velocity dispersion. These dispersive effects can distort ultrashort optical pulses in the linear as well as in nonlinear regimes. Another important fiber parameter is the measure of power loss during the transmission of optical signals inside the fiber, given by the attenuation constant α.
The first nonlinear term represents the self-phase modulation (SPM), which results from the intensity dependence of the refractive index. It is responsible for a large variety of phenomena, such as spectral broadening or optical solitons. The term proportional to a_1 results from the intensity dependence of the group velocity and causes self-steepening and shock formation at the pulse edge. The last term considers the intrapulse Raman scattering and originates from the delayed response, which causes a self-frequency shift. $a_2 = \gamma T_R$, where T_R is related to the slope of the Raman gain. The intrapulse Raman scattering becomes a dominant perturbation for ultrashort pulses and is one of the most important limitations for ultrashort pulse propagation in optical fibers.

In [1] we have derived the NLSE (1) from the Maxwell equations in a non-standard way, showing that the neglect of the 2nd derivative with respect to z is no approximation as often claimed in the literature. In general a numerical approach is needed for an investigation of the generalized NLSE. For the numerical solution we have developed a code based on a standard dealiased pseudospectral method with a Runge-Kutta integration scheme ([1]). This scheme differs from the most commonly used split-step Fourier method and guarantees a higher accuracy, because no further approximations to (1) are used. Using our code we have investigated the impact of the various terms in (1) separately as well as their interplay, where we could reproduce previous analytical as well as experimental data ([1]). As the most prominent application we have studied the propagation of optical solitons. As an example the temporal evolution of a third-order soliton over one soliton period is drawn in Figure 1 (left). Perturbations caused by self-steepening and intrapulse Raman scattering break the degeneracy of solitons. The higher-order solitons decompose then into their constituents, which propagate at different speed. In the case of the intrapulse Raman scattering the low-intensity pulse is advanced, Figure 1 (right), whereas in the case of self-steepening both pulses are delayed.
Moreover, we have investigated the phenomenon of supercontinuum (SC) generation, where ultrabroad optical spectra are generated during the propagation of femto- or high-power picosecond pulses through dispersive nonlinear media ([2]). We have demonstrated that the primary mechanism for SC generation is the modulation instability (MI), accompanied by four-wave mixing. Higher-order effects, such as the self-steepening effect and the Raman effect were shown to be of minor influence on the generation of broad spectra. Raman scattering affects mainly the shape of the spectra. Because higher-order effects are not a prerequisite for the generation of SC, it is not restricted only to ultrashort sub-picosecond pulses. The MI enhances when higher-order dispersive terms are present, such that it can appear also in the normal dispersion regime ($\beta_2 > 0$), if the fourth-order dispersion coefficient β_4 is negative.

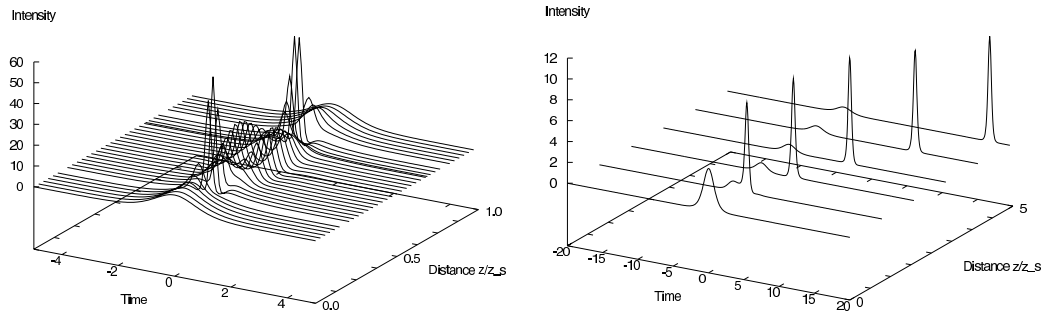

Fig. 1: Spatio-temporal evolution of a 3rd-order soliton in an optical fiber (left) and of a soliton decay induced by Raman scattering (right)

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

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WIAS-TeSCA simulations of laser diodes

Collaborators: U. Bandelow, H. Gajewski, A. Glitzky, R. Hünlich

Cooperation with: F. Heinrichsdorff, N. Kirchstädter (LUMICS GmbH Berlin)

Supported by: LUMICS GmbH Berlin

The static and dynamic performance of laser diodes is analyzed on the basis of different models. The device simulator `WIAS-TeSCA`, [3], uses two-dimensional models in the transverse cross section combined with rate equations in the longitudinal direction. Numerical solutions of these equations allow for an exploration of a wide spectrum of lasing effects.

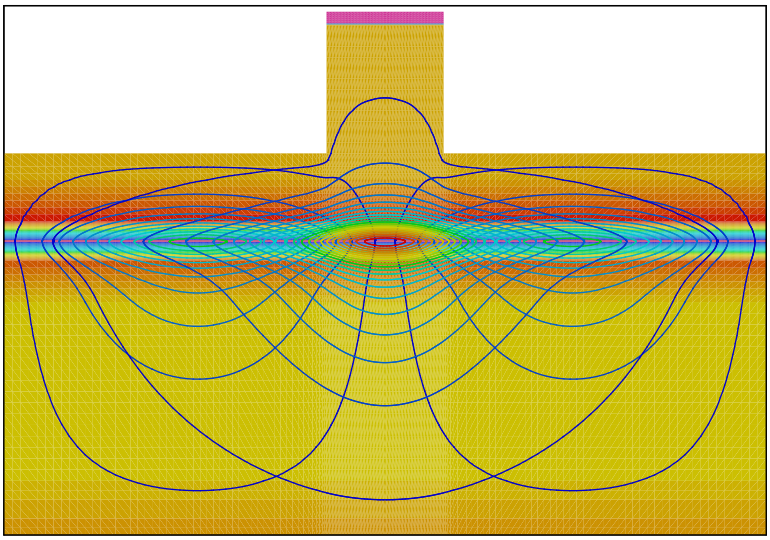

Fig. 1: Schematic transverse cross section of a ridge waveguide semiconductor laser diode

Figure 1 shows a schematic transverse cross section of a GaAs-based high-power laser diode. The colors indicate different materials, the lines represent the intensity distribution of two optical modes.

The underlying model equations for the relevant electronic, thermodynamic, and optical phenomena form a system of nonlinear partial differential and ordinary differential equations. The electronic processes are described by continuity equations for electrons and holes, and a Poisson equation for the electrostatic potential (drift-diffusion model). Thermodynamic behavior is modeled by a heat flow equation for the device temperature (or equivalently by balance equations for the density of the entropy or the internal energy), [1]. Finally, Helmholtz equations for different modes of the transverse optical field and corresponding photon balance equations in longitudinal direction characterize the optical behavior, [2].

In this project we used our simulation tool `WIAS-TeSCA` to calculate stationary characteristics for laser diodes of the company LUMICS GmbH. For this purpose we solved the stationary equations to obtain *IU* characteristics and *PI* characteristics. To give hints for the development of new lasing structures we varied in our simulations the geometry of the device, the doping and the composition of the material of relevant layers in the active zone, especially the number of quantum wells.

Important parameters for laser operation are derived from the *PI* characteristics (see left upper picture in Figure 2). Relevant properties are, firstly, the threshold current which is the minimum injection current that is required for lasing to occur and, secondly, the differential quantum efficiency which means the slope of the characteristics near threshold. These parameters depend strongly upon the temperature in the active zone of the laser which has to be calculated, too.

Figure 2 illustrates simulation results for a test structure for which the half transverse cross section is given in the middle of the last line of pictures. The left upper picture shows the *PI* characteristics. Here the second optical mode does not give a relevant contribution to the optical

output power. The right upper picture contains the temperature profile on the half transverse cross section. The middle upper curve represents the optical gain along the quantum well. Here already the saturation of gain under the ridge can be observed. The left lower diagram contains the densities of electrons and holes in a cross section along the y-axis of the adjacent picture. The right lower picture gives the electrostatic potential (black), the position of the valence band and of the conduction band (green and red), and the quasi-Fermi potentials of electrons and holes (blue and orange) along the same cross section.

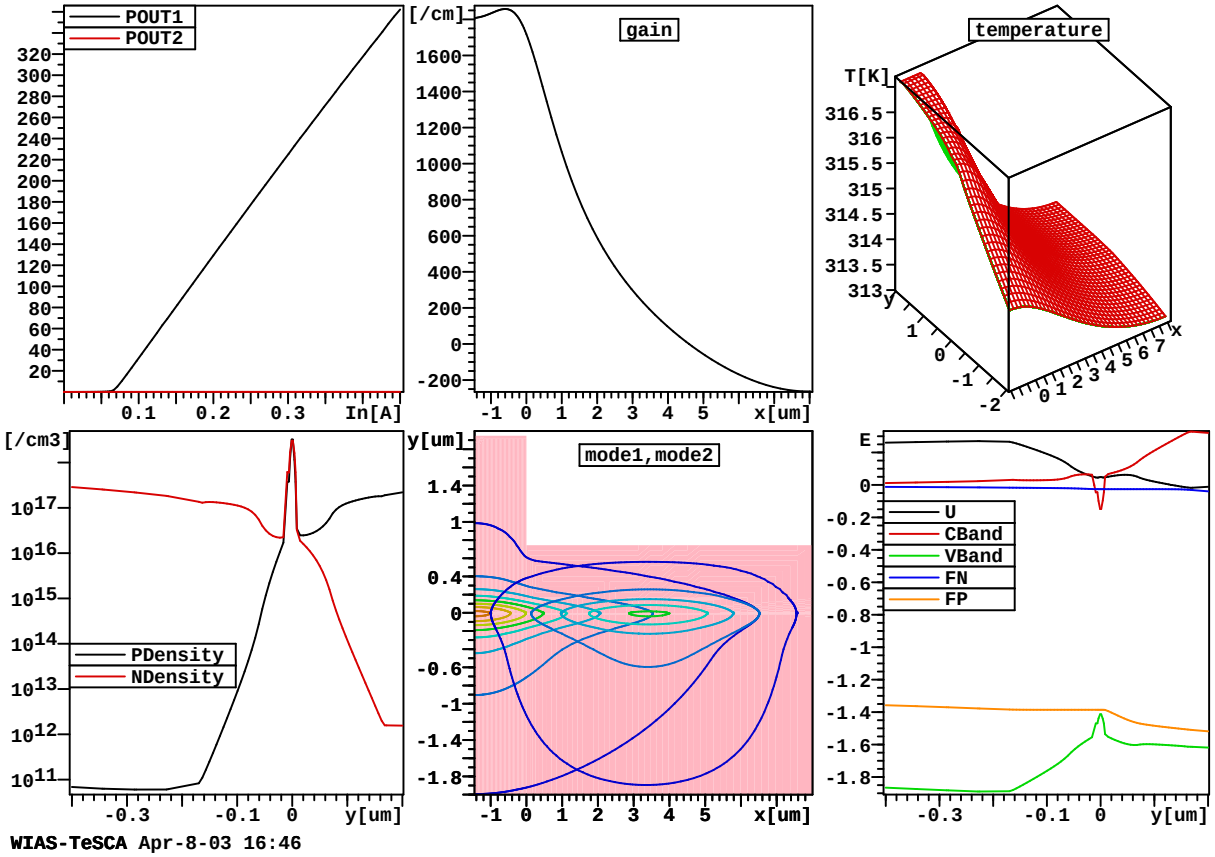

Fig. 2: WIAS-TeSCA simulation of a ridge waveguide laser diode

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1. U. BANDELOW, H. GAJEWSKI, R. HÜNLICH, *Thermodynamics-based modeling of edge-emitting quantum well lasers*, in preparation.

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3. WIAS-TeSCA. http://www.wias-berlin.de/software/tesca, 2003.

Thermodynamics-based modeling of semiconductor lasers

Collaborators: U. Bandelow, H. Gajewski, R. Hünlich

Cooperation with: H. Wenzel (Ferdinand-Braun-Institut für Höchstfrequenztechnik (FBH) Berlin)

In modern semiconductor devices such as high power transistors or lasers, thermal effects caused by strong electric and optical fields and by strong recombination play an important role and have to be included in the mathematical models. Indeed, there is a large variety of energy models for semiconductor devices. Typically, these models base on the usual state equations and continuity equations for the carrier densities, and on the balance of the total energy expressed by the equation

$$\partial_t u + \nabla j_u = -\gamma \tag{1}$$

for the density u and the current density j_u of this total energy, where γ counts for the radiation which is emitted from the device. Furthermore, differential relations for u and general thermodynamic relations for j_u are used to transform the energy balance equation (1) into a heat flow equation

$$c_h \partial_t T - \nabla \cdot (\kappa_L \nabla T) = H, \tag{2}$$

where c_h is the heat capacity and κ_L the heat conductivity. While the heat flow equation (2) with the description of the source term H is well established, the discussion about its relation to the conservation law of energy is still ongoing.
In our model, the transport of electrons and holes is ruled by the drift-diffusion equations

$$-\nabla(\varepsilon \nabla \varphi) = C + p - n\,, \tag{3}$$

$$\partial_t n - \nabla \cdot \mathbf{j}_n = -R\,, \qquad \partial_t p + \nabla \cdot \mathbf{j}_p = -R \tag{4}$$

for the densities of electrons n and holes p, and the electrostatic potential φ in the transverse cross section Ω of the laser. The recombination rate R in (4) involves all non-radiative and radiative recombination processes. The current densities $\mathbf{j}_n$ and $\mathbf{j}_p$ are driven by the gradients of the quasi-Fermi potentials f_n and f_p, which are linked with the carrier concentrations by means of Fermi-Dirac statistics:

$$n = N_c \mathcal{F}_{1/2}\left(\frac{\varphi - f_n - e_c}{T}\right), \quad p = N_v \mathcal{F}_{1/2}\left(\frac{e_v + f_p - \varphi}{T}\right). \tag{5}$$

The optical field distribution $\chi(\mathbf{r})$ within Ω is governed by the waveguide equation

$$\left[\nabla^2 + \frac{\omega^2}{c^2}\varepsilon_{opt}(\omega, \mathbf{r}) - \beta^2\right]\chi(\mathbf{r}) = 0 \tag{6}$$

where the optical response function $\varepsilon_{opt}(\omega, \mathbf{r})$ contains the refractive index and the material gain, which depends on almost all properties of the device and its operating state, in particular on n, p, and T. The respective (complex) eigenvalue β readily counts the number N_s of photons in the laser by a corresponding photon rate equation

$$\dot{N}_s = v_g(2\Im m\beta - \alpha_0 - \alpha_m)N_s + r^{sp}. \tag{7}$$

The field intensity $N_s \cdot |\chi(\mathbf{r})|^2$ times the material gain enters the radiative recombination rate in R in (4), which self-consistently completes our model ([1]). Based on an expression for the density of the free energy

$$\begin{aligned} f &= \frac{\varepsilon}{2}|\nabla\varphi|^2 + c_L T(1-\log T) + u_{rad} - T s_{rad} \\ &\quad + n[T(\log\frac{n}{N_c} - 1) + e_c] + p[T(\log\frac{p}{N_v} - 1) - e_v], \end{aligned} \tag{8}$$

we extended (3)–(7) to a thermodynamics-based system (2)–(7) of evolution equations for semiconductor lasers in a deductive way. Here, we only apply first principles like the entropy maximum principle and the principle of partial local equilibrium as well as the Onsager symmetry relations ([2]). In particular we could show that the heat source term H in (2) is

$$\begin{aligned} H &= T\nabla P_n \cdot \mathbf{j}_n - T\nabla P_p \cdot \mathbf{j}_p + T\nabla\cdot(\mathbf{j}_n - \mathbf{j}_p) \\ &\quad - \mathbf{j}_n \cdot (\nabla f_n - P_n \nabla T) - \mathbf{j}_p \cdot (\nabla f_p + P_p \nabla T) \\ &\quad + (u_n + u_p)R - \partial_t u_{rad} - \gamma, \end{aligned} \tag{9}$$

with the thermoelectric powers P_n, P_p, and the energy density of the optical field $u_{rad} = \bar{h}\omega|\chi|^2 N_s$. The current densities $\mathbf{j}_n$ and $\mathbf{j}_p$ are now driven by the gradients of the temperature T, too. Moreover, a continuity equation for the entropy density s

$$\frac{\partial s}{\partial t} + \nabla\cdot\mathbf{j}_s = d/T, \tag{10}$$

with the entropy current density $\mathbf{j}_s$ could be derived. The dissipation rate d

$$\begin{aligned} d &= \frac{\kappa_L}{T}|\nabla T|^2 + \sigma_n|\nabla f_n - P_n\nabla T|^2 + \sigma_p|\nabla f_p + P_p\nabla T|^2 \\ &\quad + \sigma_{np}|\nabla(f_n - f_p) - (P_n + P_p)\nabla T|^2 + (f_p - f_n)R - \gamma \end{aligned} \tag{11}$$

appears to be always positive for a device which is isolated from the outside world ($\gamma = 0$). Therefore, by partial integration of (10) and supposing no-flux boundary conditions, and $\gamma = 0$, it follows, according to the second law of thermodynamics,

$$\frac{dS}{dt} = \int_\Omega \frac{ds}{dt}\, d\Omega = \int_\Omega \frac{d}{T}\, d\Omega \geq 0\,. \tag{12}$$

In conclusion, as a feature, we are able to prove the thermodynamic correctness of our model in view of the second law of thermodynamics (12).
The complete energy transport model has been implemented in WIAS-TeSCA ([3]), a numerical code for the simulation of semiconductor devices. On this base, we have demonstrated the simulation of long-wavelength edge-emitting quantum well lasers, with a special focus on the self-heating of the device and the modulation response ([2]).

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3. WIAS-TeSCA. http://www.wias-berlin.de/software/tesca, 2003.

A quantum transmitting Schrödinger-Poisson system

Collaborators: M. Baro, H.-Chr. Kaiser, H. Neidhardt, J. Rehberg

Cooperation with: A. Jüngel (Johannes Gutenberg-Universität Mainz), P. Degond, N. Ben Abdallah (Université Paul Sabatier, Toulouse, France), V.A. Zagrebnov (Université de la Méditerranée, Aix-Marseille II and Centre de Physique Théorique, France), P. Exner (Academy of Sciences of the Czech Republic, Prague)

Supported by: DFG: DFG-Forschungszentrum "Mathematik für Schlüsseltechnologien" (Research Center "Mathematics for Key Technologies"), project D4; "Kopplung von van Roosbroeck- und Schrödinger-Poisson-Systemen mit Ladungsträgeraustausch" (Coupling between van Roosbroeck and Schrödinger-Poisson systems with carrier exchange); DAAD (PROCOPE): "Numerics of hybrid models for quantum semiconductors"

This project is part of a long-term investigation of quantum mechanical models for semiconductor nanostructures, cf. [2, 9, 10, 11, 12, 13, 14], and their embedding into macroscopic models, like drift-diffusion and energy models, cf. [15] and p. 26, for semiconductor devices, in particular optoelectronic ones, cf. [1, 3] and pp. 22, 24.
We investigate, from a mathematical point of view, a basic quantum mechanical model for the transport of electrons and holes in a semiconductor device. More precisely, our subject is the distribution of electrons and holes in a device between two reservoirs within a self-consistent electrical field, thereby taking into account quantum phenomena such as tunneling and the quantization of energy levels in a quantum well. These very quantum effects are the active principle of many nanoelectronic devices: quantum well lasers, resonant tunneling diodes et cetera, cf., e.g., [17]. We look for stationary states of a quasi-two-dimensional electron-hole gas in a semiconductor heterostructure which is translationally invariant in these two dimensions. Thus, neglecting any magnetic field induced by the carrier currents, we are dealing with an essentially one-dimensional physical system. The transport model for a single band, electrons or holes, in a given spatially varying potential v is as follows: The potential v as well as the material parameters of the physical system are constant outside a fixed interval (a,b), cf. [7, 16]. The possible wave functions are given by the generalized solutions of

$$K_v\psi_k = \lambda(k)\psi_k$$

where

$$K_v = -\frac{\hbar^2}{2}\frac{d}{dx}\frac{1}{m}\frac{d}{dx} + v \tag{1}$$

is the single-particle effective-mass Hamiltonian in Ben-Daniel-Duke form, $\hbar$ is the reduced Planck constant, $m = m(x) > 0$ is the spatially varying effective mass of the particle species under consideration, and $\lambda = \lambda(k)$ is a dispersion relation, e.g.,

$$\lambda(k) = \begin{cases} \frac{\hbar^2 k^2}{2m_a} + v_a & \text{for } k > 0, \\ \frac{\hbar^2 k^2}{2m_b} + v_b & \text{for } k < 0; \end{cases}$$

m_a, m_b are the effective masses, and v_a, v_b are the potentials in the asymptotic regions $x < a$ and $x > b$, respectively. If there are no bounded states, then the particle density u is a composition

of the wave functions ψ_k weighted by values of a distribution function f:

$$u(x) = c\int_0^\infty dk\, f(\lambda(k)-\varepsilon_a)|\psi_k(x)|^2 + c\int_{-\infty}^0 dk\, f(\lambda(k)-\varepsilon_b)|\psi_k(x)|^2, \quad x\in(a,b). \tag{2}$$

ε_a and ε_b is the quasi-Fermi potential of the reservoir in the asymptotic region $x<a$ and $x>b$, respectively, and c is the two-dimensional density of states. The distribution function is

$$f(\xi) = \begin{cases} \exp\left(-\frac{\xi}{k_BT}\right) & \text{for Boltzmann statistics,} \\ \ln\left(1+\exp(-\frac{\xi}{k_BT})\right) & \text{for Fermi-Dirac statistics,} \end{cases}$$

where T is the temperature and k_B Boltzmann's constant. (2) can be written in the following way: Let $\widehat{\rho}$ be the multiplication operator on $\mathsf{L}^2(\mathbb{R})$ induced by the function

$$\rho(k) = \begin{cases} c\, f(\lambda(k)-\varepsilon_a) & \text{for } k>0, \\ c\, f(\lambda(k)-\varepsilon_b) & \text{for } k<0, \end{cases} \tag{3}$$

and let $\mathcal{F}_v : \mathsf{L}^2(\mathbb{R}) \to \mathsf{L}^2(\mathbb{R})$ be the Fourier transform which diagonalizes the operator K_v on $\mathsf{L}^2(\mathbb{R})$, that means $\mathcal{F}_v K_v \mathcal{F}_v^* = \widehat{\lambda}$, where $\widehat{\lambda}$ is the maximal multiplication operator induced by the dispersion relation $\lambda = \lambda(k)$. Then the operator

$$\rho(v) = \mathcal{F}_v^* \widehat{\rho}\, \mathcal{F}_v \tag{4}$$

is a steady-state, that means a self-adjoint, positive operator on the Hilbert space $\mathsf{L}^2(\mathbb{R})$ which commutes with K_v. Moreover, any steady state can be expressed in the form (4) by means of a function $\rho = \rho(k)$. The particle density u, defined by (2), is the Radon-Nikodým derivative of the (Lebesgue) absolutely continuous measure $(a,b) \supset \omega \mapsto \mathrm{tr}\big(\rho(v)M(\chi_\omega)\big)$ ($M(\chi_\omega)$ denotes the multiplication operator induced by the characteristic function χ_ω of the set ω) that means

$$\int_\omega u(x)dx = \mathrm{tr}\big(\rho(v)M(\chi_\omega)\big), \tag{5}$$

for all Lebesgue measurable subsets ω of (a,b). By replacing the real-valued distribution function (3) by a generalized distribution function with 2×2-matrix values, this concept of particle density carries over to the setup we investigate in this project, cf. [4, Section 5.1]. It should be noted that the species current density between the reservoirs also can be expressed in terms of the ψ_k, cf. [4, Section 5.2].

In the asymptotic regions $x<a$ and $x>b$ the generalized eigenfunctions ψ_k can be written as a superposition of plane waves. This allows to define boundary conditions at a and b, with respect to the dispersion relation $\lambda = \lambda(k)$, by means of the quantum transmitting boundary method, cf. [7, 16]. The corresponding homogeneous boundary conditions are

$$\frac{\hbar}{m(a)}\psi'(a) = -i\,\mathfrak{v}(k)\psi(a), \quad \frac{\hbar}{m(b)}\psi'(b) = i\,\mathfrak{v}(-k)\psi(b), \quad k\in\mathbb{R}, \tag{6}$$

where $\mathfrak{v}(k)$, $k\in\mathbb{R}$, is the group velocity defined by $\mathfrak{v} = \frac{1}{\hbar}\frac{d\lambda}{dk}$. The differential expression (1), together with the boundary conditions (6), sets up a family of maximal dissipative operators on the Hilbert space $\mathsf{L}^2(a,b)$. We call this family, in the style of [16], the *quantum transmitting boundary operator family* (QTB operator family), cf. [4, Section 2]. The QTB operator

family already contains all the information needed to define, in conjunction with a generalized distribution function ρ, physical quantities such as the particle density, the current density, and the scattering matrix.
The interaction between an electric field and carriers of charge within a semiconductor device can be modeled by Poisson's equation, cf. [8] and the references cited there:

$$-\frac{d}{dx}\varepsilon(x)\frac{d}{dx}\varphi(x) = q\left(C(x) + \mathcal{N}^+(v^+)(x) - \mathcal{N}^-(v^-)(x)\right), \quad x \in (a,b), \tag{7}$$

where q denotes the elementary charge, C is the density of ionized dopants in the semiconductor device, $\varepsilon > 0$ is the dielectric permittivity function, and φ is the electrostatic potential, $v^\pm = \mp w^\pm \pm q\varphi$ are the potential energies of electrons ("$-$") and holes ("$+$"), and w^-, w^+ are the conduction and valence band offset, respectively. The quantum transmitting Schrödinger-Poisson system is a Poisson equation (7) with nonlinear electron and hole density operators $\mathcal{N}^-$ and $\mathcal{N}^+$ defined as the map of a potential v to the density (5) with steady states $\rho^-(v)$ and $\rho^+(v)$, respectively. In [4, Section 6] we have demonstrated that the thus defined carrier density operators are continuous; the corresponding currents are uniformly bounded for all potentials v. We have proved that the quantum transmitting Schrödinger-Poisson system comprising electrons and holes always admits a solution provided the function inducing the steady states has reasonable decay properties with increasing energy. Furthermore, we give a priori estimates for the solutions. The a priori bounds for the electrostatic potential and the electron and hole density of solutions are explicit expressions in the data of the problem. Ben Abdallah, Degond, and Markowich have investigated a special case of this model in [6] and prove the existence of solutions for the unipolar case. Unfortunately, the mathematical techniques used in their proof do not apply to the bipolar case, which we treat in this project.
The quantum transmitting Schrödinger-Poisson system is closely related to the dissipative Schrödinger-Poisson system, which we have investigated in [5], cf. Annual Research Report 2002, pp. 26–28. In particular, the dissipative Schrödinger-Poisson system and the quantum transmitting Schrödinger-Poisson system coincide for fixed energy, modulo a unitary transformation.

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Nonlocal phase separation problems for multicomponent systems

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To describe phase separation processes we consider a closed multicomponent system with interacting particles of type $k \in \{0,1,\dots,n\}$ occupying a spatial domain. In our model we assume that the particles jump around on a given microscopically scaled lattice following a stochastic exchange process (see [2]). On each lattice site sits exactly one particle (exclusion principle). Two particles of type k and l change their sites x and y with probability $p_{kl}(x,y)$ due to *diffusion* and *nonlocal interaction*. The hydrodynamical limit leads to a system of conservation laws for $k \in \{0,1,\dots,n\}$,

$$u_k' + \nabla \cdot j_k = 0 \text{ in } (0,T)\times\Omega, \quad \nu \cdot j_k = 0 \text{ on } (0,T)\times\partial\Omega, \quad u_k(0) = g_k \text{ in } \Omega, \tag{1}$$

for (scaled) *particle densities* $u_0,u_1,\dots,u_n$, their *initial values* $g_0,g_1,\dots,g_n$, and *current densities* $j_0,j_1,\dots,j_n$. Here, $(0,T)$ denotes a time interval and ν is the outer unit normal on the boundary $\partial\Omega$ of the bounded m-dimensional Lipschitz domain Ω. Due to the exclusion principle of the stochastic process we can assume $\sum_{k=0}^n u_k = 1$, $\sum_{k=0}^n g_k = 1$, and $\sum_{k=0}^n j_k = 0$, that means, only n of the $n+1$ equations in (1) are independent of each other. Hence, we can drop out one equation, say the equation for the zero component, and describe the state of the system by n-component vectors $u = (u_1,\dots,u_n)$ having in mind the notation $u_0 = 1 - \sum_{k=1}^n u_k$.
To establish thermodynamical relations between current densities, particle densities, and their conjugated variables, we minimize the free energy functional under the constraint of particle number conservation. In contrast to the classical Cahn–Hilliard theory we consider diffuse interface models and free energy functionals with nonlocal expressions. As a straightforward generalization of the nonlocal phase separation model for binary systems (see [1]) we define a *free energy functional* $F = F_1 + F_2$ by

$$F_1(u) = \int_\Omega f(u(x))\,dx, \quad F_2(u) = \frac{1}{2}\sum_{k=0}^n \int_\Omega (Ku)_k(x)\,u_k(x)\,dx, \tag{2}$$

$$f(u) = \sum_{k=0}^n u_k \log(u_k), \quad (Ku)_k(x) = \sum_{l=0}^n \int_\Omega \kappa_{kl}(x,y)\,u_l(y)\,dy. \tag{3}$$

The convex function f and the symmetric $(n+1)\times(n+1)$-matrix kernel κ define the *chemical* part F_1 and the *nonlocal interaction* part F_2 of the functional F, respectively. Minimizing F under the constraint of particle number conservation, we identify the conjugated variables of the densities as *grand chemical potential differences*

$$\lambda_k = \frac{\partial F}{\partial u_k} = \mu_k + w_k, \quad k \in \{1,\dots,n\},$$

where μ_k and w_k are *chemical* and *interaction potential differences*, respectively,

$$\mu_k = \frac{\partial F_1}{\partial u_k} = \log(u_k) - \log(u_0), \quad w_k = \frac{\partial F_2}{\partial u_k} = (Ku)_k - (Ku)_0, \quad k \in \{1,\dots,n\}. \tag{4}$$

The hydrodynamical limit process (see [2]) yields current densities

$$j_k = -\sum_{l=1}^n a_{kl}(u)\nabla\lambda_l, \quad k \in \{1,\dots,n\},$$

where the *mobility* has the form $a(u) = d(u)(D^2 f(u))^{-1}$, and $d(u)$ denotes the *diffusivity*. Hence, we can interpret the above nonlocal phase separation model as a system of *drift-diffusion equations* with semilinear diffusion and nonlinear nonlocal drift terms, if we rewrite the currents as

$$j_k = -\sum_{l=1}^{n} d_{kl}(u)\nabla u_l - \sum_{l=1}^{n} a_{kl}(u)\nabla w_l\,, \quad k \in \{1,\dots,n\}\,.$$

In [4] we consider the case $d_{kl} = \delta_{kl}$. Then, an elementary computation of the inverse Hessian matrix $(D^2 f(u))^{-1}$ yields the following expressions for the mobility coefficients

$$a_{kl}(u) = \delta_{kl}\, u_k - u_l u_k\,, \quad k,l \in \{1,\dots,n\}\,.$$

For the functional analytic formulation of our problem we use standard spaces

$$H = [L^2(\Omega)]^n\,, \quad V = [H^1(\Omega)]^n\,, \quad L^\infty = [L^\infty(\Omega)]^n\,,$$

respectively, and their generalizations suitable for evolution systems,

$$\mathcal{H} = L^2((0,T);H)\,, \quad \mathcal{V} = L^2((0,T);V)\,, \quad \mathcal{L}^\infty = L^\infty((0,T);L^\infty)\,, \quad \mathcal{W} = \{u \in \mathcal{V} : u' \in \mathcal{V}^*\}\,.$$

Having in mind $u_0 = 1 - \sum_{k=1}^n u_k$, we define *simplices* $S \subset L^\infty$ and $\mathcal{S} \subset \mathcal{L}^\infty$ by

$$S = \{g \in L^\infty :\, 0 \le g_0, g_1, \dots, g_n \le 1\}\,, \quad \mathcal{S} = \{u \in \mathcal{L}^\infty :\, 0 \le u_0, u_1, \dots, u_n \le 1\}\,.$$

Furthermore, we introduce the *drift-diffusion operator* $\mathcal{A} : [\mathcal{V} \cap \mathcal{L}^\infty] \times \mathcal{V} \longrightarrow \mathcal{V}^*$ by

$$\langle \mathcal{A}(u,w), \varphi \rangle = \sum_{k=1}^{n} \int_0^T \int_\Omega \nabla u_k \cdot \nabla \varphi_k \, dx\, ds + \sum_{k=1}^{n}\sum_{l=1}^{n} \int_0^T \int_\Omega a_{kl}(u)\nabla w_l \cdot \nabla \varphi_k \, dx\, ds\,,$$

for $(u,w) \in [\mathcal{V} \cap \mathcal{L}^\infty] \times \mathcal{V}$, $\varphi \in \mathcal{V}$. More general than in the above description of the model, we assume that the interaction between particles can be described by means of a (possibly nonlinear and nonlocal) Lipschitz continuous *interaction operator* $\mathcal{P} : \mathcal{H} \longrightarrow \mathcal{V}$.

Applying fixed-point arguments and comparison principles in [4], we show that for every initial value $g \in S$ there exists a *solution* $(u,w) \in [\mathcal{W} \cap \mathcal{S}] \times \mathcal{V}$ *of the evolution system*

$$u' + \mathcal{A}(u,w) = 0\,, \quad w = \mathcal{P}u\,, \quad u(0) = g\,. \tag{5}$$

Moreover, under some natural regularity assumption on the interaction operator $\mathcal{P} : \mathcal{H} \longrightarrow \mathcal{V}$ in [4] we also get the unique solvability of our problem. In fact, we additionally assume that $\mathcal{P}$ has the Volterra property and that the restriction of $\mathcal{P}$ to $\mathcal{L}^\infty$ is a Lipschitz continuous operator from $\mathcal{L}^\infty$ into a certain *Sobolev–Morrey space* $\mathcal{X}^\sigma \subset \mathcal{V}$ for some parameter $\sigma > m$. Then, our regularity theory for initial boundary value problems with nonsmooth data in Sobolev–Morrey and Hölder spaces (see [3]) enables us to prove the unique solvability of problem (5).

To illustrate our results, we consider an example of a ternary system, where the interaction operator $\mathcal{P} : \mathcal{H} \longrightarrow \mathcal{V}$ is defined by $(\mathcal{P}u)_k = (Ku)_k - (Ku)_0$, $k \in \{1,\dots,n\}$ (see (3), (4), (5)). The corresponding matrix kernel κ is chosen such that particles of the same type attract and particles of different type repel each other with the same range and strength of interaction. Figures 1 and 2 show simulation results of phase separation processes in a unit square. Notice that both initial configurations contain equal numbers of black, white, and red particles,

respectively. Moreover, the final states are local minimizers of the free energy functional F under the constraint of particle number conservation.

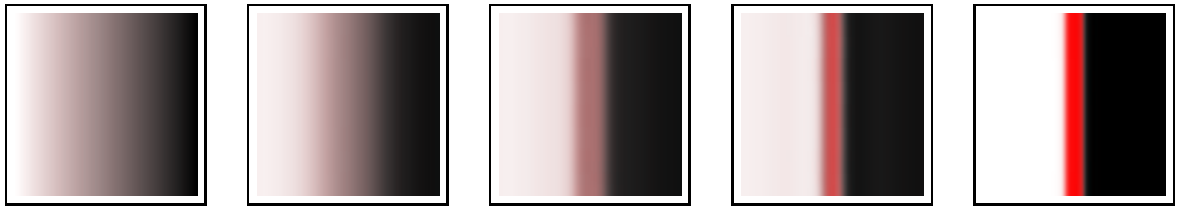

Fig. 1: Phase separation process for an initial value which is constant in the vertical direction. The stripe pattern is preserved during the whole evolution.

Fig. 2: Phase separation process for a symmetric initial value. There occur metastable states. Finally, the phases are separated by a straight line and circular arcs.

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Stationary solutions of a two-dimensional heterogeneous energy model for semiconductor devices near equilibrium

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Semiconductor devices are heterostructures consisting of various materials (different semiconducting materials, passive layers, and metals as contacts, for example). A typical situation is shown in Figure 1. Equations for the contacts are substituted by Dirichlet boundary conditions on the two parts of the boundary Γ_{D0}. In the remaining domain Ω, involving the passive layer (Ω_1) and semiconducting materials (Ω_0), we have to formulate a Poisson equation and an energy balance equation with boundary conditions on $\Gamma = \Gamma_{D0} \cup \Gamma_{N0} \cup \Gamma_{N1} \cup \Gamma_S$, where the subscripts D, N, and S indicate the parts with Dirichlet, inhomogeneous Neumann, and symmetry boundary conditions, respectively. Only in the part Ω_0, continuity equations for electrons and holes have to be taken into account, and here we must formulate boundary conditions on $\Gamma_0 = \Gamma_{D0} \cup \Gamma_{N01} \cup \Gamma_{N0} \cup \Gamma_S$. Let T and φ denote the lattice temperature and the electrostatic potential. Then the state equations for electrons and holes are given by the following expressions

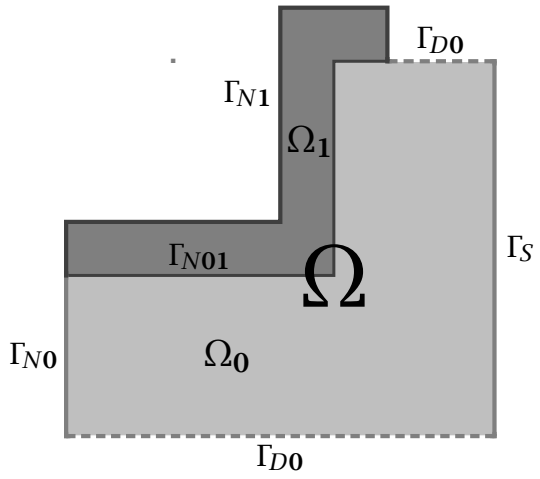

Fig. 1: Schematic picture of a modeled semiconductor device

$$n = N(\cdot,T)F\Big(\frac{\zeta_n + \varphi - E_n(\cdot,T)}{T}\Big),\ p = P(\cdot,T)F\Big(\frac{\zeta_p - \varphi + E_p(\cdot,T)}{T}\Big) \quad \text{in } \Omega_0,$$

where n and p are the electron and hole densities, N and P are the effective densities of state, ζ_n and ζ_p are the electrochemical potentials, E_n and E_p are the energy band edges, respectively. The function F arises from a distribution function (e.g., $F(y) = \mathrm{e}^y$ in the case of Boltzmann statistics, or $F(y) = \mathcal{F}_{1/2}(y)$ in the case of Fermi-Dirac statistics). The electrostatic potential φ fulfils the Poisson equation

$$-\nabla \cdot (\varepsilon \nabla \varphi) = \begin{cases} f - n + p & \text{in } \Omega_0 \\ f & \text{in } \Omega_1 \end{cases}. \tag{1}$$

Here, ε is the dielectric permittivity and f is a given doping profile. Mixed boundary conditions on Γ have to be prescribed. For the densities of the particle fluxes j_n, j_p and of the total energy flux j_e, we make the ansatz (see [1])

$$j_n = -(\sigma_n + \sigma_{np})(\nabla\zeta_n + P_n\nabla T) - \sigma_{np}(\nabla\zeta_p + P_p\nabla T) \quad \text{in } \Omega_0,$$

$$j_p = -\sigma_{np}(\nabla\zeta_n + P_n\nabla T) - (\sigma_p + \sigma_{np})(\nabla\zeta_p + P_p\nabla T) \quad \text{in } \Omega_0,$$

$$j_e = \begin{cases} -\kappa\nabla T + \sum_{i=n,p}(\zeta_i + P_i T)\, j_i, & \text{in } \Omega_0 \\ -\tilde{\kappa}\nabla T, & \text{in } \Omega_1 \end{cases},$$

with conductivities $\sigma_n = \sigma_n(x,n,p,T) > 0$, $\sigma_p = \sigma_p(x,n,p,T) > 0$, $\sigma_{np} = \sigma_{np}(x,n,p,T) \geq 0$, $\kappa = \kappa(x,n,p,T) > 0$, $\tilde{\kappa} = \tilde{\kappa}(x,T) > 0$, and transported entropies $P_n = P_n(x,n,p,T)$, $P_p = P_p(x,n,p,T)$. These flux densities fulfil the balance equations

$$\nabla \cdot j_n = -R, \quad \nabla \cdot j_p = -R \quad \text{in } \Omega_0, \quad \nabla \cdot j_e = 0 \quad \text{in } \Omega, \tag{2}$$

where the net recombination rate R has the form

$$R = r(\cdot,n,p,T)(\mathrm{e}^{(\zeta_n+\zeta_p)/T} - 1) \quad \text{in } \Omega_0.$$

Suitable boundary conditions on Γ_0 for the first two continuity equations and on Γ for the last energy balance equation have to be added.
We use the variables $z = (z_1,z_2,z_3,z_4) = (\zeta_n/T|_{\Omega_0}, \zeta_p/T|_{\Omega_0}, -1/T, \varphi)$, where z_1, z_2 are defined on Ω_0, while z_3, z_4 live on Ω. Then the stationary energy model for semiconductor devices can be written in the more compact form

$$\begin{aligned} -\nabla \cdot \begin{pmatrix} a_{11} & a_{12} & a_{13} & 0 \\ a_{21} & a_{22} & a_{23} & 0 \\ a_{31} & a_{32} & a_{33} & 0 \\ 0 & 0 & 0 & \varepsilon \end{pmatrix} \begin{pmatrix} \nabla z_1 \\ \nabla z_2 \\ \nabla z_3 \\ \nabla z_4 \end{pmatrix} &= \begin{pmatrix} -R \\ -R \\ 0 \\ f - n + p \end{pmatrix} && \text{in } \Omega_0, \\ -\nabla \cdot \begin{pmatrix} \tilde{a}_{33} & 0 \\ 0 & \varepsilon \end{pmatrix} \begin{pmatrix} \nabla z_3 \\ \nabla z_4 \end{pmatrix} &= \begin{pmatrix} 0 \\ f \end{pmatrix} && \text{in } \Omega_1, \end{aligned} \tag{3}$$

with coefficient functions $a_{ik}(x,z) = a_{ki}(x,z)$, $x \in \Omega_0$, $z \in \mathbb{R}^2 \times (-\infty,0) \times \mathbb{R}$, $i,k = 1,\ldots,3$, $\tilde{a}_{33}(x,z_3)$, $x \in \Omega_1$, $z_3 \in (-\infty,0)$, $\varepsilon(x)$, $x \in \Omega$, and R, n, and p have to be regarded as functions of $x \in \Omega_0$ and $z \in \mathbb{R}^2 \times (-\infty,0) \times \mathbb{R}$.
We consider the boundary conditions

$$\begin{aligned} & z_i = z_i^{D0}, \quad i = 1,2,3,4, \text{ on } \Gamma_{D0}, \\ & \nu \cdot \textstyle\sum_{k=1,2,3} a_{ik}(x,z)\nabla z_k = g_i^{N0}, \quad i = 1,2,3, \quad \nu \cdot (\varepsilon \nabla z_4) = g_4^{N0} \text{ on } \Gamma_{N0}, \\ & \nu \cdot \tilde{a}_{33}(z_3) = g_3^{N1}, \quad \nu \cdot (\varepsilon \nabla z_4) = g_4^{N1} \text{ on } \Gamma_{N1}, \\ & \nu \cdot \textstyle\sum_{k=1,2,3} a_{ik}(x,z)\nabla z_k = 0, \quad i = 1,2, \text{ on } \Gamma_{N01}, \\ & \nu \cdot \textstyle\sum_{k=1,2,3} a_{ik}(x,z)\nabla z_k = 0, \quad i = 1,2,3, \quad \nu \cdot (\varepsilon \nabla z_4) = 0 \text{ on } \Gamma_S. \end{aligned} \tag{4}$$

We use the vectors $z^D = (z_1^D,\ldots,z_4^D)$, $g = (g_1^{N0},\ldots,g_4^{N0},g_3^{N1},g_4^{N1})$, and the triplet of data $w = (z^D,g,f)$ and look for weak solutions of (3), (4) in the form $z = Z + z^D$, where z^D corresponds to a function fulfilling the Dirichlet boundary conditions and Z represents the homogeneous part of the solution.
We assume that the boundary values z_i^D, $i = 1,2,3,4$, are traces of $W^{1,p}$-functions, $p > 2$. Under weak assumptions on the coefficient functions a_{ij}, $\tilde{a}_{33}$, and ε (for example, Ω_0 can be composed of different semiconducting materials), we found $W^{1,q}$–formulations ($q \in (2,p]$) for that system of equations,

$$F(Z,w) = 0, \quad Z \in W_0^{1,q}(\Omega_0 \cup \Gamma_{N0} \cup \Gamma_{N01} \cup \Gamma_S)^2 \times W_0^{1,q}(\Omega \cup \Gamma_{N0} \cup \Gamma_{N1} \cup \Gamma_S)^2.$$

If $w^* = (z^{D*},g^*,f^*)$ is arbitrarily given such that the boundary values z_i^{D*}, $i = 1,2,3$, are constants, $z_1^{D*} + z_1^{D*} = 0$ and $z_3^{D*} < 0$ and $g^* = (0,0,0,g_4^{N0*},0,g_4^{N1*})$, then there exists a unique

solution Z^* of $F(Z^*, w^*) = 0$. Then $z^* = Z^* + z^{D*}$ is a thermodynamic equilibrium of (3), (4). Using techniques from [5], the operator F turned out to be continuously differentiable. For suitable $q > 2$, we proved that its linearization $\frac{\partial F}{\partial Z}(Z^*, w^*)$ is an injective Fredholm operator of index zero. For this purpose we derived new results concerning $W^{1,q}$-regularity and surjectivity for strongly coupled systems of linear elliptic equations which are defined on different domains. Here we adapted ideas of [4]. We applied the Implicit Function Theorem and obtained that for $w = (z^D, g, f)$ near w^*, the equation $F(Z, w) = 0$ has a unique solution Z near Z^*. Thus, near z^* there is a locally unique Hölder continuous solution $z = Z + z^D$ of (3), (4). For details and the precise assumptions of our investigations see [3].
In [2] we investigated an energy model with multiple species, but there the continuity equations, the energy balance equation, and the Poisson equation were defined on the same domain.

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Hysteresis operators

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Supported by: DFG: "Hysterese-Operatoren in Phasenfeld-Gleichungen" (Hysteresis operators in phase-field equations)

To be able to deal with phase transitions, one has to take into account hysteretic phenomena that are modeled by hysteresis operators. Moreover, methods derived for dealing with hysteresis operators also allow to derive results for equations formulated without a hysteresis operator.
In a number of papers (see, for instance, [1, 2, 4] and the references given therein), integrodifferential (nonlocal) models for isothermal phase transitions with either conserved or non-conserved order parameters have been studied, leading to a number of results concerning existence, uniqueness, and asymptotic behavior of solutions. In the recent papers [3, 10] the more difficult *non-isothermal* case has been treated, modeling the phase transition by considering the time evolution of an order parameter χ and of the absolute temperature θ. In these papers, one uses a free energy density containing a logarithmic part that forces the order parameter to attain values within the physically meaningful range $[0,1]$.
Within the covered research period, the results of [10] have been complemented by investigating the case when the logarithmic part is replaced by the indicator function $I_{[0,1]}$ of the interval $[0,1]$, see [8]. Considering the phase transition within a container $\Omega \subset \mathbb{R}^N$ that forms an open and bounded domain, and denoting with $T > 0$ some final time, the following system has been considered in $\Omega \times (0,T)$:

$$\mu(\theta)\,\chi_t + \theta F_1'(\chi) + F_2'(\chi) + Q[\chi] \ni -\partial I_{[0,1]}(\chi)\,, \tag{1}$$

$$Q[\chi](x,t) = \int_\Omega K(x-y)\,(1-2\chi(y,t))\,\mathrm{d}y\,, \tag{2}$$

$$C_V\,\theta_t + (F_2'(\chi) + Q[\chi])\,\chi_t - \kappa\Delta\theta = 0\,, \tag{3}$$

with a given kernel function $K : \mathbb{R}^N \to [0,\infty)$, appropriate functions μ, F_1, and F_2, and positive constants C_V and κ. In [8], this system has been investigated by introducing the *generalized freezing index*

$$w(x,t) = w_0(x) - \int_0^t \left[\frac{1}{\mu(\theta)}\,\left(\theta F_1'(\chi) + F_2'(\chi) + Q[\chi]\right)\right](x,\tau)\,\mathrm{d}\tau\,, \tag{4}$$

with some initial condition w_0, so that $\chi(x,t) = \mathfrak{s}_{[0,1]}[\chi_0(x), w(x,\cdot)](t)$ with $\mathfrak{s}_{[0,1]} : [0,1] \times C[0,T] \to C[0,T]$ being the *stop operator* for the interval $[0,1]$. This has been used to eliminate χ from (1)–(3), leading to a system for (w,θ) involving hysteresis operators, which is of the same form as the system considered in [7, 9] except for the nonlocal term. The lines of argumentation used in [7, 9] have been adapted to deal also with the nonlocal term and, in [10], this has been used to prove results concerning existence, uniqueness, and asymptotic behavior for $t \to +\infty$, resembling those established in [10] for the smooth case. The results are even more complete than those of [10] since a certain crucial assumption is not needed in [8].

It has been shown in [5, 6] that one can derive uniform estimates for the solutions to some partial differential equations involving hysteresis operators, if these operators are "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 outward have been formulated in [5, 6]. Within the covered research period, it has been tried to formulate also appropriate conditions for Preisach operators, but the derived conditions are not yet satisfactory, and further investigations are required.

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Numerical simulation and optimization of SiC single crystal growth by sublimation from the gas phase

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Supported by: BMBF: "Numerische Simulation und Optimierung der Züchtung von SiC-Einkristallen durch Sublimation aus der Gasphase" (Numerical simulation and optimization of SiC single crystal growth by sublimation from the gas phase); DFG-Forschungszentrum "Mathematik für Schlüsseltechnologien" (Research Center "Mathematics for Key Technologies"), 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. It is still a challenging problem to grow sufficiently large SiC crystals with a low defect rate. Sublimation growth of SiC bulk single crystals via *physical vapor transport (PVT)*, also known as the *modified Lely method*, has been one of the most successful and most widely used growth techniques of recent years.

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 from the powder 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.

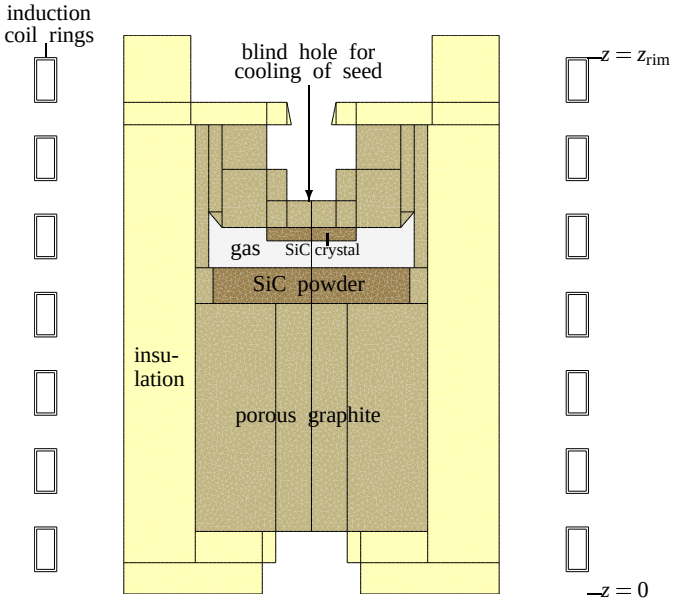

Fig. 1: Setup of growth apparatus according to [6]

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, and different kinds of chemical reactions and phase transitions. 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.

The heat sources caused by induction heating are computed via an axisymmetric complex-valued magnetic scalar potential that is determined as the solution of an elliptic PDE using the imposed voltage as input data. The scalar potential enables one to calculate the resulting current density and thus the heat sources (see [1, 2] and the references therein).

Within the covered research period, the simulation software WIAS-HiTNIHS (see p. 257) has been tested at the IKZ by comparing, for a simple version of the equations, the results derived with WIAS-HiTNIHS with results computed by other software. This has led to an enlargement of the region considered for computations and to some improvements of WIAS-HiTNIHS.
In [4], based on the numerical solution of the stationary mathematical model for the heat transport in the growth system by WIAS-HiTNIHS, a Nelder-Mead method has been used for a numerical optimization of the control parameters frequency f, power P, and coil position z_{rim} for the radio frequency (RF) induction heating of the growth apparatus. The control parameters have been determined to minimize a cost functional, being either the L^∞-norm of the radial temperature gradient on the single crystal surface or the L^2-norm $\mathcal{F}_{r,2}$ of this radial gradient, or $\mathcal{F}_{r,2}$ minus the L^2-norm $\mathcal{F}_{z,2}$ of the vertical temperature gradient between SiC source and seed. The optimizations have been subject to constraints with respect to a required temperature difference between source and seed, a required temperature range at the seed, and an upper bound for the temperature in the entire apparatus.
Several series of Nelder-Mead optimizations of (P, z_{rim}) have been performed, varying the used initial values and keeping the frequency f fixed. Moreover, also the functional dependence of the cost functional on (P, z_{rim}) as well as the restrictions imposed by the state constraints have been studied, varying the power P and the coil position z_{rim} and performing, for each (P, z_{rim}), a forward computation to compute temperature fields $T = T(f, P, z_{\mathrm{rim}})$ and the corresponding value of the cost functionals.

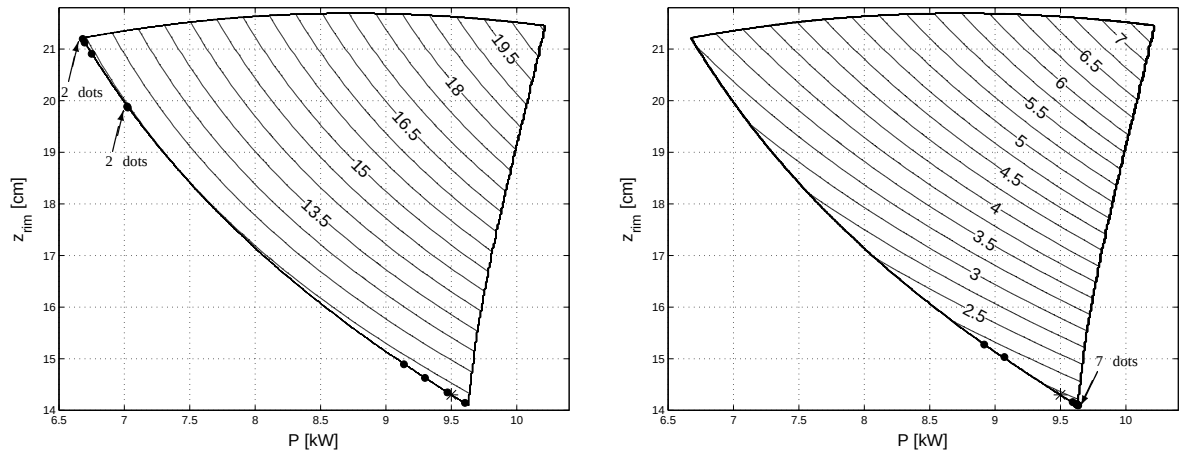

Fig. 2: Contour plots of the functionals $\mathcal{F}_{r,2}$ (left-hand side) and $\frac{1}{2}\mathcal{F}_{r,2} - \frac{1}{2}\mathcal{F}_{z,2}$ (right-hand side) restricted to the part of the (P, z_{rim})-plane where the state constraints are satisfied. Therein, a star marks the location where the smallest value of the considered objective functional occurred during the series of forward computations discussed, and the locations of results of 9 corresponding 2-dimensional Nelder-Mead computations (keeping $f = 10$ kHz fixed) are indicated by dots, which can be found on the lower edge of the respective admissible region.

Moreover, we have performed three-dimensional Nelder-Mead optimizations, controlling f in addition to P and z_{rim}. As in the two-dimensional optimizations, different objective functionals have been considered. Varying the initial values, series of 27 Nelder-Mead computations have been performed. The results for two series are shown in Figure 3.

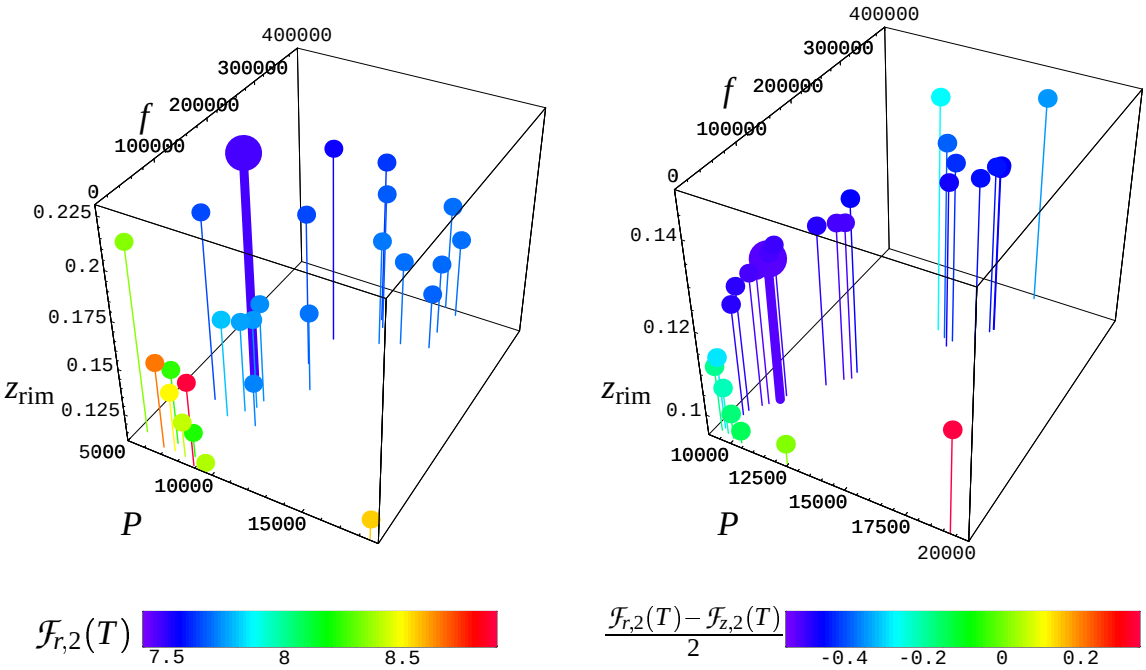

Fig. 3: Result values for (P, z_{rim}, f) for two series of three-dimensional Nelder-Mead computations, with a color presentation of the corresponding values of the objective function $\mathcal{F}_{r,2}$ (left-hand side) and $\frac{1}{2}\mathcal{F}_{r,2} - \frac{1}{2}\mathcal{F}_{z,2}$ (right-hand side). The big point in each figure corresponds to the triple with the respective lowest value of the considered objective function.

The effect of the respective minimizations of $\mathcal{F}_{r,2}(T)$ and of $\frac{1}{2}\mathcal{F}_{r,2}(T) - \frac{1}{2}\mathcal{F}_{z,2}(T)$ on the shape of the temperature distribution between SiC source and crystal is portrayed in Figure 3. Therein, one has the stationary solution for a generic, unoptimized situation, and also the solutions with the lowest values for $\mathcal{F}_{r,2}(T)$ and for $\frac{1}{2}\mathcal{F}_{r,2}(T) - \frac{1}{2}\mathcal{F}_{z,2}(T)$ found within the three-dimensional Nelder-Mead computations, which are marked in Figure 3.
As a result of the optimizations, a minimal radial temperature gradient is found to coincide with a minimal temperature at the single crystal surface, and a maximal temperature gradient between source and seed is found to coincide with a low coil position.

In [5], a quite general version of transient nonlinear and nonlocal heat transport equations has been discretized using an implicit Euler scheme in time and a finite volume method in space. For the corresponding nonlinear and nonlocal discrete scheme, the existence of a unique discrete solution has been proved and discrete L^∞-L^1 *a priori* estimates have been established. In [3], a less general version of the equations has been considered, and the existence of a unique discrete solution to the corresponding discrete scheme has been proved under weaker assumptions for the discretization, and, moreover, a discrete L^∞-L^∞ *a priori* estimate has been derived.

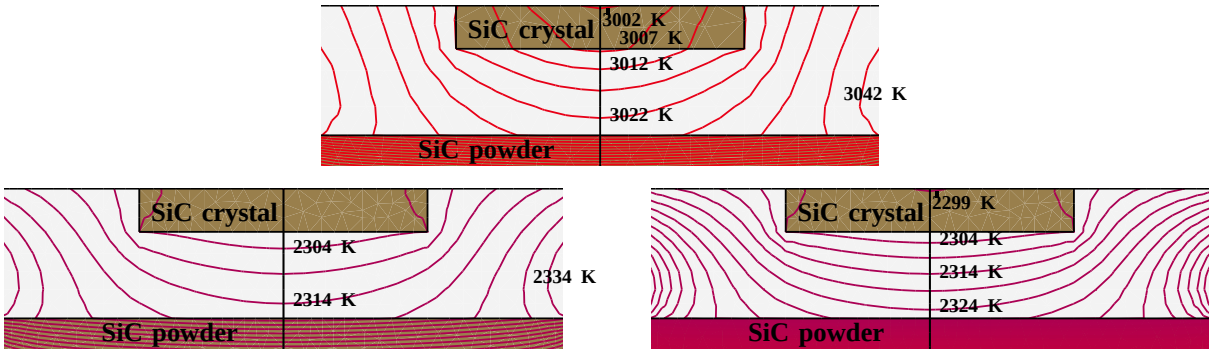

Fig. 4: The shape of the temperature distribution between SiC source and crystal. The distribution on the top corresponds to a generic, unoptimized situation, using $f = 10$ kHz, $P = 10$ kW, and $z_{\text{rim}} = 24$ cm. The lower figures present temperature distributions corresponding to those values for (f, p, z_{rim}) with the lowest values for $\mathcal{F}_{r,2}(T)$ (left-hand side) and of $\frac{1}{2}\mathcal{F}_{r,2}(T) - \frac{1}{2}\mathcal{F}_{z,2}(T)$ (right-hand side) found by the three-dimensional Nelder-Mead computations, which have been marked in Figure 3.

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Approximation and optimization of curved mechanical structures

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Supported by: DFG-Forschungszentrum "Mathematik für Schlüsseltechnologien" (Research Center "Mathematics for Key Technologies"), project C8

The work for this research project continued in several directions. We have finished paper [1] concerning the optimization of structures like curved rods and shells. This gives a rather complete theoretical treatment of the subject, under low regularity assumptions for the geometry. Numerical experiments involving three-dimensional curved rods are also included. Notice that in [3] the case of planar arches was completely solved. Paper [5] introduces a new approach, based on control theory, for the general linear elasticity system and discusses some thickness optimization problems for plates. In [2] stable approximation methods are investigated in connection with the curved rod model proposed in [4]. It is well known that differential equations involving very small parameters (in this case the "thickness" of the rod, i.e. the area of the cross section) may be very difficult to handle via standard finite element methods. This difficulty is known under the name "locking problem". We propose a method that can improve the stability properties in computations related to curved rods.
Finally, paper [6] considers a new way to obtain a model for the deformation of elastic curved rods, of asymptotic type. The new estimates that we derive allow to study curved rods with piecewise C^1 parametrization.

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Lyapunov functions for positive linear evolution problems in C^*

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Supported by: DFG: "Physikalische Modellierung und numerische Simulation von Strom- und Wärmetransport bei hoher Trägerinjektion und hohen Temperaturen" (Physical modeling and numerical simulation of current and heat transport at high carrier injection and high temperatures)

Lyapunov functions for evolution equations are important tools for their variational formulation and the asymptotic investigation of the underlying problem. As usual, for a given equation we have a special Lyapunov function. So, it is well known (see, e.g., [2]) that the classical Fokker-Planck equation

$$\frac{\partial}{\partial t}W(z,t) = (\mathbf{A}^*W)(z) \quad = \quad -\sum_{i=1}^{n}\frac{\partial}{\partial z_i}\Big(a_i(z)W\Big) + \sum_{i,j=1}^{n}\frac{\partial^2}{\partial z_i \partial z_j}\Big(b_{ij}(z)W\Big) \tag{1}$$

has the Lyapunov function

$$H(t) = H[W_1,W_2] = \int_\Gamma W_1(z,t)\log\frac{W_1(z,t)}{W_2(z,t)}\,dz, \tag{2}$$

where W_1 and W_2 are two solutions (for different initial data) to equation (1). The Lyapunov function $H(t)$ has the properties $H(t)\geq 0$, $H[W,W]=0$, and $\frac{d}{dt}H(t)\leq 0$. If we take the stationary solution $W_2 = W_\infty$, $H(t)$ has the physical meaning of a negative entropy, and $\frac{d}{dt}H(t)\leq 0$ can be understood as the second law of thermodynamics, showing (under further assumptions) that the considered physical system tends to the equilibrium state W_∞.
Equation (1) describes the evolution of the probability density $W(z,t)$ of a Markov process $z(t)$ in phase space $z(t)\subset\Gamma\subset\mathbb{R}^n$. As usual, equation (1) is considered in L_1-type spaces, for instance $L_1(\Gamma,dz)$, where it has (under certain assumptions) a unique normalized positive solution $W(z,t)\geq 0$, $\|W(\cdot,t)\|_{L_1}=1$, if the initial density $W_0(z)$ is positive and normalized.
In general, e.g., if the coefficients of (1) degenerate $b_{ij}(z)\geq 0$, the densities can vanish somewhere or they may not exist at all. In this case it is difficult to understand what is $H(t)$, defined by (2), and to show $\frac{d}{dt}H(t)\leq 0$ in a rigorous way. Furthermore, it is natural to ask if there are other Lyapunov functions of (1) and what other equations of this type have Lyapunov functions. These problems can be solved completely by an inequality for Radon measures ([3]) in the following way:
Let Γ be a compact topological Hausdorff space, $C(\Gamma)$ the space of continuous real-valued functions on Γ, and $C^*(\Gamma)$ (the dual of $C(\Gamma)$) the space of regular Radon measures, $C^{**}(\Gamma)$ the bidual of $C(\Gamma)$, and $\langle\cdot,\cdot\rangle$ their dual pairing.
Let $\mathcal{S}^* = \{p\in C^*(\Gamma)\ :\ p\geq 0, \|p\|=1\}$ be the convex set of positive and normalized (i.e. probability) measures in $C^*(\Gamma)$ and $\mathcal{S}^*_e = \big\{\delta_z \ \big|\ z\in\Gamma\big\}$ the subset of extreme points of $\mathcal{S}^*$.
Let $\mathbf{S}$ be a linear Markov operator in $C(\Gamma)$, i.e. an operator with $\mathbf{S}\geq 0$ and $\mathbf{S}\ 1 = 1$, and $\mathbf{S}^*$ its adjoint. $\mathcal{S}^*$ is invariant with respect to adjoint Markov operators.

Theorem 1: Let $p,q\in\mathcal{S}^*$, $\mathbf{S}^*$ the adjoint of a Markov operator and $F(x):\mathbb{R}_+\longrightarrow\mathbb{R}$ a convex function with $F(1)=0$. Let q/p be the Radon-Nikodym derivative of q by p and

$H[p,q] := \langle F(q/p), p\rangle$, then the following inequality holds: $0 \le H[\mathbf{S}^* p, \mathbf{S}^* q] \le H[p,q]$. Equality holds if $\mathbf{S}^*$ maps extreme points to extreme points $\mathbf{S}^* \mathcal{S}_e^* \subset \mathcal{S}_e^*$.

This result can be extended, if q/p does not exist, but $H[p,q]$ exists.
From this inequality one can derive Lyapunov functions for linear evolution equations for probability measures. Let $\mathbf{A}$ be the generator of a continuous semigroup in $C(\Gamma)$, satisfying $\mathbf{A}1 = 0$ and the maximum principle, i.e. $(\mathbf{A}g)(z_+) \le 0$ for $g \in D(\mathbf{A})$, where z_+ is the max-point of g (i.e. $g(z) \le g(z_+)$, $z \in \Gamma$). Then, it is well known ([1]) that the evolution equation

$$\dot{p}(t) = \mathbf{A}^* p(t), \;\; p(0) = p_0 \in \mathcal{S}^* \tag{3}$$

has a unique weak* solution in $\mathcal{S}^* \subset C^*(\Gamma)$ for any t.

Theorem 2: Let $p_0, q_0 \in \mathcal{S}^*$ and $H[p_0,q_0] := \langle F(q_0/p_0), p_0\rangle$ exist. Let $p(t)$ and $q(t)$ be two solutions to equation (3) with $p(0) = p_0$ and $q(0) = q_0$. Then $H[p(t),q(t)]$ exists for all times and satisfies $0 \le H[p(t_2),q(t_2)] \le H[p(t_1),q(t_1)]$, $t_2 \ge t_1$. If equation (3) is the Liouville equation of a dynamical system $\dot{z} = \Phi(z)$ with solution in $C(\Gamma)$, then equality holds, i.e. the function $H(t) = H[p(t),q(t)]$ is constant in time.

If $q = q_\infty$ is any stationary solution, we get $0 \le H[p(t_2),q_\infty] \le H[p(t_1),q_\infty]$ for $t_2 \ge t_1$.
Similar results can be obtained for non-autonomous problems and Markov chains.
If $\Gamma \subset \mathbb{R}^n$, then the general form of operators $\mathbf{A}$, satisfying the maximum principle, is

$$\big(\mathbf{A}g\big)(z) \;\; = \;\; \sum_{i=1}^n a_i(z) \frac{\partial}{\partial z_i} g + \sum_{i,j=1}^n b_{ij}(z) \frac{\partial^2}{\partial z_i \partial z_j} g + \int\!\!\!\!\!\!- _\Gamma \, Q(z,z') \Big(g(z') - g(z) \Big) dz'$$

with suitable coefficients $b_{ij} \ge 0$, $Q(z,z') \ge 0$. The mean-valued integral is a pseudo-differential operator of order less than 2. The corresponding kinetic equation is formally

$$\begin{aligned} \frac{\partial}{\partial t} W(z,t) \;\; &= \;\; -\sum_{i=1}^n \frac{\partial}{\partial z_i} \Big(a_i(z) W \Big) + \sum_{i,j=1}^n \frac{\partial^2}{\partial z_i \partial z_j} \Big(b_{ij}(z) W \Big) + \\ &+ \;\; \int\!\!\!\!\!\!- _\Gamma \Big(Q(z',z) W(z') - Q(z,z') W(z) \Big) dz' \end{aligned}$$

(if there is no density W, this equation is to be understood in a weak* sense in $\mathcal{S}^*$).
While this result holds for arbitrary convex functions $F(x)$, the second law for linear kinetic equations is not a consequence of the special definition of the entropy by the log function. Any negative entropy, defined by $H(t) = \langle F(p_\infty/p(t)), p(t)\rangle$ is constant in a deterministic system and decreases in a random system.

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4.2 Research Group Laser Dynamics

4.2.1 Overview

Im Mittelpunkt der Forschungen steht die Entwicklung analytischer und numerischer Methoden zur Analyse, Simulation und Steuerung dynamischer Systeme und deren Anwendung auf Probleme optischer Kommunikationssysteme und der Reaktionskinetik.
Forschungsschwerpunkte sind

- Modellierung, Analyse und Simulation der Dynamik von Mehrsektions-Halbleiterlasern mit verzögerter Rückkopplung,
- Verzweigungen und Stabilitätswechsel in Mehrskalensystemen.

Die Erfolge der Forschungsgruppe basieren auf enger nationaler und internationaler Kooperation, die finanziell durch das WIAS, die DFG, den DAAD und das BMBF gefördert wurde. Die Ergebnisse wurden in führenden internationalen Zeitschriften veröffentlicht.
Wir möchten erwähnen, dass die Resultate auf dem Gebiet des Stabilitätswechsels in Mehrskalensystemen, die in Zusammenarbeit mit dem Lehrstuhl für Differentialgleichungen an der Physikalischen Fakultät der Staatlichen Universität Moskau erhalten wurden, einen wesentlichen Anlass für die Verleihung des Lomonossov-Preises erster Klasse an unsere Partner Prof. V. F. Butuzov, Prof. N. N. Nefedov und Prof. A. B. Vasil'eva bildeten.
Ein weiterer Höhepunkt in der Arbeit unserer Forschungsgruppe war das internationale Echo auf die Workshops

- Multiscale Systems and Applications,
- Dynamics of Semiconductor Lasers,

die von unserer Gruppe in Zusammenarbeit mit dem DFG-Forschungszentrum „Mathematik für Schlüsseltechnologien“ und dem Sonderforschungsbereich 555 „Komplexe Nichtlineare Prozesse“ durchgeführt wurden.

The research of the group is focused on the development of analytic and numerical methods for the analysis, simulation, and control of dynamical systems and their applications to problems of optical communication systems and reaction kinetics.
The main research is concerned with the following topics

- Modeling, analysis, and simulation of the dynamics of multi-section semiconductor lasers with delayed feedback;
- Bifurcations and exchange of stabilities in multi-scale systems.

The successes of the research group are based on a close national and international cooperation financially supported by WIAS, DFG, DAAD, and BMBF. The results have been published in leading international journals.

We would like to mention that the research achievements in the field of exchange of stabilities in multiscale systems obtained in cooperation with the chair of differential equations at the Faculty of Physics of the Moscow State University essentially contributed to awarding Prof. V.F. Butuzov, Prof. N.N. Nefedov and Prof. A.B. Vasil'eva the First Class Lomonosov Prize.

A further highlight of the work of our research group was the international response to the workshops

- Multiscale Systems and Applications;
- Dynamics of Semiconductor Lasers,

organized by our group in cooperation with the DFG Research Center “Mathematics for Key Technologies” and the Collaborative Research Center 555 “Complex Nonlinear Processes”

4.2.2 Projects

Dynamics of semiconductor lasers

Collaborators: M. Radziunas, K.R. Schneider, D. Turaev (until 10/03), A. Vladimirov, M. Wolfrum, S. Yanchuk, U. Bandelow (FG 1)

Cooperation with: B. Sartorius, O. Brox, S. Bauer, B. Hüttl, R. Kaiser, M. Rehbein (Fraunhofer-Institut für Nachrichtentechnik, Heinrich-Hertz-Institut, Berlin (HHI)), H.-J. Wünsche (Institut für Physik, Humboldt-Universität zu Berlin (HU)), L. Recke (Institut für Mathematik, Humboldt-Universität zu Berlin (HU)), H. Wenzel (Ferdinand-Braun-Institut für Höchstfrequenztechnik, Berlin (FBH)), M. Umbach (u^2t Photonics AG, Berlin), S.V. Gonchenko (Institute for Applied Mathematics and Cybernetics, Nizhny Novgorod, Russia), G. Kozyreff (Mathematical Institute, Oxford University, UK)

Supported by: BMBF: "Hochfrequente Selbstpulsationen in Mehrsektions-Halbleiterlasern: Analysis, Simulation und Optimierung" (High frequency self-pulsations in multi-section semiconductor lasers: Analysis, simulations, and optimization),
DFG: DFG-Forschungszentrum „Mathematik für Schlüsseltechnologien" (Research Center "Mathematics for Key Technologies"), projects D3 and D8; SFB 555 "Komplexe Nichtlineare Prozesse" (Collaborative Research Centre "Complex Non-linear Processes")
Terabit Optics Berlin: project "Modeling and simulation of mode-locked semiconductor lasers"

Semiconductor lasers are key elements in modern telecommunication systems. Our research is focused on edge-emitting multi-section lasers, which due to their complex nonlinear dynamical behavior can be used for generating, transforming, and processing optical signals at high speed. In this project, we are concerned with a broad range of questions, including modeling and numerical simulation as well as analytical investigations of the models and their dynamical properties.
With the software `LDSL-tool`, we develop a comprehensive toolkit to simulate and analyze the spatio-temporal dynamical behavior of a broad range of multi-section lasers, including lasers with dispersive or amplified feedback, mode-locked lasers with saturable absorbers, and interaction of several coupled lasing sections.
Moreover, based on simplified models, we investigate analytically fundamental mathematical structures leading to dynamical behavior like synchronization or short pulses of high intensity.
The main subjects in the period of this report were

- Synchronization of coupled lasers;
- Mode-locking in lasers with saturable absorbers;
- Numerical mode analysis by means of `LDSL-tool`;
- Quasiperiodic regimes in multi-section lasers.

Synchronization of coupled lasers (K.R. Schneider, S. Yanchuk).
Using the model of coupled rate equations

$$\begin{aligned}
\frac{dE_1}{dt} &= i\bar{\delta}E_1 + \tfrac{1}{2}\left(\mathcal{G}_1(N_1,|E_1|^2) - \tfrac{1}{\tau_{p_1}}\right)E_1 + \kappa e^{-i\varphi}E_2(t-\bar{\tau}),\\
\frac{dN_1}{dt} &= I_1 - \tfrac{N_1}{\tau_{c_1}} - \mathrm{Re}[\mathcal{G}_1(N_1,|E_1|^2)]\cdot|E_1|^2,\\
\frac{dE_2}{dt} &= \tfrac{1}{2}\left(\mathcal{G}_2(N_2,|E_2|^2) - \tfrac{1}{\tau_{p_2}}\right)E_2 + \kappa e^{-i\varphi}E_1(t-\bar{\tau}),\\
\frac{dN_2}{dt} &= I_2 - \tfrac{N_2}{\tau_{c_2}} - \mathrm{Re}[\mathcal{G}_2(N_2,|E_2|^2)]\cdot|E_2|^2,
\end{aligned} \tag{1}$$

we study in [2] the dynamics of two face-to-face coupled semiconductor lasers with short time delay τ (see Fig. 1).

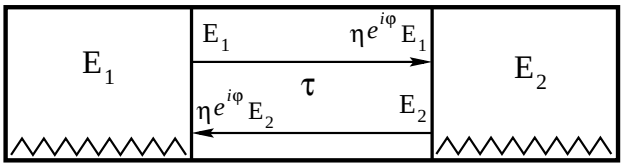

Fig. 1: Schematic configuration of two face-to-face coupled semiconductor lasers

In particular, we have obtained conditions for the stability of synchronized and antisynchronized regimes in the case of identical lasers (see Fig. 2a) as well as conditions for the existence of stable locked states for coupled systems with detuning (see Fig. 2b). The bifurcation diagram in Fig. 2a also reveals that the first destabilization threshold, i.e. the destabilization of the CW solutions by increasing coupling η for fixed φ, may occur already for a coupling strength of order τ_p/τ_c via Hopf bifurcation. Here, τ_p and τ_c ($\tau_p \ll \tau_c$) are photon and carrier lifetimes, respectively.

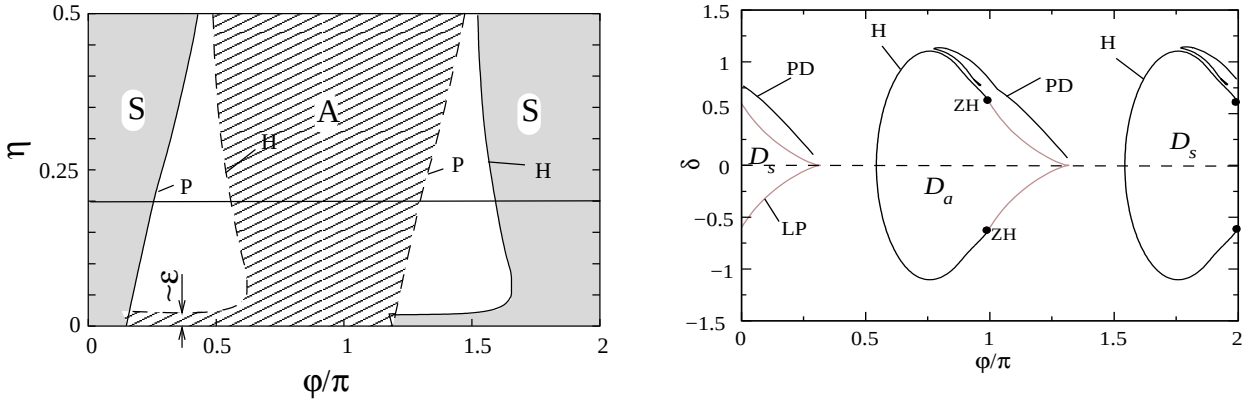

Fig. 2: (a) Region of stability for synchronous "S" and antisynchronous "A" CW solutions, respectively. "P" denotes the curves of transverse pitchfork bifurcation and "H" the curves of Hopf bifurcation. (b) Stability regions D_a, D_s for the stationary states of coupled systems with detuning. "LP" denotes saddle-node bifurcation. "ZH" is a codimension-2 bifurcation point (Guckenheimer-Gavrilov bifurcation).

In [2] we derived conditions for the complete synchronization of two symmetrically coupled identical systems of differential-delay equations

$$\begin{aligned}\frac{dx}{dt} &= f(x,x(t-1))+g(t,x,x(t-1),y,y(t-1)),\\ \frac{dy}{dt} &= f(y,y(t-1))+g(t,y,y(t-1),x,x(t-1)).\end{aligned}$$

Complete synchronization is understood in the sense that $\|x(t)-y(t)\| \to 0$ as $t \to \infty$. For the case of coupled ordinary differential equations with linear diffusive coupling we obtained an estimate of the region of attraction of the synchronized solution. We have also estimated the synchronization error for the case when the coupled systems are not identical, namely, for perturbed systems of the type

$$\begin{aligned}\frac{dx}{dt} &= f(x)+\varepsilon h_1(t,x,y)+g(t,x,y),\\ \frac{dy}{dt} &= f(y)+\varepsilon h_2(t,x,y)+g(t,y,x)\end{aligned}$$

with bounded functions $|h_i| \le m_0$. Under some additional assumptions, we have established the inequality

$$\|x(t,x_0,y_0)-y(t,x_0,y_0)\| \le 2\varepsilon\frac{m_0}{\alpha}+e^{-\alpha t}\left(-2\varepsilon\frac{m_0}{\alpha}+|x_0-y_0|\right) \quad \text{for} \quad t \ge 0, \tag{2}$$

with some positive ε and α. In the papers [3], [4], [5], we have performed mostly a numerical study of the phenomenon of complete synchronization in coupled systems of chaotic oscillators.

Passive mode-locking in semiconductor lasers (D. Turaev, A. Vladimirov).
Passive mode-locking of lasers is a very effective technique to generate high quality short pulses with high repetition rates. Monolithic semiconductor lasers, passively or hybrid mode-locked, are ideal for applications in high speed telecommunication due to their compactness, low costs, and reliability. The basic mechanism for passive mode-locking is well understood since the analysis by New [21], who showed that the differential saturation of the gain and losses in the laser cavity opens a short temporal window of net gain for pulses. A wide range of experimental, numerical, and analytical methods exist to characterize mode-locking (for an overview, see Haus [22] and Avrutin *et al.* [23]). While numerical integrations of traveling wave field equations coupled to material equations (distributed models) faithfully reproduce experimental observations, they offer little insight into the underlying dynamics. This is why analytical approaches based on lumped element models, we refer to those introduced by New [21] and Haus [22] for slow and fast saturable absorbers, are still widely used. Inevitably, though, these approaches require certain approximations (such as, e.g., small gain and loss per pass approximation) that are not satisfied for semiconductor lasers. Therefore, we have proposed a new model for passive mode-locking in a monolithic semiconductor laser which consists of a set of ordinary and delay-differential equations. Unlike the classical mode-locking theories it does not use the approximations of small gain and loss per cavity round trip and weak saturation; these are not satisfied enough in semiconductor laser devices. On the other hand, as in most lumped element models, the spatial effects inherent to a linear cavity, such as spatial hole burning and self-interference of the pulse near the mirrors, are neglected. This amounts to consider a unidirectional lasing in a ring cavity. Absorbing, amplifying, passive,

and spectral filtering segments are placed in succession in the cavity. Under the assumption of Lorentzian lineshape of the spectral filtering element the following set of equations governing the evolution of the complex envelope of the electric field, $a(t)$, and of the saturable gain and losses, $g(t)$ and $q(t)$, have been derived starting from the traveling-wave equations

$$\gamma^{-1}\dot{a}(t) + a(t) = \sqrt{\kappa} e^{\frac{1-i\alpha_g}{2} g(t-T) - \frac{1-i\alpha_q}{2} q(t-T)} a(t-T). \tag{3}$$

$$\dot{g}(t) = g_0 - \gamma_g g(t) - e^{-q(t)} \left(e^{g(t)} - 1 \right) |a(t)|^2, \tag{4}$$

$$\dot{q}(t) = q_0 - \gamma_q q(t) - s \left(1 - e^{-q(t)} \right) |a(t)|^2. \tag{5}$$

Here, the delay parameter T is equal to the cold cavity round trip time, $g(t)$ and $q(t)$ describe unsaturated gain and loss, the parameter γ stands for the spectral width of the bandwidth limiting element, s is the ratio of the saturation energies of the amplifying and absorbing sections; κ describes linear non-resonant losses per cavity round trip, $\alpha_{g,q}$ are the linewidth enhancement factors.

The model equations (3)–(5), being more general than the classical mode-locking models by New and Haus, can be reduced to these models in certain particular limits. New's results [21] can be obtained by setting $\gamma^{-1} = 0$ in the left-hand side of (3) and expanding the exponentials on the right-hand side of (3), (4), and (5) up to the first-order terms in g and q**.** If, on the other hand, we neglect all relaxation terms in (4) and (5), substitute their solutions in (3), expand to second order in pulse energy, and finally assume periodicity with period $T + \delta T$, using the expansion $a(t) \approx a(t-T) + \delta T \dot{a}(t-T)$ in the right-hand side of (3), then the Haus sech solution [22] can be recovered in the limit $\gamma \to \infty$.

One advantage of this new formulation of the mode-locking problem is that it allows us to make use of techniques that have been developed for delay-differential systems. In particular, we have used the package DDE-BIFTOOL [24] in order to study bifurcations leading to the appearance and break-up of a mode-locking regime.

The constant intensity (cw) solution of (3)–(5) exists above the linear threshold, $g_0/\gamma_g > \left(q_0/\gamma_q - \ln \kappa \right)$. We have studied bifurcations of this solution. The bifurcation diagram is shown in Fig. 1a in the (g_0, q_0) plane for the parameter values given in the figure caption. The curves H_n indicate Andronov-Hopf bifurcations to time-periodic intensities with periods close to T/n. The curve H_1 corresponds to the fundamental mode-locking regime with pulse repetition frequency close to $\Omega_1 = 2\pi/T$, while the curves H_n with $n = 2, 3, 4$ signal the onset of multiple pulse ML regimes with the repetition frequencies close to $n\Omega_1$. On the other hand, H_Q is an Andronov-Hopf bifurcation with a frequency approximately eight times smaller than Ω_1. This

bifurcation is responsible for the Q-switching instability.

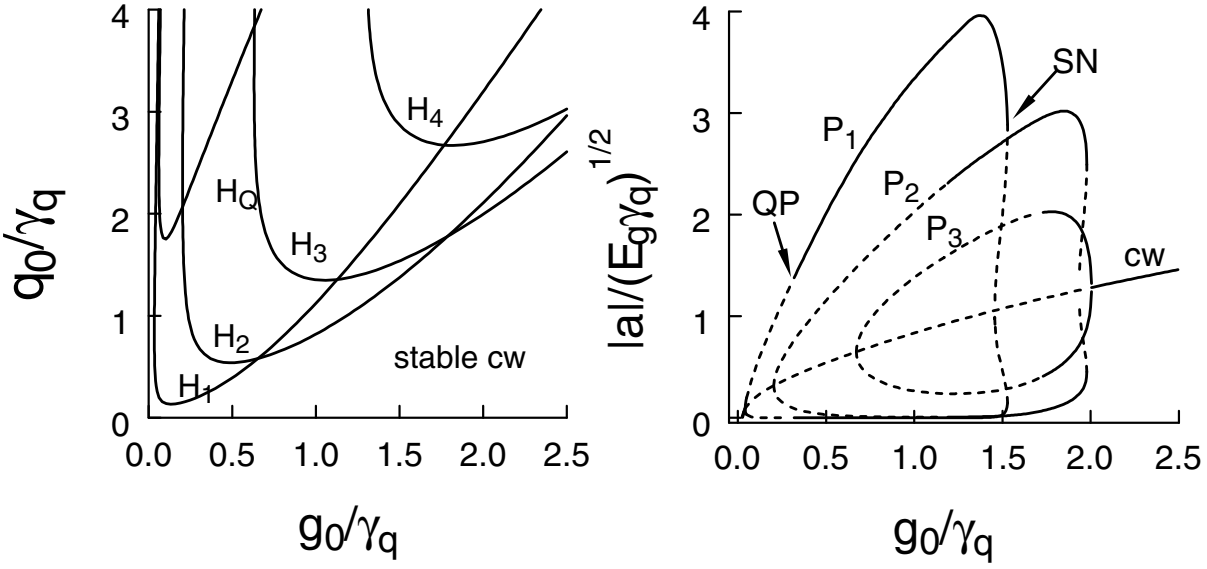

Fig. 3: (a) Andronov-Hopf bifurcations of the cw solution of Eqs. (3)–(5).
(b) Branches of ML solutions bifurcating from the Andronov-Hopf bifurcation curves shown in Fig. 1a. Solid (dotted) lines indicate stable (unstable) solutions. The branch of constant intensity solutions is labeled *cw*.

Similarly to the Andronov-Hopf bifurcation curves, the branches of periodic solutions and their stability have been calculated numerically using DDE-BIFTOOL. An example is shown in Fig. 1b. The branch P_1 corresponding to the fundamental mode-locking regime has a stability range limited by two bifurcation points. The left one of these two points is a secondary Andronov-Hopf bifurcation point labeled *QP*. This bifurcation produces a solution with quasiperiodic laser intensity that corresponds to a mode-locking regime modulated by the Q-switching frequency. With the decrease of the pump parameter g_0 below the *QP* point, the modulation depth grows for the quasiperiodic solution. Another bifurcation point, labeled *SN*, is a saddle-node bifurcation where two periodic intensity solutions, one stable and the other unstable, merge and disappear. The solutions corresponding to multiple pulse mode-locking are labeled P_2 and P_3 in Fig. 1b. These solutions undergo bifurcations similar to those of the fundamental branch P_1. In a certain parameter range a bistability exists between different mode-locking regimes.

The proposed model can be extended to study active or hybrid mode-locking and to include additional microscopic effects, e.g., carrier heating. This model is easy to simulate and analyze. Unlike the classical mode-locking theories developed by New and Haus it can describe asymmetric pulses with “unstable” background that can appear in the case of large cavity losses per pass, i.e. in a situation typical of semiconductor lasers. A derivation and a more detailed description of the proposed model are given in [25, 26, 27].

New features of `LDSL-tool`: Mode analysis (M. Radziunas).
During the last years we were considering different aspects of the traveling wave model (a hyperbolic system of first-order one-dimensional PDEs nonlinearly coupled with ordinary differential equations)

$$\begin{aligned} \frac{\partial}{\partial t}E(z,t) &= H(z,\partial_z,\beta(z,n,|E|^2))E(z,t), \\ \frac{d}{dt}N(z,t) &= I(z,t)-R(z,N)-\Re e[E^* g(z,N(z,t),|E|^2)E], \end{aligned} \tag{6}$$

which describes the complicated nonlinear dynamics of the optical field and the polarization ($E(z,t)$ is a four-component complex vector function), and the carrier densities (real vector function $N(z,t)$) in multi-section semiconductor lasers, [6, 9, 10]. Here, the operator H contains first-order spatial derivatives ∂_z and is mainly determined by the spatially distributed complex propagation factor β. Its domain includes also the corresponding boundary conditions.
Different topics of our research such as numerical integration of the model equations, computation of eigenvalues, derivation and investigation of the reduced ODE system (mode approximation) were implemented in the software `LDSL-tool` ("Longitudinal Dynamics in Semiconductor Lasers"), [6, 10, 11, 12, 13]. These potentialities turn `LDSL-tool` into a powerful tool suited for simulations, parameter studies, and analyses of various dynamical effects in different multi-section semiconductor lasers. The application of `LDSL-tool`, together with theoretical and experimental studies, have proved to be very useful to get a better understanding of the laser behavior as well as for designing lasers with specific properties, [7, 8, 9, 13, 14].
In what follows we report on the recently implemented capacity of `LDSL-tool` to perform mode analysis (i.e. to analyze the dynamics of longitudinal modes) which allows to understand and to predict typical dynamical behavior of the optical field $E(z,t)$ and its power $|E|^2$, [7, 10, 11, 13, 14]. For this reason, we decompose the computed optical field $E(z,t)$ into modal components that are determined by the eigenfunctions $\Theta(z,\beta)$ of the operator H, that is, we solve for each computed instant distribution of the propagation factor $\beta(z,t)$ the spectral problem:

$$[H(\beta)-i\Omega(\beta)]\,\Theta(z,\beta)=0 \qquad \Rightarrow \qquad E(z,t)=\sum_{k=1}^{\infty} f_k(t)\Theta_k(z,\beta). \tag{7}$$

Here, $\Re e\Omega$ and $\Im m\Omega$ determine the modal wavelength (or angular velocity) and the damping of the mode, respectively, [6, 7, 10, 11]. Squared modulus of the complex modal amplitudes $|f(t)|^2$ (after an appropriate normalization of the eigenfunctions $\Theta(z,\beta)$) represents the contribution of the corresponding mode at the laser facet. Figures 4a and 4b represent results of the mode analysis in a three-section laser with two distributed feedback sections.

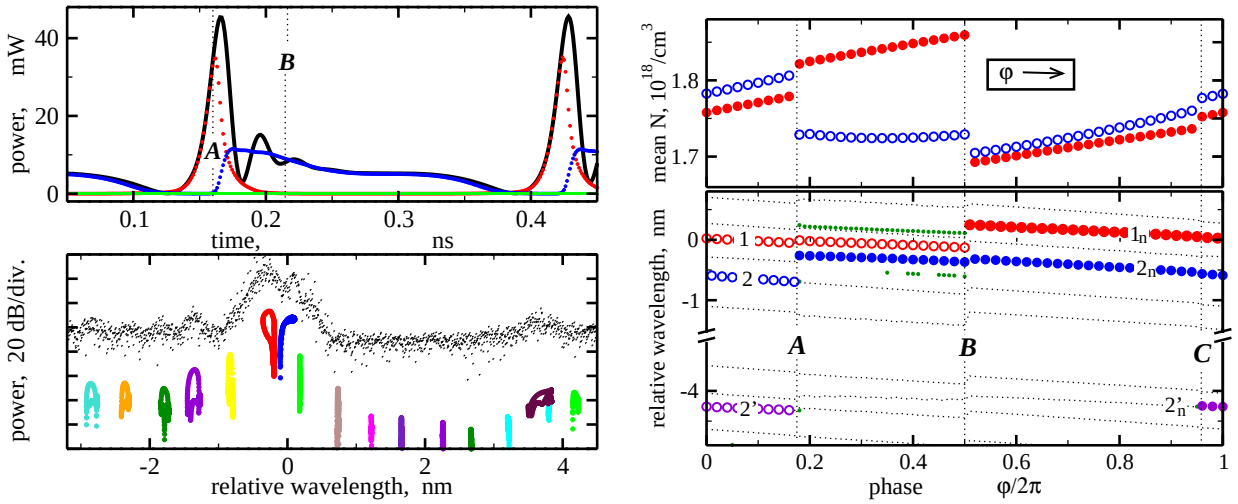

Fig. 4: a (left side): Outgoing optical field (black) and its decomposition into modes (colored) in time (above) and frequency (below) domain.
b (right side): Sectionally averaged N (above) and modal wavelengths (dotted lines below) as a function of the face $\varphi/2\pi$. Thick and thin bullets in the lower diagram represent main and side peak positions in the optical spectrum of the outgoing optical field.

A detailed description of the mode analysis can be found in [10, 13].

Quasiperiodic regimes in multi-section semiconductor lasers (D. Turaev, K.R. Schneider). Consider an edge-emitting multi-section semiconductor laser with k active sections. The longitudinal dynamics of such lasers can be described by the traveling wave model reflecting the slow dynamics of the carrier densities and the fast dynamics of the electromagnetic field

$$\begin{aligned} \frac{dE}{dt} &= H(N)E, \\ \frac{dN_j}{dt} &= \varepsilon\,(f_j(N) - E^T g_j(N) E^*),\ j = 1,\ldots,k. \end{aligned} \tag{1}$$

We suppose that there is a point N^0 in R^k such that the operator $H(N^0)$ has k simple eigenvalues located on the imaginary axis, while all other eigenvalues λ_i satisfy $\mathrm{Re}\,\lambda_i < \kappa < 0$. Under these assumptions there exists a smooth inertial manifold such that (1) represents on this manifold an ODE system of the form

$$\begin{aligned} \frac{dE_c}{dt} &= [H_c(N) - \varepsilon\alpha(N)F(E_c,N) + O(\varepsilon^2)]E_c, \\ \frac{dN}{dt} &= \varepsilon F(E_c,N) + O(\varepsilon^2), \end{aligned} \tag{2}$$

with $E_c \in C^k$, $N \in R^k$. We establish the existence of nearly identical coordinate transformations mapping (2) into some normal form that can be viewed as a small dissipative perturbation (of order $\sqrt{\varepsilon}$) of the conservative and reversible system

$$\frac{d^2u}{d\tau^2} = \hat{F}(N^0) - \hat{G}(N^0) \begin{pmatrix} e^{u_1} \\ \vdots \\ e^{u_k} \end{pmatrix}, \tag{3}$$

where $|E_{c,i}|^2 = e^{u_i}, i = 1, \ldots, k$.
Under some conditions, we can conclude from the existence of equilibria of system (3) to the existence of invariant tori of system (2) for sufficiently small ε. In case $k = 2$ we derive inequalities which implies the existence of an asymptotically stable invariant torus for system (2). For more details we refer to [20].

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Multiscale systems

Collaborators: K.R. Schneider, E.V. Shchetinina, D. Turaev (until 10/03)

Project 1: Blue-sky catastrophe in singularly perturbed systems (D. Turaev).

Cooperation with: A.L. Shilnikov (Georgia State University, Atlanta, USA), L.P. Shilnikov (Institute for Applied Mathematics and Cybernetics, Nizhny Novgorod, Russia)

One of the basic questions of dynamics concerns the structure of the regions of stability of periodic orbits. The last known stability boundary was discovered only in 1995, [1]. It corresponds to the so-called blue-sky catastrophe, a special case of a saddle-node bifurcation where a saddle periodic orbit collides with a stable one, then both disappear, and a single stable periodic orbit with very large length and period is created (the length and period tend to infinity when the bifurcational moment is approached). The global structure of the unstable set of the saddle-node for the blue-sky catastrophe appears to be rather complex. Nevertheless, it was shown in [2] that this particular configuration of the unstable set is, in fact, quite typical for singularly perturbed systems with at least two fast variables.
A singularly perturbed system, a paradigm for dynamical processes with two distinct time scales, is a system of the form

$$\begin{aligned} \dot{x} &= g(x,y,\varepsilon), \\ \varepsilon\dot{y} &= h(x,y,\varepsilon), \end{aligned}$$

where $\varepsilon > 0$ is a small parameter; x stands for the slow variables and y for the fast ones. The y equation for fixed x is called a fast system. The dynamics of singularly perturbed systems is characterized by the slow motion along the invariant manifolds corresponding to attractors of the fast system (equilibria or periodic orbits in the simplest situation) and by fast jumps between different such manifolds. The jumps happen at the values of x which correspond to bifurcations in the fast system.
In this project we show ([3]) that the blue-sky catastrophe almost inevitably accompanies the saddle-node bifurcation in the slow-fast systems, where there are jumps between invariant manifolds corresponding to fast periodic orbits and those corresponding to fast equilibria. We present and analyze three distinct specific scenarios which lead to the blue-sky catastrophe in the singularly perturbed systems. These scenarios correspond to three different types of jumps, caused either by a saddle-node bifurcation in the fast system, or by an Andronov-Hopf

bifurcation, or by a homoclinic loop.

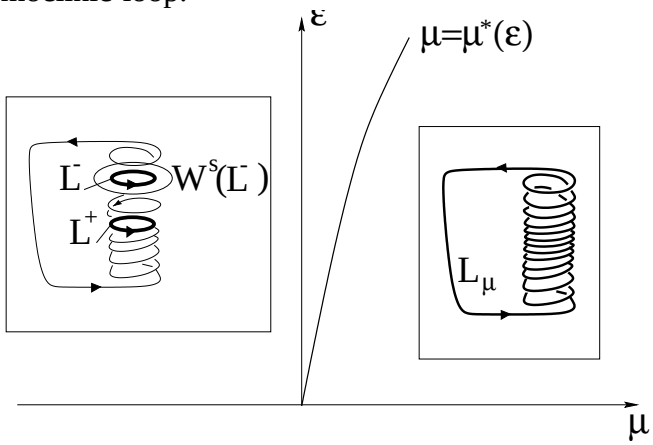

Fig. 1: At $\mu < \mu^*(\varepsilon)$ the system has two periodic orbits: a stable orbit L^+ and a saddle orbit L^-. The orbits which do not lie in the stable manifold of L^- tend to L^+ as time increases. At $\mu > \mu^*(\varepsilon)$ the system has a single and attracting limit cycle L_μ whose length tends to infinity as $\mu \to \mu^*(\varepsilon) + 0$.

We remark that the suggested mechanisms of the blue-sky catastrophe in singularly perturbed systems have indeed been reported in models of neuronal activity, for example, describing the dynamics of the leach heart interneurons ([4]). The transition (illustrated in Fig. 1) from one type of self-sustained oscillations (a round stable periodic orbit L^+) to the regime where the attractor is the "long" stable orbit L_μ can be interpreted as a transition from periodic tonic spikes to periodic bursting oscillations of the neuron.
Note as well that even before the transition to the bursting oscillations the spiking mode is in an excitable state here: a perturbation which drives the initial point outside the saddle limit cycle L^- results in a long calm phase before the sustained spiking restores.

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Project 2: Exchange of stabilities in multiscale systems (E.V. Shchetinina, K.R. Schneider).

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

Supported by: DFG: 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

Consider a dynamical system of the type $dx/dt = f(x,\lambda)$ and assume that the parameter λ slowly changes in time. Setting $\lambda \equiv \varepsilon\tau$ we obtain after rescaling t the singularly perturbed non-autonomous differential equation

$$\varepsilon \frac{du}{dt} = f(u,t),\ 0 < \varepsilon \ll 1. \tag{1}$$

We suppose that the solution set $f^{-1}(0)$ of the degenerate equation of (1)

$$0 = f(u,t)$$

consists in the (t,u)-plane of two curves $k_1(u \equiv 0)$ and k_2 intersecting transversally for $t = 0$. If the solution $\overline{u}(t,u^0,\varepsilon)$ of (1), satisfying $u(t_0) = u^0$ for $t_0 < 0$, exists for $t > 0$, then the behavior near $t = 0$ can be characterized by one of the following cases:

(i) $\overline{u}(t,u^0,\varepsilon)$ follows immediately the stable branch of k_2,

(ii) $\overline{u}(t,u^0,\varepsilon)$ follows for some $O(1)$-time interval (not depending on ε) the unstable part of k_1 and then jumps either to the stable part of k_2 or to infinity (blowing up).

The case (i) is called an immediate exchange of stabilities, the case (ii) is referred to as delayed exchange of stabilities or as delayed loss of stability. These cases cannot be treated by applying the standard theory of singularly perturbed systems. In [1], [2], [3], we have developed a theory based on the method of asymptotic upper and lower solutions to characterize and to distinguish immediate and delayed exchange of stabilities. In the project under consideration we study equation (1) under the assumption that the curves k_1 and k_2 intersect in at least two different points. By means of the method of asymptotic upper and lower solutions we derive conditions on f guaranteeing that the solution of the initial value problem exhibits the phenomena of immediate as well as of delayed exchange of stabilities. It is important to emphasize that it is not possible to prove this result by only verifying the assumptions for immediate and delayed exchange of stabilities. In fact, we have to look for an appropriate modification of the method of asymptotic upper and lower solutions. We also study the case that f is periodic in t. In order to be able to prove the existence of a harmonic solution which represents a periodic forced canard we have to construct asymptotic upper and lower solutions which are discontinuous and contain boundary layer functions.

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Project 3: Integral manifolds loosing their attractivity (E.V. Shchetinina, K.R. Schneider).

Cooperation with: V.A. Sobolev, E.A. Shchepakina (Samara State University, Russia)

We consider slow-fast systems that can be transformed into the form

$$\begin{aligned} \frac{dy}{dt} &= \varepsilon Y(t,y,z,\varepsilon), \\ \frac{dz}{dt} &= B(t)z + Z(t,y,z,a(y,\varepsilon),\varepsilon) + a(y,\varepsilon), \end{aligned} \tag{1}$$

where $y \in R^n$, $z \in R^2$, ε is a small positive parameter, a is a two-dimensional vector function, and $B(t)$ is the matrix

$$B(t) = \begin{pmatrix} \alpha t & \beta \\ -\beta & \alpha t \end{pmatrix} \quad 0 < \alpha, \beta < +\infty.$$

The eigenvalues of the matrix $B(t)$ are $\alpha t \pm i\beta$, that is $B(0)$ has purely imaginary eigenvalues, and therefore (1) is a nonhyperbolic system.

The aim of this project is to investigate the integral manifolds loosing their attractivity and, especially, to study their relations with the phenomenon of delayed loss of stability. In the hyperbolic case the existence of the integral manifolds of the form $z = h(t,y,\varepsilon)$ has been known for a long time (see, e.g., [1]).

It is proved that under some general assumptions on the functions Y and Z, there exists a control function $a(y,\varepsilon)$ such that system (1) has an integral manifold $z = h(t,y,\varepsilon)$, where h is uniformly bounded. We note that this manifold is attractive for $t < 0$ and repulsive for $t > 0$. We call these manifolds loosing as manifolds their attractivity.

The question of the smoothness of the integral manifold and of the control function is investigated. By the induction method it is shown that if the functions $Y(t,y,z,\varepsilon)$, $Z(t,y,z,a,\varepsilon)$ have continuous and uniformly bounded partial derivatives with respect to the variables y,z,a,ε up to the order k, then the integral manifold $h(t,y,\varepsilon)$ and the control function $a(y,\varepsilon)$ have continuous and uniformly bounded partial derivatives with respect to y up to the order $k-1$.

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Project 4: Maximal temperature of safe combustion in case of an autocatalytic reaction (K.R. Schneider).

Cooperation with: E.A. Shchepakina (Samara State University, Russia)

We consider the problem of thermal explosion of a gas mixture in case of an autocatalytic combustion reaction in a homogeneous medium. As a mathematical model we use the differential system

$$\begin{aligned} \varepsilon \frac{d\Theta}{dt} &= \eta(1-\eta)e^{\Theta} - \alpha\Theta, \\ \frac{d\eta}{dt} &= \eta(1-\eta)e^{\Theta}. \end{aligned} \tag{1}$$

Here, Θ denotes the temperature, η is the depth of conversion of the gas mixture, $-\alpha\Theta$ describes the volumetric heat loss, and ε is a positive parameter which is small in case of a highly exothermic reaction. There exists an exponentially small α-interval $A_\varepsilon := (\alpha_0(\varepsilon), \alpha_1(\varepsilon))$ containing $\alpha^*(\varepsilon)$, where

$$\alpha^*(\varepsilon) = \alpha_0 + \alpha_1\varepsilon + O(\varepsilon^2),\ \alpha_0 = e/4,\ \alpha_1 = -e/\sqrt{2},$$

such that for $\alpha > \alpha_1(\varepsilon)(\alpha < \alpha_0(\varepsilon))$ belongs to the slow regime (explosive regime). The interval A_ε characterizes the critical regime. For $\alpha \in A$, there are canard trajectories $\sum_{\alpha,\varepsilon}(t)$ of system (1) starting at $\Theta = \Theta_0 = 0,\ \eta = \eta_0 < 0.5$, and satisfying $\sum_{\alpha,\varepsilon}(t) \to (\eta = 1,\ \Theta = 0)$ as $t \to \infty$. Our goal is to estimate the maximal temperature $\Theta^\varepsilon_{\max}$ of the canard solution $\sum_{\alpha,\varepsilon}(t)$ for $\alpha = \alpha^*(\varepsilon)$ and ε sufficiently small. We derive an estimate and an asymptotic relation for $\Theta^\varepsilon_{\max}$ as $\varepsilon \to 0$ by means of a result on delayed exchange of stabilities in singularly perturbed systems derived by one of the authors ([1]).

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4.3 Research Group Numerical Mathematics and Scientific Computing

4.3.1 Overview

Die Forschungsgruppe erarbeitet numerische Verfahren für Systeme von partiellen Differentialgleichungen und Algebro-Differentialgleichungen, analysiert diese Methoden und wendet sie auf relevante Fragestellungen der Praxis an. Dabei sind die Forschungen naturgemäß langfristig angelegt. Besondere Bedeutung kommt der Entwicklung und Implementierung numerischer Software zu. Hier stellt die Forschungsgruppe moderne und effiziente Werkzeuge bereit.

The group develops numerical procedures for systems of partial differential equations and differential–algebraic equations, analyzes these methods, and applies them to practical problems of interest. The research projects are, by their nature, long-term studies. Of particular importance is the development and implementation of numerical software, to which the group creates and provides modern and efficient tools.

Die Methoden bewähren sich bei konkreten Anwendungen in Projekten mit Partnern aus der Industrie und experimenteller Forschung. Diese Kontakte wiederum stimulieren weitere mathematisch-numerische Forschungen.

The methods are applied to real-world problems in collaborative projects with partners from industry and experimental research. These contacts in turn stimulate further mathematics-based numerical research.

Die thematischen Schwerpunkte waren:

- Numerische Verfahren und Softwarekomponenten für die Lösung von Systemen partieller Differentialgleichungen,
- Simulation von Höchstfrequenzschaltungen,
- Statische und dynamische Simulation verfahrenstechnischer Prozesse.

The main research topics were:

- Numerical procedures and software modules for the solution of systems of partial differential equations;
- Simulation of high-frequency circuits;
- Stationary and dynamic simulation in process engineering.

Ein Schwerpunkt der Arbeiten in der Forschungsgruppe im Jahre 2003 war die Überarbeitung des Designs der Toolbox `pdelib` zur numerischen Lösung partieller Differentialgleichungen.

The new design of the toolbox for solving partial differential equations `pdelib2` was one of the objectives the group focused on.

`pdelib2` ist als nochmals verbesserte Brücke zwischen neuen algorithmischen Entwicklungen und deren effizienter Implementierung innerhalb und außerhalb des WIAS und Anwendungen gedacht.

`pdelib2` is designed to bridge the gap between new algorithmic developments and their fast and efficient implementation inside and outside WIAS.

pdelib2 bietet Programmierschnittstellen zu Geometriebeschreibung, Gittergenerierung, paralleler Assemblierung, Lösungsverfahren für lineare und nichtlineare Probleme, sowie interaktiver Visualisierung, welche es dem Nutzer erlauben sollen, sich auf den problemspezifischen Code zu konzentrieren.

pdelib2 offers interfaces to describe geometries, generate grids, assemble functions and Jacobian matrices in parallel, and solution procedures for linear and nonlinear equations. Together with the interactive visualization possibilities pdelib2 will allow the user to stay focused on her or his special application code.

Neue Features sind u. a.

- Cache-Effizienz und Parallelisierung für Shared-Memory-Architekturen auf der Basis spezieller Gitterpartitionierungen,
- Einbindung der Gittergeneratoren triangle (2D, J. R. Shewchuk, University of California, Berkeley) und TetGen (H. Si, WIAS Berlin),
- Basis-Datenstruktur für alle algorithmisch relevanten Objekte sind ein- oder zweidimensionale Felder. Damit lassen sich alle diese Objekte aus verschiedenen Programmiersprachen ansprechen.
- Ein großer Teil der Programmierschnittstellen ist sowohl in C als auch in der Extensionssprache Lua vorhanden, um eine einfache Problembeschreibung mittels einer Skriptsprache zu ermöglichen.

New features:

- Improved cache efficiency and portable parallelization for shared memory architectures using special grid partitioning and coloring algorithms;
- Integration of grid generators: triangle (2D, J.R. Shewchuk, University of California, Berkeley), TetGen (H. Si, WIAS Berlin);
- Multilingual support, the basic data structures for all objects relevant for any algorithm are one- or two-dimensional arrays, that guaranties freedom of choice for programming languages per algorithm;
- A large fraction of the interfaces is defined in C and the extension language Lua, to make problem description easily possible by using a scripting language.

In der Forschungsgruppe werden zudem die folgenden institutsweiten Querschnittsaufgaben bearbeitet:

- Aktive Unterstützung anderer Gruppen bei der numerischen Umsetzung von Projekten mit pdelib, z. B.
  - Numerische Simulation und Optimierung der Züchtung von SiC-Einkristallen durch Sublimation aus der Gasphase (siehe S. 40),
  - Spannungsanalyse in einer dünnen Wafer-Platte,

In addition, the group works on the following cross-sectional tasks:

- Active support for other groups in converting mathematical problems to forms compatible with pdelib, e.g.,
  - Numerical simulation and optimization of SiC single crystal growth by sublimation from the gas phase (see page 40);
  - Stress analysis of a thin wafer plate;

– Optimierung diffraktiver Strukturen und Rekonstruktionsmethoden für stark schlechtgestellte Probleme (siehe Seite 101).

- Entwicklung spezieller Moduln und Features für `pdelib`, allgemeine Beratung in numerischen Fragen,
- Gittergenerierung,
- Visualisierung.

– Optimization of diffractive structures and reconstruction methods for severely ill-posed problems (see page 101).

- Development of special modules and features for `pdelib`, general advice for questions on numerical issues;
- Grid generation;
- Visualization.

4.3.2 Projects

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, und Max-Planck-Institut für extra-terrestrische Physik, Garching)

The main goal is the development of improved algorithms for the numerical solution of degenerate systems of elliptic and parabolic partial differential equations based on discretizations, fulfilling qualitative stability properties, known from the analytic equations, too.
The semiconductor device equations can be seen as an example out of a much larger class of problems, but they are well understood in many respects, sufficiently hard to solve and of practical interest—hence a good candidate to deal with. The interest starts with grid generation, includes properties of the equations and their discretization, effective algorithms for the solution, and ends with solving some selected real-world problems.
The present status of the work is roughly characterized by:

- A basic level of the models (for recombination, transport phenomena, etc.);
- A general geometry and boundary descriptions using tetrahedral Delaunay grids;
- Three different Newton methods based on different decoupling techniques together with the use of iterative and direct simulation methods (`PARDISO`, see page 69) to solve the stationary equations and to compare their efficiency and robustness;
- The use (expansion) of 2D numerically given doping profiles is possible now.

The present results are:

- A 3D prototype code (SMP parallel in the essential parts, using a completely weak formulation of the finite volume discretization) for discussing and investigating some issues of interest in the more general `pdelib2` (see page 96) design, including basic algorithms;
- The transfer of specific algorithms to `WIAS-TeSCA`;
- And some contribution by “insight” into computed potential and density distributions to the design of a DEPFET sensor at the Semiconductor Laboratory in Munich.

To illustrate the status from the application point of view, a summary of the device function is given: the DEPFET combines detection and amplification within one device, [1]. A p-channel MOSFET or JFET (junction field effect transistor, contacts SOURCE, GATE, DRAIN) is integrated onto a silicon detector substrate, which becomes fully depleted by the application of a sufficiently high negative voltage to a backside p+ contact (BACK). By means of sideward depletion, a potential minimum is formed which is shifted directly underneath the transistor channel at a depth of about $1\,\mu m$ below the GATE contact. Incident photons and particles generate electron-hole pairs within the fully depleted bulk. While the holes drift into the back contact, electrons are accumulated in the potential minimum, called the internal gate. The

resulting change of the JFET current is a measure of the collected amount of charge and the deposited energy, respectively.
The readout of the device is non-destructive and can be repeated several times. For removing signal electrons and thermally generated charges from the internal gate, a clear structure is integrated into the device (contacts CLEAR and CLEAR-GATE). The efficiency of the clear process determines the readout noise essentially. Understanding this process is the point where 3D device simulations enter. Due to the very low input capacitance the inherent noise during amplification becomes very low. Equivalent noise charges of about two electrons were measured at room temperature on recently fabricated structures.
DEPFET detectors can be applied for XRAY spectroscopy, e.g., in space or biomedical experiments ([2], [3]) as well as for particle detection, for instance, in vertex detectors ([4]).
The pictures (generated by `gltools`) show the electron and hole density ($\log_{10}$) in a section of a sensor element. The grid is highly anisotropic and has a resolution of order 10 *nm* close to the contacts. The computational domain of 18x28x50 μm^3 size is discretized by 156000 nodes. The numerical challenges are introduced by the floating regions and the very small recombination, resulting in density variations of 25 orders of magnitude.
The I-V curves show some properties of the detector for different boundary and doping conditions. The device performance depends strongly on doping concentration, geometric parameters, and boundary conditions.
Numerical challenges for the future are, for instance, faster algorithms to allow higher resolution and time-dependent computations on better grids (TetGen, see page 71). Investigations of the interaction of two or more pixel sensor elements may be another task introducing a new level of complexity.

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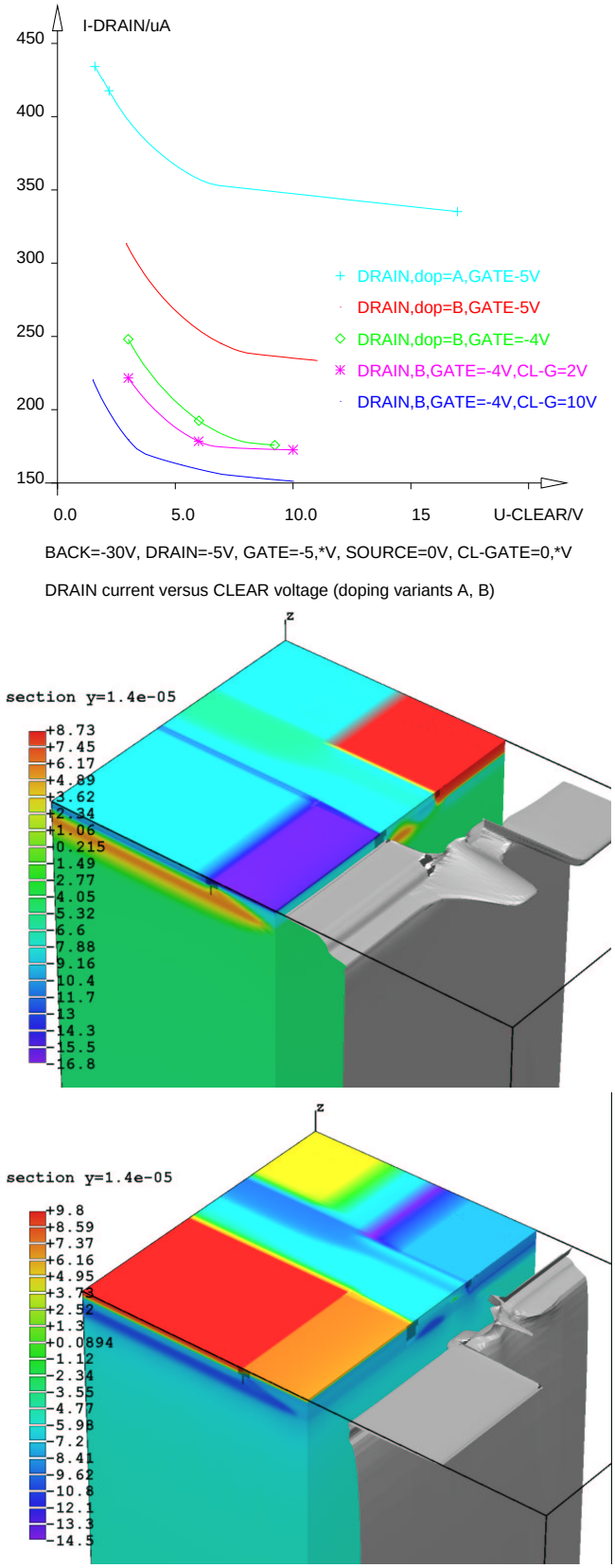

Fig. 1: I-V curves (top), $\log_{10}$ of the electron (middle) and hole densities (bottom) at the top and a vertical cut (cut at $y = 14\,\mu m$, grey relief) of the detector.
(The contact areas on top of the device can be identified by the following codes (e, h: color), where e denotes the electron density and h the holes density pictures above: CLEAR (e: red), CLEAR-GATE (e, h: light blue), DRAIN (in the cut of region), GATE (h: orange), SOURCE (h: red), floating region (h: yellow).)

Optimization of the sparse direct solver `PARDISO` for use in the Intel Math Kernel Library

Collaborator: K. Gärtner

Cooperation with: O. Schenk (Universität Basel, IFI, Switzerland), B. Greer (Intel Corporation, Hillsboro, Oregon, USA)

After passing the evaluation process at Intel Hillsboro, the incorporation of the solver into the Intel Math Kernel Library (MKL) was stated as project goal. The interplay of `PARDISO` [1, 2, 3] with the Intel compilers and other Math Kernel Library routines (especially BLAS3 routines) was further improved. Intel took care of the questions arising from the programming interface conditions of the MKL and the problems related to redistributing the libraries for different processors and operating systems.
A MKL user interface introducing an additional abstraction layer is provided and, for experienced users, the original one is maintained, too. Because `PARDISO` involves large sets of matrices with very different sizes, it will be used as one of the performance measurement tools at Intel. Future MKL development will particularly pay attention to the behavior in a parallel environment and will assure that especially the DGEMM implementation works as well as possible for small and large matrices.
Just now in January 2004 Intel announced the β release of `PARDISO` within MKL
(see http://www.intel.com/software/products/mkl/beta/features.htm).
The distribution via the vendor library will benefit internal simulation needs and provide users outside academia with a stable code basis.

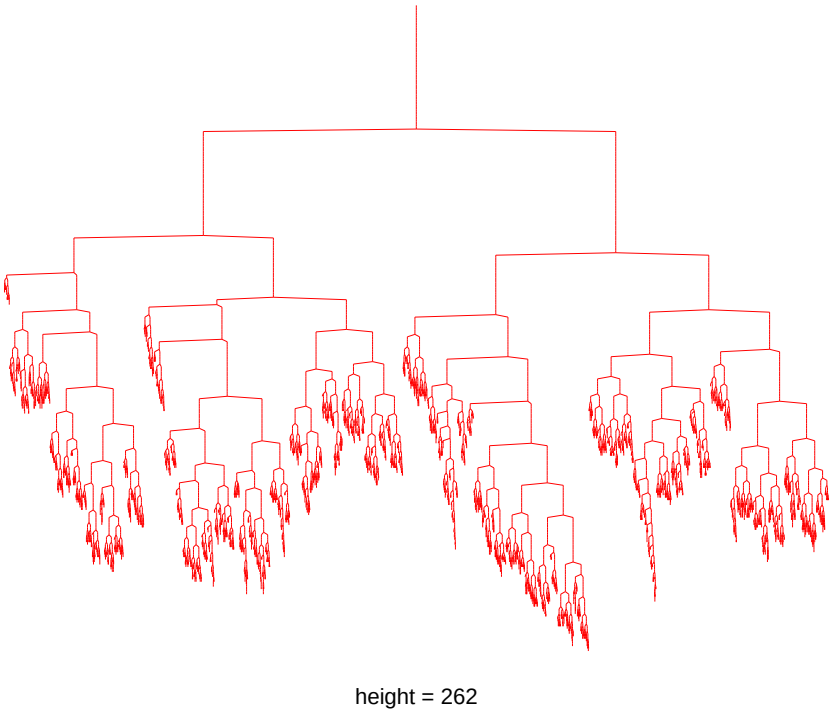

Fig. 1: Elimination tree after permutation for four processors

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Three-dimensional 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. The purpose of this research at WIAS is to provide a reliable and efficient three-dimensional mesh generation tool based on the up-to-date technologies, including newly developed algorithms. TetGen, a 3D Delaunay mesh generator and TetView, a geometry and mesh visualization and debugging program shall be reviewed here.

TetGen TetGen is a 3D tetrahedral mesh generator. It creates tetrahedral meshes conforming to the Delaunay criteria (so-called conforming Delaunay tetrahedralizations, or CDT) for arbitrary 3D domains with piecewise linear boundary. It has various options to refine CDTs and produces high-quality Delaunay meshes which are suitable for finite element and finite volume methods. TetGen is written in C++. It is freely available at http://tetgen.berlios.de (open source). A lot of people are interested in using TetGen (about 150 downloads per month). Clearly, this produces feedback and contacts from all over the world. Very different applications and the related requirements contribute to quality improvement.
In the year 2003, the development of TetGen can be divided into two parts: the release of version 1.2c, and the development of new meshing algorithms.
TetGen Version 1.2c is an improved version of version 1.2, especially with respect to stability and efficiency. In detail, it has the following features:

- Improved algorithms for geometric predications using finite precision arithmetic;
- Detection and handling of two degenerate cases: cospherical points, coplanar points;
- The input/output user interface “tetgenio” was complemented;
- A new boundary edge recovery algorithm for constrained Delaunay tetrahedralization was included;
- Various quality checking and refinement routines have been added to improve the quality of the resulting mesh.

TetView TetView is a 3D mesh and geometry viewer. It can be used to view and manipulate tetrahedral meshes and surface triangular meshes. It views geometries like piecewise linear complexes, too. The driving force for developing TetView is the need for efficient visualization working on algorithmic issues of TetGen. TetView is distributed in executable form for many operating systems. Figure 3 shows the interactive graphical user interface of TetView. It uses OpenGL as the kernel for efficiently rendering 3D objects. Experienced users can exploit the scripting possibilities provided by Lua to generate animations. The WIAS tools LDF (Lua Data Framework) and `gltools` provided the basis for the TetView development.

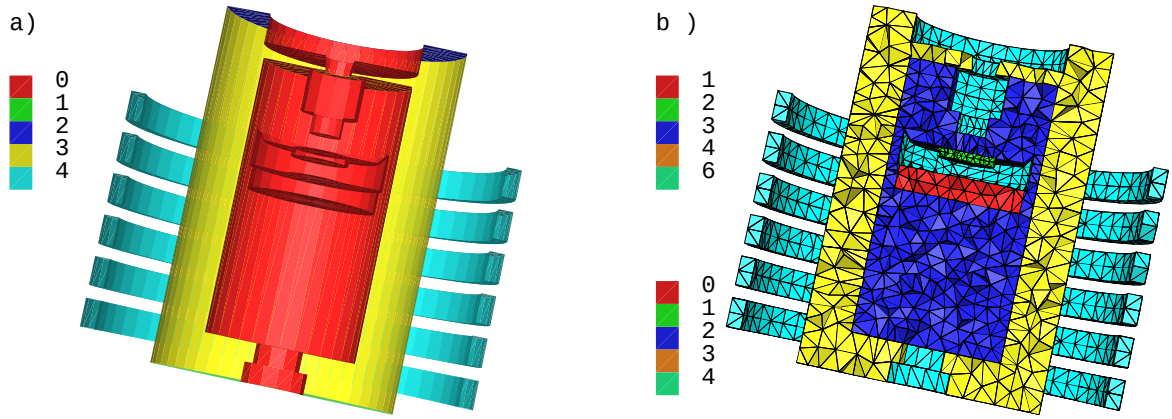

Fig. 1: Mesh of a crystal growth apparatus. (a) shows the input model (a piecewise linear complex) with different boundary markers; (b) the resulting mesh (cut in the middle to show a view accordingly to (a), different materials are displayed in different colors; the model is due to the WIAS crystal growth simulation project, see page 40).

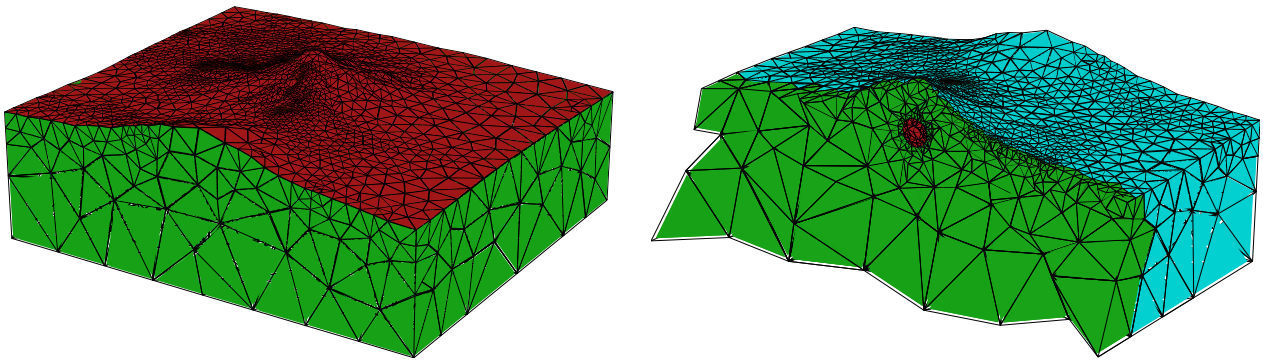

Fig. 2: Quality mesh of a geological model of volcano Merapi (Java/Indonesia, model provided by C. Rücker, Institute for Geophysics and Geology of the University of Leipzig).

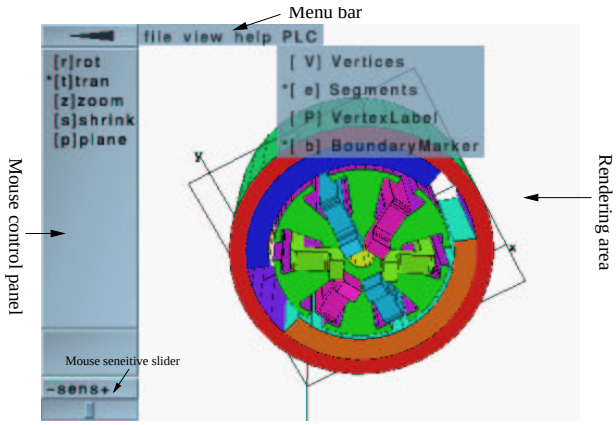

Fig. 3: Example view of the graphic user interface of TetView

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

Like in many other process industries, the numerical process simulation plays an important role in today's gas turbine engineering. Here, the simulation is used for process design, safety management, efficient operation and control of single components of industrial gas turbines (Fig. 1) as well as entire combined-cycle power plants. In complex and highly nonlinear modeling, large-scale simulation problems may arise. Thus, using concentrated physical models, high-dimensional systems of nonlinear or differential–algebraic equations (DAEs) have to be solved in static or dynamic process simulation, respectively. For their solution, robust and fast numerical simulation tools are needed.

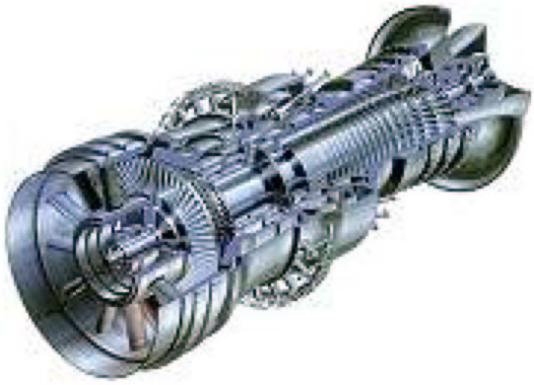

Fig. 1: Industrial gas turbine (source: www.power.alstom.com)

At the Weierstrass Institute we have developed a simulation concept which exploits the modular structure of the process, that in most cases corresponds to the hierarchical unit structure of the underlying plant (see, e.g., the right part of Fig. 2). With it the corresponding system of equations is structured into subsystems according to the units and can be portioned into blocks, which can then be treated almost concurrently within appropriately modified numerical methods. The approach is based on divide and conquer techniques and has been implemented in the Block Oriented Process simulator BOP 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). Within this approach a block-partitioned system of equations

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

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

is solved, 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. For static problems the system of

DAEs degenerates to a system of nonlinear equations. Efficiently parallelizable block-structured Newton-type methods, [1], can be applied in both cases.
In the period under report, the simulation approach of BOP was successfully adapted to the process simulation of industrial gas turbines. Improvements of the numerical methods in combination with a more efficient implementation have led to a remarkable speedup of simulation time in this field. Simulations of numerous industrial gas turbine problems have shown that the simulation runs with BOP are between two and five times faster than those performed with the Aspen Custom Modeler^{TM} (ACM), a worldwide leading commercial simulation tool of Aspen Technology (USA). For about 95 % of these simulation problems, the steady state solution was found with the standard numerical control parameters of the BOP solver. In almost all of the remaining cases, the solution was found after modification of some control parameters. After the implementation of a subset of the modeling language of ACM, BOP can now handle three different types of model descriptions. Beside a description with MLPE, descriptions with language subsets of SPEEDUP and ACM are possible as well, where the two subsets correlate to the scope of MLPE. Additionally, we implemented techniques that allow an exchange of parameters (fixed) and variables (free) of a simulated process without the necessity either to generate a new data interface or to recompile model functions before a new simulation run of the modified sample can be performed. This holds also for repeated fixed-free changes.

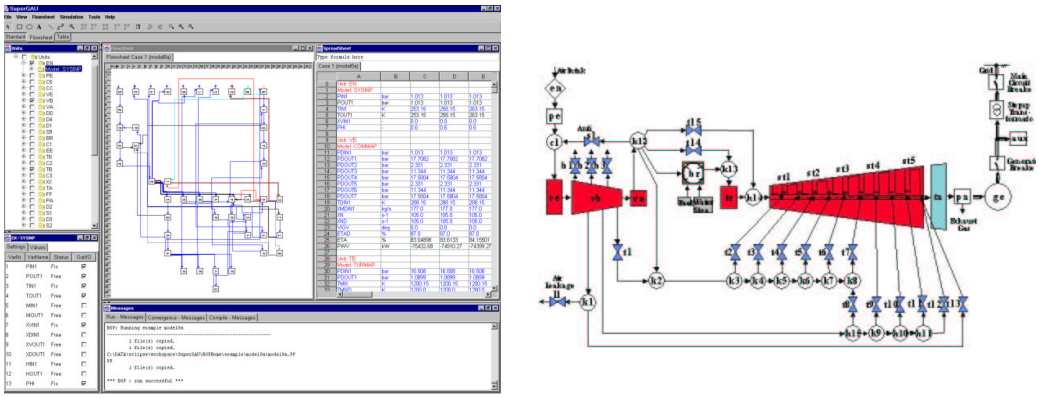

Fig. 2: Graphical user interface *SuperGAU* and a modular model of a gas turbine (ALSTOM (Switzerland) Ltd.)

As a result of these achievements, a license of the simulator has been sold to ALSTOM (Switzerland) Ltd., a leading gas turbine producer. Currently, BOP is used here for single steady state simulation as well as parameter verification problems. It runs under the Windows XP operating system on PCs, where it is called by the graphical user interface *SuperGAU* (see the left part of Fig. 2) developed by our cooperation partner at ALSTOM Power.
Lately, a second contract between WIAS and ALSTOM has been signed which aims at an enlargement of the functionality of BOP as well as a further adaptation to industrial needs. In this context we started the implementation of advanced elements of the modeling language of ACM, which are currently not included in MLPE. Beside this we provided the simulator with a Java Native Interface (JNI) and a binary input/output. The interface is needed for a direct data transfer between the Java GUI and the simulator, now realized by a dynamic link library.
The numerical methods realized within BOP require a repeated solution of linear systems with the same pattern structure of sparse, unsymmetric coefficient matrices. This is done with an

adapted version of our linear solver *GSPAR*, [3], which uses a modified Gaussian elimination with column reordering, partial pivoting, and pseudo code generation for refactorization (so-called *fast second factorization*). The basic (non hierarchical) version can be used as a stand-alone linear solver as well. Its newest version *GSPAR2* has recently been compared with the solver *UMFPACK Version 4.1 (Apr. 30, 2003)* (Timothy A. Davis, CISE Department, University of Florida, USA). Results concerning the computing time on an *HP AlphaServer GS1280 7/1150* are given in Table 1. For the linear systems with matrices arising from different real-world applications, the numbers *N* and *NNZ* denote the order and the number of nonzeros of the coefficient matrix, respectively.

Table 1: *CPU times (in sec.) for factorization using GSPAR2 and UMFPACK V4.1*

Matrix			*GSPAR2*		*UMFPACK V4.1*	
	N	NNZ	First Factoriz.	Fast second Factoriz.	Symbolic Factoriz.	Numeric Factoriz.
bayer01	57 735	277 774	0.696	0.105	0.32	0.45
lhr34c	35 152	764 014	4.977	1.042	0.53	0.83
circuit_4	80 209	307 604	1.202	0.035	2.65	2.20
shermanACb	18 510	145 149	0.211	0.034	0.13	0.27

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Numerical simulation of non-Newtonian fluids of Oldroyd type

Collaborator: N.D. Scurtu

This work is realized in the framework of my dissertation under the supervision of Prof. Dr. E. Bänsch. In nature, there are many fluids that do not satisfy the Newtonian constitutive law. This is also the case of many fluids created for industrial purposes. Fluids like multi-grade oils, liquid detergents, shampoos, dyes, adhesives, biological fluids like blood, paints, greases, printing inks, industrial suspensions, polymer solutions, and polymer melts, fall within the category of non-Newtonian fluids.

The numerical simulation of many industrial problems has been carried out using viscoelastic models of the Oldroyd kind. The aim of this work is to develop a mixed finite element method for the computation of instationary, incompressible non-Newtonian fluid flow. Viscoelastic fluid models of Oldroyd type are considered. The dimensionless constitutive, momentum, and continuity equations, respectively, for the Oldroyd fluid model are:

$$\begin{cases} We\left(\dfrac{\partial \tau}{\partial t}+(\mathbf{u}\cdot\nabla)\tau+\beta_a(\tau,\nabla\mathbf{u})\right)+\tau-2\alpha D=0 \\ Re\left(\dfrac{\partial \mathbf{u}}{\partial t}+(\mathbf{u}\cdot\nabla)\mathbf{u}\right)-2(1-\alpha)divD-div\tau+\nabla p=\mathbf{f} \\ div\,\mathbf{u}=0 \end{cases}$$

where $\beta_a(\tau,\nabla\mathbf{u}) := \frac{1-a}{2}(\tau\nabla\mathbf{u}+\nabla\mathbf{u}^T\tau)-\frac{1+a}{2}(\nabla\mathbf{u}\tau+\tau\nabla\mathbf{u}^T)$, $a\in[-1,1]$

($a=1$ corresponds to the Oldroyd-B model).

The unknown fields are the symmetric stress tensor $\tau:\mathbb{R}_+\times\Omega\longrightarrow\mathbb{R}_s^{N^2}$, the velocity field $u:\mathbb{R}_+\times\Omega\longrightarrow\mathbb{R}^N$, and the pressure field $p:\mathbb{R}_+\times\Omega\longrightarrow\mathbb{R}$, where $\Omega\subset\mathbb{R}^N$, $N=2,3$.
Initial conditions and boundary conditions of Dirichlet type for the velocities and a condition for the stresses on the upstream boundary section have to be added.
Three parameters characterize the flow: the Reynolds number $Re\geq 0$, the fraction of viscoelastic viscosity $\alpha\in[0,1]$, and the Weissenberg number $We\geq 0$. This system includes the Navier-Stokes system as a particular case ($We=0,\alpha=0$), so it is favorable to develop a numerical method which can generalize an existing one used for the Navier-Stokes system.

There are two aspects which must be discussed for this system: the finite element spatial discretization and the time discretization.
The solution of Oldroyd's problem by the finite element method presents a difficulty due to the hyperbolic character of the constitutive equation.
This hyperbolic character implies that some upwinding is needed. The choice of the upwinding technique depends on the choice of the finite element space used to approximate τ. Since no continuity requirement is needed on τ at interfaces between elements, as shown in [2], this will be done by using the discontinuous Galerkin method, which allows the computation of each component of τ on an element-by-element basis. For fixed τ the last two equations are a Stokes system in the variables $\mathbf{u}$ and p. To solve the Stokes system, a mixed finite element method was used: the stable Taylor-Hood element on unstructured simplicial grids, i.e. piecewise-quadratic basis functions for the velocity and piecewise-linear for the pressure.

Major numerical problems for the instationary Oldroyd system arise due to the incompressibility condition, the strong nonlinearity in the momentum equation, the transport of the stress, the strong coupling of the unknowns, and stability versus accuracy of the numerical scheme.
The decoupled computation of stress, velocity, and pressure is performed with an algorithm involving a time approximation based on the fractional θ-scheme ([3]) and on the splitting method introduced by Saramito ([6]). As an operator splitting method, the θ-scheme was used, e.g., by Bänsch for the Navier-Stokes equations ([1]). The method consists of splitting each time interval $[t_n, t_{n+1}]$ of length Δt into three subintervals $[t_n, t_n+\theta\Delta t]$, $[t_n+\theta\Delta t, t_n+(1-\theta)\Delta t]$, and, $[t_n+(1-\theta)\Delta t, t_{n+1}]$, and integrating the equations on each of these subintervals.

For the Navier-Stokes equations this scheme is second-order accurate, non-dissipative, and A-stable. Stability and convergence analysis of the fractional step θ-scheme for the unsteady Navier-Stokes equations are proven in [4] and [5]. Due to the complexity of the splitting method for the Oldroyd system, only the stability in the linearized case could be proved. The spectral analysis of the splitting scheme for the linearized equation system in Fourier space shows very good properties of this scheme (ξ = wave vector):

- (local) stability: the eigenvalues of the asymptotic damping factor fulfill $|\lambda_i(\Delta t, |\xi|)| \leq 1$;
- strong stability: the eigenvalues fulfill
  - $\lim_{\Delta t\to\infty} |\lambda_i(\Delta t, |\xi|)| < 1$, ξ is the wave vector,
  - $\forall\varepsilon > 0\ \exists\Delta t_0,\ \xi_0 :\ |\lambda_i(\Delta t, |\xi|)| \leq q+\varepsilon,\ q<1\ \forall\Delta t \geq \Delta t_0,\ \forall|\xi| \geq |\xi_0|$;
- accuracy: second-order accurate if $\theta = 1-\frac{\sqrt{2}}{2}$, else only first-order accurate.

For the numerical realization of the algorithm, the following subproblems and solvers are used: in the first and third step, a Stokes problem (CG), for the second step, a Burgers-like subproblem (GMRES) and a stress-transport problem (GMRES discontinuous Galerkin FEM scheme) are to be solved.
To prove the correctness of the algorithm implementation, the experimental order of converges (EOC) was calculated. The EOC is defined by:

$EOC_h := \dfrac{ln(\frac{Err_h}{Err_{h/2}})}{ln(2)}$, with errors $Err_h = \lim\limits_{t\to\infty} \|u(\cdot,t) - u_h(\cdot,t)\|$ and grid size h.

The table below contains EOC tests for different norms of the unknown of the Oldroyd system. The numerical results are presented for two examples. For each example, computations with $Re = 1.0$, $\alpha = 0.89$, and different values of We are presented. $\|\cdot\|_{dg}$ is the norm used in the discontinuous Galerkin method for error estimation.

We	$\|p-p_h\|_{L_2}$	$\|p-p_h\|_{H_1}$	$\|u-u_h\|_{L_2}$	$\|u-u_h\|_{H_1}$	$\|\tau-\tau_h\|_{L_2}$	$\|\tau-\tau_h\|_{dg}$
1.0	2.2563	1.1283	2.3071	1.3095	2.1580	1.6599
4.0	2.4671	1.1959	2.3036	1.3586	2.1354	1.6317
40.0	2.1266	1.0343	2.5759	1.5868	2.0295	1.4994
0.5	2.0734	1.0306	2.7892	1.7899	2.1941	1.8746
1.0	2.1578	1.078	2.9616	1.9939	2.036	1.5056
10.0	2.2528	1.1113	3.4107	2.5078	2.0345	1.4937

The numerical algorithm is implemented in ALBERT, an adaptive hierarchical finite element toolbox ([7]).
The described method is applied to the computation of the flow in a plane 4:1 contraction, subject to specified boundary conditions. Such a flow is of interest from both a theoretical and a practical point of view (e.g., in relation to polymer processing problems). Experiments show increasing recirculating zones when the Weissenberg number *We* increases. Similarly growth of the recirculating zones may be expected also in numerical experiments.
Figure 1 shows the streamlines in the upper half part of the 4:1 contraction flow and Figure 2 the recirculating zone in the right upper corner.

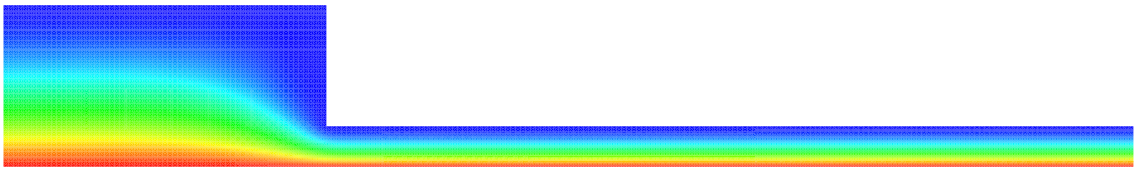

Fig. 1: Streamlines

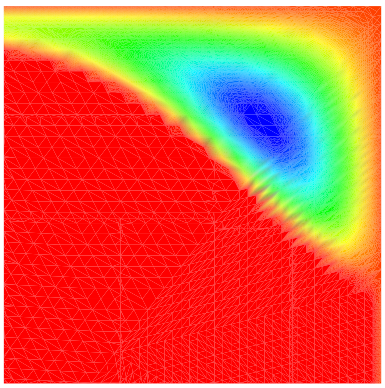

Fig. 2: Streamlines in the right upper corner

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Two-phase flow with evaporation

Collaborators: R. Krahl, E. Bänsch

Cooperation with: M. Dreyer (Universität Bremen, ZARM), M. Adamov, M. Lozano Avilés (Technische Universität Berlin)

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

The prediction of the dynamic behavior of liquids with free capillary surfaces in partly filled containers is of importance for the construction of space vehicles using liquid propulsion. In the case of cryogenic propellants, this behavior is influenced to a large extent by thermal effects, such as evaporation. As a first step for simulations, a model for two-phase flow with evaporation has been developed.
To model the situation mathematically, balance equations for mass, momentum, and energy in the bulk of the phases and on the phase boundary, respectively, were established, assuming gas and liquid to be incompressible Newtonian fluids and using the Boussinesq approximation to model buoyancy. In the bulk of both phases this leads to the Navier-Stokes equations with convection-diffusion equations for heat and vapor:

$$\begin{aligned}
\rho(\partial_t \mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u}) - \mu\Delta\mathbf{u} + \nabla p &= \rho\mathbf{g} - \rho\beta_T(\vartheta-\vartheta_0)\mathbf{g}, && (1)\\
\nabla\cdot\mathbf{u} &= 0, && (2)\\
\rho c_p(\partial_t\vartheta + \mathbf{u}\cdot\nabla\vartheta) - \lambda\Delta\vartheta &= \tau : (\nabla\mathbf{u}), && (3)\\
\partial_t\rho_v + \mathbf{u}\cdot\nabla\rho_v - \varsigma\Delta\rho_v &= 0. && (4)
\end{aligned}$$

On the phase boundary, we get the following jump conditions:

$$\begin{aligned}
[\rho\,(\mathbf{u}\cdot\mathbf{n} - u_\Gamma)] &= 0, && (5)\\
[\rho\mathbf{u}\,(\mathbf{u}\cdot\mathbf{n} - u_\Gamma) - \mathbf{T}\mathbf{n}] &= -(\sigma(\nabla_S\cdot\mathbf{n})\mathbf{n} - \sigma_T\nabla_S\vartheta), && (6)\\
[\rho c_p\vartheta(\mathbf{u}\cdot\mathbf{n} - u_\Gamma) - \lambda\partial_\mathbf{n}\vartheta] &= j\Lambda, && (7)\\
\rho_v(\mathbf{u}_g\cdot\mathbf{n} - u_\Gamma) - \varsigma\partial_\mathbf{n}\rho_v &= j. && (8)
\end{aligned}$$

Further conditions are needed to determine the evaporation rate j. Thus, we add the assumption that the temperature ϑ is continuous and is always equal to the saturation temperature ϑ_{eq} given by the partial pressure of vapor $\psi(\vartheta,\rho_v)$ on the phase boundary. Note that in a precise physical sense this assumption is contradictory to a non-vanishing evaporation rate, since it is the statement of equilibrium. However, the difference $\vartheta - \vartheta_{eq}$ is negligible in many practical cases. This assumption yields a Dirichlet boundary condition for the temperature in both phases that is sufficient to solve the heat transport equation (3). Equation (7) may then be used to calculate j. This approach results in a fully coupled two-phase flow problem.
In general, viscosities in gas are much smaller than in liquid and thus $\mathbf{T}_g\mathbf{n} \ll \mathbf{T}_l\mathbf{n}$. Using this assumption, one may decouple the flow problems from both phases by neglecting the shear stresses from the gaseous phase on the boundary. The flow from the gaseous phase does not have any direct influence on the shape of the free surface then. The flow problems in the two phases are only weakly coupled by the temperature and the mass flux.

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Thermocapillary instability in full-zone liquid bridges

Collaborator: D. Davis

Cooperation with: F. Smith (University College London, UK)

This work has addressed some aspects of the stability of steady axisymmetric melt flows occurring in cylindrical floating-zone configurations, and is the continuation of a project first described in the WIAS 2001 yearly report ([1]). The initial aim of the project was to investigate flow and thermal effects nonlinearly for low Prandtl number (Pr) within a sub-critical framework. In [2] full numerical results from direct simulation (based on solving the *unsteady* incompressible axisymmetric Navier-Stokes and heat-transport equations) were presented for a wide range of domain aspect ratios; it was found that for both sufficiently "wide" domains (that is, having a radius-to-height ratio r_c exceeding 2, roughly) and "narrow" domains ($r_c < 0.3$, approx.) the results showed very good agreement with corresponding results obtained from (asymptotically) reduced models in each case.
Moreover, the (slender-flow) approximation for narrow domains provided considerable insight into the structure of the flow solution, especially in the case of Marangoni convection under zero buoyancy; as the thermo-capillary stress (proportional to the dynamic Reynolds number, Re_D) is increased at the liquid/gas interface, a strong jet-like flow regime is found to emerge around the mid-zone, where the two counter-rotating, axially-aligned tori (which characterize the basic flow) merge.

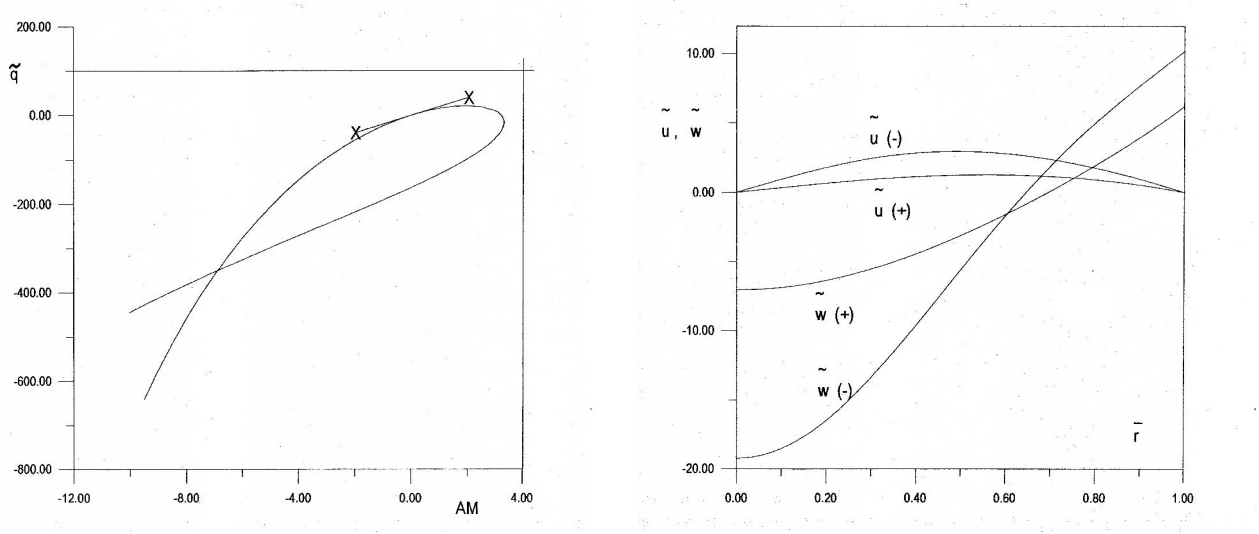

Fig. 1: Sub-critical mid-zone-analysis result from a slender-flow model depicting scaled local pressure gradient (q) versus scaled dynamic Reynolds number (AM), in the left-hand plot; radial profiles of radial ($\tilde{u}$) and axial ($\tilde{w}$) velocity components at the mid-height on the upper ('+') and lower ('-') branches, for $AM = 2.43$, in the right-hand plot; see [2] for further details.

Numerical analysis of the (nonlinear) *reduced-model mid-zone equations* reveals several important properties: (a) if the system has a solution, then it is not generally unique; (b) the flow cannot remain steady and axisymmetric, beyond a critical value of $AM := r_c^3 Re_D$ (≈ 3.31), the scaled dynamic Reynolds number (see Fig. 1). However, the (transient) DNS solutions were

found to be exclusively “upper branch” in type, regardless of the initial conditions used, which would seem to suggest that the “lower branch” is a less probable solution form, in practice.
To investigate the possible solution forms beyond the critical Reynolds number, a series of supercritical flows were simulated (with a fixed Prandtl number of 0.02 and zero buoyancy). The following variational system

$$\frac{d}{dt}\int_\Omega \mathbf{u}\cdot\mathbf{v}\,d\Omega + \int_\Omega \nabla\mathbf{u}:\nabla\mathbf{v}\,d\Omega - \int_\Omega p\nabla\cdot\mathbf{v}\,d\Omega$$
$$+\int_\Omega [(\mathbf{u}\cdot\nabla)\mathbf{u}]\cdot\mathbf{v}\,d\Omega - \int_{\Gamma_{LG}} (\mathbf{u}\cdot\hat{\mathbf{e}}_\theta)(\mathbf{v}\cdot\hat{\mathbf{e}}_\theta)\,dS \;=\; -Re_D r_c \int_{\Gamma_{LG}} \nabla T_D\cdot\mathbf{v}\,dS \tag{1a}$$

$$\int_\Omega (\nabla\cdot\mathbf{u})w\,d\Omega = 0, \tag{1b}$$

$$\frac{d}{dt}\int_\Omega TX\,d\Omega + \frac{1}{Pr}\int_\Omega \nabla T\cdot\nabla X\,d\Omega + \int_\Omega [(\mathbf{u}\cdot\nabla)T]X\,d\Omega = 0, \tag{1c}$$

which is derived from the governing equations and boundary conditions for the floating-zone configuration ([2]), was solved by a standard finite element method using P_2-P_1 Taylor–Hood tetrahedra. To discretize in time, a three-step operator-splitting scheme for the momentum part, combined with a Crank-Nicholson scheme for the heat transport equation, was applied. Here Ω denotes the volume of melt while Γ_{LG} is the liquid-gas interface; also $\mathbf{u}$ is the melt velocity, p the melt pressure, T the melt temperature, T_D the (imposed) temperature on Γ_{LG}, and t time, whereas $\mathbf{v}$, w, and X are appropriate test functions. Our numerical results have indicated that the melt flow undergoes a transition from a steady axisymmetric state to a non-oscillatory *three-dimensional* one, for any given aspect ratio of the bridge. This result is wholly consistent with well-established half-zone results ([3], [4]) and suggests that certain characteristics of the instability mechanism are essentially unchanged for the more realistic full-zone model.

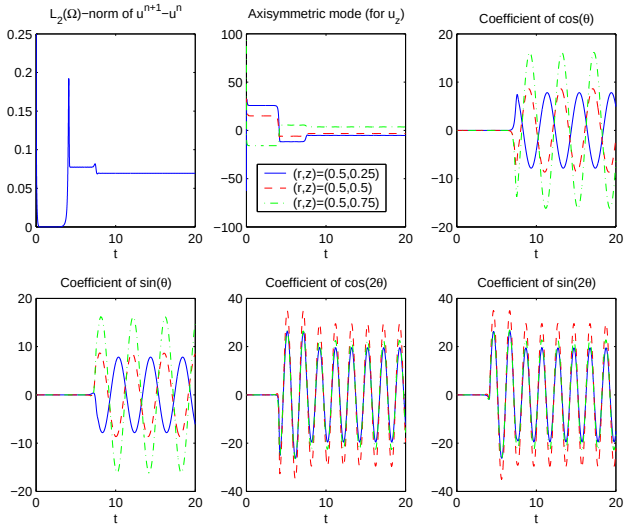

Fig. 2: Fourier-mode transient behavior for $Re_D = 2500$, $Pr = 0.02$, $r_c = 0.5$ indicating the coefficients of axial velocity
($(r,z) = (0.5, 0.25)$ blue solid line, $(0.5, 0.5)$ red dash line, $(0.5, 0.75)$ green dash-dot line.)

In Figure 2, computational results are shown for $Re_D = 2500$, $Pr = 0.02$, and $r_c = 0.5$ with $T_D \equiv sin(\pi z)$ and a zero solution as input. The transient behavior of the *Fourier (angle) modes for axial velocity* at selected points in the domain is mainly portrayed, and from these plots several distinct phases are discernible: (a) the switch to an (unstable) axisymmetric state, at the start; (b) the brief, dominant linear growth of the $m = 2$ mode; (c) the subsequent weakly-nonlinear interaction of the $m = 0$ and $m = 2$ modes, which stabilizes both modes; (d) the later linear growth of the $m = 1$ mode, leading to a significantly asymmetric state. From numerical *linear* instability analysis for half zones ([3], [4]), it is known that for aspect ratios lying between 0.3 and 0.68 approximately, the $m = 2$ mode dominates, which is consistent with the example shown; moreover, in general, the azimuthal number of the most dangerous mode tends to increase with increasing aspect ratio, again in line with half-zone findings.

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Two- and three-dimensional unsteady melt-flow simulation in Czochralski InP crystal growth

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

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

As a result of recent semiconductor technology, there is currently much interest in the growth of high-quality indium phosphide (InP) crystals. This is especially true in the fields of optoelectronics and radio frequency electronics. There it is known, for example, that InP-based electronic components can perform much more efficiently than the hitherto favored gallium arsenide (GaAs) or silicon, mainly because InP can operate at higher frequencies.
Since May 2003 we have been engaged in a collaborative project with the Institute for Crystal Growth (IKZ) in Berlin, which has involved comparison of 2D and 3D numerical transient-flow simulations performed with different solvers at each institute, as a precursor to experimental growth using the vapor-pressure-controlled Czochralski (VCz) equipment at IKZ (http://www.ikz-berlin.de/groups/ag.czhl/pview.php?lang=EN&opt=0&no=07). This method of growth is a variant on the liquid-encapsulated Czochralski (LEC) growth method; an important additional feature of the VCz method is that the crystal, melt, and encapsulant are placed in an insulated inner chamber, which can significantly reduce potentially damaging thermal stresses within the grown crystal. We have previously applied the method to modeling the growth of GaAs crystals, as documented in last year's report [1]. Subsequent results can be found in [2], [3]. A similar model to the one described therein can be applied to InP growth, i.e. the liquid mechanics are again described by a coupled thermo-hydrodynamic system comprising the incompressible Navier-Stokes equations and the heat-transport equation. A fundamental difference applies to the boundary conditions for temperature, specifically on the encapsulant/melt interface Γ_E and the crucible wall Γ_C. For the InP study, we have applied a Dirichlet condition on both boundary sections, based on advection-free global simulation data supplied by IKZ. This contrasts with the more simplified conditions of adiabaticity on Γ_E and Dirichlet value dependence derived from simple functions on Γ_C, as assumed for the GaAs study.

R_C	76.7 mm	ν	1.62×10^{-7} m^2/s
ρ	5.05×10^3 kg/m^3	δT	1 K
Ω_C	up to 30 rpm	Ω_X	up to 15 rpm
Pr	0.015	Ro	1

Table 1: Geometric/parametric values used to simulate Czochralski InP growth

In our mathematical model, the flow variables are non-dimensionalized in a standard fashion, mainly using the crucible radius R_C (as characteristic length), the melt kinematic viscosity ν, the melt density ρ, the temperature difference δT between the crystal/melt interface Γ_X and the rim of the crucible, and the angular velocities of the crystal and crucible (Ω_X and Ω_C, in turn). Industry-relevant values of these quantities are shown in Table 1 above, as well as the Prandtl number Pr and thermal Rossby (or Richardson) number Ro. Finally, a non-dimensional crystal radius $r_X = 0.5$ and a non-dimensional height $h_T = 0.6$ were chosen. As with the GaAs project, we have performed computations using both cylindrical and realistic geometry. Also our initial

efforts have been directed towards the case of iso-rotation, with $\Omega_C = \Omega_X$, and *this holds for the examples shown below*. The Reynolds number is appropriately defined as: $Re = \Omega_C R_C^2/\nu$. First, in the case of cylindrical geometry, we have performed axisymmetric, and more recently, three-dimensional (3D) melt-flow simulations for Reynolds numbers ranging from 1000 to 8000, all with $Ro = 1$, $Pr = 0.015$. Although these values are typically well below those required by industry (whose values lie inside the turbulent regime), the rich structure in the resultant flow behavior seems worthy of analysis in its own right. Moreover, it provides a good basis for comparing results obtained with our finite element solver NAVIER, and those provided by STHAMAS3D, a finite-volume code with upwinding implemented at IKZ. The latter is more dissipative than ours and may be better suited to computing flow properties more relevant to industry, especially time-averaged quantities such as crystal/melt interface shape, and mean frequencies. On the other hand, NAVIER seems to be better suited to capturing transient effects accurately. As in the case for the GaAs research, the steady axisymmetric state was found to be most unstable to 3D oscillatory instabilities; for iso-rotation with $\Omega_X = \Omega_C$ for example, we have found that, while the 2D solver first exhibits transient behavior for $Re \approx 4500$ (corresponding to 1.18 rpm), in the 3D simulation this value is just below 3000 (around 0.79 rpm).

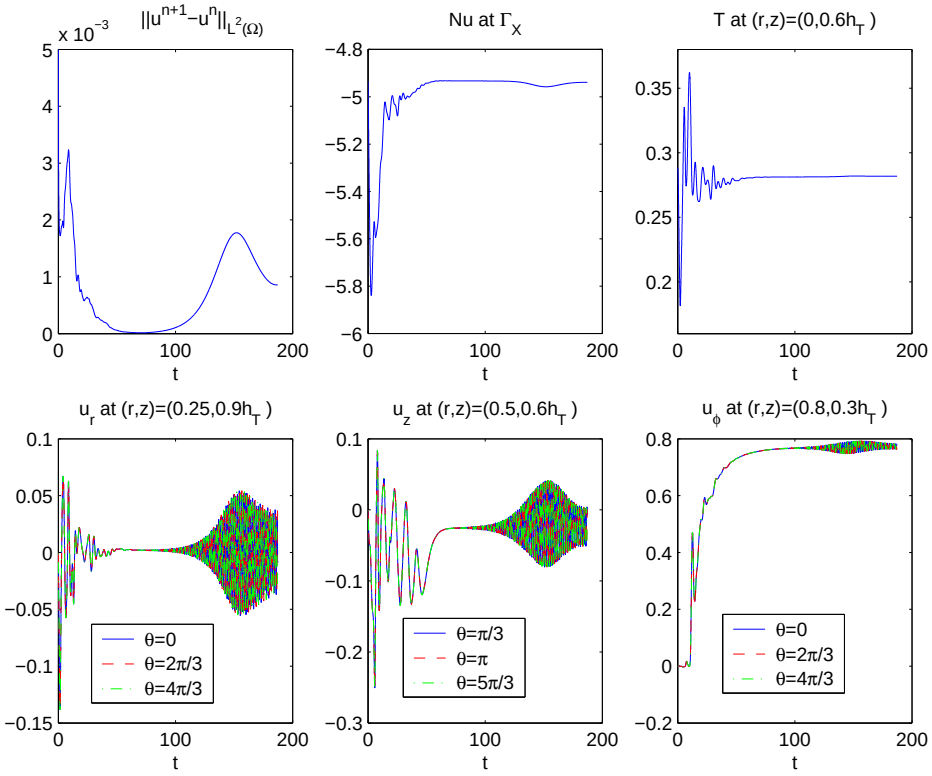
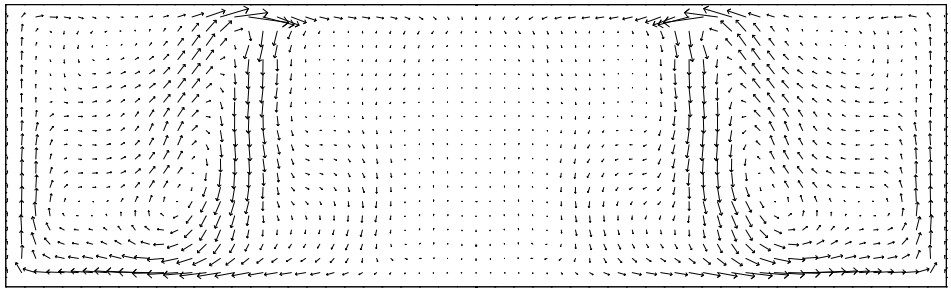


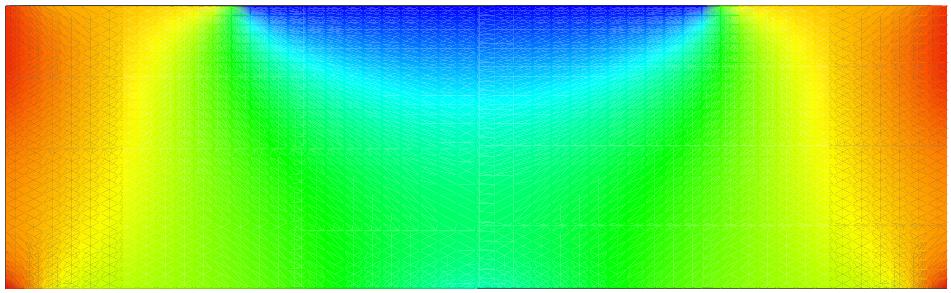
Fig. 1: Time-history behavior of various quantities in a cylindrical crucible with $Re = 3000$, $Ro = 1$; top (from left to right): mean difference of successive solutions, Nusselt number at crystal/melt interface, temperature at an axial location; bottom (left to right): Radial, axial, and azimuthal velocity components at various non-axial locations. Here $h_T = 0.6$.

In Figure 1, we can see the time history plots for a selection of point data, as well as the Nusselt number on the crystal/melt interface and the mean difference between successive solutions; the relatively long "swing-in" phase which precedes oscillatory motion may suggest nearness to the critical Reynolds number. It is also noticeable from these plots that the high frequencies at this stage are purely associated with the three-dimensionality, with two-dimensional frequencies being very short, in comparison.

Figure 2 depicts the time-averaged flow and temperature profiles in an (almost) arbitrary vertical plane passing through the crucible and containing the axis. Here the time averaging was based on using a non-dimensionalized end time of 200 (or equivalently, running for 31.8 revolutions in dimensional terms). In fact, this solution is very similar to the axisymmetric component of the flow and reinforces the point regarding the relatively weak three-dimensional presence. Examination of the Fourier angle modes for various flow quantities reveals that the mode with azimuthal wavenumber 4 is the dominant 3D mode, although this is virtually indiscernible from cross-sectional slices of the crucible, so dominant is the axisymmetry. Another conclusion is that the flow is dominantly rotational with buoyancy playing a minor rôle here; the strongest non-rotational influence appears to stem from the large temperature gradient near the crystal/melt/encapsulant triple line (annulus).



(a)



(b)

Fig. 2: Time-averaged behavior in a typical vertical slice through the crucible showing (a) projected velocity (b) temperature for the test case $Re = 3000, Ro = 1$

We have also recently applied our axisymmetric solver to simulating melt flows in crucibles of a more realistic design. The geometry here principally consists of a cylindrical flat-topped rim section joined to a spherical section, which itself is joined to a spherical cap of relatively large radius. Although similar qualitative features are found in comparison with using cylindrical geometry, early indications suggest that the former type is more de-stabilizing. In Figure 3, for example, the solution is presented for $Pr = 0.015, Ro = 1$, and $Re = 3500$ (0.92 rpm, approx.) portraying the *time-averaged* temperature and projected-velocity fields, based on a dimensionless end time of 100 (15.9 revolutions).

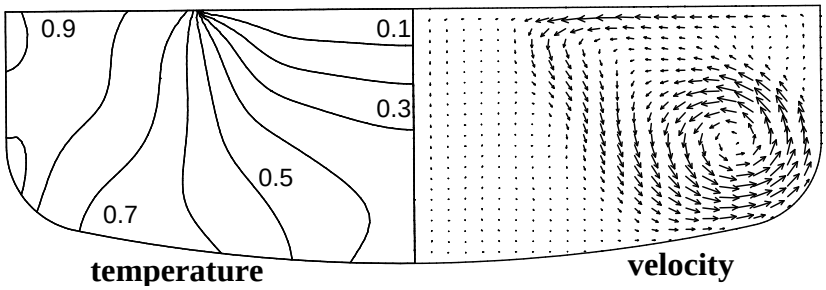


Fig. 3: Time-averaged solution for melt flow in a curve-based crucible for $Re = 3500$, $Ro = 1$, showing temperature contours to the left of the axis; projected velocity vectors to the right of the axis

In conclusion then, we have computed axisymmetric and 3D steady/transient melt-flow solutions for crucibles with cylindrical geometry, and axisymmetric steady/transient solutions using realistic geometry. In general, all of the results tend to suggest that, for Reynolds numbers up to 8000 at least, the flow is dominantly rotational, with the strongest non-rotational influence stemming from the triple line. For future work, we are principally interested in simulating transient 3D solutions using realistic geometry (in parallel with IKZ). Before this however, a realistic design of the meniscus at the triple line will be added, and suitable 3D meshes constructed.

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Simulation of microwave and laser structures using rectangular grids and tetrahedral nets

Collaborators: G. Hebermehl, F.-K. Hübner, R. Schlundt

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

Field-oriented methods which describe the physical properties of microwave circuits and optical structures are an indispensable tool to avoid costly and time-consuming redesign cycles. 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, [7]. The computational domain is truncated by electric or magnetic walls; open structures are treated using the Perfectly Matched Layer (PML) ([11]) absorbing boundary condition.

The subject under investigation are three-dimensional structures of arbitrary geometry which are connected to the remaining circuit by transmission lines. Ports are defined at the transmission lines' outer terminations. In order to characterize their electrical behavior the transmission lines are assumed to be infinitely long and longitudinally homogeneous. Short parts of the transmission lines and the passive structure (discontinuity) form the structure under investigation, [7].

The equations are discretized with orthogonal grids using the Finite Integration Technique (FIT), [1, 4, 16]. Maxwellian grid equations are formulated for staggered non-equidistant rectangular grids and for tetrahedral nets with corresponding dual Voronoi cells.

A three-dimensional boundary value problem can be formulated using the integral form of Maxwell's equations in the frequency domain in order to compute the electromagnetic field:

$$\begin{aligned} \oint_{\partial\Omega} \vec{H}\cdot d\vec{s} &= \int_{\Omega} j\omega[\varepsilon]\vec{E}\cdot d\vec{\Omega}, & \oint_{\cup\Omega} ([\varepsilon]\vec{E})\cdot d\vec{\Omega} &= 0, \\ \oint_{\partial\Omega} \vec{E}\cdot d\vec{s} &= -\int_{\Omega} j\omega[\mu]\vec{H}\cdot d\vec{\Omega}, & \oint_{\cup\Omega} ([\mu]\vec{H})\cdot d\vec{\Omega} &= 0, \end{aligned}$$

$$\vec{D} = [\varepsilon]\vec{E}, \quad \vec{B} = [\mu]\vec{H},$$

with

$$[\varepsilon] = \varepsilon_0 \mathrm{diag}\,(\varepsilon_x, \varepsilon_y, \varepsilon_z), \quad [\mu] = \mu_0 \mathrm{diag}\,(\mu_x, \mu_y, \mu_z)$$

for rectangular grids and

$$[\varepsilon] = \varepsilon_0 \varepsilon_r, \quad [\mu] = \mu_0 \mu_r$$

for tetrahedral grids. This results in a two-step procedure: an eigenvalue problem for complex matrices and the solution of large-scale systems of linear algebraic equations with indefinite symmetric complex matrices.

(1) Eigenmode problem ([2]): The interesting modes of smallest attenuation are found solving a sequence of eigenvalue problems of modified matrices with the aid of the invert mode of the Arnoldi iteration using shifts implemented in the package ARPACK, [9]. To reduce the execution time for high-dimensional problems, a coarse and a fine grid are used. The use of the linear sparse solver PARDISO ([13]) and two levels of parallelization results in an additional

speed-up of computation time. The eigenvalue problem for rectangular grids is described in [5–8]. The mode fields at the ports of a transmission line, which is discretized by means of tetrahedral grids, are computed interpolating the results of the rectangular discretization. The PML influences the mode spectrum. Modes that are related to the PML boundary can be detected using the power part criterion [15].

(2) 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. In general, these matrix problems have to be solved repeatedly for different right-hand sides, but with the same coefficient matrix. The number of right-hand sides depends on the number of ports and modes. Independent set orderings, Jacobi and SSOR pre-conditioning techniques, [10], and a block quasi-minimal residual algorithm, [3], are applied to solve the systems of the linear algebraic equations. Details are given in [7] and [14]. In comparison to the simple lossy case, the number of iterations of Krylov subspace methods increases significantly in the presence of PML. Moreover, overlapping PML conditions at the corner regions of the computational domain lead to an increase of the magnitude of the corresponding off-diagonal elements in comparison to the diagonal ones of the coefficient matrix. This downgrades the properties of the matrix, [7].

Using rectangular grids, a mesh refinement in one point results in an accumulation of small elementary cells in all coordinate directions. In addition, rectangular grids are not well suited for the treatment of curved and non-rectangular structures. Thus, tetrahedral nets with corresponding Voronoi cells are used for the three-dimensional boundary value problem. The primary grid is formed by tetrahedra and the dual grid by the corresponding Voronoi cells, which are polytopes, [12]. The gradient of the electric field divergence at an internal point is obtained considering the partial volumes of the appropriate Voronoi cell.

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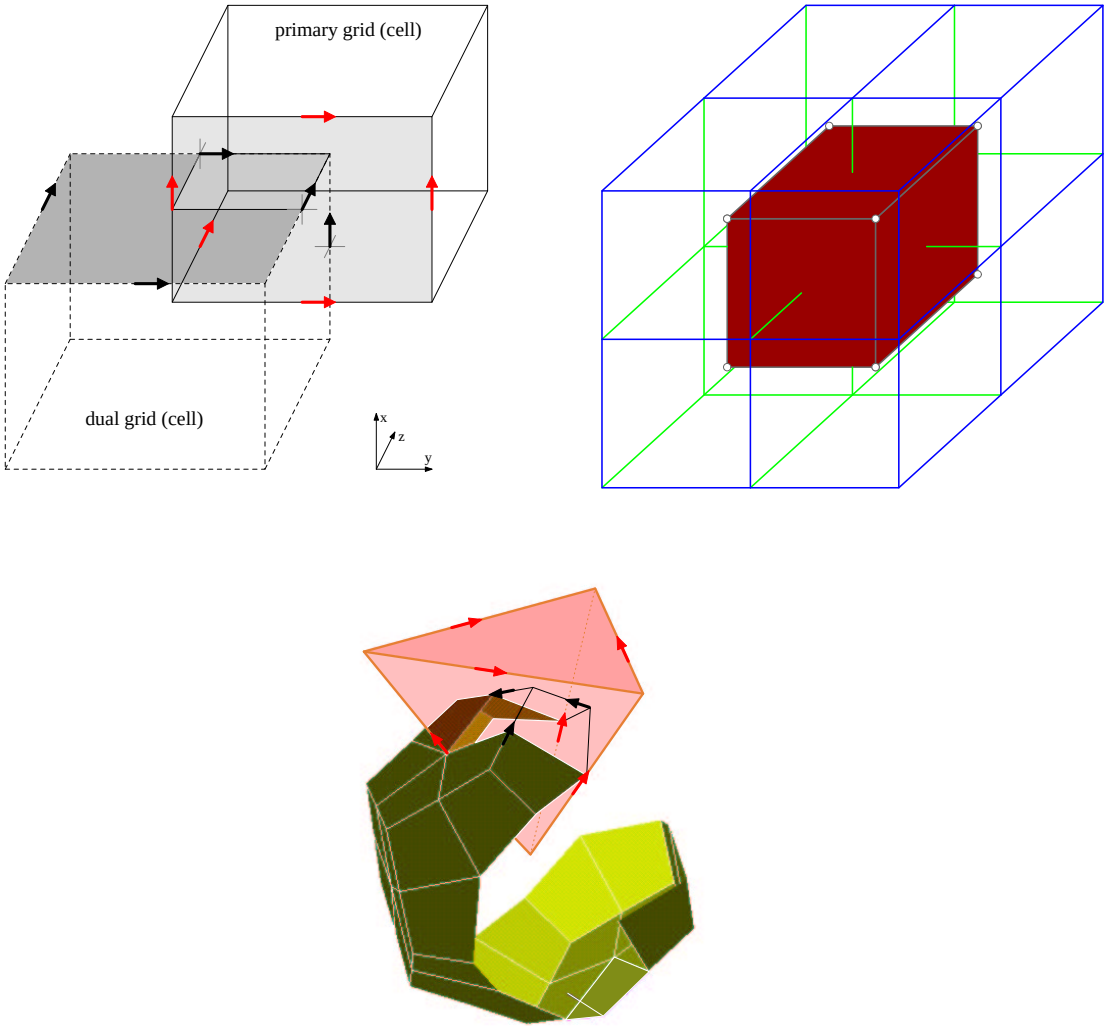

Fig. 1: Primary and dual grid; An eight-cell primary grid and its one interior dual cell; Voronoi cell and single tetrahedron. The electric field intensity components marked with red color are located at the centers of the edges, and the magnetic flux density components marked with black color are normal to the cell faces.

Visualization of numerical simulations and production of presentations

Collaborators: G. Reinhardt, F.-K. Hübner

Visualization for numerical simulations, in particular video animation for time-dependent problems, has been the main task in the period since the last review. This has been especially important for 3D problems, where visualization is a vital tool for interpretation and verification of numerical results.

Due to the generally higher performance of the computers, the production of videos has been focused on computer animation such as Animated GIFs, AVI animation (Microsoft) and MPEG videos. The creation of VHS/SVHS videos was not required.
The configuration of the computer with a Fire Wire and/or USB 2 interface enables direct transfer from online visualization and computer animation to a digital video recorder.

An important part of the support provided for all research groups of the institute was the conversion of differing image formats, notably the conversion of file formats from the “PC world” to the “workstation world”. For this reason it has also been necessary to handle visualization software for the operating system Windows, such as Power Point or Adobe Photoshop.

With the development of a new corporate identity for our institute, it has been necessary to realize the technical transfer of the designer’s outlines from typographic PC software to the workstation software environment (UNIX) of the institute. This included the creation of macros for LaTeX (together with J. Fuhrmann), the installation of postscript fonts, and the adaptation and optimization of files in the UNIX environment.
Software was thereby subsequently developed for the new layout of posters and flyers from our institute. Active support for the production of new posters and flyers for all of the research groups was provided.
The “Numerical Modeling” group of the Institute of Crystal Growth (IKZ) presented results on crystal melt-flow simulation from an ongoing collaborative project with the WIAS research group “Numerical Mathematics and Scientific Computing” at the “Long Night of Sciences” in Berlin/Potsdam (“Lange Nacht der Wissenschaften”). The graphics were presented in the form of Animated GIFs, which were produced at WIAS.

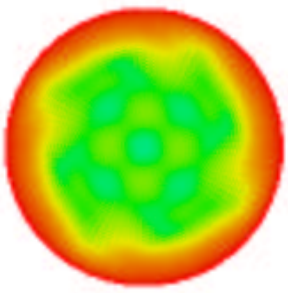

Fig. 1: A picture of the melt-flow simulation

Numerical simulation of Direct Methanol Fuel Cells

Collaborators: J. Fuhrmann, K. Gärtner

Cooperation with: J. Bloch (Freie Universität Berlin (FU-FZT 86))

Supported by: DFG-Forschungszentrum “Mathematik für Schlüsseltechnologien” (Research Center “Mathematics for Key Technologies” (FZT 86)), project C1

The project has been continued with the following focuses:

Improvement of the solver kernel The corresponding work is closely related to the `pdelib2` project. The aim is to be able to handle efficiently calculations in the two- and three-dimensional cases.

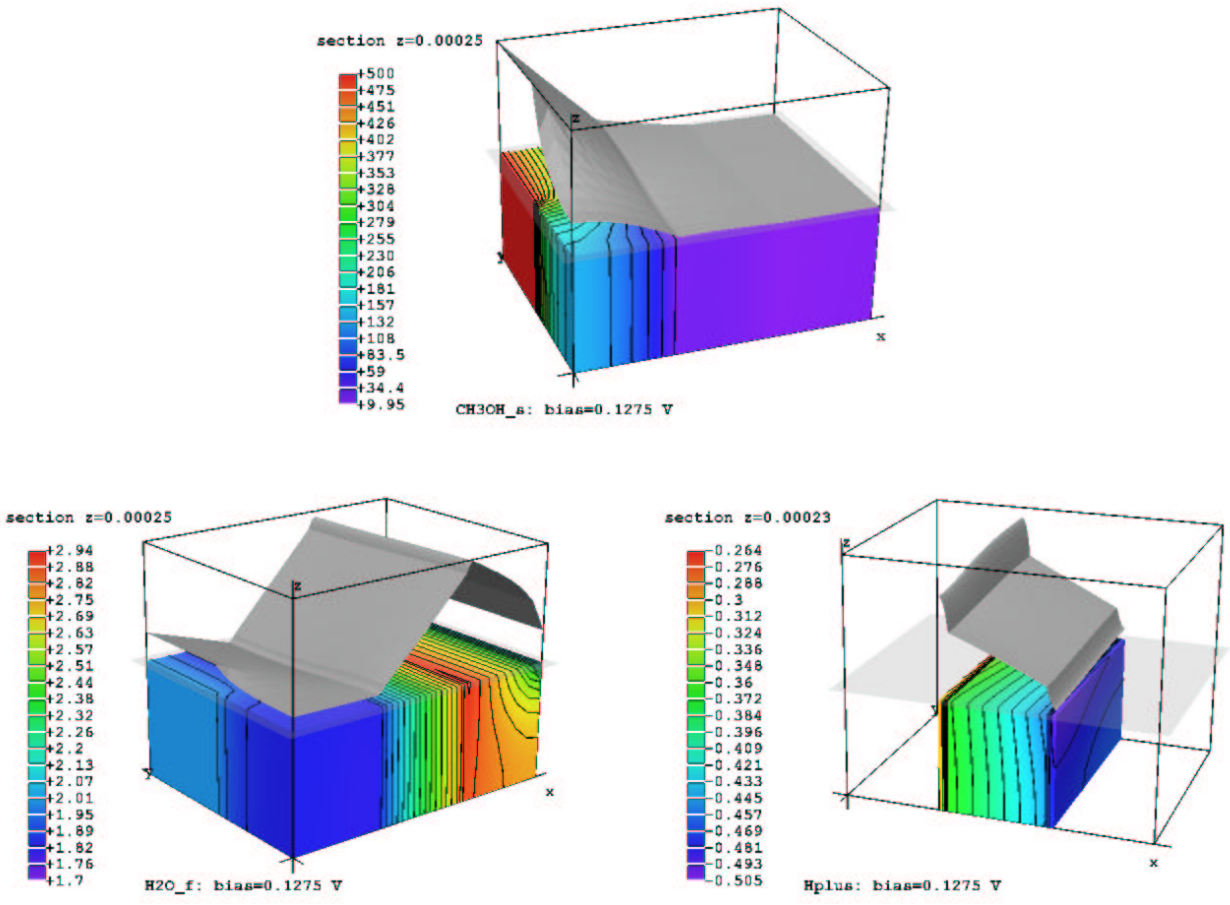

Fig. 1: Three-dimensional simulation results for an elementary cell in the case of crossing diffusion channels.
Top: methanol concentration (mol/l), bottom: water pressure (bar) and proton potential (V)

Development of tools for bifurcation analysis In close cooperation with project C1 of the DFG Research Center we started the development of tools for path-following and bifurcation detection for systems of partial differential equations. Once available, this tool shall help to understand under which conditions a fuel cell can have several steady states.
Currently, we are able to handle sufficiently well model problems like the Brusselator equations.

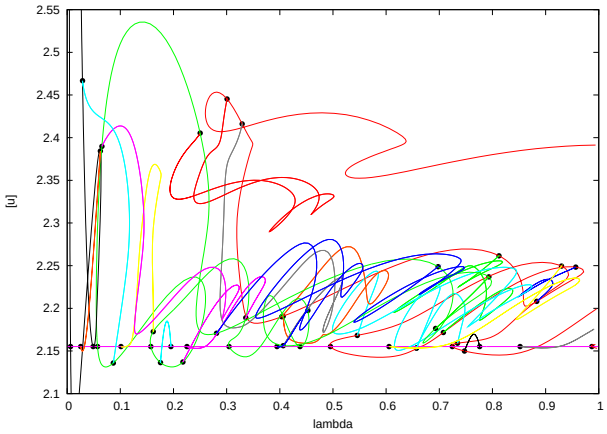

Fig. 2: Bifurcation diagram of a 1D Brusselator system in dependency of the reactor length λ

Project presentation We have been able to present our results at the Computational Fuel Cell Dynamics II workshop in Banff, Canada, and—jointly with the Micro fuel cell group of Fraunhofer IZM Berlin—at the H_2 Expo 2003 fair in Hamburg.

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

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

Cooperation with: A. Linke (Freie Universität Berlin (FU-FZT 86))

Supported by: DFG-Forschungszentrum “Mathematik für Schlüsseltechnologien” (Research Center “Mathematics for Key Technologies” (FZT 86)), project C1

The purpose of this project is the further development of `pdelib`, a toolbox of software components for the numerical solution of partial differential equations. Current project works focus on the re-design of the whole code.

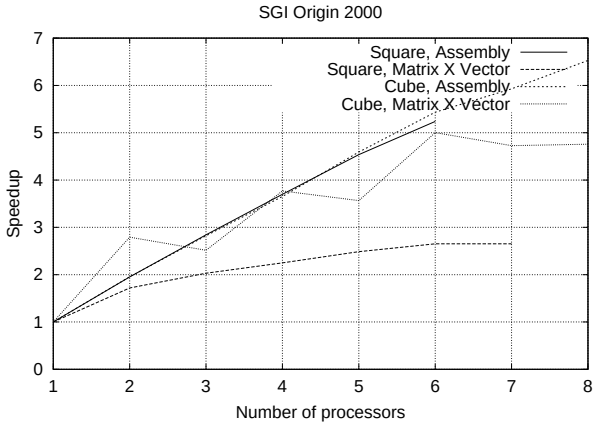

Fig. 1: Preliminary results for parallel speedup for Laplace operator

The main features being implemented are

- Solver kernel which runs efficiently on single processor workstations and multiprocessor SMP architectures using OpenMP or pthreads. The API is targeted at ease of use of the parallel features while not giving up code efficiency;
- Support for a wide class of problems including finite volumes for systems of convection/diffusion/reaction equations, Navier-Stokes equations, and higher order finite elements;
- 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;
- Parameter input and solver control can use the Lua [3] extension language;
- Online visualization of the solution process based on OpenGL.

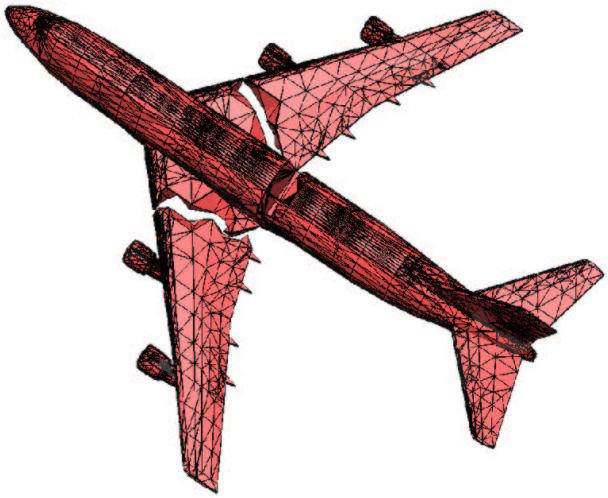

Fig. 2: Mesh subdivided for running calculations on four processors with separators removed

The main aim of the efforts during the reporting period was to bring the `pdelib2` code into a state where it can be used in application projects. We focused on the following issues:

Grid partitioning We assume that grid generators produce grids which are described by an array of node coordinates, an array of cells characterized by the adjacent node numbers, an array of cell *region* numbers, an array of boundary faces characterized by the adjacent node numbers, and an array of *boundary region* numbers.
Grid partitioning in `pdelib2` has the following aims:

- Given a number of processors `nproc`, subdivide the sets of cells, resp. boundary faces resp. nodes into *partitions*. To each of the partitions we assign a color in such a way that neighboring partitions appear in different colors. If possible, `nproc` partitions shall correspond to each of the colors.

  This is motivated by the assumption that all partitions with one color can be processed in parallel without write conflicts by `nproc` processors during assembly and preconditioning.

- Given a number `ncache` of cells, re-arrange cells and boundary faces into homogeneous *zones* stored consecutively. Homogeneity means that each zone belongs to exactly one region and exactly one partition.

  Behind this lies the assumption that all data for assembly on `ncache` elements fit into the cache and can be processed utilizing superscalar features of modern processor architectures.

Partitioning is performed recursively in several steps with the help of the METIS [4] package. A loop over the grid after partitioning then has the following hierarchical structure:

```
loop over all partition colors
      #pragma omp parallel
            loop over all partitions with given color
            loop over all zones of the partition
                  loop over all elements of a zone
```

The user needs to write code for the inner two loops while the outer loop and the parallel loop are hidden, opening the possibility for varying the implementation.

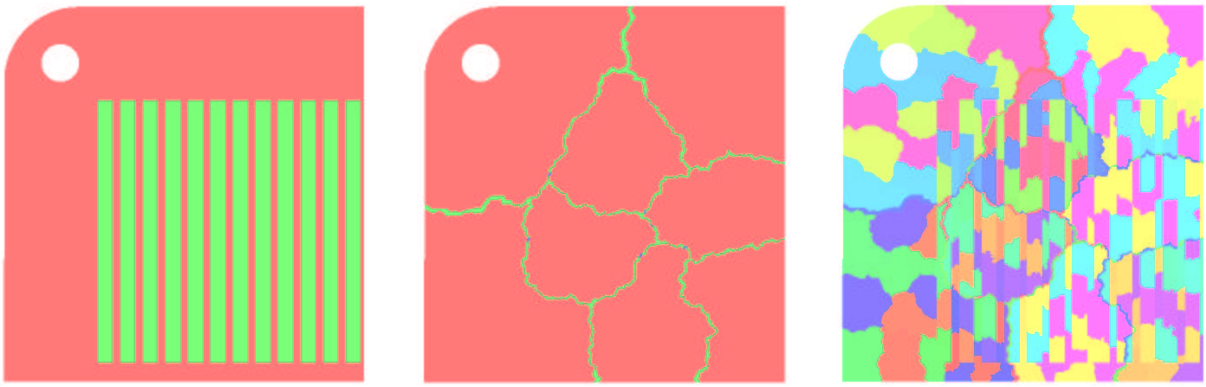

Fig. 3: Regions, partitions, and zones for a DMFC contact plate

Higher order FEM On top of the partitioned grid structure, currently, structures for assembly of higher order finite elements are being implemented.

FVSystem problem class As a first problem class available, a system of coupled nonlinear reaction-diffusion-convection equations as described in [6] has been implemented on top of the grid kernel.

Online graphics Visualization for partitioned grids and functions defined on them has been implemented using OpenGL and the `gltools` framework.
The `gltools` framework has been re-implemented on top of the FLTK [2] GUI toolkit. The portability of FLTK to MacOSX and Microsoft Windows allows now to make `pdelib2` available for these systems, including graphics and GUI.

Clean-up of the API documentation The application programming interface has been cleaned up so that it can be well understood by the users. Documentation using the Doxygen [5] documentation tool has been started.

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4.4 Research Group Nonlinear Optimization and Inverse Problems

4.4.1 Overview

Die Arbeit der Forschungsgruppe konzentrierte sich auf die analytische und numerische Behandlung hochdimensionaler Optimierungsaufgaben und inverser Probleme, die in aktuellen ingenieurtechnischen Anwendungen auftreten. Sie umfasste Grundlagenforschung zur Analysis und Numerik dieser Probleme bis hin zur Entwicklung von effizienten Algorithmen und Software und wurde finanziell durch Industriepartner, das BMBF und die DFG gefördert.

Unsere Forschungsschwerpunkte waren:

- Optimierung diffraktiver Strukturen,
- Optimale Steuerung von Oberflächenwärmebehandlungen,
- Optimierungsprobleme bei der industriellen Einsatzplanung.

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

- Optoelektronische Sensoren (zusammen mit der Forschungsgruppe „Partielle Differentialgleichungen und Variationsgleichungen“),
- Enveloppenfunktionsapproximation für elektronische Zustände in Halbleiter-Nanostrukturen (zusammen mit den Forschungsgruppen „Partielle Differentialgleichungen und Variationsgleichungen“ und „Numerische Mathematik und Wissenschaftliches Rechnen“),
- Quasilineare nichtglatte Evolutionssysteme in L^p-Räumen in dreidimensionalen Gebieten (zusammen mit der Forschungsgruppe „Partielle Differentialgleichungen und Variationsgleichungen“).

The work of the group concentrated on the analytical and numerical treatment of large-scale optimization and inverse problems occurring in current engineering applications. It ranged from basic research on analysis and numerics to the development of efficient algorithms and software, and was financially supported by industrial partners, BMBF, and DFG.

The main research topics were:

- Optimization of diffractive structures;
- Optimal control of surface heat treatments;
- Optimization problems related to industrial resource scheduling.

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”);
- 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”),
- Quasilinear nonsmooth evolution systems in L^p-spaces on three-dimensional domains (in cooperation with research group “Partial Differential Equations and Variational Equations”).

4.4.2 Projects

Optimization of diffractive structures and reconstruction methods for severely ill-posed problems

Collaborators: G. Bruckner, J. Elschner, A. Rathsfeld, G. Schmidt

Cooperation with: B. Kleemann (Carl Zeiss Oberkochen), R. Güther (Ferdinand-Braun-Institut für Höchstfrequenztechnik Berlin), G. Bao (Michigan State University, East Lansing, USA), G.C. Hsiao (University of Delaware, Newark, USA), M. Yamamoto (University of Tokyo, Japan), CiS Institut für Mikrosensorik gGmbH (Erfurt)

Supported by: BMBF: "Modellierung und Optimierung mikrooptischer Oberflächenstrukturen" (Modeling and optimization of microoptical surface structures), DFG: "Scientific cooperation with Japan: Inverse problems in electromagnetics and optics"

1. Accurate FEM and BEM simulation of diffraction by binary and polygonal gratings (A. Rathsfeld, G. Schmidt).

The diffraction of light waves by optical gratings can be reduced to boundary value problems for the Helmholtz equation on a rectangular domain which contains one period of the surface structure. In case of complicated surface geometries, the FEM is the natural method for the numerical solution. We continued to develop our FEM program package `DiPoG`, versions 1.4 and 2.0 (cf. [16], [17]), which treats the outgoing wave conditions at infinity by coupling with BEM and which includes a generalized FEM approach for high frequency solutions.
`DiPoG`-1.4, which is used to simulate and optimize binary and multilevel structures, now includes all modifications which were developed due to requirements of the industrial partners from Carl Zeiss and CiS Erfurt. This concerns the possibility to model homogeneous layers of any thickness also within the grating structure, to choose different output formats for the computed diffracted fields and related values, and the improved GMRES-based iterative solver. Most of these extensions have been included into the programs for solving optimal design problems. In particular, in version 1.4 we implemented new functionals, which take into account prescribed polarizations of the incoming waves, and we introduced a new solver for the direct and dual problems based on the PARDISO library. Both of the implemented optimization algorithms, a conjugate gradient and an interior point method, can now be controlled by the same set of parameters.
In `DiPoG`-2.0 we implemented in accordance with the requirements of our cooperation partners from Carl Zeiss a new presentation of the computed results, a graphical display of the far-field solution, and an improved output of efficiency data for the conical diffraction. Since a simple handling of geometric data is essential for a user-friendly operation of `DiPoG`, we increased the number of standard gratings which can be generated by simple code words and a few parameters. In particular, two types of echelle gratings, of sine-shaped, lamellar, and coated trapezoidal gratings have been realized and a stack of such profiles can now easily be assembled. Finally, based on our FEM code and on simulated annealing, we developed a first version of a global optimization algorithm to design polygonal grating profiles. This work is to be continued next year.
For gratings with a single transition profile and, possibly, a single coated layer, a boundary integral equation method like the IESMP (owned by Carl Zeiss, cf. [13]) turns out to be more efficient. However, in order to treat thin coatings and corner profiles, the simple combination

of trigonometric collocation for the main part operator and of a Nyström quadrature for the remainder within IESMP is not sufficient. We changed the basic discretization scheme of the integral equation method to spline collocation over graded meshes and developed an adapted quadrature algorithm. Further we implemented an extension of Ewald's method for computing the kernel functions of the integral operators. The acceleration method for these infinite sums implemented in IESMP breaks down if the kernel is nearly singular, whereas Ewald's method allows to extract the main singularity and to handle it separately. For special profile curves, the resulting method converges and the numerical error diminishes in accordance with theoretically predicted orders. This work is to be continued next year.

2. Inverse problems for diffraction gratings: Uniqueness results and reconstruction methods (G. Bruckner, J. Elschner, A. Rathsfeld, G. Schmidt).

The reconstruction of the shape of periodic structures from measurements of scattered electromagnetic waves is a problem of great practical importance in modern diffractive optics, [2]. We studied the scattering of monochromatic plane waves by a two-dimensional diffraction grating, i.e. a periodic curve (the grating profile) which separates two regions with different optical materials. Let $k^+ > 0$ be the refractive index (or wave number) above the grating, whereas the refractive index below the interface satisfies $\Re k^- > 0$, $\Im k^- \geq 0$. The direct diffraction problem is modeled by a transmission problem for the periodic Helmholtz equation.
Let the profile of the diffraction grating be given by the curve $\Lambda_f := \{(x_1, x_2) \in \mathbb{R}^2 : x_2 = f(x_1)\}$ where f is a 2π-periodic Lipschitz function. Suppose that a plane wave given by

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

is incident on Λ_f from the top, where $\theta \in (-\pi/2, \pi/2)$ is the incident angle. The *inverse problem* or the *profile reconstruction problem* can be formulated as follows.
(IP): Consider a fixed refractive index k^- below Λ_f, and let θ be a fixed incident angle. Determine the profile function f from incident waves u^{in}, given for several wave numbers k^+, and the knowledge of the corresponding scattered fields on two straight lines $\{x \in \mathbb{R}^2 : x_2 = b^\pm\}$ above and below the structure.
Note that this problem also involves near-field measurements since the evanescent modes cannot be measured far away from the grating profile. The uniqueness with a single arbitrary wave number k^- in problem (IP) is presently only known for reflection gratings, i.e. for $\Im k^- > 0$ ([8]). General uniqueness results with a single wave number are also available for perfectly reflecting diffraction gratings with polygonal profiles ([10]).
In the practically important case of transparent gratings ($k^- > 0$), we were recently able to show uniqueness for a finite number of refractive indices, where this number only depends on the maximal value $k_{\max}$ of k^-, k^+, θ, and the amplitude h of the profile function f ([9]). In particular, if $h\sqrt{(k^+)^2 + (k^-)^2} < \pi$, i.e. the refractive indices are sufficiently small, then uniqueness with a single wave number holds. The proof is based on the Courant-Weyl min-max principle for the eigenvalues of a fourth-order elliptic problem.
The efficient numerical solution of the profile reconstruction problem is challenging due to the fact that it is both nonlinear and severely ill-posed. For the reconstruction of perfectly reflecting periodic interfaces leading to the inverse Dirichlet problem, several inversion algorithms based on iterative regularization ([12]), linear sampling ([1]), and the Kirsch-Kress optimization method ([4], [6]) became recently available. The latter approach was originally developed for acoustic obstacle scattering and avoids the solution of direct diffraction problems. In [5] a

corresponding reconstruction method for the inverse transmission problem (IP) was developed and analyzed for the first time.
As in [4], [6], this method splits the inverse problem into a linear ill-posed part to reconstruct the scattered field and a nonlinear well-posed part to find the profile curve. The minimization of the Tikhonov functional for the linear problem and the defect minimization of the transmission conditions are then combined into one cost functional. We obtained convergence results in the general case of Lipschitz grating profiles, extending the variational approach for the perfectly reflecting case. However, in the transmission case, it is harder to establish convergence of the cost functional. The proof of this is based on nontrivial continuity and solvability properties of layer potentials on periodic Lipschitz graphs.
The reconstruction algorithm was implemented as a two-step method. Two unknown density functions are first computed from near-field data measured above and below the grating structure, which allows us to represent the scattered and transmitted fields as single layer potentials. Then these density functions are used as inputs to a nonlinear least squares problem, which determines the unknown profile as a curve where the associated transmission conditions are fulfilled. After discretization, the least squares problem is solved iteratively by the Gauss-Newton method. Numerical results with exact and noisy data demonstrated the efficiency of the inversion algorithm, [5].

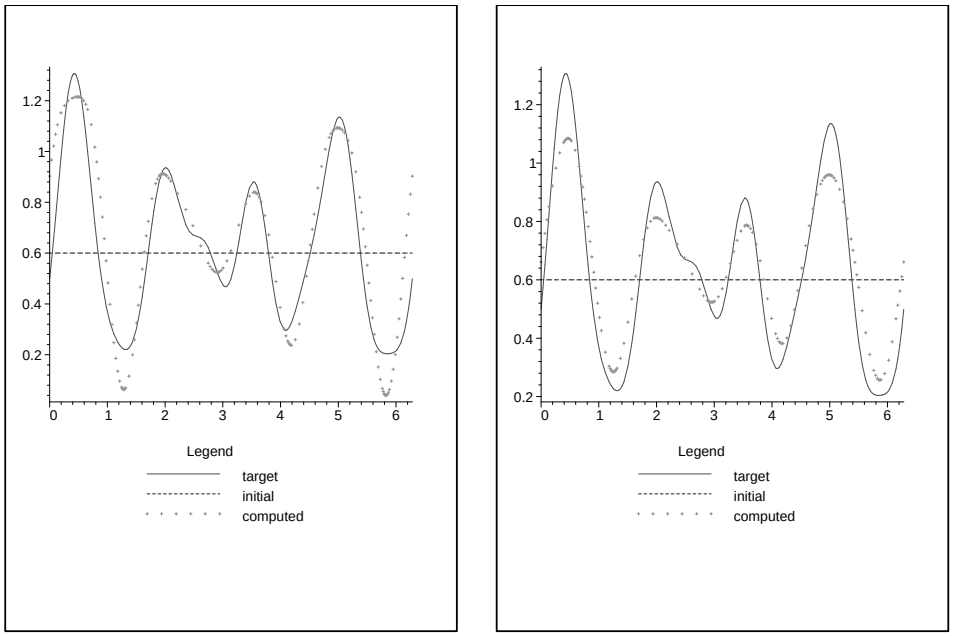

Fig. 1: Given and reconstructed profile using 100 and 800 Gauss-Newton iterations

3. Optimal design of nonlinear diffraction gratings (G. Schmidt).

If a plane wave of frequency ω_1 illuminates on a grating or periodic structure ruled on some nonlinear optical material, then the nonlinear optical interaction gives rise to diffracted waves at frequencies ω_1 and $\omega_2 = 2\omega_1$. This process represents the simplest situation in nonlinear optics, the so-called second harmonic generation (SHG). An exciting application of SHG is to obtain coherent radiation at a wavelength shorter than that of the available lasers. Unfortunately, it is well known that nonlinear optical effects from SHG are generally so weak that their observation requires an extremely high intensity of laser beams. The effective enhancement of nonlinear optical effects presents one of the most challenging tasks in nonlinear optics. It has been announced recently that SHG can be greatly enhanced by using diffraction gratings or periodic structures, and the PDE model can predict the field propagation accurately.
The joint paper [3] with Gang Bao and Kai Huang (Michigan State University) is concerned with some aspects of the systematic design of surface (grating) enhanced nonlinear optical effects. We give the mathematical foundation of optimization methods for solving the optimal design problem of nonlinear periodic gratings. By conducting a perturbation analysis of the grating problems that arise from smooth variations of the interfaces, we derive explicit formulas for the partial derivatives of the reflection and transmission coefficients. Such derivatives allow us to compute the gradients for a general class of functionals involving the Rayleigh coefficients.

4. Reconstruction of curve source profiles from boundary measurements in a 2D wave equation model (G. Bruckner).

Generalizing earlier investigations, [7], where point sources in a one-dimensional vibrating string were identified from dislocations at one fixed point, here a corresponding 2D problem is investigated: the identification of curves in a plane domain from measurements at the boundary, where excitations are governed by the 2D wave equation. This can be considered as a first step towards a reduced earthquake model. A second step could be replacing the wave equation by the Lamé system. In [11] the Lamé system has been considered with an L^2 source function, while here H^{-1} sources are asked for. In our case a main difficulty consists in finding an adequate distance for curves in a 2D domain. So far, this problem could be solved by the authors only for pieces of straight lines. The stability estimate is of logarithmic type, and in the proofs, Duhamel's principle and Carleman estimates are essential.
A paper is in preparation.

5. New solution method for volume integral equations of scattering theory (G. Schmidt).

Scattering of incoming plane waves by inhomogeneous media can be described by Lippmann-Schwinger-type integral equations, which contain the diffraction potential over the volume of the scatterer. Especially in the case of high wave numbers, the approximation of the diffraction potential is very expensive. In [14] the cubature approach which had been developed in [15] was extended to the numerical solution of Lippmann-Schwinger equations. We considered a collocation method where the unknown is sought as a linear combination of scaled and shifted Gaussians. Then the discrete system could be obtained from the semi-analytic representation. We proved spectral convergence rates of the method, which were confirmed in one-dimensional numerical tests.

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Optimal control of surface heat treatments

Collaborators: E. Bänsch (FG 3), M.H. Farshbaf Shaker, D. Hömberg, W. Weiss

Cooperation with: A. Khludnev (Lavrentyev Institute of Hydrodynamics, Novosibirsk, Russia), J. Sokołowski (IECN/INRIA Lorraine, Vandoeuvre-lès-Nancy, France), F. Tröltzsch (Technische Universität Berlin), S. Volkwein (Karl-Franzens-Universität Graz, Austria)

Supported by: DFG-Forschungszentrum "Mathematik für Schlüsseltechnologien" (Research Center "Mathematics for Key Technologies"), project C11

1. Thermomechanical models of phase transitions in steel (E. Bänsch, D. Hömberg, W. Weiss).

While the interplay between temperature and phase volume fractions is well understood, the incorporation of mechanical effects is still a challenging task. The metallurgical phases have material parameters with different thermal characteristics, hence their effective values have to be computed by a mixture ansatz. The different densities of the metallurgical phases result in a different thermal expansion. This thermal and transformation strain is the major contribution to the evolution of internal stresses during heat treatments. Experiments with phase transformations under applied loading show an additional irreversible deformation even when the equivalent stress corresponding to the load is far below the normal yield stress. This effect is called *transformation-induced plasticity*. The irreversible deformation leads to a mechanical dissipation that acts as a source term in the energy balance.

Neglecting the influence of internal stresses on the transformation kinetics, a consistent mathematical model which takes care of all these effects has been developed and analyzed in [1]. The new model has been implemented in an existing adaptive finite element code, [9]. In a simplified situation without inelastic dissipation term in the energy balance, an optimal control problem has been investigated, [8].

In [2] a thermoelastic contact problem with phase transitions has been studied.

2. Optimal control of laser surface treatments (M.H. Farshbaf Shaker, D. Hömberg, W. Weiss).

Besides of the reduced order approach to tackle the optimal control problem of laser surface hardening, which has been considered in [4, 5], the emphasis of last year's work lay on the development of new nonlinear PID control algorithms for two- and three-dimensional situations. The results are published in [3] and [7].

Figure 1 shows the result of a simulation with constant laser energy (top) in comparison with the application of a linear PID control of subsurface temperature (bottom left) and the result of a simulation with the new nonlinear PID algorithm (bottom right).

Fig. 1: Control of laser surface hardening to achieve a constant hardening depth: uncontrolled (top); linear PID subsurface control (bottom left); nonlinear PID subsurface control (bottom right).

3. Laser-induced thermotherapy (M.H. Farshbaf Shaker, D. Hömberg, W. Weiss).

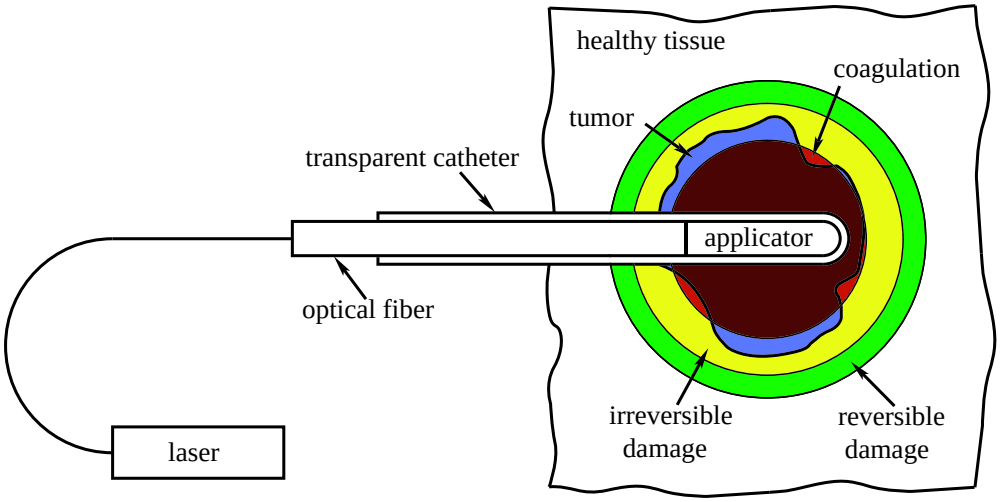

Fig. 2: Mechanism of laser thermotherapy

In a first step towards life sciences applications we have started to apply our laser hardening model to the case of laser-induced thermotherapy (Fig. 2). This is a cancer therapy in which laser light is guided through a transparent catheter into a tumor. The absorbed light leads to a heating of the tissue. In contrast to hyperthermia cancer treatments where the temperature does not exceed, say, 43 ^{o}C, in this process the tissue is heated up to more than 60 ^{o}C leading to a coagulation of the tumor tissue and thus a destruction of the tumor.
In [6] our software `WIAS-SHarP` has been used to simulate this process using an Arrhenius ansatz to model the tissue damage due to coagulation.
Future work will concern improved models for tissue damage and the investigation of optimal control problems related to therapy planning and the design of applicators.

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Optimization problems related to industrial resource scheduling

Collaborators: I. Bremer, R. Henrion

Cooperation with: W. Römisch (Humboldt-Universität (HU) zu Berlin), T. Szántai (Technical University of Budapest, Hungary), J. Outrata (Institute of Information Theory and Automation (UTIA) Prague, Czech Republic), A. Jourani (Université de Bourgogne, Dijon, France), D. Dentcheva (Stephens Institute of Technology, New Jersey, USA), A. Seeger (Université d'Avignon, France)

Supported by: DFG-Forschungszentrum "Mathematik für Schlüsseltechnologien" (Research Center "Mathematics for Key Technologies"), project C7;
Rücker Ges.m.b.H, Graz, Austria

1. Path planning for industrial robots and human models in automotive industry (I. Bremer).

The VR tool of Rücker for production planning in automotive industry uses a large number of externally created 3D models in different formats. The models which are usually generated from CAD are not optimized with respect to memory and/or speed performance. Hence, real-time animations of complete shop floors with a lot of moving materials, robots, and humans become very difficult.
On the basis of OpenGL Performer [5], which offers several possibilities to improve performance, i.e. the frame rate, we provided a tool for automatic model conversion such that the visual impression for the user is not affected but the cost of rendering is reduced as much as possible.
In particular, we have considered the problem of removing holes and the development and implementation of active surface definitions (ASD). There ASDs are hierarchical multigrid structures. Based on the distance between viewer and object each object is visualized on a certain grid level. For distance changes, the corresponding change in visualization is realized by a smooth morphing between the respective grid levels.
See also the results of the year before[3,4].

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

A typical feature of optimization problems arising in engineering sciences is the presence of random and nonsmooth parameters. In this research project, modeling, solution procedures, and investigations on structure and stability of such problems are the main objective. It is embedded into a cooperation with other scientific institutions in Berlin via the DFG Research Center (with HU), a joint research seminar (with HU and Konrad-Zuse-Zentrum für Informationstechnik (ZIB)), and the joint organization of a yearly course for chemical engineers supported by DECHEMA (with Technische Universität (TU) and ZIB). The focus of research is on stochastic optimization problems.

The following subjects were considered:

[3] http://www.wias-berlin.de/publications/annual-reports/2002/node60.html
[4] http://www.wias-berlin.de/publications/annual-reports/2002/node50.html

1. Scenario reduction: The solution of power management problems is typically based on a scenario tree formulation. The complexity of such trees requires a drastical reduction to subtrees without much loss of information. A general theoretical framework to do so on the basis of suitable probability metrics was developed in [1]. For mixed-integer models to be considered in this project, certain discrepancy distances have to be used. As a first step, an explicit formula for scenario reduction could be obtained in case of the "closed-set" discrepancy and a linear programming reformulation in case of the interval discrepancy.

2. Chance constraints: One possibility to model risk in stochastic optimization is to use probabilistic (chance) constraints. Due to the discretization process in power management, possibly continuous distributions are approximated by discrete ones. This raises the question of solution stability for problems with chance constraints. An extensive analysis was provided in [2] and [3].

3. Error bounds: The concept of error bounds is a key concept in nonlinear optimization (numerical solution, constraint qualifications, stability) and is itself a special instance of the more general calmness concept for multifunctions. A detailed characterization in the framework of nonsmooth optimization including relations to the above research project is contained in [4].

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4.5 Research Group Interacting Random Systems

4.5.1 Overview

Das Hauptinteresse unserer mathematischen Forschung galt weiterhin der stochastischen Dynamik, wobei eine Anzahl bemerkenswerter Resultate erzielt werden konnte. Diese betreffen zufällige Störungen von schnell-langsamen dynamischen Systemen, unendlichdimensionale Diffusionsprozesse, wechselwirkende Verzweigungsprozesse und Koagulations-Fragmentations-Prozesse. Zum Thema der ungeordneten Spin-Systeme im Gleichgewichtszustand konnte eine vollständige Analyse erzielt werden für eine Klasse von Modellen, die auf Gauß'schen Prozessen mit hierarchischer Kovarianzfunktion basieren. Interessanterweise spielen in dieser Untersuchung reellwertige Verzweigungsprozesse eine wesentliche Rolle, eine Tatsache, die die vielfältigen Beziehungen zwischen den verschiedenen in der Gruppe untersuchten Fragestellungen illustriert. Im Rahmen des durch das DFG-Forschungszentrum finanzierten Projekts ist unserem Profil durch die Anwendung von Methoden aus dem Gebiet der interagierenden Teilchensysteme auf mikroskopische Modelle in der Finanzmathematik eine neue Facette hinzugefügt worden.

The focus of our mathematical research has continued to be on stochastic dynamics, where a number of remarkable results could be obtained. These concern stochastic perturbations of slow-fast dynamical systems, infinite dimensional diffusion processes, interacting branching diffusion processes, and coagulation-fragmentation processes. In the analysis of the equilibrium properties of disordered spin systems, a complete analysis of a class of models based on Gaussian processes with hierarchical covariance function could be achieved. Interestingly, in this analysis continuous-state branching processes play a crucial role, highlighting the mathematical coherence of the different areas of activity within the group. Within the project funded by the DFG Research Center, applications of methods from interacting particle systems to microscopic models in finance have added a new facet to our application profile.

Während das DFG-Schwerpunktprogramm „Interagierende stochastische Systeme von hoher Komplexität“ im Jahr 2003 zum Abschluss kam, wird ein Teil dieser Aktivitäten fortgeführt in Form einer ”Dutch German Bilateral Research Group“, die gemeinsam von der DFG und der NWO finanziert wird. Die Forschungsgruppe war stark vertreten während des Halbjahresprogramms “Interaction and Growth in Complex Stochastic Systems” am Isaac-Newton-Institut in Cambridge. Auch die Beteiligung am Programm “Population Genetics and Statistical Mechanics” am Erwin-Schrödinger-Institut in Wien gab Impulse für neue Anwendungen der Kompetenzen der Forschungsgruppe auf dem Gebiet der biologischen Fragestellungen.

While the DFG Priority Program “Interacting Stochastic Systems of High Complexity” came to a close in 2003, part of the activities are continued in the framework of a Bilateral Dutch-German Research Group that is jointly financed by the DFG and the NWO. The research group was strongly present at a semester on “Interaction and Growth in Complex Stochastic Systems” organized at the Isaac Newton Institute in Cambridge. Also, the participation in the program “Population Genetics and Statistical Mechanics” at the Erwin Schrödinger Institute in Vienna brought new impulses for applications of the expertise of the group in biological problems.

Im Berichtsjahr habilitierte sich Barbara Gentz an der Technischen Universität Berlin, und Ingo Matheis schloss seine Dissertation ab.

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

In 2003, Barbara Gentz passed her habilitation at the Technical University of Berlin, and Ingo Matheis completed his Ph.D. thesis.

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

4.5.2 Projects

Low temperature phases in models with long-range interactions

Collaborators: A. Bovier, C. Külske

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Supported by: DFG Priority Program „Interagierende Stochastische Systeme von hoher Komplexität" (Interacting stochastic systems of high complexity)

Models of statistical mechanics with weak long-range interactions have been introduced by V. Kac half a century ago to obtain a rigorous version of the van der Waals mean field theory. Today we see these models anew as interesting candidates to reach a better understanding of disordered spin systems and in particular the relation between mean field theory and lattice models in the context of disordered systems. In this project, whose funding through the DFG ended with the termination of the Priority Program "Interacting stochastic systems of high complexity" in 2003, we have undertaken a long-term effort to investigate such models and to develop appropriate mathematical tools for their analysis. An detailed review of the results obtained here can be found in [1].

In a joint paper with Merola, Presutti, and Zahradník, we have addressed in this context a classical question from statistical mechanics, that of the *Gibbs Phase Rule*. "In the abstract space of all potentials, phase transitions are an exception". This statement by Ruelle in his classical textbook, [6], suggests the validity of the Gibbs phase rule, but the notion must be accepted only very cautiously, as a complete proof of the Gibbs rule would require to show that in the space of the thermodynamically relevant parameters, phase transitions occur on regular manifolds of positive co-dimension. But, as stated again by Ruelle in a recent review on open problems in mathematical physics, [7], the proof of such a statement must be regarded as one of the main challenges in statistical mechanics.

In the Pirogov-Sinai regime where configurations can be described by contours which satisfy Peierls conditions, the situation is definitely better, as the theory provides tools for a very detailed knowledge on the structure of Gibbs measures in a region in the relevant parameters space. The traditional Pirogov-Sinai theory is a low temperature expansion which enables to control the entropic fluctuations from the ground states, its natural setup being the lattice systems. But the theory is not limited to such cases and it has been applied to a great variety of situations, covering various types of phase transitions. One is the case of Kac potentials, which are seen as a perturbation of mean field, where the small parameter is the inverse interaction range of a Kac potential. According to van der Waals, the theory becomes then well suited for investigating the liquid-vapor branch of the phase diagram and, as shown in [5], its applications are not restricted to lattice models, [3], [4], but continuum particle systems can be treated as well.

All the above cases have a common structure. There is a term in the Hamiltonian of the form $-\lambda\alpha$, where α is an extensive quantity and $\lambda \in \mathbb{R}$ is its conjugate variable: in the case of spins, λ is an external magnetic field and α the spin magnetization; for particles, λ is the chemical potential and α the particles number. Our main assumption is that at a value, say $\lambda = 0$, of the intensive parameter there is phase coexistence with α an order parameter, and that defining contours in terms of the variable α, the contours satisfy the Peierls bounds with

suitable coefficients. Under this assumption the process described in terms of the variable α has the typical features of a low temperature Ising model. We will thus have a class of "plus" measures where α is typically positive (as well as its expectation) and a class of "minus" measures with α typically negative. We are talking of classes of plus and minus measures and not just of plus and minus measures, because we are not ruling out the possibility of other phase transitions, described by other order parameters.
These assumptions imply that at $\lambda = 0$ there are two distinct classes of DLR measures, the plus and minus ones, for which the expected value of α is positive, respectively negative, and which are obtained by thermodynamic limits with plus, respectively minus, boundary conditions. Under this assumption (plus some technical conditions of super-stability type if the variables are unbounded) we prove that there is a finite interval I of values of λ, centered at $\lambda = 0$, where coexistence occurs only at $\lambda = 0$. More precisely, if $\lambda > 0$ (or $\lambda < 0$) and in I, then any translational invariant DLR measure has positive (negative) expectation, and both plus and minus boundary conditions produce in the thermodynamic limit the same class of states.

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Stochastic dynamics

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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 microscopically 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*. 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. Over the last years, we have developed a novel approach to the analysis of both probabilistic (distribution of transition times) and spectral (eigenvalues and eigenfunctions of the generator) quantities and their relations. This approach allows in particular to obtain rigorous results that have a far greater precision than the standard exponential estimates obtained in the Wentzell-Freidlin theory. In a collaboration with F. den Hollander and F. Nardi we are currently applying these methods to 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 [3] and den Hollander, Olivieri, Scoppola, and Nardi [4] in dimensions two and three, respectively, using the conventional large deviation-type methods. By a detailed analysis of the energy landscape of the model, they obtained the logarithmic asymptotics of the nucleation time in the limit as the temperature tends to zero. In a forthcoming paper ([5]), 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 pre-factors 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. While in this paper we remain in the regime of very low temperatures, we see a perspective to move to the physically more interesting regimes of moderately low temperatures, and we intend to pursue this line actively in the coming years.

The investigation of more complex systems with an infinity of metastable states leading to the phenomenon of "ageing" ([1]) has continued rather intensely. One of the main goals here is to extend the analysis performed in [6], [7] for the random energy model to the much more complicated generalized random energy models. The issue is to reduce the dynamics on the space of spin configurations to the dynamics of an effective trap model. Work has continued in collaboration with G. Ben Arous and V. Gayrard, and first significant results can be expected soon. Another line of work concerns the analysis of trap models as such. Here, J. Černý, in collaboration with G. Ben Arous and T. Mountford ([8]), has been able to precisely analyze various autocorrelation functions for Bouchaud's trap model on the two-dimensional lattice $\mathbb{Z}^2$. In an attempt to better understand the signature of ageing in terms of spectral properties, we have returned to the analysis of Bouchaud's REM-like trap model. It turns out that in this case the generator can be diagonalized explicitly, and precise expressions for eigenvalues and eigenfunctions can be obtained, which allows to recover all dynamical properties purely from this spectral information. One also realizes a clear connection between aging exponents and the singularity in the limiting spectral density of the model.

Over the last years, in collaboration with Nils Berglund, we developed a new approach to random perturbations of dynamical systems, evolving on two well-separated time scales. After detailed studies of noise-induced phenomena in one-dimensional slowly time-dependent systems, [10], [11], [12], first results on fully coupled multidimensional slow-fast systems were obtained last year. These results provide estimates on the fluctuations of the fast variables near slow or centre manifolds of the corresponding deterministic system, thus allowing to study a reduced system ([13]).
This year we turned our attention towards truly multidimensional effects in non-gradient systems. As a first step we studied the random dynamics near periodic orbits of the deterministic dynamics, in particular the first-passage time through an unstable periodic orbit. Passage through an unstable periodic orbit plays a key role in many applications, in particular in those showing stochastic resonance or synchronization. Examples include climate models, phase slips in noisy systems of coupled oscillators, and stochastic resonance in lasers.
While on the exponential scale, accessible to the classical Wentzell-Freidlin theory, all points on an unstable orbit are equally likely to occur as first-exit points, the subexponential asymptotics of the distribution of first-exit points or times reflects the fact that the unstable orbit is generally not uniformly repelling. As discovered by Day ([15]), "cycling" occurs: The distribution of first-exit *points* rotates around the unstable orbit, periodically in the logarithm of the noise intensity, and thus does not converge in the zero-noise limit. In [14], we study the distribution of first-exit *times* for a class of model equations. A rich picture emerges, showing cycling most prominently in a metastable time regime, but also during the transitional initial phase and in the asymptotic regime. Our results cover a large range of possible values for the period of the unstable orbit, thus providing insight into the transition from the stochastic-resonance regime into the synchronization regime.

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Gibbs measures of highly disordered systems

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The investigation of the Generalized Random Energy Models (GREM) described in last year's report ([1], [2]) has been continued this year in [3]. Our aim was to give a more explicit description of the limiting Gibbs measure of these models. To this end we introduced the notion of a flow of probability measures and its associated genealogy. In fact, embedding the Gibbs measure of spin systems together with all its coarse graining in the unit interval, one obtains naturally such a flow of measures, time playing the role of the scale of the coarse graining. It turns out that the associated genealogical structure is precisely equivalent to the multi-overlap structure of the original Gibbs measures. Based on the results of [2] we could then show this flow converges (in the sense that its genealogy converges) to a flow of probability measures associated to a particular continuous-state branching process, introduced by J. Neveu (incidently the same process that was considered in a recent paper by K. Fleischmann and A. Sturm in another project of our group this year). This yields finally a very satisfactory probabilistic and geometric description of Gibbs measures of disordered models and highlights an intimate connection between branching processes and continuous-state branching process.

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Microscopic modeling in financial markets

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The main goal of this new project, that is part of the application area E of the DFG Research Center “Mathematics for Key Technologies”, is to develop and investigate more realistic models for the dynamics of stock prices 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 theory of price processes in finance ([2]).
An approach based on a Markovian evolution in a space of opinions of traders is presented in the paper [1]. We have developed an interactive simulation tool that allows to experiment with a rather large class of model parameters, and some rather interesting features emerge even with rather simple models involving few parameters. One can, for instance, study the effect of time-dependent changes in parameters (modeling a changing macro-economic environment) on the stock price. For example, the following graph shows the reaction to a sequence of bursts of optimism followed by neutral periods.

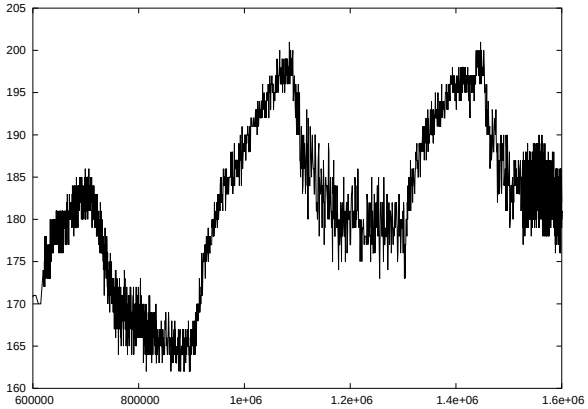

Fig. 1: A sequence of “bubbles”

It also emerges that one can identify a number of very challenging mathematical problems in the context of interacting particle systems that are relevant and so far little understood. The further development of the model, its numerical and analytical investigation, and comparison of statistical properties of the model price processes with real data, offer interesting perspectives for continued research over the next years.

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Interacting catalytic branching processes

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Pairs of interacting catalytic branching processes describe the evolution of two types of materials, which randomly move, split, and possibly disappear in space. The point is the interaction in the system: The branching behavior of each material is dependent on the other one.

A main result this year is the construction and investigation of a so-called *symbiotic branching process,* [3]. This model generalizes three well-known interacting models: the mutually catalytic branching model in $\mathbb{R}$ of Dawson and Perkins (1998), [2], and Mytnik (1998), [11], the continuous stepping-stone model of Shiga (1988), [13], and the continuous space Anderson model (see, for instance, Mueller (1991), [10]). Compared with mutually catalytic branching, the two types might now be somehow correlated. Basic tools such as self-duality, particle system moment duality, measure case moment duality, and moment equations are shown to be still available in this generalized context. As an application, the *compact interface property* is derived: Starting from complementary Heaviside states, the interface is compact almost surely at each time. For the stepping-stone model, such property was known earlier by Tribe (1995), [15], but for mutually catalytic branching, for instance, this is the first result on the interface at all. Techniques from [15] are essentially used, except the ones which have been based on the boundedness of states. Instead of this, some exponential grow of certain moments could be established, which are now used as a replacement for the original boundedness of states.

Superprocesses under a Brownian flow are studied in [16]. Such processes were first considered by Skoulakis and Adler (2001), [14], by a moment duality method. As they indicated, it is natural to study the process under a fixed environment and to make use of the related *conditional log-Laplace* transform. This idea is now confirmed in [16]. The conditional log-Laplace functional is in fact shown to be the unique solution to a nonlinear stochastic partial differential equation by making use of a particle system representation developed by Kurtz and Xiong (1999), [8]. This approach has many potential applications.

In [9] the model is governed by a white noise in space-time. Therefore, it also involves spatial interaction. Further, an immigration mechanism is introduced to the model. In this case, the conditional log-Laplace functional is the unique solution to a nonlinear SPDE driven by space-time white noise. As an application, the long-term limit is obtained.

A uniqueness problem raised in Fleischmann and Xiong (2001), [6], for critical cyclically catalytic super-Brownian motions is solved in [1] in the simplified spaceless case, that is, for cyclically catalytic branching diffusions $\mathbf{X}$, where, moreover, any correlation between the

components is allowed (in the sense of symbiotic branching). More precisely, $\mathbf{X}$ is characterized as the *unique strong solution of a singular stochastic equation.*

A *spatial version of Neveu's* (1992), [12], *continuous-state branching process* is constructed in [4]. Opposed to earlier superprocesses, here the branching has infinite mean. Construction is provided by starting from certain supercritical (α, d, β)-superprocesses $X^{(\beta)}$ with symmetric α-stable motion and $(1+\beta)$-branching and proving convergence on path space of finite measure-valued cadlag paths as $\beta \downarrow 0$. The log-Laplace equation related to the new process X, say, has the locally non-Lipschitz function $u \log u$ as nonlinear term (instead of $u^{1+\beta}$ in the case of $X^{(\beta)}$). It can nevertheless be shown to be well posed. X behaves quite differently from usual supercritical spatial branching processes. In fact, it is immortal at all finite times, propagates mass instantaneously everywhere in space also in the Brownian case $\alpha = 2$, and it has locally countably infinite biodiversity.

The phenomenon of *multi-scale clustering* is verified in [5] for a non-Markovian branching particle system in $\mathbb{R}^d$ in the critical dimension $d = \alpha/\beta$, where particles move according to a symmetric α-stable motion, have a lifetime distribution of finite mean, and branch with an offspring law of index $1+\beta$, $0 < \beta \leq 2$. This is expressed in an fdd scaling limit theorem, where initially one starts with an increasing localized population or with an increasing homogeneous Poissonian population. The limit state is uniform, but its intensity varies in line with the scaling index according to a continuous-state branching process of index $1+\beta$. The case $\alpha = 2$ of Brownian particles was due to Klenke (1998), [7], where PDE methods had been used which are not available in the present setting.

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Stochastic models for Boltzmann-type equation

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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

$$v^* = v + e(e,w-v), \quad w^* = w + e(e,v-w). \tag{2}$$

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 according to (2). Here $\mathcal{S}^2$ denotes the unit sphere in the Euclidean space $\mathcal{R}^3$, and B is called the collision kernel, containing information about the assumed microscopic interaction potential.
A nonlinear equation of similar structure as equation (1) is Smoluchowski's coagulation equation

$$\frac{\partial}{\partial t} c(t,x) = \frac{1}{2} \sum_{y=1}^{x-1} K(x-y,y)\, c(t,x-y)\, c(t,y) - \sum_{y=1}^{\infty} K(x,y)\, c(t,x)\, c(t,y), \tag{3}$$

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 (non-negative and symmetric) coagulation kernel K representing properties of the physical medium. The phenomenon of the 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 (3). 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. Stochastic numerical methods provide results that are subject to random fluctuations. Thus, the construction of algorithms with reduced fluctuations is an important issue (variance reduction problem).

In recent years a new approach to the variance reduction problem for the Boltzmann equation (1), called SWPM (stochastic weighted particle method), has been developed. The new method, which uses a system of weighted particles, has been successfully applied to situations with strong density gradients (cf. [1]). In [2] convergence of SWPM was studied. First the method was extended by introducing new stochastic reduction procedures, in order to control the number of simulation particles. Then, under rather general conditions, convergence to the solution of the Boltzmann equation was proved. Finally, numerical experiments illustrated both convergence and considerable variance reduction for the specific problem of calculating tails of the velocity distribution. The assumptions of the convergence theorem were significantly weakened in [3], in order to cover deterministic reduction procedures. First steps towards a new field of applications were taken in [4]. A new stochastic numerical algorithm was derived for the Boltzmann equation for rarefied granular flows, where collisions between particles are inelastic.

The topic of studying stochastic models for Boltzmann-type equations has attracted much interest in recent years. An interesting direction of research is the consideration of more physical effects. In [5] the stochastic approach to nonlinear kinetic equations (without gradient terms) has been presented in a unifying general framework, which covers many interactions important in applications, like coagulation, fragmentation, inelastic collisions, as well as source and efflux terms. Conditions for the existence of corresponding stochastic particle systems in the sense of regularity (non-explosion) of a jump process with unbounded intensity are provided. Using an appropriate space of measure-valued functions, relative compactness of the sequence of processes is proved, and the weak limits are characterized in terms of solutions to the nonlinear equation. As a particular application, existence theorems for Smoluchowski's coagulation equation with fragmentation, efflux and source terms, and for the Boltzmann equation with dissipative collisions are derived. Some results concerning clusters containing several chemical species are presented in [6], [7]. For sufficiently fast increasing coagulation kernels, there exists the phenomenon of gelation. At the level of the macroscopic equation (3), 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 [8].

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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

Collaborators: D. Belomestny, V. Essaoulova, A. Hutt, P. Mathé, D. Mercurio, H.-J. Mucha, J. Polzehl, V. Spokoiny

Cooperation with: F. Baumgart (Leibniz-Institut für Neurobiologie, Magdeburg), R. Brüggemann, Ch. Heyn, U. Simon (Institut für Gewässerökologie und Binnenfischerei, Berlin), P. Bühlmann, A. McNeil (ETH Zürich, Switzerland), C. Butucea (Université Paris 10, France), M.-Y. Cheng (National Taiwan University, Taipeh), A. Daffertshofer (Free University of Amsterdam, The Netherlands), A. Dalalyan (Université Paris 6, France), J. Dolata (Johann Wolfgang Goethe-Universität Frankfurt am Main), L. Dümbgen (University of Bern, Switzerland), J. Fan (Princeton University, USA), J. Franke (Universität Kaiserslautern), R. Friedrich (Universität Münster), F. Godtliebsen (University of Tromsø, Norway), H. Goebl, E. Haimerl (Universität Salzburg), A. Goldenshluger (University of Haifa, Israel), I. Grama (Université de Bretagne-Sud, Vannes, France), J. Horowitz (Northwestern University, Chicago, USA), B. Ittermann (Physikalisch-Technische Bundesanstalt (PTB), Berlin), A. Juditsky (Université de Grenoble, France), I. Molchanov (University of Bern, Switzerland), K.-R. Müller (Fraunhofer FIRST, Berlin), M. Munk (Max-Planck-Institut für Hirnforschung, Frankfurt am Main), S.V. Pereverzev (RICAM, Linz, Austria), H. Riedel (Universität Oldenburg), B. Röhl-Kuhn (Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin), R. von Sachs (Université Catholique de Louvain, Belgium), A. Samarov (Massachusetts Institute of Technology, Cambridge, USA), M. Schrauf (DaimlerChrysler, Stuttgart), S. Sperlich (University Carlos III, Madrid, Spain), U. Steinmetz (Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig), P. Thiesen (Universität der Bundeswehr, Hamburg), G. Torheim (Amersham Health, Oslo, Norway), C. Vial (ENSAI, Rennes, France), Y. Xia (National University of Singapore, Singapore), S. Zwanzig (Uppsala University, Sweden)

Supported by: DFG: DFG-Forschungszentrum “Mathematik für Schlüsseltechnologien” (Research Center “Mathematics for Key Technologies”), project A3; SFB 373 “Quantifikation und Simulation Ökonomischer Prozesse” (Quantification and simulation of economic processes), Humboldt-Universität zu Berlin; Priority Program 1114 “Mathematische Methoden der Zeitreihenanalyse und digitalen Bildverarbeitung” (Mathematical methods for time series analysis and digital image processing)

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 (D. Belomestny, V. Essaoulova, A. Hutt, D. Mercurio, H.-J. Mucha, J. Polzehl, V. Spokoiny).

The investigation and development of adaptive smoothing methods have been driven by interesting problems from imaging and time series analysis. Applications to imaging include

signal detection in functional Magnet Resonance Imaging (fMRI) and tissue classification in dynamic Magnet Resonance Imaging (dMRI) experiments, image denoising, analysis of images containing Poisson counts or binary information or the analysis of Positron Emission Tomography (PET) data.

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

The models and procedures proposed and investigated at WIAS are based on two main approaches, the pointwise adaptation, originally proposed in [46] for estimation of regression functions with discontinuities, and adaptive weights smoothing, proposed in [33] in the context of image denoising.

The main idea of the pointwise adaptive approach is to search, in each design point, for the largest acceptable window that does not contradict to 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.

The general concept behind adaptive weights smoothing is structural adaptation. The procedure attempts to recover the unknown local structure from the data in an iterative way while utilizing the obtained structural information to improve the quality of estimation. This 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 is applicable to high-dimensional situations.

Both ideas have been investigated and applied in a variety of settings.

- *Imaging problems*: The *pointwise adaptive approach* has been extended and theoretically investigated for the denoising of 2D images in [32]. The procedure delivers an optimal (in rate) quality of edge recovering and demonstrates a reasonable numerical performance. Adaptive weights smoothing has been generalized to cover locally smooth images in [36], see Figure 1 for an example, and local likelihood estimation for exponential family models in [35]. The latter allows, e.g., to handle images containing Poisson counts, binary or halftone images or images with intensity-dependend gray value distributions.

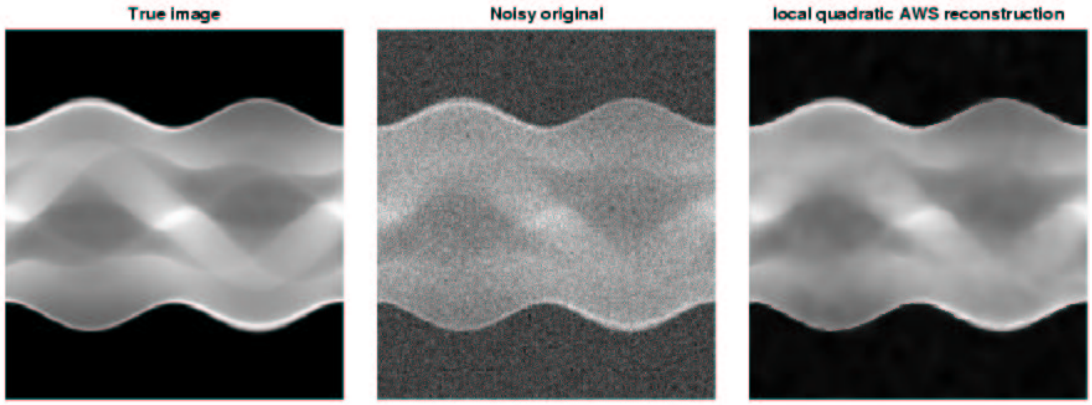


Fig. 1: Reconstruction of a piecewise smooth image by local polynomial AWS

- *Adaptive wavelet thresholding*: Modifications of the AWS procedure have been developed for denoising one- and two-dimensional data via wavelet thresholding. The estimates

obtained by the AWS procedure turn out to be spatially adaptive. They attain the near optimal rate of estimation over Besov classes $B^s_{p,q}$. The procedure performs well in terms of the mean absolute error as well as visually. The use of AWS for wavelet thresholding allows for improved compression rates.

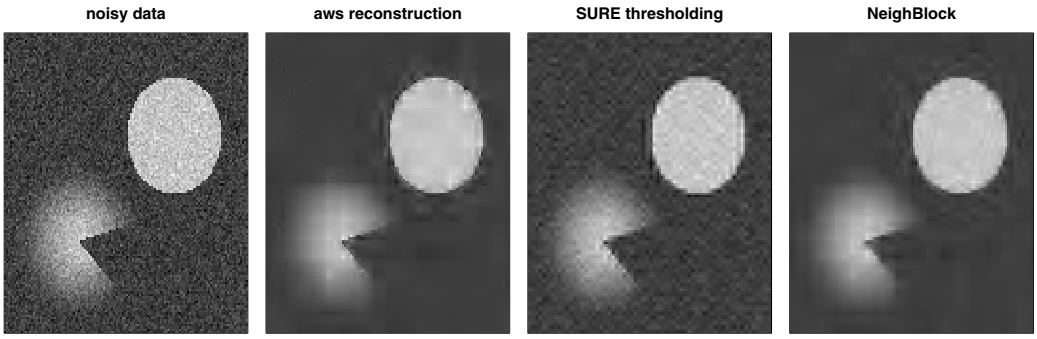


Fig. 2: Reconstruction of an artificial image by wavelet thresholding using AWS (Compression rate (CR): 0.031), SURE thresholding (CR: 0.188), and the NeighBlock method of Cai and Silverman ([4]) (CR: 0.087)

- *Functional and dynamic magnetic resonance experiments*: Adaptive weights smoothing allows for the analysis of spatio-temporal structures. The methods proposed in [34] have been tested on fMRI data and dMRI datasets from cardiology.

  The use of spatially adaptive smoothing methods allows, in comparison to a voxelwise decision, for an improved sensitivity and specitivity of signal detection and, in contrast to nonadaptive approaches, to preserve information about the shape of regions of interest. Figure 3 provides a comparison for one fMRI series.

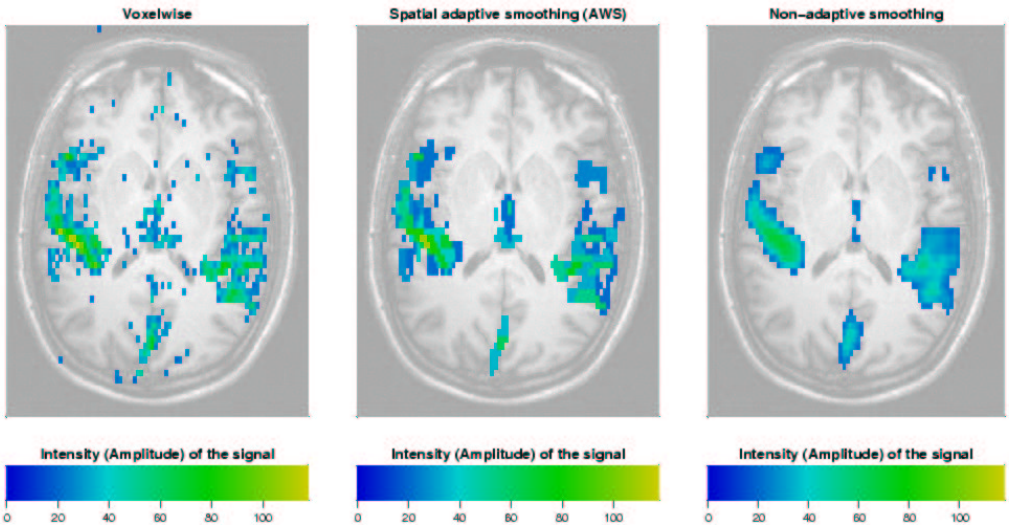


Fig. 3: Comparison of signal detection methods in fMRI: voxelwise decision (left), adaptive spatial smoothing (AWS) (center), and nonadaptive spatial smoothing (right)

- *Analysis of bio-signals*: Synchronization effects are supposed to play the key role in information processing in the brain. These effects have been observed in invasive and non-invasive experimental data ([49]). In order to improve the understanding of intrinsic neural activity, we study phase synchronization effects in empirical multivariate brain

signals by a novel segmentation method ([19]). It allows the detection of mutually phase-synchronized states in multivariate signals. The algorithm combines the k-means cluster algorithm for toroidal topologies and the statistical estimation of the synchronization strength [18, 19]. Applications to simulated metastable multivariate time series from stochastic and chaotic systems reveal its properties successfully. First applications to brain signals are successful.

- *Modeling of financial time series and volatility estimation*: Time series models with varying coefficients are appropriate for a wide range of financial time series. In [26], a pointwise adaptive approach for volatility modeling of financial time series is developed. [16] extends this procedure to the case of multidimensional financial time series. Appropriate methods for locally stationary time series are investigated in [9] and [10]. In [27], the pointwise adaptive approach is applied for the estimation and forecasting of the volatility of financial time series. The approach is based on the assumption of local homogeneity: for every time point there exists an interval of time homogeneity in which the parameters of the volatility model can be well approximated by a constant. The procedure recovers for each point the maximal interval of homogeneity from the data using a local change point analysis. Afterwards the estimate of the volatility is simply obtained by local averaging. The performance of the procedure is investigated both from a theoretical point of view and through Monte Carlo simulations. The new procedure is applied to some data sets and compared with the LAVE procedure from [26] and a standard GARCH model. The numerical results demonstrate a very reasonable performance of the new method.

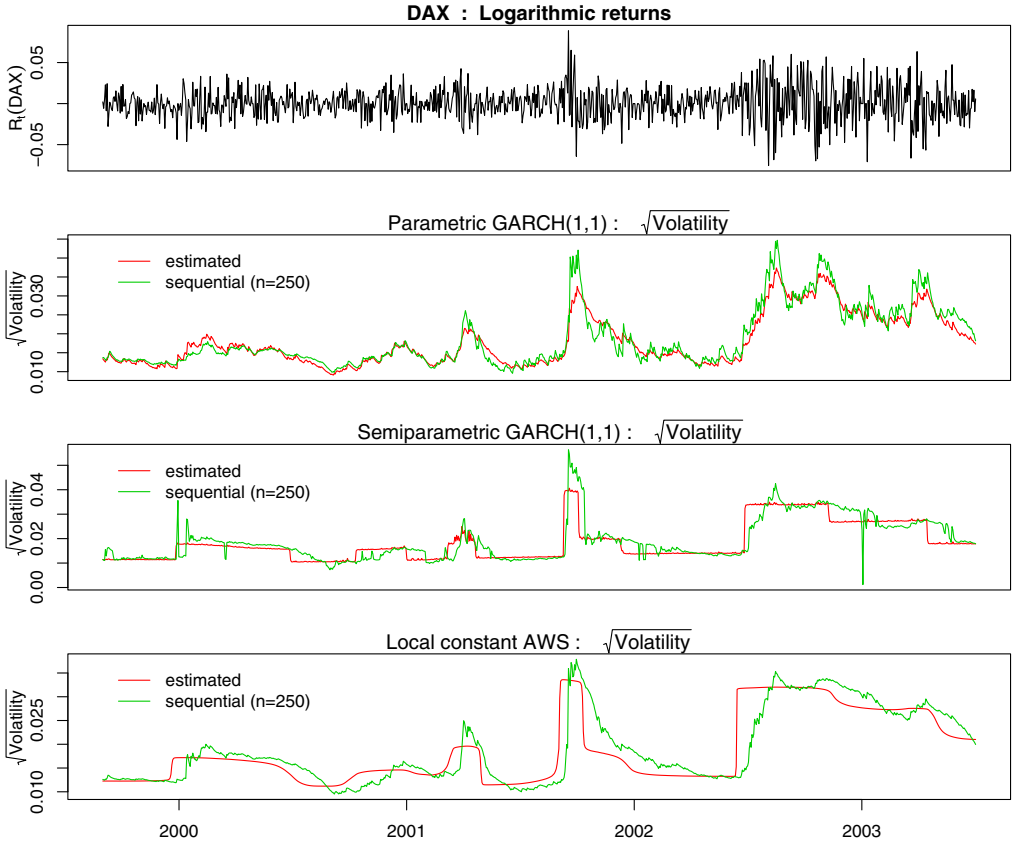


Fig. 4: Volatility modeling of the DAX data from 1999 to 2003 by parametric GARCH(1,1), AWS for semiparametric GARCH(1,1), and local constant volatility AWS

The adaptive weights smoothing approach has been generalized to time varying GARCH

models and semiparametric GARCH models in [37]. The procedure involves new ideas on localization of GARCH models. Simulations and applications on financial data show that phenomena like long-range dependence and heavy tails, which are often considered as inherent to financial time series, can as well be interpreted by nonstationarity.

Both the semiparametric GARCH(1,1) and the local constant AWS volatility model can be used to analyze the local stationarity structure. They allow for an improved volatility prediction and explain the observed heavy tails of the logarithmic returns. Applications of the methodology are intended in cooperation with the project *Applied mathematical finance*.

Figure 4 illustrates volatility estimates obtained for the time series of DAX values.

Nonparametric filters often involve some filtering parameters. These parameters can be chosen to optimize the performance locally at each time point or globally over a time interval. In [5], the filtering parameters are obtained minimizing the prediction error for a large class of filters. Under a general martingale setting, with mild conditions on the time series structure and virtually no assumption on filters, the adaptive filter with filtering parameter chosen on the basis of historical data is shown to perform nearly as well as the one with the ideal filter in the class, in terms of filtering errors. The theoretical result is also verified via intensive simulations. The approach can be used to choose the order of parametric models such as AR or GARCH processes. It can also be applied to volatility estimation in financial economics.

- *Tail index estimation*: The tail index is used to characterize the tail behavior of a distribution. This is important, e.g., for extreme value statistics and risk assessment. The results on tail index estimation will be used in cooperation with the project *Applied mathematical finance.*

  In [14], the pointwise adaptive approach is extended to tail index estimation. The approach is based on approximation by an exponential model. The proposed procedure adaptively selects the number of upper order statistics used in the estimation of the tail of the distribution function. The selection procedure consists in consecutive testing the hypothesis of homogeneity of the estimated parameter against the change-point alternative. The selected number of upper order statistics corresponds to the first detected change-point. The main results are non-asymptotic and state optimality of the proposed method in the “oracle” sense.

  A similar idea is used for tail index estimation by adaptive weights smoothing in [35].

- *Classification*: In [35], a spatially adaptive discriminant analysis procedure based on the local likelihood AWS for binary regression is proposed. This approach is currently extended using the specific bias-variance decomposition of classification problems. First simulation results show potential for improvements over [35] and classical procedures. Figure 5 provides results of a simulation study for three types of classifiers. Illustrated is

the dependence of the classification error on the main parameter of the procedures.

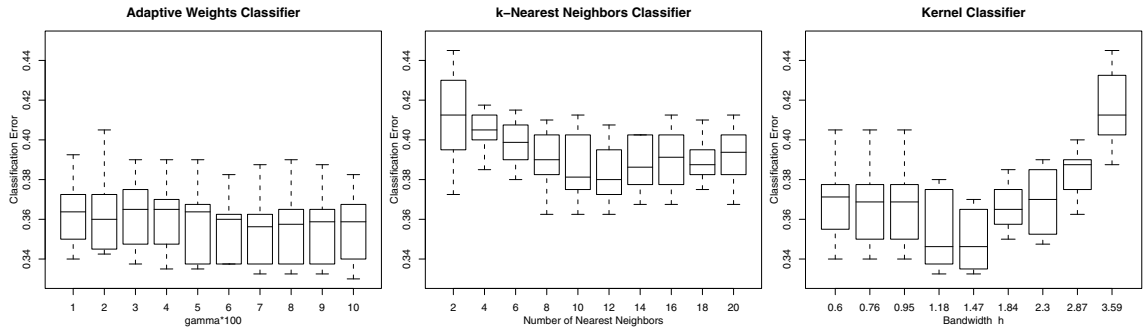
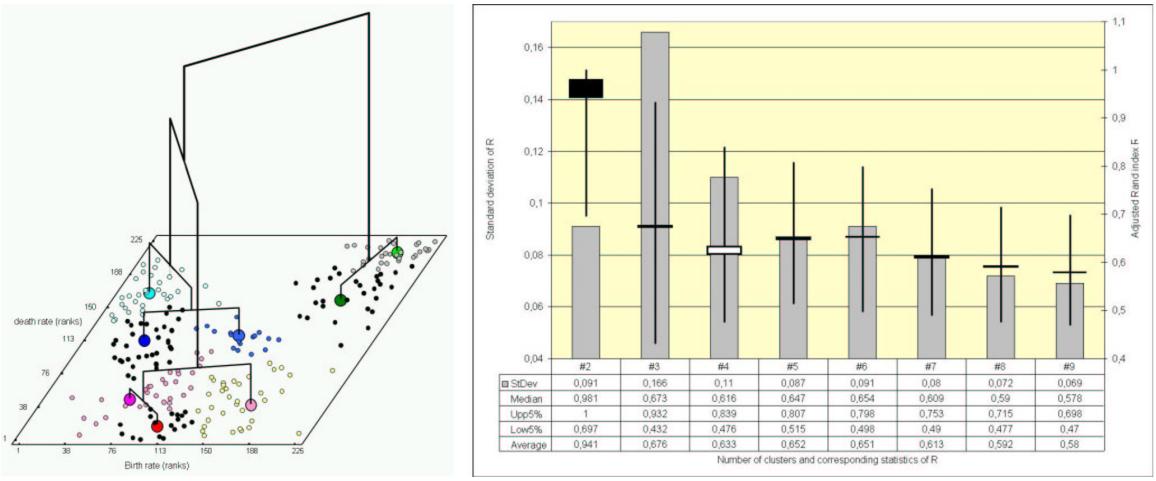


Fig. 5: Comparison of classification errors for a simulated example

- *Density estimation*: An adaptive weights procedure for density estimation has been obtained using the asymptotic equivalence of density estimation and Poisson regression ([35]). This approach is currently extended to cover piecewise smooth densities, see [15].

- *Cluster analysis and data mining*: The research has been focused on the validation of cluster analysis results ([30]). An automatic validation technique that becomes a general validation tool for all hierarchical clustering methods available in the statistical software `ClusCorr98`® is under development. This built-in validation via resampling techniques is based on the adjusted Rand index applied to contingency tables, which are obtained by crossing two partitions. Both the appropriate number of clusters can be validated and the stability of each cluster can be assessed.

  Bootstrap samples and subsets are equivalent to the choices of weights of observations. This is used to make resampling computationally effective. The built-in validation is an automatic technique with default values for the parameters of the simulations.



	#2	#3	#4	#5	#6	#7	#8	#9
StDev	0,091	0,166	0,11	0,087	0,091	0,08	0,072	0,069
Median	0,981	0,673	0,616	0,647	0,654	0,609	0,59	0,578
Upp5%	1	0,932	0,839	0,807	0,798	0,753	0,715	0,698
Low5%	0,697	0,432	0,476	0,515	0,498	0,49	0,477	0,47
Average	0,941	0,676	0,633	0,652	0,651	0,613	0,592	0,58

Fig. 6: Obtained clusters and summary of validation results for *Ward*'s method

For illustration purposes observed birth and death rates from 225 countries are investigated. Ranks are used for hierarchical clustering by *Ward*'s minimum variance method. The stability of the result is investigated by random weighting of observations. In doing so, 200 such replicates were clustered by *Ward*'s method.

Figure 6 illustrates the obtained clusters (left) and the statistics used to validate the result (right). The unique solution is compared with results from the bootstrap samples by the

adjusted Rand index R. The axis at the left-hand side and the bars in the graphic are assigned to the standard deviation of R, whereas the axis at the right-hand side scales box-plots showing median, mean, upper, and lower 5 percent quantile of R. The median of R for $K = 2$ is near to its theoretical maximum value 1. That means, the two cluster solution is stable. It can be confirmed to a high degree for almost all samples. For more than two clusters, the median (or mean) of the adjusted Rand values is much smaller. Therefore the number of clusters $K = 2$ is the most likely one.

2. Dimension reduction (J. Pohlzehl, V. Spokoiny).

Data sets from economy or finance are often high dimensional. Usually many characteristics of a firm or an asset are monitored without knowledge which characteristics are needed to answer specific questions. Data structures often do not allow for simple parametric models. Nonparametric statistical modeling of such data suffers from the curse of dimensionality problem (high-dimensional data are very sparse). Fortunately, in many cases structures in complex high-dimensional data live in low-dimensional, but usually unknown subspaces. This property can be used to construct efficient procedures to simultaneously identify and estimate the structure inherent to the data set. The most common models in this context are additive models, single- and multi-index models and partial linear models. These models focus on index vectors or dimension reduction spaces which allow to reduce the dimensionality of the data without essential loss of information. They generalize classic linear models and constitute a reasonable compromise between too restrictive linear and too vague pure nonparametric modeling.

Indirect methods of index estimation like the nonparametric least squares estimator, or nonparametric maximum likelihood estimator have been shown to be asymptotically efficient, but their practical applications are very restricted. The reason is that their evaluation leads to an optimization problem in a high-dimensional space, see [20]. In contrast, computationally straightforward direct methods like the average derivative estimator, or sliced inverse regression behave far from optimally, again due to the “curse of dimensionality” problem.

[17] developed a structural adaptive approach to dimension reduction using the structural assumptions of a single-index and multi-index model. The method allows for an asymptotically efficient estimation of the dimension reduction space and of the link function. [47] improves on these procedures for single- and multi-index models and generalizes it to the case of partially linear models and partially linear multi-index models.

[45] proposes a new method for partially linear models whose nonlinear component is completely unknown. The target of analysis is identification of regressors which enter in a nonlinear way in the model, and complete estimation of the model including slope coefficients of the linear component and the link function of the nonlinear component. The procedure allows for selecting the significant regression variables. As a by-product, a test that the nonlinear component is M-dimensional for $M = 0, 1, 2, \ldots$ is developed. The proposed approach is fully adaptive to the unknown model structure and applies under mild conditions on the model. The only important assumption is that the dimensionality of the nonlinear component is relatively small. Theoretical results indicate that the procedure provides a prescribed level of the identification error and estimates the linear component with an accuracy of order $n^{-1/2}$. A numerical study demonstrates a very good performance of the method even for small or moderate sample sizes.

3. Statistics for inverse problems (P. Mathé, 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.

The problem of reconstructing a planar convex set from noisy observations of its moments is considered in [12] . An estimation method based on pointwise recovering of the support function of the set is developed. We study intrinsic accuracy limitations in the shape-from-moments estimation problem by establishing a lower bound on the rate of convergence of the mean squared error. It is shown that the proposed estimator is near-optimal in the sense of the order. An application to tomographic reconstruction is discussed, and it is indicated how the proposed estimation method can be used for recovering edges from noisy Radon data. This constitutes a first step to adaptive estimation procedures for Positron Emission Tomography (PET).

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 is compact in some Hilbert space, 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 $x = \varphi(A^*A)v$, $\|v\| \le R$, for some increasing function φ, $\varphi(0) = 0$. This approach allows to treat regularly and severely ill-posed problems in the same way. The deterministic theory for such equations was developed in [23, 24], including discretization and adaptation to unknown source conditions. The statistical setup is more complicated. However, based on the seminal work by [31], we could also extend this, including several ill-posed problems as studied by [13, 50]. One is often not interested in the calculation of the complete solution x, but only in some functional, say, $\langle z,x\rangle$ of it, where z is given afore-hand. If this is the case, then the linear functional strategy, as proposed by Anderssen ([1]) is important. Previous analysis of this strategy is extended, as carried out in [25] to the present setup.

The analysis of ill-posed problems under general source conditions raises many new issues and bridges between approximation theory and interpolation theory in function spaces.

Natural inference problems for parameters in stochastic processes lead to ill-posed inverse problems. A first instance is the problem of nonparametric estimation of the weight measure a in the stochastic delay differential equation

$$dX(t) = \left(\int_{-r}^{0} X(t+u)\,da(u)\right)dt + \sigma\,dW(t), \quad 0 \le t \le T,$$

where $\sigma > 0$ is constant and W denotes Brownian motion. In [40], it is shown that this inference problem for $T \to \infty$ is equivalent to an integral equation with stochastic errors in the kernel and in the right-hand side, which can be regularized and solved by the Galerkin method. An adaptive wavelet thresholding method is proposed in [41], which attains the minimax rates for classes of weight measures a with Lebesgue densities in Besov spaces. An algorithm based on the wavelet-Galerkin method for general ill-posed linear problems is proposed in [6]. The problem of estimating the length of the delay in models with continuous weight densities is treated in [42], where it is related to change-point detection in ill-posed settings.
A surprising fact is that in the classical scalar diffusion model

$$dX(t) = b(X(t))\,dt + \sigma(X(t))\,dW(t), \quad 0 \le t \le T,$$

ill-posedness arises due to the lack of continuous-time observations. Assuming that b has regularity $s-1$ and σ has regularity s, estimators based on the low-frequency observations

$(X(n\Delta))_{0\le n\le N}$ with large N, but arbitrary $\Delta > 0$ are constructed in [11]. They attain the optimal minimax rate $N^{-s/(s+3)}$ for σ and $N^{-(s-1)/(2s+3)}$ for b. The significant loss compared to the situation of high-frequency or continuous-time observations is due to the loss of information about the continuous path properties. The estimators are based on spectral estimation of the underlying Markov transition generator and are modified to a larger model class in [43].

4. Monte-Carlo methods and related topics (D. Belomestny, J. Polzehl, V. Spokoiny).

In cooperation with the project *Applied mathematical finance* a root–N consistent Monte Carlo estimator for a diffusion density ([28]) has been developed. The approach has been applied to an environmental problem ([3]) and extended to a large class of models for stochastic processes in discrete time ([29]). These models allow in particular for realistic estimation of ruin probabilities in finance.

In [2], new algorithms for the evaluation of American options using consumption processes are proposed. The approach is based on the fact that an American option is equivalent to a European option with a consumption process involved. A new method of sequential improvement of an initial approximation based on step-by-step interchanging between lower and upper bounds is developed. Various smoothing techniques are used to approximate the bounds in each step and hence to reduce the complexity of algorithm. The results of numerical experiments confirm efficiency of the algorithms proposed. Applications are intended within the project *Applied mathematical finance*.

Simulation-extrapolation-type estimators in errors-in-variables models are investigated in [38, 39]. These estimates generalize and improve proposals from [7, 48].

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Applied mathematical finance

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Reuters Financial Software, Paris

The central theme of the project *Applied mathematical finance* is the quantitative treatment of problems raised by the financial industry, based on innovative methods and algorithms developed in accordance with fundamental principles of mathematical finance. These problems include stochastic modeling of financial data, valuation of complex derivative instruments (options), and risk analysis. The methods and algorithms developed benefit strongly from the synergy with the projects *Statistical data analysis* and *Numerical methods for stochastic models*.

1. Methods for pricing and hedging of non-standard derivatives (D. Belomestny, A. Kolodko, G.N. Milstein, O. Reiß, J. Schoenmakers).

The valuation of financial derivatives based on arbitrage-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), [6]. 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. In general, the fair price of an American- or Bermudan-style derivative can be represented as the solution of an optimal stopping problem.

- *American options*: For the multidimensional American option in a generalized Black-Scholes framework, this optimal stopping problem can be converted into a free boundary value problem (Stefan problem). In this context we have developed in [22] a pure Monte Carlo algorithm for determining the (free) exercise boundary of an American option. Due to the thus constructed exercise boundary, the option may be priced and hedged by well-known Monte Carlo simulation of a respective Cauchy boundary value problem. As such we have a pure Monte Carlo procedure for the solution of a Stefan problem which may be considered remarkable. For one dimension the main idea is as follows. Let us suppose that the exercise curve $x = g'(t)$ is known from $\bar{t} \le t \le T$. By using the free boundary conditions and taking boundary limits of the Black-Scholes PDE and its time derivative in the continuation region, we have shown that the derivative $g'(\bar{t})$ can be expressed in $u_{xxx}(\bar{t}, g'(\bar{t})+)$ and known quantities $u_x(\bar{t}, g'(\bar{t})+)$, $u_{xx}(\bar{t}, g'(\bar{t})+)$ which can be expressed in the PDE coefficients and the pay-off function f. As a result we may compute numerically the third derivative u_{xxx} via a Taylor expansion by an accurate enough computation of $u(\bar{t}, \bar{x} + \rho h^q)$ in a neighborhood point in the continuation region. The latter can be done by standard Monte Carlo simulation using the *known* exercise curve for $\bar{t} \le t \le T$, see Figure 1. Having $g'(\bar{t})$, the exercise curve can be extended one step, $g(\bar{t} - h) \approx g(\bar{t}) - g'(\bar{t})h$, and then we proceed in the same way. In [22] this method is generalized to the multidimensional case.

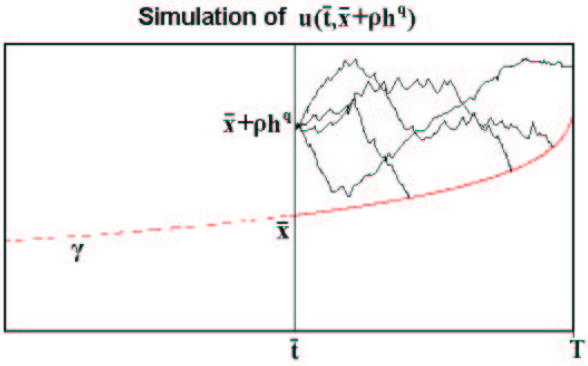

Fig. 1: Backward construction of the exercise boundary in one dimension

- *American options in time-delayed models*: In [10] we have started to consider optimal stopping rules for models driven by stochastic delay differential equations. A natural application is the valuation of American options where the volatility depends on the past. For instance the choice

$$\sigma_t = \sigma\Big(\Big\|X_t - \int_{-\infty}^{0} X_{t+s}\rho e^{\rho s}\, ds\Big\|\Big)$$

postulates that the volatility is driven by the deviation of the current price from an exponentially weighted average over the past, which is close in spirit to classical chart techniques. In certain particular cases the models can be described by higher dimensional Markov diffusion processes with singular diffusion matrix. We study the singular free boundary value problem occurring in the analytical description of the solution.

- *Bermudan-style products*: For Bermudan options we have constructed in [18] an efficient Monte Carlo method for computing a price upper bound. The method is based on a duality approach for Monte Carlo construction of a Bermudan price upper bound via the Doob-Meyer martingale part of an approximation of the respective Snell envelope process,

[15], [36]. In our approach we enclose the theoretical upper bound by approximating from above with an "up-up" estimator due to Haugh & Kogan and from below by a newly developed lower estimator, called "up-low" estimator. Both the "up-up" estimator and the "up-low" estimator require in general simulations in simulations and, as a consequence, tend to be time-consuming. However, we show that by taking a suitable convex combination of the lower and upper estimator we can obtain a combined estimator which requires only a very low number of inner simulations and, as a result, this estimator has a higher computational efficiency. For an application to the Bermudan swaption, approximated by the maximum of "still alive" swaptions, see Figure 2, and for more details, see [18].

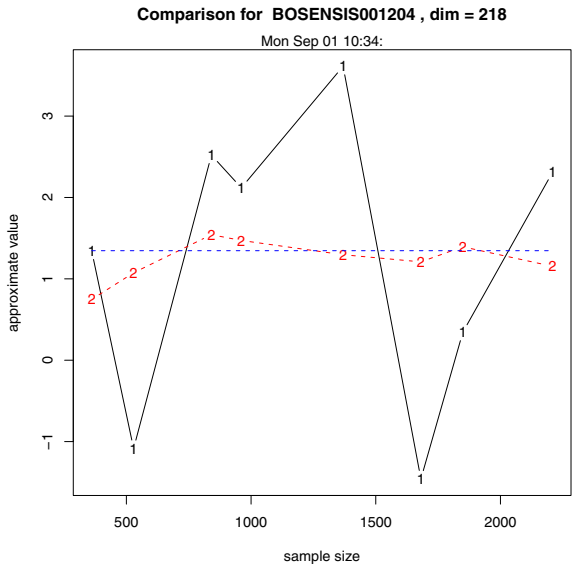

Fig. 2: Bias of different estimators as function of K inner simulations. The dashed line is the combined estimator

Another new method for constructing an upper bound of the Bermudan/American price using some lower bound is currently in development. This approach is based on the fact that an American option is equivalent to a European option with a consumption process involved. The value of the upper bound $V(t,x)$ at a position (t,x) is constructed by the Monte Carlo method. Our attention focuses on constructing new numerical procedures and their practical implementation. The results of numerical experiments confirm efficiency of the algorithms proposed ([3]).

In an initiated 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. The Greenian kernels are connected with the (high-dimensional) LIBOR process and integration with respect to these kernels will be implemented on sparse grids.

- *Monte Carlo evaluation of Greeks by finite differences*: In many cases the price of an option can be represented as the solution of a Cauchy boundary value problem for a parabolic PDE. As a consequence, option prices can be computed by Monte Carlo simulation of a respective system of stochastic differential equations. Derivatives of the solution, in financial terms called "Greeks", can in principal be computed by finite

differences of solutions obtained by Monte Carlo simulation. In [26] it is shown that this method is effective when in the Monte Carlo simulation the method of dependent realizations is exploited. An error analysis is given, and numerical experiments are in agreement with the developed theory. A related Monte Carlo method for computation of Greeks was previously constructed in [23], see also [35].

2. Robust interest rate (LIBOR) modeling and calibration (O. Reiß, J. Schoenmakers).

Robust calibration of the LIBOR market model, a popular benchmark model for effective forward interest rates ([5], [17], [28]), to liquidly traded instruments such as *caps* and *swaptions* has been a challenging problem for several years. In particular, calibration methods which avoid the use of historical data are very desirable, both from a practical and a more fundamental point of view. The dynamics of the LIBOR model is given by

$$dL_i = -\sum_{j=i+1}^{n-1} \frac{\delta_j L_i L_j \sigma_i \sigma_j \rho_{ij}}{1+\delta_j L_j}\, dt + L_i \sigma_i dW_i^{(n)}, \tag{1}$$

where the LIBOR/EurIBOR processes L_i are defined in $[t_0, T_i]$, with $\delta_i = T_{i+1} - T_i$ being day count fractions and σ_i being scalar deterministic volatility functions. Further, $(W_i^{(n)}(t) \mid t_0 \le t \le T_{n-1})$ are correlated Wiener processes under the so-called terminal measure $\mathbb{P}_n$, with deterministic local covariance structure

$$< dW_i^{(n)}, dW_j^{(n)} >= \rho_{ij} dt.$$

In order to construct a stable calibration procedure, we first introduce the following economically motivated parametrization of the scalar volatility and correlation function,

$$\begin{aligned} \sigma_i(t) &:= c_i g(T_i - t) \\ \rho_{ij}(t) &:= \rho^{(0)}_{i-m(t),\, j-m(t)}, \qquad m(t) := \min\{m : T_m \ge t\}, \end{aligned}$$

with a simple parametric function $g(s) := g_\infty + (1 - g_\infty + as)\exp(-bs)$, and, for example, one of the correlation structures developed by Schoenmakers & Coffey in [40], [41], based on some semi-parametric framework, [19], [39].

$$\begin{aligned} \rho_{ij} &= \exp\left[-\frac{|j-i|}{m-1} (-\ln \rho_\infty + \right. \\ &\quad \left. + \eta \frac{i^2 + j^2 + ij - 3mi - 3mj + 3i + 3j + 2m^2 - m - 4}{(m-2)(m-3)} \right)\Bigg], \\ &\quad \eta > 0,\ 0 < \eta < -\ln \rho_\infty. \end{aligned}$$

The thus designed volatility structure relies on sensible assumptions regarding the behavior of forward rates and implies a kind of time shift invariance when $c_i \equiv c$. Calibration of this volatility structure to a set of market cap and swaption volatilities comes down to fit the *model* cap and swaption volatilities to a rather flat surface of market quotes, see the first picture in Figure 3.

The LIBOR model is in a sense designed to price cap(let)s in closed form. Indeed, for any function g and correlation structure $\rho^{(0)}$, caps can be matched perfectly by appropriate choice of the coefficients c_i. However, since caps are in fact one period swaptions, the *model* swaption

volatility surface intersects with the market volatility surface at the 1 period swaption line, regardless of the choice of g and $\rho^{(0)}$. See the second picture in Figure 3 for a model swapvol surface for some rather arbitrary choice of g and $\rho^{(0)}$. This is in fact an intrinsic stability problem (see also [37]), since basically two explaining powers are available determining one rotation angle. We have resolved this problem by introducing economically motivated regularizations of the least squares object function and implemented the so developed stable procedures for testing against market data. Meanwhile our calibration methods are gaining interest, appearing from consulting requests (Reuters FS, Bankgesellschaft Berlin AG) and a currently developing book project ([38]).

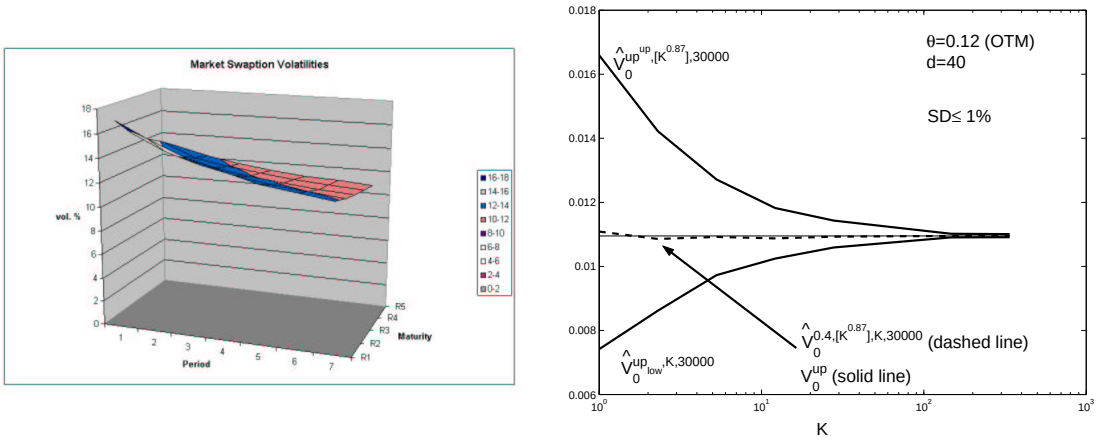

Fig. 3: Market swaption vols and model vols for some typical but arbitrary choice of $g, \rho^{(0)}$

3. Volatility estimation of financial time series (D. Mercurio, V. Spokoiny).

In cooperation with the project *Statistical data analysis*, new techniques for the volatility estimation for financial time series have been developed, [12], [21], [30].

- *Locally time-homogeneous volatility estimation*: The usual approach to volatility estimation starts from the definition of a parametric model, such as GARCH, and then fits this model to the data, globally, for example, by maximum likelihood estimation. On the other hand, practitioners usually prefer to focus on the most recent data, which are perceived as more informative. Therefore, exponentially weighted moving average and window estimators are often applied in practice. However, the results of these techniques strongly depend on the choice of the smoothing parameters. The attempt of the technique proposed in [21] is precisely to put the window estimator on a sound statistical basis. The most recent window of data on which the estimation is performed is selected through a multiple testing procedure, where the probability of rejecting a homogeneous interval is specified. Applications to exchange rate data show good results. The method is successfully applied to problems of volatility forecasting and

Value at Risk evaluation.

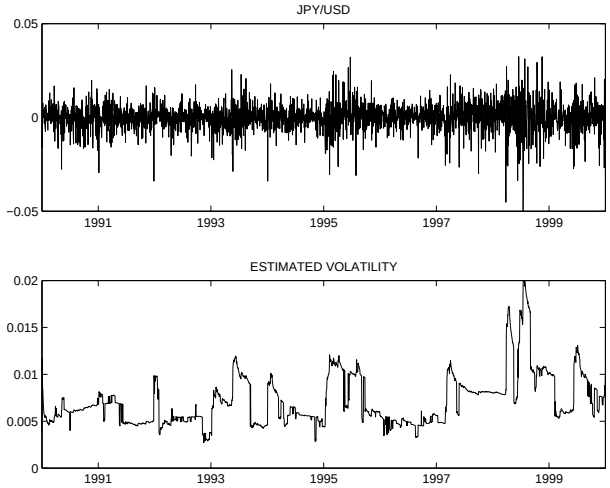

Fig. 4: Returns and estimated volatility for the JPY/USD exchange rate

- *Volatility estimation from discrete observations*: Since many artifacts are observed in high-frequency or tick data during the day, one often uses daily data in historical financial time series to draw inference on the underlying model parameters. In mathematical finance the underlying models are, however, usually formulated in continuous time. Nevertheless, classical methods for estimating the volatility in diffusion-type models are only asymptotically consistent for observation distances tending to zero. In [12] and [30], we studied the prototype problem of estimating the drift and diffusion (volatility) coefficient in a scalar diffusion X from the observation $(X_{n\Delta})_{0\le n\le N}$ for arbitrary $\Delta > 0$. We prove optimality of our nonparametric estimation method in a minimax sense for fixed $\Delta > 0$ and the asymptotics $N \to \infty$. First simulation results indicate that already for relatively small observation distances Δ our method outperforms classical procedures based on quadratic variation estimation.

4. Methods for risk management (S. Jaschke, D. Mercurio, O. Reiß, J. Schoenmakers, V. Spokoiny, J.-H. Zacharias-Langhans).

Since the Basel Committee's proposal for "An internal model-based approach to market risk capital requirements" (1995) was implemented in national laws, banks have been allowed to use internal models for estimating their market risk and have been able to compete in the innovation of risk management methodology. Since all banks are required to hold adequate capital reserves with regard to their outstanding risks, there has been a tremendous demand for risk management solutions. A similar "internal ratings-based approach" is planned for the controlling of credit risk in the "Basel II" process, which is due to be implemented in national laws by 2006. Meanwhile, credit derivatives play an important role as vehicle for banks to transform credit risk into de jure market risk and to potentially lower the required reserves. Such problems of risk measurement and risk modeling are the subject of the research on "Mathematical methods for risk management". This research is supported by the BMBF project "Efficient methods for valuation of risk measures", which continued in 2003 in cooperation with the Bankgesellschaft Berlin AG. Problems of both market and credit risk from the viewpoint of supervisory authorities are being worked on in cooperation with the BAFin.

Although the basic principles of the evaluation of market risks are now more or less settled, e.g., [2], [8], [9], [29], in practice many thorny statistical and numerical issues remain to be solved.

Specifically the industry standard, the approximation of portfolio risk by the so-called "delta-gamma normal" approach, can be criticized because of the quadratic loss approximation and the Gaussian assumptions. Further, in the context of the "Basel II" consultations fundamental questions arise in the area of Credit Risk Modeling.

- *Evaluation of market portfolio risk*: A procedure is constructed, where a small set of scenarios is carefully generated according to a target distribution, which approximates the *optimal* importance sampling measure adapted to this portfolio, but still reflects small variations in the components accurately, and is therefore perfectly suited to calculate the derivatives on a small sample of scenarios. The sample can be generated by a simple rejection algorithm on a previously generated large sample set, but also by a Markov chain, similar to the annealed importance sampling scheme with Metropolis-Hastings kernel, which is also used in the alternative approach. Here, the target distribution is determined by a weight of the form $\exp(-\theta(L-VaR_\alpha)^2)$, approximating for large θ the condition $L = VaR_\alpha$, see Figure 5.

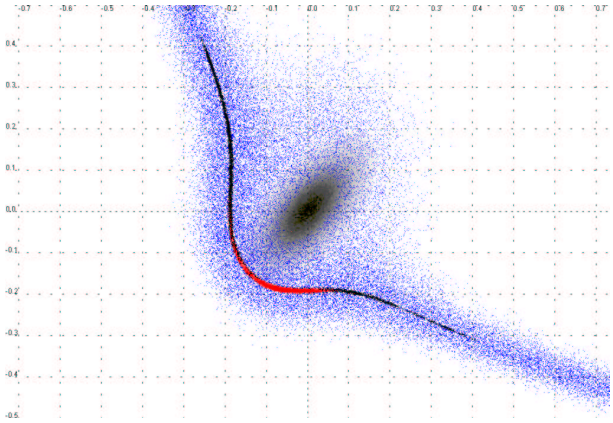

Fig. 5: Sampling in the area of certain losses

- *Evaluation of credit portfolios*: The results obtained in cooperation with the BMBF project "Efficient methods for evaluation of risk measures" for the problem of evaluating market portfolio risk were our starting point for the study of credit risk portfolios. In particular, the enhanced Fourier inversion method is adapted for application to the popular credit risk portfolio model CreditRisk$^+$, proposed by Credit Suisse First Boston (1997) ([7]). CreditRisk$^+$ is a *default-mode* model which distinguishes between two states, *default* or *survival* of an obligor within a one-year period. The popularity of CreditRisk$^+$ is due to the following features. The input data and parameters are readily available. For instance, default probabilities and recovery rates are required in the context of the *Internal Ratings-Based Approach* of the *Basel II* framework on the regulatory treatment of credit risk. Furthermore, CreditRisk$^+$ is very appealing from a computational point of view due to its analytical tractability. In particular, the loss distribution is discrete and its probability generating function is explicitly known,

$$\begin{aligned} G(z) &= \sum_{n=0}^{\infty} P[\tilde{X}=n]\, z^n \qquad (2)\\ &= \exp\left(\sum_{i=1}^{N} w_{0,i}\, p_i\, (z^{\nu_i}-1) - \sum_{k=1}^{K} \frac{1}{\sigma_k^2} \ln\left[1-\sigma_k^2 \sum_{i=1}^{N} w_{k,i}\, p_i\, (z^{\nu_i}-1)\right]\right), \end{aligned}$$

where ν_i is the loss exposure of obligor i with average loss probability p_i, and $w_{k,i}$ and σ_k are economic sector weights and volatilities, respectively. In [32], [33], Fourier inversion techniques are applied successfully to CreditRisk$^+$ and generalizations of it. Moreover, in [31], [34], a unified model is proposed which incorporates CreditRisk$^+$ and Delta-normal as special cases. Further, in [13] we present an alternative numerical recursion scheme for computing the loss probabilities in (2) of the standard CreditRisk$^+$ model, based on well-known expansions of the logarithm and the exponential of a power series. We show that it is advantageous to the Panjer recursion advocated in the original CreditRisk$^+$ document, in that it is numerically stable whereas the Panjer algorithm is known to suffer from stability problems. Also we show that this stable recursion method can be extended to a model which incorporates stochastic exposures as proposed by Tasche ([42]).

Based on knowledge of the complete loss distribution one can easily compute different risk measures such as *Value at Risk* and *Expected shortfall*. These risk measures are also important in the context of stochastic optimization ([14]).

5. Monte Carlo methods in finance (G.N. Milstein, J. Schoenmakers, V. Spokoiny).

Monte Carlo methods are very important in the field of applied mathematical finance, and we present here some interesting applications.

- *Forward-reverse simulation of worse case probabilities*: Previously, Milstein, Schoenmakers and Spokoiny ([25]) developed in cooperation with the project *Statistical data analysis* a new transition density estimator for diffusion processes which is basically root-N consistent for any dimension of the diffusion process. This estimator,

$$\hat{p}(t,x,T,y) = \frac{1}{MN\delta^d} \sum_{m=1}^{M} \sum_{n=1}^{N} K\left(\frac{X_{t,x}^{(n)}(t_1) - Y_{t_1,y}^{(m)}(T)}{\delta} \right) \mathcal{Y}_{t_1,y}^{(m)}(T), \tag{3}$$

  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. For estimating worst-case scenario probability densities in financial applications it is desirable to have a variation of the method in [25] for discrete time models, which have basically more potential for modeling heavy tails. To this end we have constructed in [24] the discrete adjoint process for a large class of discrete time Markov processes such that the forward-reverse density estimator (3) goes through for such processes as well. Several financial applications are currently studied in cooperation with the project *Statistical data analysis*.

- *Variance reduction by Stratification*: In cooperation with the project *Numerical methods for stochastic models* we have been considering the following problem in [20]. 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 $\{I_t^1, I_t^2, \ldots, I_t^m\}$, of m underlyings with respective shares $w_1, w_2, \ldots, w_m$, determining the present value $V_t = \sum_{j=1}^m w_j I_t^j$. There are many numerical schemes for the valuation

of such financial products. Often a reasonable approximation is obtained using the $\Delta-\Gamma$-normal-method for the forecast of V_{t+1} at a future time knowing V_t, given by

$$V_{t+1} \approx V_t + \theta + \Delta y + \langle \Gamma y, y \rangle, \tag{4}$$

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 this situation, the ANOVA decomposition of the integrand in (4) admits only up to bivariate contributions, such that it makes sense to apply Monte Carlo methods, which intrinsically use this information. For the situation at hand, we propose the use of *randomized orthogonal arrays* of strength 2 ([4]), which are known to show *super-convergence*, i.e. converge faster than usual Monte Carlo. Test calculations based on real-world data provided by the *Bankgesellschaft Berlin AG* actually show superiority above conventional simulations, see Figure 6.

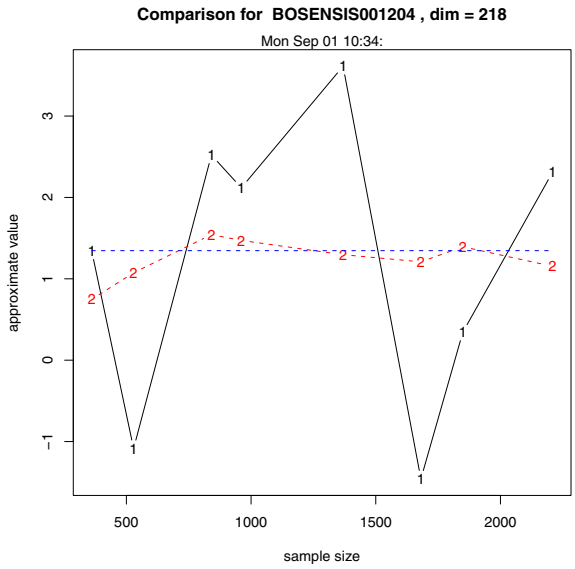

Fig. 6: Convergence Monte-Carlo (1) vs. orthogonal arrays (2)

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Numerical analysis of complex stochastic models

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In 2003, the main research was concentrated on the development of new stochastic models, methods, and simulation techniques for solving high-dimensional boundary value problems with random parameters (involving Wiener processes and log-normal random fields). The developed approach was successfully applied to the transport of gases and particles within plant canopies and statistically isotropic porous media, potential and elasticity problems, and to the numerical solution of Smoluchowski equation governing ensembles of diffusing, nucleating, and coagulating particles under free molecular collision regime. A particular case of interactions analyzed is related to stochastic Hamiltonian systems and Langevin-type equations based on symplectic integrators. This approach results in effective numerical methods for stochastic differential equations used in mathematical finance. Remarkably, the constructed stochastic Lagrangian model for porous media appears to be the first one developed while the discussion and different attempts to construct such a model have a long history in the literature. This work is a result of the cooperation with the Jülich Forschungszentrum (H. Vereecken) and the Free University of Brussels (O. Smidts). The results of the research of 2003 have been published in the refereed papers [1], [5], [7], [8], [9], [10], [13], [14], [18], [22], seven WIAS preprints, and presented in eight talks at international conferences.

In 2003, the EU project INTAS-99-1501 has been successfully finished. In this project, seven groups from five countries (Finland, Denmark, Germany, Russia, Turkmenistan) have been working on the development of new measurement instruments for monitoring the gas-aerosol exchange in the plant canopies. The build-up of the measurement technique was coordinated by Professor T. Vesala (Helsinki University), and K.K. Sabelfeld (WIAS) was the scientific coordinator in the simulation models development. A special issue of the journal *Boundary-layer Meteorology* with papers stemming from this project is to appear in 2004.

The group has organized (Chairman K.K. Sabelfeld) the IVth IMACS Seminar on Monte Carlo Methods (September 15–19, 2003, Berlin) which was co-sponsored by WIAS, the Konrad-Zuse-Zentrum and the DFG. This Seminar is the world's largest international forum on stochastic simulation (see also p. 239).

1. Eulerian and Lagrangian stochastic models for the transport in porous media (K.K. Sabelfeld, D. Kolyukhin).

Lagrangian stochastic model

The Langevin-type models assume that the trajectory $(\mathbf{X}(\mathbf{t}),\mathbf{V}(\mathbf{t}))$ of a particle is governed by a stochastic differential equation of Ito type

$$\begin{aligned} dX_i(t) &= V_i\,dt, \\ dV_i(t) &= a_i(\mathbf{X}(t),\mathbf{V}(t),t)\,dt+\sigma_{ij}(\mathbf{X}(t),\mathbf{V}(t),t)\,dB_j(t), \qquad i=1,2,3. \end{aligned} \tag{1}$$

The summation convention over the repeated indices is used. Here a_i are the drift, and σ_{ij} the diffusion terms, and B_j are standard independent Wiener processes.

This kind of models is widely used in atmospheric turbulence simulations (see, e.g., [4], [11], [15]). The motivation comes from the fact that the characteristic time of the acceleration correlations is much less than that for the velocity correlations which is the case for the turbulent flow.

In a porous medium, when dealing with laminar flows we cannot treat the velocity as turbulent. However, the acceleration direction is highly varying because of the pore structure inhomogeneity. Therefore, the acceleration and velocity fields can be considered as random flows, and the Langevin-type equations can be used to describe the Lagrangian dynamics. The main difference, compared to the turbulence, is that the flow in porous media is extremely anisotropic, which results in a much more complicated form of the drift and diffusion terms. In particular, here we do not have this nice and simple diffusion term in the form of a constant C_0 coming from the Kolmogorov theory of fully developed turbulence.

Compared to random displacement models (RDM) ([2], [3]), the Langevin-type models involve more information about the statistics of velocity, e.g., they naturally use the information about the probability density function (pdf) of the Eulerian velocity field. Indeed, in case the velocity is incompressible, it is known that the Eulerian pdf p_E is related to the coefficients of the Langevin equation through the well-mixed condition

$$\frac{\partial p_E}{\partial t}+u_i\frac{\partial p_E}{\partial x_i}+\frac{\partial}{\partial u_i}(a_i p_E)=\frac{1}{2}\frac{\partial^2(b_{ij}\,p_E)}{\partial u_i\partial u_j}\ , \tag{2}$$

where $b_{ij}=\sigma_{ik}\sigma_{jk}$.

This complicates the model, but wins very important gains: the model is able to describe the transport in detail for scales inside or compared to the Lagrangian time scale where the dispersion is not linear, so generally we deal here with a super-diffusion phenomenon ([17]). It is important that the model enables to evaluate the concentration field not far from the source. Thus, these models are free of the Fickian hypothesis.

The derivation of the drift and diffusion terms is not simple. So far, even in the well-studied atmospheric turbulence, there is no theoretical approach which derives uniquely the expressions for these terms. Therefore, experimental and heuristical information is used to determine the model. In our case we evaluated the diffusion term from the numerical solution of the flow equations. We have derived the drift term and the tensor σ_{ij} from the well-mixed condition (2), and via the numerical solution of the following boundary value problem with random coefficients

$$\nabla\left[K(\mathbf{r})\,\nabla\phi(\mathbf{r})\right]=0\ ,\mathbf{r}\in\mathcal{D} \tag{3}$$

with the following boundary conditions over the outer surface $\mathcal{S}$

$$\phi(\mathbf{r}) = F_D(\mathbf{r}) \ , \quad \frac{\partial \phi(\mathbf{r})}{\partial n} = F_N(\mathbf{r}) \ , \mathbf{r} \in \mathcal{S}_N \ . \tag{4}$$

Here, $\mathcal{S}_D$ and $\mathcal{S}_N$ are parts of $\mathcal{S}$ where the Dirichlet and Neumann boundary conditions are used, respectively. F_D and F_N are given functions over $\mathcal{S}_D$ and $\mathcal{S}_N$. The solution $\phi(\mathbf{r})$ of the flow equation (3) with the boundary conditions (4) determines entirely the time-independent flow problem in a saturated porous medium because the knowledge of the hydraulic potential $\phi(\mathbf{r})$, everywhere in $\mathcal{D}$ and over $\mathcal{S}$, yields the groundwater velocity by applying Darcy's law.
The hydraulic conductivity K in (3) is a random field, the hydraulic potential $\phi(\mathbf{r})$ is therefore also a random field, and the velocity is a random vector field as well.
A validation of the model developed was made through a comparison of various statistical characteristics obtained with our method with those known from measurements and direct numerical simulations. The backward trajectory approach we suggest in [24] for finance models is used here for variance reduction purpose.

Eulerian stochastic model

Under the assumption of smallness of fluctuations in the hydraulic conductivity we construct a stochastic Eulerian model for the incompressible flow as a divergence-free Gaussian random field with a spectral tensor of a special structure derived from Darcy's law. A randomized spectral representation is then used to simulate this random field. Numerical results are compared with the analytical results obtained by the small perturbation expansion in [2], [3]. A series of test calculations confirmed the high accuracy and computational efficiency of the method. Comparisons with asymptotically exact results show a good agreement.

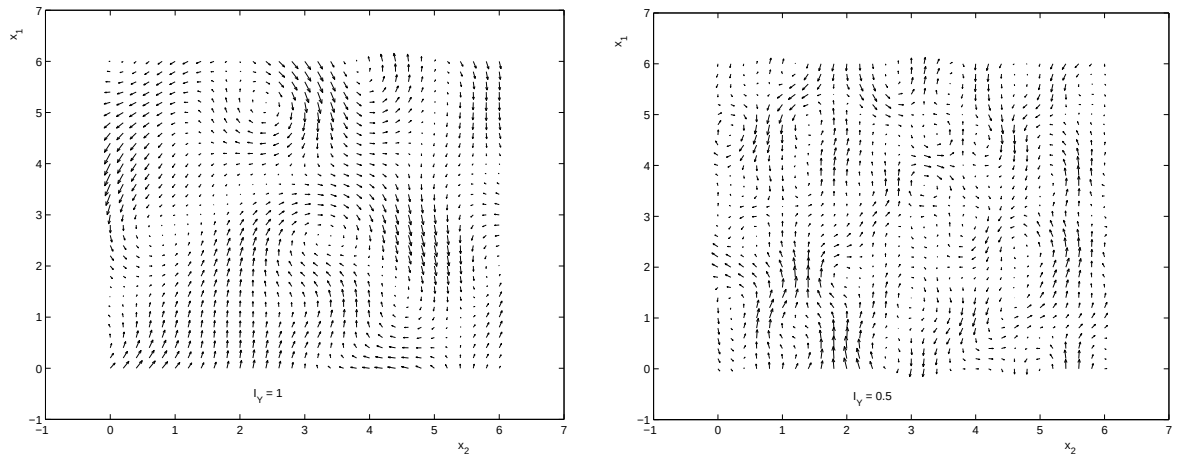

Fig. 1: Samples of specific discharge perturbation random fields q_1, q_2, for the isotropic hydraulic conductivity. Left picture: the correlation length $I_Y = 1$, right picture: $I_Y = 0.5$. The number of harmonics was $N = 100$.

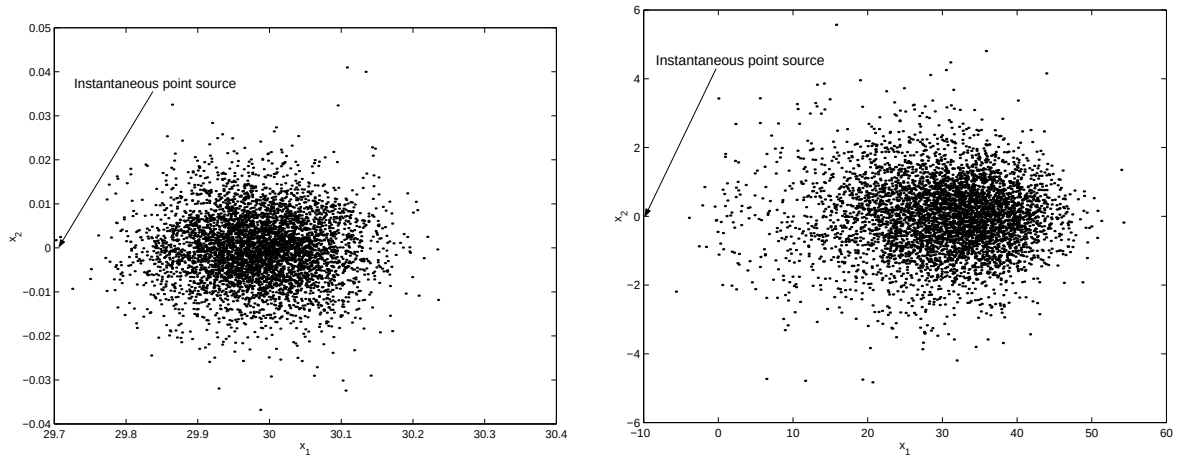

Fig. 2: A cloud of 5000 particles ejected by an instantaneous point source at the origin, shown at the time instant $t' = 30$, $\sigma_Y^2 = 10^{-2}$ (left picture) and $\sigma_Y^2 = 1$ (right picture)

The samples of the velocity field are constructed by a very fast spectral randomization method ([16]). For illustration, we show here two samples of such a field in Figure 1. The particle scattering by this velocity field is shown in Figure 2.
The work is done in cooperation with ULB, Brussels, and FZ Jülich, Institute of Chemistry and Dynamics of the Geosphere, the results are presented in [8], [10]. The backward trajectory technique developed in our project was also usefully applied by our colleagues in the *Statistical data analysis* project.

2. Random Walk methods for the iterative solution of high-dimensional boundary value problems (K.K. Sabelfeld).

Suppose a homogeneous isotropic medium G with a boundary Γ is given, whose state in the absence of body forces is governed by the Lamé equation, see, e.g., [16], [21]:

$$\Delta \mathbf{u}(x) + \alpha \,\mathrm{grad}\,\mathrm{div}\,\mathbf{u}(x) = 0, \quad x \in G, \tag{5}$$

where $\mathbf{u}(x) = (u_1(x_1,\ldots,x_n),\ldots,u_n(x_1,\ldots,x_n))$ is a vector of displacements, whose components are real-valued regular functions. The elastic constant α is expressed through the Lamé constants of elasticity λ and μ: $\alpha = \frac{\lambda+\mu}{\mu}$.
The first boundary value problem for the Lamé equation consists in finding a vector function $\mathbf{u} \in C^2(G) \cap C(\bar{G})$ satisfying the boundary condition

$$\mathbf{u}(y) = \mathbf{g}(y), \quad y \in \Gamma\ , \tag{6}$$

where $\mathbf{g} \in C(\Gamma)$ is a given vector function.

The stochastic algorithm is based on the spherical mean value relation for the general n-dimensional case, see, e.g., [21].
The regular solutions to the system (5) satisfy the following spherical mean value relation in $S(x,r)$

$$u_i(x) = \frac{n}{2(n+\alpha)\omega_n} \sum_{j=1}^{n} \int\limits_{\Omega} \Big((2-\alpha)\delta_{ij} + \alpha\,(n+2) s_i s_j \Big) u_j(x+rs)\ d\Omega(s), \tag{7}$$

$i = 1, \ldots, n$, δ_{ij} is the Kronecker symbol, s_i are the cosine directions of the unit vector s, and $\omega_n = 2\pi^{n/2}\Gamma(n/2)$ is the area of the surface of $\Omega = S(0,1)$, a unit sphere of dimension n.
Standard Monte Carlo walk on spheres process uses this relation so that the transition in the Markov chain goes from the center of the sphere to its surface ([21]).
We suggest a further development of the method proposed in [23] which is based on a generalization of the spherical mean value relation for an arbitrary point inside the sphere. This generalization is written

$$u(x) = \int\limits_{S(x_0,R)} p(y;x)\, Bu(y)\, dS(y)\,,$$

where $p(y;x)$ is the probability density for a Wiener process starting in an arbitrary point x inside the sphere to the point $y \in S(x_0,R)$, and the kernel B is given explicitly in 2D and 3D cases.
It can be shown that the new method converges much faster compared to the standard walk on spheres method. Namely, the cost of the new method is $log\, log(|\varepsilon|)/\varepsilon^2$ while for the standard method it is $log(|\varepsilon|)/\varepsilon^2$. Remarkably, the cost is very weakly dependent on n, the dimension of the problem. Different modifications of this approach are discussed in [19], [23], [24].
In a cooperation with the group of Professor M. Mascagni (Florida State University, Tallahassee, USA), the permeability for a complicated geometry of a porous medium is studied to find the distribution of the velocity field. The methods used are the Decentred Random Walk on Spheres (DRWS) suggested by K.K. Sabelfeld and I. Shalimova ([24]). In a cooperation with the Institute of Computational Mathematics and Mathematical Geophysics, Russian Academy of Sciences, Novosibirsk (Dr. I. Shalimova), an additional validation of the model based on the DRWS method is made by applying the Random Walk on Boundary process ([20]).

3. Stochastic particle method for the evaluation of Footprint functions (K.K. Sabelfeld).

Forward and backward stochastic Lagrangian trajectory simulation methods are developed to calculate the footprint and cumulative footprint functions of concentration and fluxes in the case when the ground surface has an abrupt change of the roughness height. The statistical characteristics of the stochastic model are extracted numerically from a closure model we developed for the atmospheric boundary layer. The flux footprint function is perturbed in comparison with the footprint function for a surface without change in properties. The perturbation depends on the observation level as well as the roughness change and the distance from the observation point. It is concluded that the footprint function for a horizontally homogeneous surface, widely used in the estimation of sufficient fetch for measurements, can be seriously biased in many cases of practical importance.
Over a horizontally homogeneous surface the flux measured by micrometeorological technique equals to the surface flux. This principle is used to determine the surface exchange by the eddy covariance (EC) technique ([4]). The flux footprint function links the surface emissions to the observed fluxes above surface at EC measurement level. The footprint function is therefore used to estimate a distance required to make reliable EC measurements, i.e. if the horizontal extent of underlying surface of interest is sufficient to determine its exchange rate. Extended tower measurements of fluxes over forests have been used during the last ten years to obtain detailed information on carbon and water exchanges between forest canopies and atmosphere. Large areas of forest, however, are not common in Europe nor in the USA. The footprint models based on analytical diffusion theory as well as Lagrangian stochastic simulation of an ensemble of fluid parcel trajectories assume a horizontally homogeneous surface. For forest canopies the

footprint models involve a number of uncertainties originating from the parametrization of the canopy turbulence features. Such models are frequently applied to estimate the contribution of an area of certain upwind distance, or to estimate the fetch to ensure that the given area contributes a certain percent to the observed flux, by vaguely assuming that the footprint function for a horizontally homogeneous surface is a good approximation for a more complex situation with changes in the surface properties. In reality changes in the surface roughness can be very drastic, for example in the case of forest and field interface. Also the thermal inhomogeneities induced by albedo and repartitioning of available energy into sensible and latent heat fluxes can be significant, this will be analyzed, however, in the future work. So we deal here with pure mechanical turbulence caused by the surface roughness.
The governing equations involve the closure model for the mean flow and stochastic differential equations for the Lagrangian trajectories. There exists a variety of closure models for turbulent mixing, ranging from constant eddy coefficient parametrization to detailed Large Eddy Simulations and Direct Numerical Simulation. We assume that the mean profiles in the boundary layer of atmosphere are described by the following system:

$$\begin{aligned} u\frac{\partial u}{\partial x}+w\frac{\partial u}{\partial z} &= \frac{\partial}{\partial z}k\frac{\partial u}{\partial z}+f(v-G\sin\alpha), \\ u\frac{\partial v}{\partial x}+w\frac{\partial v}{\partial z} &= \frac{\partial}{\partial z}k\frac{\partial v}{\partial z}-f(u-G\cos\alpha) \end{aligned} \tag{8}$$

is the momentum equation, where the Coriolis parameter is given by $f = 2\Omega\sin\varphi$, $\Omega = 7.29\,10^{-5}s^{-1}$, G is the geostrophic wind, and φ is the angle between the x-axis and the isobare; α is the angle between the x-axis and the direction of the geostrophic wind. Further,

$$\frac{\partial u}{\partial x}+\frac{\partial w}{\partial z}=0$$

is the continuity equation, where k is the turbulent exchange coefficient for the momentum.
The balance of the kinetic energy is written as

$$u\frac{\partial b}{\partial x}+w\frac{\partial b}{\partial z}=\alpha_b\frac{\partial}{\partial z}k\frac{\partial b}{\partial z}+k\left[\left(\frac{\partial u}{\partial z}\right)^2+\left(\frac{\partial v}{\partial z}\right)^2\right]-\bar{\varepsilon}, \tag{9}$$

where $\bar{\varepsilon}=\frac{cb^2}{k}$ is the mean rate of dissipation of the turbulent energy, $c = 0.0286$, $\alpha_b \approx 0.7$.
The functions k and b are related through

$$l=\left(\frac{1}{\kappa z}+\frac{1}{l_0}\right)^{-1}, \quad k=C_k l\sqrt{b}, \tag{10}$$

with $\kappa \approx 0.4$, $l_0 = 100$ m, $C_k = 0.41$. Thus our system of governing equations consists of (8), (9), and the relation (10).
The functions vary in the layer $z_0 \le z \le h$, h being the height of the boundary layer, and z_0 the roughness height. The system of equations is considered with the following boundary conditions:

$$\begin{aligned} &u=0, v=0, w=0, \quad \text{at } z=z_0, \\ &u=G\cos\alpha, v=G\sin\alpha \quad \text{at } z=h,\ x\le 0, \\ &\tfrac{\partial u}{\partial z}=\tfrac{\partial v}{\partial z}=0 \text{ at } z=h,\ x>0\ , \\ &\tfrac{\partial b}{\partial z}=0 \text{ at } z=z_0, \quad \text{and } b=0 \text{ at } z=h\ . \end{aligned}$$

At $z = z_0$, we take $l = \kappa z_0$.
We present the backward estimators for the evaluation of footprint functions in the case of the boundary layer with the sources uniformly distributed over the strips D_i, $i = 1, \ldots, n_{sr}$. For simplicity, we have taken the x-axis coincident with the direction of the geostrophical wind, i.e. $\alpha = 0$.
The backward trajectory starts at time t, at the detector point with the velocity sampled from the Eulerian velocity pdf $p_E(u,x)$ which is assumed to be Gaussian. Below, we denote by $\bar{u}_{Ek}$ the k-th component ($k = 1,2,3$) of the mean Eulerian velocity vector, and the hat over the symbols x and u is to indicate that this is a finite-difference approximation to the true Lagrangian trajectory.
The backward trajectory simulation is conveniently carried out through the semi-implicit Euler scheme, which can be written for one time step as follows:

$$\begin{aligned} \hat{x}_k(t-\Delta t) &= \hat{x}_k(t) - (\hat{u}'_k(t) + \bar{u}_{Ek}(t, \hat{x}(t))\,\Delta t, \\ \hat{u}'_k(t-\Delta t) &= \hat{u}'_k(t) - \hat{a}'_k(t, \hat{x}(t-\Delta t), \hat{u}(t))\,\Delta t + \sqrt{C_0 \bar{\varepsilon}(t-\Delta t, \hat{x}(t-\Delta t))\,\Delta t}\,\eta_{tk}, \end{aligned}$$

where η_{tk}, $k = 1,2,3$, are independent standard Gaussian random variables. Here for a reason of practical convenience, we work in the "primed" velocity variables $\hat{u}'_k = \hat{u}_k - \bar{u}_{Ek}$, so that

$$\begin{aligned} d\hat{x}_k &= (\hat{u}'_k + \bar{u}_{Ek})\,ds\ , \\ d\hat{u}'_k &= \hat{a}'_k\,ds + \sqrt{C_0 \bar{\varepsilon}}\ \overleftarrow{d}\ W_k(s), \quad s < t,\ k = 1,2,3, \end{aligned}$$

with the condition that the trajectory starts at the detector position with the velocity sampled from the Gaussian pdf p_E. The form of all the input function is given explicitly, see [9], and $\overleftarrow{d}\ W_k(s)$ stands for the backward Wiener differential (see [11]) which implies for the Euler scheme that the increments are taken back in time.
Let τ_{ij} be the time at which the trajectory $(\hat{\mathbf{x}}(s), \hat{\mathbf{u}}(s))$, $s \le t$, reaches the ground surface and touches the i-th strip: the first touchdown at τ_{i1}, the second (after a reflection from the boundary) at τ_{i2}, etc., and the last one at τ_{iN_i}. The random estimators have the following form, for the concentration,

$$c_i = \left\langle \sum_{j=1}^{N_i} \frac{2}{\Delta_i} \frac{1}{|\hat{u}_3(\tau_{ij})|} \right\rangle\ ,$$

and for the vertical flux:

$$q_{iz} = \left\langle \sum_{j=1}^{N_i} \frac{2}{\Delta_i} \frac{\hat{u}_3(t)}{|\hat{u}_3(\tau_{ij})|} \right\rangle\ , \quad i = 1, \ldots, n_{sr}.$$

Here Δ_i are the widths of the surface strips ejecting the particles, and the angle brackets stand for the averaging over the ensemble of independent backward trajectories.
A sensitivity analysis is made for the footprint functions under perturbation of the roughness height; two cases are considered: (1) smooth-to-rough, and (2) rough-to-smooth change of the roughness height. The calculations show that the footprint function of concentration is more sensitive than that of the vertical flux.
It is concluded that the footprint and cumulative footprint functions of concentration for a horizontally homogeneous surface, widely used in the estimation of sufficient fetch for

measurements, can be seriously biased in many cases of practical importance. The calculations show that the footprint area based on the cumulative concentrations, if estimated through the homogeneous case, can be essentially under- or overestimated, compared to the true inhomogeneous case.
The work is done in cooperation with Prof. Dr. T. Vesala and Dr. U. Rannik (Helsinki University, Finland), N.O. Jensen (Risoe National Laboratory, Denmark), V. Kukharets (Obukhov Institute of Atmospheric Physics, Moscow, Russia), O. Kurbanmuradov (Physical Technical Institute, Turkmenian Academy of Sciences, Ashkhabad, A. Levykin (Institute of Computational Mathematics and Mathematical Geophysics, Russian Academy of Sciences, Novosibirsk).

4. New stochastic particle methods for the Smoluchowski coagulation equation: Variance reduction and error analysis (A. Kolodko, K.K Sabelfeld).

In the stochastic models for the simulation of coagulation equation it is well known that the decrease of the number of particles in a model system is the main source of the variance increase ([6]). To overcome it, H. Babovsky has suggested to transform the standard Smoluchowski equation (governing the particle concentration) to the mass-flow equation

$$\frac{\partial g_l(t)}{\partial t} = \sum_{i=1}^{l-1} \frac{1}{i} K_{i(l-i)} g_i g_{l-i} - g_l \sum_{i\geq 1} \frac{1}{i} K_{li} g_i,\ l \geq 1; \quad \text{where} \quad g_l(t) = l u_l(t).$$

Stochastic algorithms for this equation keep the number of particles fixed during the whole time. This approach has also another nice property: the number of large particles decreases slower than in the traditional Bird's algorithm. One may expect that these features should drastically increase the variance.
However, the distribution of small and large particles in mass-flow systems is still far from being uniform. In fact, even in the case of constant coagulation coefficients $K_{ij} = 1$ the decrease of particle concentration with the growth of size l (for any fixed time t) is exponential:

$$u_l(t) = (1+0.5t)^{-2} \left(1 - \frac{1}{1+0.5t}\right)^{l-1}.$$

Note that for the unbounded coagulation kernels the relative number of large particles is even smaller.
Therefore, it is reasonable to introduce a weight function $w(l)$ increasing with the growth of l, and to transform the original Smoluchowski equation to a "weight equation" for the new variable, the weighted concentration $z_l(t) = w(l)u_l(t)$. This weight equation reads obviously

$$\frac{\partial z_l(t)}{\partial t} = \frac{1}{2} \sum_{i+j=l} \hat{K}_{ij} z_i z_j - z_l \sum_{i\geq 1} \hat{K}_{li} \frac{w(l)}{w(i+l)} z_i, \quad l \geq 1; \qquad \hat{K}_{ij} = K_{ij} \frac{w(i+j)}{w(i)w(j)}\ .$$

To solve this equation, we develop a generalization of the method of fictitious jumps (MFJ). Together with this algorithm, we construct a generalization of the method of majorant frequencies (MMF). Though the latter algorithm can be treated as the particular case of the former, it is very important itself.
We apply the method developed to simulate a coagulation-evaporation process of aerosol particles in free molecule collision regime.

Consider a coagulation-evaporation process in a free molecule regime, which is governed by the equation

$$\frac{\partial u_1(t)}{\partial t} = -u_1 \sum_{i\geq 1} K_{i1}u_i + \sum_{i\geq 3} E_i u_i + 2E_2 u_2,$$

$$\frac{\partial u_l(t)}{\partial t} = \frac{1}{2}\sum_{i+j=l} K_{ij}u_i u_j - u_l \sum_{i\geq 1} K_{li}u_i - E_l u_l + E_{l+1}u_{l+1}, \quad l \geq 2$$

with

$$K_{ij} = \left(\frac{3}{4\pi}\right)^{\frac{1}{6}} \left(\frac{6kT}{\rho_p}\right)^{\frac{1}{2}} \left(\frac{1}{i}+\frac{1}{j}\right)^{\frac{1}{2}} \left(i^{\frac{1}{3}}+j^{\frac{1}{3}}\right)^2;$$

$$E_j = EK_{1j}\exp\left(A\left(j^{\frac{2}{3}} - (j-1)^{\frac{2}{3}}\right)\right).$$

Here k is Boltzmann's constant, T is the absolute temperature, ρ_p is the particle density, and we suppose monodisperse initial conditions:

$$u_1(0) = u^{(0)}; \quad u_l(0) = 0,\ l > 1.$$

The question we are interested in is how the values of the evaporation parameters influence the behavior of the process, in particular, we study the total concentration of all particles whose sizes are larger than a given size j_*: $c_{j_*}(t) = \sum_{i\geq j_*} u_i(t)$.

The work is done in cooperation with W. Wagner (WIAS, Research Group 5) and A. Onishuk (Institute of Chemical Kinetics and Combustion, Russian Academy of Sciences, Novosibirsk).

5. A probabilistic approach to the solution of complicated problems of mathematical physics (G.N. Milstein).

The numerical evaluation of Wiener integrals is an important and difficult task. Many approaches are proposed for solving this problem. As a rule, the known numerical methods reduce a path integral to a high-dimensional integral which is then approximated using either conventional deterministic or Monte Carlo methods. The high dimension of these integrals makes the calculations of the Wiener integrals extremely difficult.

We developed a numerical integration of stochastic differential equations together with the Monte Carlo technique to evaluate conditional Wiener integrals of exponential-type functionals. An explicit Runge-Kutta method of order four and implicit Runge-Kutta methods of order two were constructed. The corresponding convergence theorems are proved. To reduce the Monte Carlo error, a variance reduction technique is considered. The effectiveness of the constructed algorithms allowed us to evaluate the conditional Wiener integrals for a large dimension. Results of numerical experiments are in good agreement with the theory.

Nonlinear PDEs are mostly investigated by numerical methods, which are traditionally based on deterministic approaches. In [1] we propose an approximation method based on a probabilistic approach for the three-dimensional system of Navier-Stokes equations with spatial periodic boundary conditions. The method exploits the ideas of weak-sense numerical integration of stochastic differential equations. Despite the probabilistic nature, this method is nevertheless deterministic. The probabilistic approach takes into account a coefficient dependence on the space variables and a relationship between diffusion and advection in an intrinsic manner. In

particular, the derived method allows us to avoid difficulties stemming from highly varying coefficients and strong advection.
Numerical methods for stochastic Hamiltonian systems and Langevin-type equations based on symplectic integrators were further developed with an analysis of stability problems of stochastic dynamics.
In [13], [14], specific methods for stochastic Hamiltonian systems and Langevin-type equations are proposed. Stochastic Hamiltonian systems, like deterministic Hamiltonian systems, possess the property of preserving symplectic structure (symplecticness). A lot of attention in deterministic numerical analysis has been paid to the symplectic integration of Hamiltonian systems. This interest is motivated by the fact that symplectic integrators in comparison with usual numerical schemes allow us to simulate Hamiltonian systems for very long time intervals with high accuracy. Symplectic methods for stochastic Hamiltonian systems proposed in [13] have significant advantages over standard schemes for SDEs as well.
It is natural to expect that making use of numerical methods, which are close, in a sense, to symplectic ones, also has some advantages when applying them to stochastic systems close to Hamiltonian ones. An important and fairly large class of such systems is the Langevin-type equations. The Langevin-type equations have a widespread occurrence in models from physics, chemistry, and biology. In [14] we construct special numerical methods which preserve some specific properties of the Langevin-type equations. The proposed methods are such that they degenerate to symplectic methods when the system degenerates to a Hamiltonian one, and their law of phase volume contractivity is close to the exact one. The presented numerical tests of both symplectic and quasi-symplectic methods clearly demonstrate superiority of the proposed methods for very long time intervals in comparison with existing standard methods. Different examples of stochastic differential equations used in mathematical finance are now analyzed by this approach to find an optimal numerical method with small variance.

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4.7 Research Group Continuum Mechanics

4.7.1 Overview

In der Forschungsgruppe „Kontinuumsmechanik“ wurde die Forschung in zwei Problemklassen fortgeführt:

- Modellierung deformierbarer poröser Medien,
- Thermodynamische Modellierung und Simulation von Phasenübergängen.

Within the research group “Continuum Mechanics” there has been a continuation of studies on two different classes of problems:

- Modeling of deformable porous media;
- Thermodynamic modeling and simulations of phase transitions.

Auf dem Gebiet der Modellierung von porösen Medien konzentrierte sich die Forschung auf zwei Probleme:

1. Ausbreitung von Oberflächenwellen in gesättigten poroelastischen Körpern.
Der gesamte Frequenzbereich $(0,\infty)$ wurde numerisch untersucht.

2. Thermodynamische Grundlagen für die Modellierung gesättigter poroelastischer Körper.
Es wurde ein nichtisothermes, nichtlineares Modell mit einer Porositätsbilanz für solche Materialien konstruiert.

Within the field of modeling of porous media the research concentrated on two problems:

1. Propagation of surface waves in saturated poroelastic bodies.
The full frequency regime (0,∞) has been investigated numerically.

2. Thermodynamic foundations for modeling saturated poroelastic bodies.
The full nonisothermal nonlinear model of such materials with a porosity balance equation has been constructed.

Im Bereich *Thermodynamische Modellierung und Simulation von Phasenübergängen* gab es folgende Aktivitäten:

1. Phasenübergänge, teilweise gefördert im BMBF-Programm Neue Mathematische Verfahren in Industrie und Dienstleistungen *unter 03DRM3B5.*
Die Studien über Phasenübergänge wurden an drei Unterprojekten durchgeführt: 1. Das bisher benutzte Phasenfeldmodell zur Simulation von morphologischen Phasenänderungen in Lotmaterialien, die in mikroelektronischen Bauteilen eingesetzt werden, wurde geändert und erweitert. 2. Das Modell zur Bestimmung von thermodynamischen Gleichgewichten, Diffusionsprozessen und der Simulation von arsenischen Ausscheidungen in semiisolierendem GaAs wurde vervollständigt. 3. Wir haben mit einer sorgfältigen Studie über die Grinfeld-Instabilität begonnen.

Within the area of Thermodynamic modeling and simulations of phase transitions, there have been the following activities:

1. Phase transitions, partly funded within the BMBF program New Mathematical Methods in Industry and Services *under 03DRM3B5.*

The study on phase transitions has focused on three subprojects: 1. The previously used phase-field model to simulate morphological phase changes in solder materials for microelectronic devices has been changed and extended. 2. The model for the determination of thermodynamic equilibria, diffusion processes, and the simulation of arsenic precipitations in semi-insulating GaAs has been completed. 3. We have started a careful study on the Grinfeld instability.

2. Multiskalen Modellierung, Mikro-Makro-Übergänge in der atomaren Kette für verschiedene Skalierungen, *gefördert im DFG-Schwerpunktprogramm SPP 1095* Analysis, Modellbildung und Simulation von Mehrskalenproblemen.
Die Studie zur Multiskalenmodellierung ist ein gemeinsames Projekt mit J. Sprekels, und es gibt eine Kooperation mit A. Mielke (Universität Stuttgart). Die atomare Kette dient als Beispiel, wo die Möglichkeit rigoroser Multiskalenübergänge diskutiert wird.

3. Hyperbolische Erhaltungsgleichungen, Kinetische Lösungen der Boltzmann-Peierls-Gleichung und ihrer Momentensysteme, *gefördert im DFG-Schwerpunktprogramm* ANumE — Analysis und Numerik von Erhaltungsgleichungen.
Die Behandlung von hyperbolischen Anfangs- und Randwertproblemen wurde vervollständigt mit einer Studie der Boltzmann-Peierls-Gleichung und der relativistischen Euler-Gleichungen.

4. Stabilität entnetzender Polymerfilme.
In dieser Berichtsperiode haben wir verschiedene Studien über dünne Filme begonnen, insbesondere wurde die Stabilität von Entnetzungsprozessen im Detail untersucht.

5. Numerische Untersuchungen der von Karman'schen Plattengleichungen.
Das industriell geförderte Projekt zur Spannungsanalyse von dünnen Platten hatte als Schwerpunkte (i) Spannungsanalyse von rechtwinkligen Platten, und (ii) Numerische Subtilitäten betreffend das Babuska-Paradox.

2. Multiscale modelling, Micro-macro-transition in the atomic chain for various scalings, *funded within the DFG Priority Program SPP 1095* Analysis, Modelling and Simulations of Multiscale Problems.
The study on multiscale modeling is a joint project with J. Sprekels and his group and a collaboration with A. Mielke (University of Stuttgart). The atomic chain serves as an example, where the possibility of rigorous micro-macro transitions for various scalings is discussed.

3. Hyperbolic conservation laws, Kinetic solutions of the Boltzmann Peierls equation and its moment systems, *funded within the im DFG Priority Program* ANumE — Analysis and Numerics of Conservation Laws.

The treatment of hyperbolic initial and boundary value problems has been completed with a study of the Boltzmann Peierls equation and of the relativistic Euler equations.

4. Stability of dewetting polymer films.
During the period of this report we have started various studies on thin films, in particular the stability of dewetting polymer films was investigated in detail.

5. Numerical aspects of the von Karman plate equations.
The industry supported project on *Stress analysis of thin plates* focused on (i) stress analysis of rectangular plates and (ii) numerical subtleties regarding the Babuska paradox.

4.7.2 Projects

Wave properties of four models describing poroelastic media

Collaborators: B. Albers, K. Wilmanski

Cooperation with: C. Lai (European Centre for Training and Research in Earthquake Engineering, Pavia, Italy), R. Lancellotta (Politecnico di Torino, Italy)

In this project (see: [1]) we investigate the propagation of bulk waves within the frame of four different linear two-component models of poroelastic materials. In the last year it has been shown by Wilmanski [3] that Biot's model may follow from a general nonlinear thermodynamical model solely in the case when such a nonlinear model contains a constitutive dependence on the porosity gradient and, if needed, on some other higher gradients. A full linear model following from such a generalization is as follows.
We have the set of balance equations

$$\begin{aligned}
\frac{\partial \rho^S}{\partial t} &= -\rho_0^S \operatorname{div} \mathbf{v}^S, \quad \frac{\partial \rho^F}{\partial t} = -\rho_0^F \operatorname{div} \mathbf{v}^F, \\
\rho_0^S \frac{\partial \mathbf{v}^S}{\partial t} &= \operatorname{div} \mathbf{T}^S + \hat{\mathbf{p}} + \rho_0^S \mathbf{b}^S, \\
\rho_0^F \frac{\partial \mathbf{v}^F}{\partial t} &= \operatorname{div} \mathbf{T}^F - \hat{\mathbf{p}} + \rho_0^F \mathbf{b}^F, \\
\frac{\partial (n - n_E)}{\partial t} &= -\Phi \operatorname{div} \left(\mathbf{v}^F - \mathbf{v}^S \right) + \hat{n}.
\end{aligned}$$

The index 0 refers to a reference value of a quantity. In these equations the symmetric tensors $\mathbf{T}^S, \mathbf{T}^F$ are partial Cauchy stresses, $\hat{\mathbf{p}}$ is the momentum source, $\mathbf{b}^S, \mathbf{b}^F$ are partial body forces, n_E is the so-called equilibrium porosity, Φ is the transport coefficient of porosity, and $\hat{n}$ is the porosity source.
These balance equations transform into field equations if we add constitutive relations. For poroelastic materials they are assumed to have the form

$$\mathbf{T}^S = \mathbf{T}_0^S + \lambda^S e \mathbf{1} + 2\mu^S \mathbf{e}^S + Q\varepsilon \mathbf{1}, \quad e := \operatorname{tr} \mathbf{e}^S, \quad \varepsilon := \frac{\rho_0^F - \rho^F}{\rho_0^F},$$

$$\mathbf{T}^F = \mathbf{T}_0^F + \rho_0^F \kappa \varepsilon \mathbf{1} + Qe\mathbf{1}, \quad n_E = n_0 (1 + \delta e),$$

$$\hat{\mathbf{p}} = \pi \left(\mathbf{v}^F - \mathbf{v}^S \right) - N \operatorname{grad} n.$$

Certainly, the effective (macroscopic) parameters λ^S, μ^S correspond to classical Lamé constants, κ describes the macroscopic compressibility of the fluid, δ is a parameter coupling equilibrium changes of porosity with volume changes of the skeleton e, and Q is the coupling parameter introduced by Biot. The permeability coefficient π is related to the permeability appearing in the Darcy model of seepage. If the contribution of the porosity gradient which is characterized by the material parameter N is zero, the model is identical with the one proposed by Biot provided that we neglect in Biot's model added mass effects (relative accelerations). It has been shown that, for a class of granular materials for which one can apply Gassmann relations between macroscopic and microscopic (true) material parameters, Biot's model as a particular

case with $N = 0$ is thermodynamically admissible. Consequently we may describe a porous material either by a model with $N \neq 0$ and corresponding generalizations of Gassmann relations or by a model with $N = 0$ (Biot) with classical Gassmann relations.
We have also two other possibilities in which Biot's coupling between partial stresses described by the material parameter Q does not appear. Such a model has been introduced some ten years ago (see, e.g., [4], where both the model and some results for waves are presented) and its structure is similar to the so-called *simple mixtures* of fluids [2]. This model follows from Biot's model in which we substitute $Q = 0$ or from the full model with $Q = 0, N = 0$. The results are not the same because the simplified model does not admit simple tests yielding Gassmann relations. Consequently, we may use either classical Gassmann relations if we consider the simplified model to be a particular case of Biot's model or generalized Gassmann relations if we consider the simplified model to be a particular case of the full model.
Wave analysis within the simplified model is much simpler than within Biot's model or the full model. This concerns particularly surface waves. It is desirable to know whether such an analysis may describe—at least qualitatively—wave properties which would follow from more general models.
We compare numerical results for the above-mentioned four possibilities. It is demonstrated that both speeds of propagation of $P1$, S, and $P2$ waves and their attenuations differ qualitatively but not quantitatively for different models. For porosities appearing in applications to soils ($n_0 \sim 0.15 \div 0.4$), these numerical differences are smaller than 10 % (see figure below). Due to a rather poor accuracy of dynamical measurements in real soils, this discrepancy seems to be acceptable.

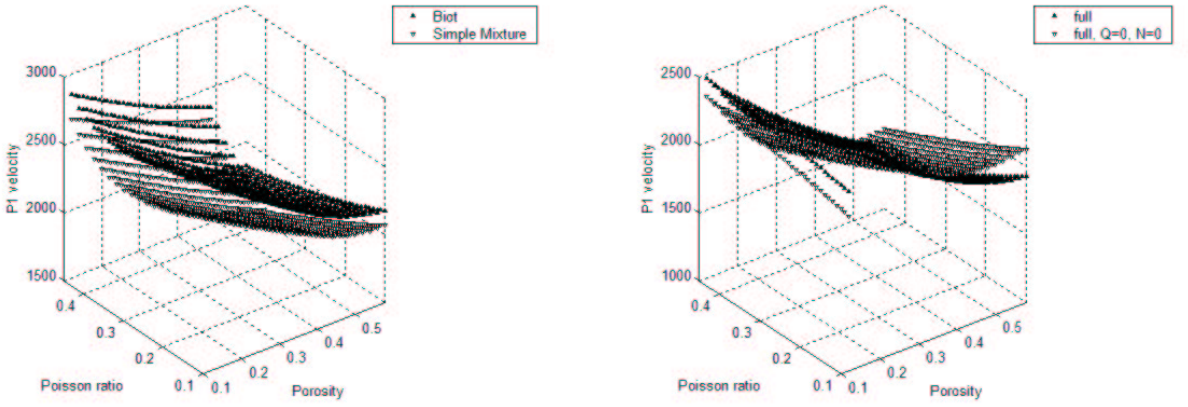

Fig. 1: Front velocity of the $P1$ wave for four different models

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Numerical analysis of surface waves on impermeable boundaries of a poroelastic medium

Collaborators: B. Albers, K. Wilmanski

Cooperation with: C. Lai (European Centre for Training and Research in Earthquake Engineering, Pavia, Italy), R. Lancellotta, S. Foti (Politecnico di Torino, Italy)

The project is the continuation of the theoretical research on surface waves on the basis of the model by Wilmanski [5]. Here, the dispersion relation for surface waves on an impermeable boundary of a fully saturated poroelastic medium is investigated numerically in the whole range of frequencies. To this aim the linear simplified model of a two-component poroelastic medium is used. Similarly to the classical Biot model, it is a continuum mechanical model but it is much simpler due to the lack of coupling of stresses. The general dispersion relation has been ascertained, and results of an earlier work [6] for the high and low frequency approximations have been recalled. The main part of the project concerns numerical aspects: first we indicate the applied numerical procedure and then we illustrate the numerical results for the normalized velocities and attenuations of the Rayleigh and Stoneley waves, [1, 2]. It is known that surface modes of propagation in linear models result from the combination of bulk modes. Physically, this means that at any point of the boundary classical longitudinal and shear waves combine into the Rayleigh wave which must be slower than both bulk waves. The presence of the second longitudinal bulk wave P2 yields the existence of the second surface mode—the Stoneley wave which should be slower than the P2 wave—the slowest of bulk waves. Both quantities, velocities and attenuations, are shown for different values of the bulk permeability coefficient π, in different ranges of frequencies. A decay of the Rayleigh wave velocity, mentioned in [3], has been confirmed in the range of small frequencies in spite of the lack of static coupling between components. Moreover, we compare the behavior of the two types of surface waves with the behavior of two bulk waves: P1 and P2.
Here, we only show a part of the project, namely the governing equations, the boundary conditions, and the numerical results for a chosen value of the permeability coefficient:

Model
Within the linear model of a two-component poroelastic saturated medium the process is described by the macroscopic fields $\rho^F(\mathbf{x},t)$ – partial mass density of the fluid, $\mathbf{v}^F(\mathbf{x},t)$ – velocity of the fluid, $\mathbf{v}^S(\mathbf{x},t)$ – velocity of the skeleton, $\mathbf{e}^S(\mathbf{x},t)$ – symmetric tensor of small deformations of the skeleton and the porosity n. These fields satisfy the following set of linear equations

$$
\begin{aligned}
&\frac{\partial \rho^F}{\partial t} + \rho_0^F \operatorname{div} \mathbf{v}^F = 0, \quad \left| \frac{\rho^F - \rho_0^F}{\rho_0^F} \right| \ll 1, \\
&\rho_0^F \frac{\partial \mathbf{v}^F}{\partial t} + \kappa \operatorname{grad} \rho^F + \beta \operatorname{grad}(n - n_E) + \hat{\mathbf{p}} = 0, \quad \hat{\mathbf{p}} := \pi \left(\mathbf{v}^F - \mathbf{v}^S \right), \\
&\rho_0^S \frac{\partial \mathbf{v}^S}{\partial t} - \operatorname{div} \left(\lambda^S \left(\operatorname{tr} \mathbf{e}^S \right) \mathbf{1} + 2\mu \mathbf{e}^S + \beta (n - n_E) \mathbf{1} \right) - \hat{\mathbf{p}} = 0, \\
&\frac{\partial \mathbf{e}^S}{\partial t} = \operatorname{sym} \operatorname{grad} \mathbf{v}^S, \quad \left\| \mathbf{e}^S \right\| \ll 1, \quad n_E := n_0 \left(1 + \delta \operatorname{tr} \mathbf{e}^S \right), \\
&\frac{\partial (n - n_E)}{\partial t} + \Phi \operatorname{div} \left(\mathbf{v}^F - \mathbf{v}^S \right) + \frac{n - n_E}{\tau} = 0, \quad \left| \frac{n - n_0}{n_0} \right| \ll 1.
\end{aligned}
$$

Here ρ_0^F, ρ_0^S, n_0 denote constant reference values of partial mass densities, and porosity, respectively, and $\kappa, \lambda^S, \mu^S, \beta, \pi, \tau, \delta, \Phi$ are constant material parameters. The first one describes the macroscopic compressibility of the fluid component, the next two are macroscopic elastic constants of the skeleton, β is the coupling constant, π is the coefficient of bulk permeability, τ is the relaxation time, and δ, Φ describe equilibrium and nonequilibrium changes of porosity, respectively. For the purpose of this work we assume $\beta = 0$.

Boundary conditions

In order to determine surface waves in a saturated poroelastic medium we need conditions for $z = 0$. In the general case of a boundary between a saturated porous material and a fluid the boundary conditions were formulated by Deresiewicz & Skalak. We quote them here in a slightly modified form and for an impermeable boundary

$$T_{13}|_{z=0} \equiv T_{13}^S\Big|_{z=0} = \mu^S \left(\frac{\partial u_1^S}{\partial z} + \frac{\partial u_3^S}{\partial x} \right)\Bigg|_{z=0} = 0, \quad \frac{\partial}{\partial t}\left(u_3^F - u_3^S \right)\Big|_{z=0} = 0,$$

$$T_{33}|_{z=0} \equiv (T_{33}^S - p^F)\Big|_{z=0} = c_{P1}^2 \rho_0^S \left(\frac{\partial u_1^S}{\partial x} + \frac{\partial u_3^S}{\partial z} \right) - 2c_S^2 \rho_0^S \frac{\partial u_1^S}{\partial x} - \kappa\left(\rho^F - \rho_0^F\right)\Big|_{z=0} = 0,$$

where u_1^S, u_3^S are x and z components of the displacement $\mathbf{u}^S$, respectively, and u_3^F the z component of the displacement $\mathbf{u}^F$.

Results for velocities and attenuations

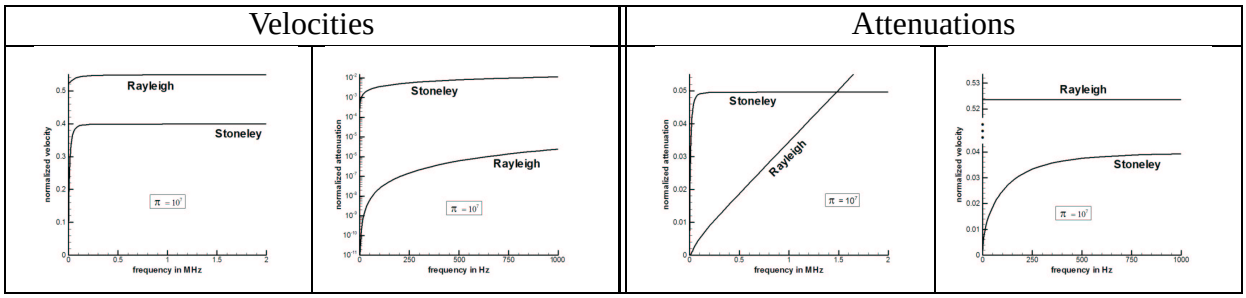

Fig. 1: Numerical results for normalized velocities and attenuations of Rayleigh and Stoneley waves, each for a small frequency range (left) and a large frequency range (right) for the permeability coefficient: $\pi = 10^7 \ \frac{\mathrm{kg}}{\mathrm{m^3 s}}$

Conclusions

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 approx. 4.7 % higher than the low frequency limit. The wave is always slower than the *S* wave. As a function of ω it possesses an inflection point and it is slightly nonmonotonous.
- This nonmonotonicity appears in the range of small frequencies. The velocity possesses in this range a minimum whose size is very small. Interestingly, the minimum value remains constant for the different values of π. This means that the decay is not driven by the diffusion. Such a behavior is also observed within Biot's model.
- The attenuation of this wave grows from zero for $\omega = 0$ to infinity as $\omega \to \infty$. In the range of large frequencies it is linear (a constant positive quality factor). This means that it is a leaky wave.

STONELEY

- The velocity of this wave grows monotonically from the zero value for $\omega = 0$ to a finite limit which is slightly smaller than the velocity 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 Stoneley wave approach zero as $\sqrt{\omega}$.
- The attenuation of the Stoneley wave grows monotonically to a finite limit for $\omega \to \infty$ (zero quality factor). It is slightly smaller than the attenuation of $P2$ waves. Consequently, in contrast to the claims in the literature, the Stoneley wave is attenuated.

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Phase transitions

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Cooperation with: W.H. Müller (Technische Universität Berlin), P. Colli, G. Gilardi (Università di Pavia, Italy), S. Eichler, G. Jurisch (Freiberger Compound Materials GmbH), T. Hauck (Motorola, München/Berlin), B. Niethammer (Humboldt-Universität zu Berlin)

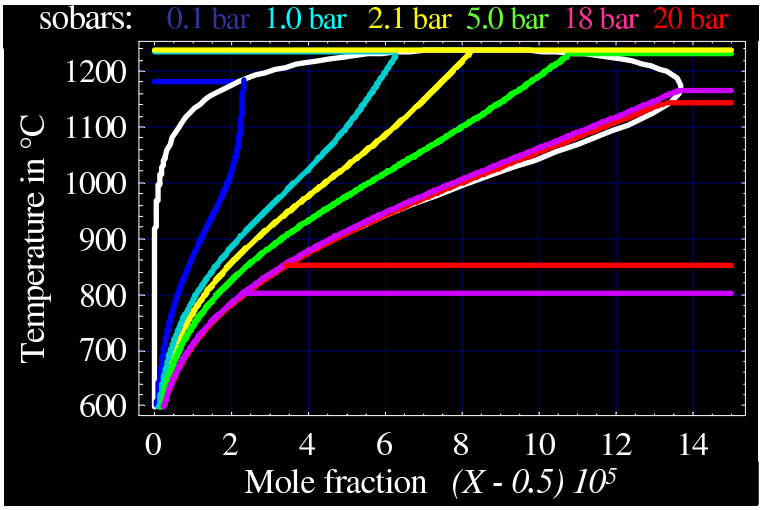
Supported by: BMBF: "Mathematische Modellierung und Simulation der Entstehung, des Wachstums und der Auflösung von Arsenausscheidungen in einkristallinem Galliumarsenid" (Mathematical modeling and simulation of the formation, growth and dissolution of arsenic precipitation in single crystal gallium arsenide)

1. Improvement of the existing phase model for morphological changes in solder materials A careful study of a sharp interface limit of the existing phase field model, that was used in the past to describe morphological changes in eutectic tin/lead alloys, exhibited that anisotropic surface energies can only be generated due to mechanical effects. This is one of the reasons that the diffusion flux was reformulated by W. Dreyer and B. Wagner. The resulting thermodynamically consistent form now reads

$$\begin{aligned} J_k \;=\; & -\frac{B_{ki}}{T}\frac{\partial}{\partial X_i}\Big(\frac{\partial \psi(c,\varepsilon_{rs})}{\partial c} - 2A_{jl}(c,\varepsilon_{rs})\frac{\partial^2 c}{\partial X_j \partial X_l} - \frac{\partial A_{jl}(c,\varepsilon_{rs})}{\partial c}\frac{\partial c}{\partial X_j}\frac{\partial c}{\partial X_l} \\ & -2\frac{\partial A_{jl}(c,\varepsilon_{rs})}{\partial \varepsilon_{mn}}\frac{\partial c}{\partial X_j}\frac{\partial \varepsilon_{mn}}{\partial X_l} - \frac{\partial^2 a_{jl}(c,\varepsilon_{rs})}{\partial \varepsilon_{mn}\partial \varepsilon_{op}}\frac{\partial \varepsilon_{op}}{\partial X_j}\frac{\partial \varepsilon_{mn}}{\partial X_l} - \frac{\partial a_{jl}(c,\varepsilon_{rs})}{\partial \varepsilon_{mn}}\frac{\partial^2 \varepsilon_{mn}}{\partial X_j \partial X_l}\Big). \end{aligned} \tag{1}$$

The variables are the (tin) concentration c and the strain ε_{rs}. B_{ki} gives the mobility tensor and T is the temperature. The functions $\psi(c,\varepsilon_{rs})$, $A_{jl}(c,\varepsilon_{rs})$, and $a_{jl}(c,\varepsilon_{rs})$ are explicitly known, see [3]. In the sharp interface limit of this model there results a surface tension that can be calculated from the gradient coefficients $A_{jl}(c,\varepsilon_{rs})$.
In the first numerical treatment of the resulting phase field equation, B. Wagner ignored the mechanical contributions and developed a non-stiff boundary integral formulation to efficiently simulate the long-time evolution of precipitates during coarsening.

2. Completion of the model for the chemistry and arsenic precipitation in semi-insulating GaAs The description of semi-insulating GaAs, which includes thermo-mechanical coupling, diffusion, interface motion, precipitation of arsenic droplets, and the determination of various thermodynamic equilibria, has been completed. The material parameters have been tested and make it possible to calculate the phase diagram of GaAs, which is in exact agreement with the experimental data.



The Figure shows a region of the phase diagram of GaAs, where the doping substances are distributed randomly over the three sublattices. Outside this region, precipitation of arsenic droplets sets in. The upper endpoints of the isobars are triple points, where solid, liquid, and gas phase are in equilibrium.
For an illustration of the involved field equations in non-equilibrium processes, we give, as an example, the diffusion equation, which describes the concentration field $y(t,r)$ of the interstitial arsenic in the vicinity of a spherical arsenic droplet.

$$\frac{\partial y}{\partial t} = D\left(\frac{\partial}{\partial r}\left(r^2\frac{\partial y}{\partial r}\right) + \frac{y(1-y)}{RT}\frac{180MGb^2}{\bar{\rho}_S r^8}\right) - \frac{D}{RT}\frac{\partial y(1-y)}{\partial r}\frac{36MGb^2}{\bar{\rho}_S r^7}. \tag{2}$$

Herein, D denotes the diffusion constant, R and T are the gas constant and the temperature, respectively, M is the molecular weight of the arsenic, G denotes the shear modulus, and $\bar{\rho}_S$ is the mass density of the solid. The quantity b measures the phenomenon that the liquid droplet needs more space than a solid of the same number of particles, leading to a multiaxial stress field in the vicinity of the droplet. Note that b depends implicitly on time via the evolving radius $r_I(t)$ of the droplet. More details can be found in [4].

3. Various initial- and boundary problems for interface motions are due to the Grinfeld instability, which is a phenomenon of growing interest. The Grinfeld instability states that a plane interface between a solid and its melt may become unstable if multiaxial stress fields appear in the solid. Surface tension and gravity provoke a stabilization of a plane interface. We found a further phenomenon in the competition of these effects. It is important whether the creation/annihilation of the melt decreases or increases the volume that is occupied by the two-phase mixture. This has the consequence that the stability of a plane interface depends on further conditions, which are:
(i) Do we consider an infinite system without mass conservation or a finite system with mass conservation?
(ii) Do we control the total volume or the total pressure of the considered system?
Our study of the Grinfeld instability relies on the solution of a quasistatic elastic problem for the stresses in the solid and the pressure in the melt. Both are used to calculate the interfacial normal speed w_ν, which is given by (see [1])

$$w_\nu = M_I(\mu_L - \mu_S + \frac{1}{\rho_S}\sigma^{<ij>}\nu^i\nu^j). \tag{3}$$

Here $M_I > 0$ denotes the interfacial mobility, μ_L and μ_S are chemical potentials of the melt and the solid, respectively, ρ_S is the mass density of the solid at the interface, $\sigma^{<ij>}$ denote the trace-free components of the stress tensor, and ν^i are the components of the interfacial normal. This equation becomes a nonlinear and nonlocal PDE determining the geometry of the interface, if the liquid pressure and the stress fields of the mechanical boundary value problem have been inserted. The main results can be found in [2].

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Stability of dewetting polymer films

Collaborator: B. Wagner

Cooperation with: A. Münch (Humboldt-Universität zu Berlin, since Nov. 2003 also Heisenberg Fellow at the WIAS), C. Neto, K. Jacobs (Universität des Saarlandes, Saarbrücken), R. Seemann (Universität Ulm)

Dewetting of thin liquid films has attracted considerable attention due to its importance for technological applications and because it is a macroscopically observable process that is driven and influenced by the microscopic physics. Hereby, the focus has shifted from considering the stationary patterns that result from the dewetting to understanding the dynamical processes that lead to these states. This has introduced slippage as a relevant influence on the patterns that evolve ([3], [4], [5]); in particular, the appearance of finger instabilities at dewetting fronts has been associated with the possibility of even relatively short chain polymer films to slip on the substrate. Theoretical progress here depends strongly on the ability to develop, analyze, and solve lubrication-type models for the film dynamics, thereby addressing the presence of highly separated scales (in space as well as in time) and the fourth order of the involved partial differential equations. To this end, 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, [1].
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, [2]. Additional computations that solve the lubrication model for the full three-dimensional flow confirm that these findings carry over into the nonlinear regime and are in good agreement with the experimental findings by C. Neto, K. Jacobs, and R. Seemann.
We are currently using 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.

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Kinetic schemes for selected initial and boundary value problems

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Cooperation with: G. Warnecke, M. Kunik (Otto-von-Guericke-Universität Magdeburg)

Supported by: DFG: Priority Program "Analysis und Numerik von Erhaltungsgleichungen" (ANumE — Analysis and numerics for conservation laws)

Within the DFG Priority Program "Analysis and numerics of conservation laws" we have developed and exploited a kinetic approach to solve initial and boundary value problems for some selected class of hyperbolic conservation laws. In this class there are hyperbolic conservation laws that have an underlying kinetic equation. In particular we have studied (i) the nonrelativistic Euler equations for gases, (ii) the hyperbolic system for heat conduction at low temperatures, (iii) the relativistic Euler equations with a special focus on the ultra-relativistic case. The kinetic approach relies on the *Maximum Entropy Principle* (MEP) and its strategy is as follows: The variables of the hyperbolic system are represented by so-called moment integrals of a corresponding phase density, which solves the underlying kinetic equation. The temporal evolution of the variables is decomposed into periods of free flight and update times. During the periods of free flight, the particles of the kinetic regime evolve according to a collision-free kinetic equation. At the update times we restart a new free flight period by maximizing the entropy of the particles.
Within the final period of the DFG Priority Program we have mainly compared the MEP method with the conventional kinetic flux-splitting schemes. We considered first-order accurate schemes as well as second-order schemes. Kinetic flux-splitting schemes also rely on the moment representation of the variables of the hyperbolic system. Here the moment integrals are decomposed into two parts with particles moving in positive and negative direction, respectively. The whole space which the particles have at their disposal is decomposed into small cells and the objective is to calculate all fluxes across the cell boundaries. In 1D the scheme is as follows: The conservation laws have the form

$$\frac{\partial \mathbf{W}}{\partial t} + \sum_{i=1}^{d} \frac{\partial F^i(\mathbf{W})}{\partial x^i} = 0\,,$$

where $\mathbf{W}$ is the vector of conserved variables and F^i are their corresponding fluxes, along each direction (d is the number of spatial dimensions).
In the one-dimensional case we decompose the x-axis into cells $I_i = \left[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}\right]$ and study the following semi-discrete kinetic upwind scheme

$$\frac{dW_i}{dt} = -\frac{F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}}}{\Delta x}.$$

Thus a first-order scheme which is fully discrete in space and time is given by

$$W_i^{n+1} = W_i^n - \lambda \frac{F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}}}{\Delta x},$$

where $\lambda = \frac{\Delta t}{\Delta x}$, $F_{i+\frac{1}{2}}$ is the fluxes at the cell boundary $x_{i+\frac{1}{2}}$. Here W_i^n are the piecewise constant cell average values of the conserved variables at time t^n, and Δx represents the cell width.

This scheme is only first-order accurate in space. To get high-order accuracy, the initial reconstruction strategy must be applied to interpolate the cell-averaged variables W_i^n.

For example,

$$W(t^n,x) = W_i^n + W_i^{n,x}\frac{(x-x_i)}{\Delta x}$$

can be constructed to approximate the cell-averaged variables W_i^n at the beginning of each time step t^n, where $W_i^{n,x}$ is an approximate slope. The extreme points $x=0$ and $x=\Delta x$ in local coordinates correspond to the intercell boundaries in general coordinates $x_{i-\frac{1}{2}}$ and $x_{i+\frac{1}{2}}$, respectively. The values W_i at the extreme points are

$$W_i^{n,L} = W_i^n - \frac{1}{2}W_i^{n,x}, \quad W_i^{n,R} = W_i^n + \frac{1}{2}W_i^{n,x}. \tag{1}$$

To avoid oscillations in the reconstructed data, the slope $W_i^{n,x}$ is obtained from the min-mod limiter as follows

$$W_i^x = MM\left(\theta\Delta W_{i+\frac{1}{2}}, \frac{\theta}{2}(\Delta W_{i-\frac{1}{2}} + \Delta W_{i+\frac{1}{2}}), \theta\Delta W_{i-\frac{1}{2}}\right).$$

Here, Δ denotes the central differencing, $\Delta W_{i+\frac{1}{2}} = W_{i+1} - W_i$, and MM denotes the min-mod nonlinear limiter

$$MM\{x_1,x_2,...\} = \begin{cases} \min_i\{x_i\} & \text{if } x_i > 0 \quad \forall i, \\ \max_i\{x_i\} & \text{if } x_i < 0 \quad \forall i, \\ 0 & \text{otherwise}. \end{cases}, \tag{2}$$

where $1 \le \theta \le 2$ is a parameter. Based on the above reconstruction, a high spatial resolution kinetic solver becomes

$$\frac{dW_i}{dt} = -\frac{F_{i+\frac{1}{2}}(W_{i+1}^L, W_i^R) - F_{i-\frac{1}{2}}(W_i^L, W_{i-1}^R)}{\Delta x}, \tag{3}$$

where W^l, W^R are given by (1).
To improve the temporal accuracy, we use a second-order TVD Runge-Kutta scheme to solve (3). Denoting the right-hand side of (3) as $L(W)$, a second-order TVD Runge-Kutta scheme updates W through the following two stages:

$$W^{(1)} = W^n + \Delta t L(W^n), \tag{4}$$

$$W^{n+1} = \frac{1}{2}\left(W^n + W^{(1)} + \Delta L(W^{(1)})\right). \tag{5}$$

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4.8 Projects interconnecting research groups

Quasilinear nonsmooth evolution systems in L^p-spaces on three-dimensional domains

Collaborators: J. Elschner (FG 4), J. Rehberg (FG 1), G. Schmidt (FG 4)

Cooperation with: V. Maz'ya (Linköping University, Sweden)

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. and 2002 p. 39 et sqq.). In particular, we are interested in quasilinear systems of the form

$$u_k' - \nabla \cdot (\mu_k J_k(\mathbf{u}) \nabla u_k) = R_k(\mathbf{u}, \nabla \mathbf{u}) \, , \, \mathbf{u}(T_0) = \mathbf{u}_0 \, ; \, \mathbf{u} = (u_1, \ldots, u_m) \tag{1}$$

which comprise—among others—reaction-diffusion systems and heat conduction, see [1] or [4] and the references cited therein. The focus is on the case of spatially three-dimensional nonsmooth domains and discontinuous coefficients μ_k, which occur in modeling heterogeneous media. Over the past years various tools for the study of such equations have been developed at the Weierstrass Institute, see [13, 14, 15, 19]. In particular, the result of Gröger [15] is of great use in many applications, see [2, 4, 7, 11, 18] to name only a few. Gröger's result states that

$$\nabla \cdot \mu \nabla : H^{1,q}_\Gamma(\Omega) \mapsto (H^{1,q'}_\Gamma(\Omega))' \tag{2}$$

is a topological isomorphism for $q \in]2, q_0[$ in case of Lipschitz domains, (elliptic) L^∞ coefficient functions, and mixed boundary conditions. Unfortunately, it is well known that in general q_0 exceeds 2 only slightly. Thus, in view of embedding theorems generically only the case of two space dimensions is covered. However, for many applications it is not sufficient to study only equations in two space dimensions, that means physical systems which are—in one space direction—translational or circular invariant, see, e.g., [2] or [9]. The increasing structural complexity of technical devices requires to perform simulations and the corresponding mathematical analysis on three-dimensional domains, see [10, 16].
In our recent paper [22] we study the Dirichlet problem for (1) with piecewise constant coefficients μ_k in a polyhedral domain $\Omega \subset \mathbb{R}^3$. We give conditions under which the problem admits a unique solution from a space

$$C([T_0, T], L^p(\Omega; \mathbb{R}^m)) \cap C^1((T_0, T], L^p(\Omega; \mathbb{R}^m)).$$

The Dirichlet boundary data may depend on time, and Ω is a Lipschitz polyhedron, that means Ω is a bounded Lipschitz domain with piecewise plane boundary. Furthermore, we assume that Ω is the union of a finite number of Lipschitz polyhedra Ω_1, …, Ω_l such that the (3×3) matrix functions μ_k are constant on these subdomains. The dependence of the functions R_k on $\nabla \mathbf{u}$ is not stronger than quadratic. The main advantage of our approach in comparison to the concept of weak solutions is the strong differentiability of the solution with respect to time and that the divergence of the corresponding currents $j_k = \mu_k J_k(t, \mathbf{u}) \nabla u_k$ are functions, not only distributions. In a strict sense, only this justifies the application of Gauss' theorem to calculate the normal components of the currents over boundaries of (suitable) subdomains. Our main result, [22, Theorem 6.10], ensures the continuity of the normal fluxes across interfaces. This property is also very important in the numerical analysis of finite volume methods for heterostructures.

The local existence result for (1) rests upon the classical theorem of Sobolevskii on abstract quasilinear parabolic equations in Banach spaces and estimates for elliptic transmission problems. The problem is to find an adequate function space with respect to which the hypotheses of Sobolevskii's theorem can be verified. In the three-dimensional case one has to ensure that the linear operators in (2) are topological isomorphisms for some $q > 3$, if the matrices $\mu = \mu_k$ in (1) are piecewise constant. The operator (2) corresponds to an interface (or transmission) problem for the Laplacian, with different anisotropic materials given on the polyhedral subdomains Ω_1, …, Ω_l of Ω, with Dirichlet conditions given on $\partial\Omega$.

In contrast to the pure Laplacian on a Lipschitz domain, see [17, Theorem 0.5], the gradients of solutions to the transmission problems only belong to $L^{2+\varepsilon}$ for some $\varepsilon > 0$. In the vicinity of vertices and edges, ε may be arbitrarily small, even for polygonal interface problems with only four isotropic materials meeting in a vertex, see [20]. In the case of complex material coefficients, which corresponds to some special anisotropy, even two materials can produce strong singularities near vertices (see [5, 6], where similar problems are studied for Helmholtz equations). Therefore, a large part of our investigation, [22], is devoted to the optimal regularity for (2). This result inherently applies to elliptic systems describing heterostructures on three-dimensional domains.

It is well known that the singularities of solutions to elliptic boundary value problems near vertices and edges can be characterized in terms of the eigenvalues of certain polynomial operator pencils on domains of the unit sphere or the unit circle. We refer to [21] for the case of the Dirichlet and Neumann problem and to [12] for the polyhedral Laplace interface problem with two isotropic materials. The corresponding analysis for several anisotropic materials has not been performed so far and is the subject of our investigation in [22].

To avoid the cumbersome analysis of optimal regularity near vertices, see [3], we use the somewhat surprising fact that if the solution of the interface problem belongs to L^q for some $q > 3$ near each interior point of the interface and boundary edges, then the operator (2) is an isomorphism. Thus, the regularity result for (2) can be reduced to that for an interface problem on dihedral angles with one common edge. The proof relies essentially on sharp pointwise estimates of Green's function, which we perform in [22].

The main result of our linear regularity theory is that the operator (2) is an isomorphism for some $q > 3$ provided that a parameter $\widehat{\lambda}_\Omega$, which depends on the decomposition of Ω into the subdomains Ω_j, satisfies the inequality

$$\widehat{\lambda}_\Omega > \frac{1}{3}\,. \tag{3}$$

This number is the minimum over all edges of spectral parameters, which can be expressed in terms of the eigenvalues of certain transmission problems on the unit circle. These problems are obtained applying the partial Fourier transform along an edge and the Mellin transform with respect to the radial direction. The regularity result is sufficient for the treatment of the quadratic gradient terms in (1), if the Banach space is the space L^p with $p = q/2$. However, condition (3) imposes a rather strong assumption on the geometry of the subdomains Ω_j and the coefficient μ_k, or equivalently, on the eigenvalues of certain pencils of ordinary differential operators. These conditions can be checked for many heterostructures of practical interest. Though at this point our results are restricted to Dirichlet boundary conditions, it should be possible to extend the result to mixed boundary conditions, which occur, e.g., in modeling semiconductor devices ([8]). This problem will be investigated in 2004.

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Micro-macro transitions in the atomic chain

Collaborators: W. Dreyer (FG 7), M. Herrmann (FG 7), J. Sprekels (FG 1)

Cooperation with: A. Mielke (Universität Stuttgart)

Supported by: DFG: Priority Program "Analysis, Modellbildung und Simulation von Mehrskalenproblemen" (Analysis, modelling and simulation of multiscale problems)

During the period of this report, we have studied micro-macro transitions for the (nonlinear) atomic chain in the context of modulation theory. We have focused on the following problems.

1. We apply the ideas of classic modulation theory to the nonlinear atomic chain.
2. We study the thermodynamic properties of the resulting modulation equations including an equation of state and a corresponding Gibbs equation.
3. We consider special atomic interaction potentials and derive the corresponding modulation equations.

In this project we closely collaborate with the group of A. Mielke, University of Stuttgart.

The atomic chain consists of N identical particles, labeled by $\alpha = 1..N$, which are located at their positions $x_\alpha(t)$. The dynamics of the chain is described by Newton's equation

$$\ddot{x}_\alpha(t) = \Phi'\Big(x_{\alpha+1}(t) - x_\alpha(t)\Big) - \Phi'\Big(x_\alpha(t) - x_{\alpha-1}(t)\Big), \tag{1}$$

where Φ denotes a convex interaction potential. In order to pass to the thermodynamic limit $N \to \infty$, we introduce a *scaling* parameter $\varepsilon = 1/N$ and we define the *macroscopic* time $\bar{t}$ and particle index $\overline{\alpha}$ by

$$\bar{t} = \varepsilon t, \quad \overline{\alpha} = \varepsilon\alpha. \tag{2}$$

In contrast to the macroscopic variables, we interpret t and α as the *microscopic* time and particle index, respectively.
The general strategy of modulation theory is as follows:

1. We identify a family of special solutions of (1), which are parametrized by a finite number of parameters. In the case at hand, the special solutions are *traveling waves*.
2. We modulate the parameters on the macroscopic scale, so that there result at least approximate solutions of (1). There exist modulation restrictions in form of macroscopic PDEs.

A traveling wave for the atomic chain has parameters r, v, k, ω and can be written as

$$x_\alpha(t) = r\alpha + vt + \mathbb{X}(k\alpha + \omega t), \tag{3}$$

Here, $\mathbb{X}(\varphi)$ is the 1-periodic wave profile, which describes the microscopic oscillations. Since the wave profile depends on r, v, k, and ω, we write $\mathbb{X}(r, v, k, \omega; \varphi)$.

A *modulated traveling wave* results, if we allow variations of the traveling wave parameters on the macroscopic scale. More precisely, we set

$$x_\alpha(t) = \frac{1}{\varepsilon}X(\varepsilon t, \varepsilon\alpha) + \tilde{\mathbb{X}}(\varepsilon t, \varepsilon\alpha; \frac{1}{\varepsilon}\Theta(\varepsilon t, \varepsilon\alpha;)), \tag{4}$$

$$\tilde{\mathbb{X}}(\varepsilon t, \varepsilon\alpha\varphi) = \mathbb{X}(r(\varepsilon t, \varepsilon\alpha), v(\varepsilon t, \varepsilon\alpha), k(\varepsilon t, \varepsilon\alpha), \omega(\varepsilon t, \varepsilon\alpha)), \tag{5}$$

where

$$v = \frac{\partial X}{\partial \bar{t}}, \quad r = \frac{\partial X}{\partial \bar{\alpha}}, \quad \omega = \frac{\partial \Theta}{\partial \bar{t}}, \quad \text{and} \quad k = \frac{\partial \Theta}{\partial \bar{\alpha}}. \tag{6}$$

The modulation equations govern the macroscopic evolution of the fields r, v, k, and ω and ensure that the ansatz (4) provides approximate solutions satisfying (1) up to order $O(\varepsilon^2)$. The modulation equations read

$$\frac{\partial}{\partial \bar{t}}\begin{pmatrix} r \\ v \\ k \\ S \end{pmatrix} + \frac{\partial}{\partial \bar{t}}\begin{pmatrix} -v \\ +p \\ -\omega \\ +g \end{pmatrix} = 0. \tag{7}$$

There is an immediate physical interpretation of all quantities: r – specific length, v – mean velocity, p – pressure, k – wave number, ω – frequency, S – specific entropy density, g – entropy flux. Consequently, the four equations in (7) are the *macroscopic conservation laws* for mass, momentum, wave number, and entropy. The system is closed by means of a Gibbs equation

$$\mathrm{d}E = v\,\mathrm{d}v + \omega\,\mathrm{d}S - p\,\mathrm{d}r - g\,\mathrm{d}k. \tag{8}$$

Here, E abbreviates the specific total energy, which is given by an equation of state $E = E(r, v, k, \omega)$. Unfortunately, the equation of state is given only implicitly, and thus a complete understanding of the modulation equations needs more insight into the structure of traveling waves. However, there exist some special atomic interaction potentials Φ, for which the equation of state can be calculated explicitly:

1. the harmonic potential;
2. the case of hard sphere collisions;
3. a model of elastic collision that combines the cases 1 and 2;
4. the limit of small amplitudes.

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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 über 60 000 Bände (Bücher, Preprints und Reports) und ungefähr 90 abonnierte Zeitschriften (40 auch als elektronische Zeitschriften). Den wissenschaftlichen Zielen und den aktuellen Projekten des Instituts wird dabei 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, which encompasses more than 60,000 volumes (books, preprints, and reports), and approximately 90 current journals (subscriptions, 40 also as e-journals), also takes into account neighboring areas of science and engineering, according to the scientific objects and actual projects of the institute:

- 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 zehn Jahren erworben wurde. Zur Vorbereitung der elektronischen Ausleihe und der elektronischen Nutzerkonten werden die älteren Teile des Bestandes schrittweise hinzugefügt. 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.

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 ten years, approximately. For preparing electronic lending, including the electonic administration of reader accounts, the elder parts of the stock are added step by step. 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.

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.

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 2003 / Statistical information about the year 2003

Erwerbungen:
126 Bücher
142 gebundene Zeitschriftenbände
786 Preprints und Reports
51 Loseblattsammlungen

Acquisitions:
126 books
142 bound volumes of journals
786 preprints and reports
51 loose-leaf collections

Entleihungen und Verlängerungen aus der WIAS-Bibliothek:
8663 Bücher

Lent and renewed from the WIAS library:
8663 books

Aus anderen Bibliotheken beschaffte Literatur:
829 Bücher
421 Artikel

Literature provided from other libraries:
829 books
421 articles

Übergabe an das Erwin-Schrödinger-Zentrum der Humboldt-Universität:
30 Jahrgänge des Journal of Algebra
25 Jahrgänge des Journal of Number Theory

Transfer to the Erwin Schrödinger Center of the Humboldt University:
30 annual volumes of Journal of Algebra
25 annual volumes of Journal of Number Theory

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/publications/. 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/publications/. 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-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 (HyperWave, WWW, FTP).

Folgende Projekte bestimmten die Entwicklung der Rechentechnik des WIAS im Jahr 2003:

1. Corporate Network

Einige Institute des FVB haben ein gemeinsames Datensicherungskonzept entwickelt. Dieses erhöht die Sicherheit der Datenbestände durch deren Sicherung an einem entfernten Standort. Dazu wird das Corporate Network genutzt. Dieses Konzept wurde in den vollen Routinebetrieb übernommen und hat sich seither voll bewährt.

2. LAN

Mit der Erweiterung des LAN wurde begonnen. Es wird das Backbone auf Gigabit-Ethernet umgestellt. Außerdem werden die Anschlussmöglichkeiten für Computer in den Arbeitsräumen wesentlich 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 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 (HyperWave, WWW, FTP).

The following projects have determined the development of the Computer Department in the year 2003:

1. Corporate Network

Some institutes of Forschungsverbund Berlin e.V. (FVB) have developed a common data protection concept. The Corporate Network is used to increase the security of the stored data by backing them up at a remote place. The concept was realized and taken into routine use. Since then it has proved its worth.

2. LAN

We started to extend the LAN. We changed the backbone to gigabit ethernet. The number of connectors for computers in the offices is essentially increased.

3. Computeserver

Die Beschaffung des neuen Computeservers HP GS1280 mit acht Prozessoren und 32 GB Hauptspeicher wurde realisiert. Er wurde in den Routinebetrieb übernommen und von den Nutzern sehr gut angenommen. Dadurch hat sich die Computeserverkapazität des WIAS wesentlich erweitert.

4. Fileserver

Der Fileserver wurde durch ein HP DS25-Cluster sowie ein HP Enterprise Virtual Array mit einer Kapazität von ca. 2 TByte ersetzt. Dadurch wurde die Leistungsfähigkeit des zentralen Datenspeichers wesentlich erweitert.

3. Compute server

The new compute server HP GS1280 with eight processors and 32 GB main memory was installed. It operates to the complete satisfaction of the users. Thereby, the compute capacity of WIAS was substantially increased.

4. File server

The file server was replaced by a cluster of HP DS25 computers and an HP Enterprise Virtual Array with a capacity of about 2 TByte, considerably increasing the power of the file server.

6 Publications, Scientific Life[1]

6.1 Publications

6.1.1 Monographs

E. BÄNSCH, ed., *Challenges in Scientific Computing — CISC 2002*, vol. 35 of Lecture Notes in Computational Science and Engineering, Springer, Berlin [u. a.], 2003.

V. BARBU, I. LASIECKA, D. TIBA, C. VARSAN, eds., *Analysis and Optimization of Differential Systems, IFIP TC7/WG7.2 International Working Conference on Analysis and Optimization of Differential Systems, September 10–14, 2002, Constanta, Romania*, Kluwer Academic Publishers, Boston, 2003.

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G. SCHMIDT, *Electromagnetic scattering by periodic structures (in Russian)*, in: Proceedings of the International Conference on Differential and Functional Differential Equations, Moscow, Russia, August 11–17, 2002, vol. 3 of Sovrem. Probl. Mat. Fund. Naprav., 2003, pp. 113–128.

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J. SPREKELS, D. TIBA, *Optimization of differential systems with hysteresis*, in: Analysis and Optimization of Differential Systems, IFIP TC7/WG7.2 International Working Conference on Analysis and Optimization of Differential Systems, September 10–14, 2002, Constanta, Romania, V. Barbu, I. Lasiecka, D. Tiba, C. Varsan, eds., Kluwer Academic Publishers, Boston, 2003, pp. 387–398.

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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.].

W. DREYER, F. DUDERSTADT, *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.].

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H.J. MUCHA, H.G. BARTEL, *ClusCorr98 – Adaptive clustering, multivariate visualization, and validation of results*, in: Proceedings of the 27th Annual Conference of the GfKl, Springer.

6.2 Preprints, Reports

6.2.1 WIAS Preprints Series

Preprints 2003[2] [3]

P. GWIAZDA, A. SWIERCZEWSKA, *An L^1-stability and uniqueness result for balance laws with multifunctions: A model from the theory of granular media*, Preprint no. 815, WIAS, Berlin, 2003.

P. GWIAZDA, A. ZATORSKA-GOLDSTEIN, *An existence result for the Leray-Lions type operators with discontinuous coefficients*, Preprint no. 811, WIAS, Berlin, 2003.

Y.I. INGSTER, I.A. SUSLINA, *Minimax nonparametric hypothesis testing for small type I errors*, Preprint no. 867, WIAS, Berlin, 2003.

P.-Y. LOUIS, *Convergence towards equilibrium of Probabilistic Cellular Automata*, Preprint no. 823, WIAS, Berlin, 2003.

A. SHILNIKOV, L. SHILNIKOV, D. TURAEV, *On some mathematical topics in classic synchronization*, Preprint no. 892, WIAS, Berlin, 2003.

H. ZÄHLE, *Heat equation with strongly inhomogeneous noise*, Preprint no. 824, WIAS, Berlin, 2003.

B. ALBERS, *Surface waves in two-component poroelastic media on impermeable boundaries – numerical analysis in the whole frequency domain*, Preprint no. 862, WIAS, Berlin, 2003.

B. ALBERS, K. WILMANSKI, *On modeling acoustic waves in saturated poroelastic media*, Preprint no. 874, WIAS, Berlin, 2003.

E. BÄNSCH, F. HAUSSER, O. LAKKIS, B. LI, *Element method for epitaxial growth with attachment-detachment kinetics*, Preprint no. 848, WIAS, Berlin, 2003.

E. BÄNSCH, F. HAUSSER, A. VOIGT, *Finite element method for epitaxial growth with thermodynamic boundary conditions*, Preprint no. 873, WIAS, Berlin, 2003.

E. BÄNSCH, P. MORIN, R.H. NOCHETTO, *Finite element methods for surface diffusion*, Preprint no. 805, WIAS, Berlin, 2003.

E. BÄNSCH, D. DAVIS, H. LANGMACH, G. REINHARDT, M. UHLE, *Two- and three-dimensional transient melt-flow simulation in vapour-pressure-controlled Czochralski crystal growth*, Preprint no. 852, WIAS, Berlin, 2003.

M. BARO, H.-CHR. KAISER, H. NEIDHARDT, J. REHBERG, *A quantum transmitting Schrödinger-Poisson system*, Preprint no. 814, WIAS, Berlin, 2003.

[2] http://www.wias-berlin.de/publications/preprints/index-2003.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.

M. BIRKNER, *A condition for weak disorder for directed polymers in random environment*, Preprint no. 891, WIAS, Berlin, 2003.

E. BAAKE, M. BAAKE, A. BOVIER, M. KLEIN, *An asymptotic maximum principle for essentially linear evolution models*, Preprint no. 886, WIAS, Berlin, 2003.

A. BOVIER, I. KURKOVA, *Derrida's Generalized Random Energy models 4: Continuous state branching and coalescents*, Preprint no. 854, WIAS, Berlin, 2003.

A. BOVIER, I. MEROLA, E. PRESUTTI, M. ZAHRADNÍK, *On the Gibbs phase rule in the Pirogov-Sinai regime*, Preprint no. 844, WIAS, Berlin, 2003.

A. BOVIER, C. KÜLSKE, *Coarse-graining techniques for (random) Kac models*, Preprint no. 894, WIAS, Berlin, 2003.

G. BRUCKNER, J. ELSCHNER, *The numerical solution of an inverse periodic transmission problem*, Preprint no. 888, WIAS, Berlin, 2003.

G.B. AROUS, J. CERNY, T. MOUNTFORD, *Aging in two-dimensional Bouchaud's model*, Preprint no. 887, WIAS, Berlin, 2003.

A. DEMIRCAN, U. BANDELOW, *Supercontinuum generation by the modelation instability*, Preprint no. 881, WIAS, Berlin, 2003.

N. SEEHAFER, A. DEMIRCAN, *Dynamo action in cellular convection*, Preprint no. 851, WIAS, Berlin, 2003.

W. DREYER, *On jump conditions at phase boundaries for ordered and disordered phases*, Preprint no. 869, WIAS, Berlin, 2003.

W. DREYER, F. DUDERSTADT, *Towards thermodynamic modeling of nucleation and growth of droplets in crystals*, Preprint no. 837, WIAS, Berlin, 2003.

W. DREYER, F. DUDERSTADT, S. EICHLER, M. JURISCH, *Stress analysis and bending tests for GaAs wafer*, Preprint no. 897, WIAS, Berlin, 2003.

W. DREYER, M. HERRMANN, M. KUNIK, S. QAMAR, *Kinetic schemes of selected initial and boundary value problems*, Preprint no. 880, WIAS, Berlin, 2003.

W. DREYER, S. QAMAR, *Kinetic flux-vector splitting schemes for the hyperbolic heat conduction*, Preprint no. 861, WIAS, Berlin, 2003.

——, *Second order accurate explicit finite volume schemes for the solution of Boltzmann-Peierls equation*, Preprint no. 860, WIAS, Berlin, 2003.

W. DREYER, B. WAGNER, *Sharp-interface model for eutectic alloys. Part I: Concentration dependent surface tension*, Preprint no. 885, WIAS, Berlin, 2003.

J. ELSCHNER, V. MAZ'YA, J. REHBERG, G. SCHMIDT, *Solutions for quasilinear nonsmooth evolution systems in L^p*, Preprint no. 827, WIAS, Berlin, 2003.

K. FLEISCHMANN, V.A. VATUTIN, *Multi-scale clustering for a non-Markovian spatial branching process*, Preprint no. 889, WIAS, Berlin, 2003.

K. FLEISCHMANN, J. XIONG, *Snake representation of a super-Brownian reactant in the catalytic region*, Preprint no. 847, WIAS, Berlin, 2003.

A.M. ETHERIDGE, K. FLEISCHMANN, *Compact interface property for symbiotic branching*, Preprint no. 822, WIAS, Berlin, 2003.

K. FLEISCHMANN, A. STURM, *A super-stable motion with infinite mean branching*, Preprint no. 821, WIAS, Berlin, 2003.

D.A. DAWSON, K. FLEISCHMANN, J. XIONG, *Strong uniqueness for cyclically symbiotic branching diffusions*, Preprint no. 853, WIAS, Berlin, 2003.

H. GAJEWSKI, I.V. SKRYPNIK, *On unique solvability of nonlocal drift-diffusion type problems*, Preprint no. 810, WIAS, Berlin, 2003.

N. BERGLUND, B. GENTZ, *On the noise-induced passage through an unstable periodic orbit I: Two-level model*, Preprint no. 864, WIAS, Berlin, 2003.

A. GLITZKY, *Electro-reaction-diffusion systems with nonlocal constraints*, Preprint no. 840, WIAS, Berlin, 2003.

A. GLITZKY, R. HÜNLICH, *Stationary solutions of two-dimensional heterogeneous energy models with multiple species*, Preprint no. 896, WIAS, Berlin, 2003.

F. GRUND, *Solution of linear systems with sparse matrices*, Preprint no. 816, WIAS, Berlin, 2003.

R. HENRION, *Perturbation analysis of chance-constrained programs under variation of all constraint data*, Preprint no. 804, WIAS, Berlin, 2003.

D. HÖMBERG, W. WEISS, *PID-control of laser surface hardening of steel*, Preprint no. 876, WIAS, Berlin, 2003.

A. HUTT, M. BESTEHORN, T. WENNEKERS, *Pattern formation in intracortical neuronal fields*, Preprint no. 825, WIAS, Berlin, 2003.

A. HUTT, A. DAFFERTSHOFER, U. STEINMETZ, *Detection of mutual phase synchronization in multivariate signals and application to phase ensembles and chaotic data*, Preprint no. 843, WIAS, Berlin, 2003.

F.M. ATAY, A. HUTT, *Stability and bifurcations in neural fields with axonal delay and general connectivity*, Preprint no. 857, WIAS, Berlin, 2003.

H.-CHR. KAISER, H. NEIDHARDT, J. REHBERG, *Convexity of trace functionals and Schrödinger operators*, Preprint no. 835, WIAS, Berlin, 2003.

O. KLEIN, P. PHILIP, *Transient conductive-radiative heat transfer: Discrete existence and uniqueness for a finite volume scheme*, Preprint no. 871, WIAS, Berlin, 2003.

A. KOLODKO, K.K. SABELFELD, *Stochastic particle methods for Smoluchowski coagulation equation: Variance reduction and error estimations*, Preprint no. 842, WIAS, Berlin, 2003.

A. KOLODKO, J. SCHOENMAKERS, *An efficient dual Monte Carlo upper bound for Bermudan style derivatives*, Preprint no. 877, WIAS, Berlin, 2003.

D. KOLYUKHIN, K.K. SABELFELD, *Stochastic Eulerian model for the flow simulation in porous media*, Preprint no. 836, WIAS, Berlin, 2003.

O. HÄGGSTRÖM, C. KÜLSKE, *Gibbs properties of the fuzzy potts model on trees and in mean fields*, Preprint no. 878, WIAS, Berlin, 2003.

G.N. MILSTEIN, M.V. TRETYAKOV, *Approximation of Wiener integrals with respect to the Brownian bridge by simulation of SDEs*, Preprint no. 855, WIAS, Berlin, 2003.

——, *Numerical analysis of Monte Carlo finite difference evaluation of Greeks*, Preprint no. 808, WIAS, Berlin, 2003.

R. KHASMINSKII, G.N. MILSTEIN, *Stability of gyroscopic systems under small random excitations*, Preprint no. 883, WIAS, Berlin, 2003.

G.N. MILSTEIN, O. REISS, J. SCHOENMAKERS, *Monte Carlo methods for pricing and hedging American options*, Preprint no. 850, WIAS, Berlin, 2003.

C. MEYER, P. PHILIP, *Optimizing the temperature profile during sublimation growth of SiC single crystals: Control of heating power, frequency, and coil position*, Preprint no. 895, WIAS, Berlin, 2003.

J. POLZEHL, V. SPOKOINY, *Varying coefficient regression modeling by adaptive weights smoothing*, Preprint no. 818, WIAS, Berlin, 2003.

S. QAMAR, *High order central schemes applied to relativistic multicomponent flows*, Preprint no. 875, WIAS, Berlin, 2003.

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*, Preprint no. 866, WIAS, Berlin, 2003.

H.-J. WÜNSCHE, M. RADZIUNAS, S. BAUER, O. BROX, B. SARTORIUS, *Simulation of phase-controlled mode-beating lasers*, Preprint no. 809, WIAS, Berlin, 2003.

N.N. NEFEDOV, M. RADZIUNAS, K.R. SCHNEIDER, *Analytic-numerical investigation of delayed exchange of stabilities in singularly perturbed parabolic problems*, Preprint no. 839, WIAS, Berlin, 2003.

O. BROX, S. BAUER, M. RADZIUNAS, M. WOLFRUM, *High-frequency pulsations in DFB-lasers with amplified feedback*, Preprint no. 849, WIAS, Berlin, 2003.

O. REISS, *Fourier inversion algorithms for generalized CreditRisk+ models and an extension to incorporate market risk*, Preprint no. 817, WIAS, Berlin, 2003.

H. HAAF, O. REISS, J. SCHOENMAKERS, *Numerically stable computation of CreditRisk+*, Preprint no. 846, WIAS, Berlin, 2003.

K.K. SABELFELD, E. SHKARUPA, *Random walk on spheres algorithm for biharmonic equation: Optimization and error estimation*, Preprint no. 826, WIAS, Berlin, 2003.

O. KURBANMURADOV, U. RANNIK, A. LEVYKIN, K.K. SABELFELD, *Stochastic Lagrangian footprint calculations over a surface with an abrupt change of roughness height*, Preprint no. 829, WIAS, Berlin, 2003.

K.R. SCHNEIDER, L.V. KALACHEV, *Global behavior and asymptotic reduction of a chemical kinetics system with continua of equilibria*, Preprint no. 870, WIAS, Berlin, 2003.

K.R. SCHNEIDER, N.N. NEFEDOV, *On immediate-delayed exchange of stabilities and periodic forced canards*, Preprint no. 872, WIAS, Berlin, 2003.

K.R. SCHNEIDER, E.A. SHCHEPAKINA, *Maximal temperature of safe combustion in case of an autocatalytic reaction*, Preprint no. 890, WIAS, Berlin, 2003.

D. RACHINSKII, K.R. SCHNEIDER, *Delayed loss of stability in systems with degenerate linear parts*, Preprint no. 820, WIAS, Berlin, 2003.

V.E. VOLKOVA, K.R. SCHNEIDER, *Qualitative theory and identification of a class of mechanical systems*, Preprint no. 884, WIAS, Berlin, 2003.

K.R. SCHNEIDER, S. YANCHUK, *Complete synchronization of symmetrically coupled autonomous systems*, Preprint no. 833, WIAS, Berlin, 2003.

A. SAMAROV, V. SPOKOINY, C. VIAL, *Component identification and estimation in nonlinear high-dimensional regression models by structural adaption*, Preprint no. 828, WIAS, Berlin, 2003.

M.-Y. CHENG, Y. FAN, V. SPOKOINY, *Dynamic nonparametric filtering with application to finance*, Preprint no. 845, WIAS, Berlin, 2003.

I. GRAMA, V. SPOKOINY, *Pareto approximation of the tail by local exponential modeling*, Preprint no. 819, WIAS, Berlin, 2003.

P. KREJČÍ, J. SPREKELS, *Nonlocal phase-field models for non-isothermal phase transitions and hysteresis*, Preprint no. 882, WIAS, Berlin, 2003.

J. SPREKELS, D. TIBA, *Optimal design of mechanical structures*, Preprint no. 863, WIAS, Berlin, 2003.

V. ARNĂUTU, J. SPREKELS, D. TIBA, *Optimization problems for curved mechanical structures*, Preprint no. 812, WIAS, Berlin, 2003.

D. TURAEV, *An example of a resonant homoclinic loop of infinite cyclicity*, Preprint no. 838, WIAS, Berlin, 2003.

A. SHILNIKOV, L. SHILNIKOV, D. TURAEV, *Blue sky catastrophe in singularly perturbed systems*, Preprint no. 841, WIAS, Berlin, 2003.

A. VLADIMIROV, D. TURAEV, G. KOZYREFF, *A new model for passive mode-looking in a semiconductor laser*, Preprint no. 893, WIAS, Berlin, 2003.

G. KOZYREFF, P. MANDEL, A. VLADIMIROV, *Synchronization of weakly stable oscillators and semiconductor laser arrays*, Preprint no. 806, WIAS, Berlin, 2003.

R. VODÁK, *On a decay rate for a Landau-Ginzburg system with viscosity for martensitic phase transitions in shape memory alloys*, Preprint no. 856, WIAS, Berlin, 2003.

——, *Stabilization of weak solutions of compressible Navier-Stokes equations for isothermal fluids with a nonlinear stress tensor*, Preprint no. 865, WIAS, Berlin, 2003.

W. WAGNER, *Stochastic models and Monte Carlo algorithms for Boltzmann type equations*, Preprint no. 831, WIAS, Berlin, 2003.

I.M. GAMBA, S. RJASANOV, W. WAGNER, *Direct simulation of the uniformly heated granular Boltzmann equation*, Preprint no. 834, WIAS, Berlin, 2003.

K. WILMANSKI, *Macroscopic modeling of porous and granular materials — microstructure, thermodynamics and some boundary-initial value problems*, Preprint no. 858, WIAS, Berlin, 2003.

——, *On a micro-macro transition for poroelastic Biot's model and corresponding Gassmann-type relations*, Preprint no. 868, WIAS, Berlin, 2003.

——, *On Biot-like models and micro-macro transitions for poroelastic materials*, Preprint no. 830, WIAS, Berlin, 2003.

——, *On thermodynamic modeling and the role of the second law of thermodynamics in geophysics*, Preprint no. 813, WIAS, Berlin, 2003.

B. FIEDLER, C. ROCHA, M. WOLFRUM, *Heteroclinic orbits between rotating waves of semilinear parabolic equation on the circle*, Preprint no. 832, WIAS, Berlin, 2003.

J. XIONG, *A stochastic log-Laplace equation*, Preprint no. 859, WIAS, Berlin, 2003.

S. YANCHUK, G. KRISTENSEN, I. SUSHKO, *Dynamical approach to complex regional economic growth based on Keynesian model for China*, Preprint no. 807, WIAS, Berlin, 2003.

S. YANCHUK, K.R. SCHNEIDER, L. RECKE, *Dynamics of two mutually coupled semi conductor lasers: Instantaneous coupling limit*, Preprint no. 879, WIAS, Berlin, 2003.

6.2.2 WIAS Reports Series

Reports 2003[4]

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

F. DUDERSTADT, *Anwendung der von Kármán'schen Plattentheorie und der Hertz'schen Pressung für die Spannungsanalyse zur Biegung von GaAs-Wafern im modifizierten Doppelringtest*, Report no. 24, WIAS, Berlin, 2003.

P. PHILIP, *Transient numerical simulation of sublimation growth of SiC bulk single crystals. Modeling, finite volume method, results*, Report no. 22, WIAS, Berlin, 2003.

6.2.3 WIAS Technical Reports Series

Technical Reports 2003[5]

J. SCHEFTER, *Discretisation of the Maxwell equations on tetrahedral grids*, Technical Report no. 6, WIAS, Berlin, 2003.

[4] http://www.wias-berlin.de/publications/reports/index-2003.html
[5] http://www.wias-berlin.de/publications/technicalreports/index-2003.html

6.2.4 Preprints/Reports in other Institutions

J. ELSCHNER, G. SCHMIDT, M. YAMAMOTO, *An inverse problem in periodic diffractive optics: Global uniqueness with a single wave number*, Preprint no. 5, University of Tokyo, Graduate School of Mathematical Sciences, 2003.

A. HUTT, F. ATAY, *Spontaneous and evoked activity of synaptically coupled neuronal fields with axonal propagation delay for gamma-distributed connectivity kernels*, Preprint no. 91, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, 2003.

J. POLZEHL, *On a comparison of different simulation extrapolation estimators in errors-in-variables models*, Preprint no. 17, Uppsala University, Department of Mathematics, 2003.

F. LANZARA, V. MAZ'YA, G. SCHMIDT, *Numerical solution of the Lippmann-Schwinger equation by approximate approximations*, Preprint no. 1412, The Erwin Schrödinger International Institute for Mathematical Physics, Vienna, 2003.

E. VANDEN BERG, A.W. HEEMINK, H.X. LIN, J.G.M. SCHOENMAKERS, *Probability density estimation in stochastic environmental models using reverse representations*, Report no. 03-06, Delft University of Technology, 2003.

——, *Probability density estimation in stochastic environmental models using reverse representations*, Report no. 6, TU Delft, The Netherlands, Applied Mathematical Analysis, 2003.

E. SHCHEPAKINA, E. SHCHETININA, V. SOBOLEV, *Loss of stability scenario in the Ziegler system*, Preprint no. 07, National University of Ireland, University College Cork, Boole Centre for Research in Informatics, 2003.

6.3 Membership in Editorial Boards

E. BÄNSCH, Editor, Electronic FBP News (http://fbp.lmc.fc.ul.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. 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.

V. SPOKOINY, Editorial Board, Statistics and Decisions, Oldenbourg Wissenschaftsverlag, München.

——, Editorial Board, Journal of Statistical Planning and Inference, Elsevier, Amsterdam, The Netherlands.

——, 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 Talks

B. ALBERS, *Modeling of flows in porous media with mass exchange. Part II: A modified Langmuir model of adsorption; stability of flows*, Politecnico di Torino, Department of Geo-Resources and Land, Italy, May 23.

——, *On the influence of adsorption on linear stability of a flow in porous material*, 19th Canadian Congress of Applied Mechanics, CANCAM03, June 1–6, The University of Calgary, Department of Mechanical & Manufacturing Engineering, Canada, June 4.

U. BANDELOW, *Report on WIAS activities concerning COST Action 288*, Kick-off Meeting for the Cost Action 288, COST TIST Secretariat, Brussels, Belgium, April 7.

——, *Modeling and simulation of mode-locked lasers*, WIAS Minisymposium on Pulse Generation in Laser Diodes, Berlin, June 12.

——, *Simulation of mode-locked lasers based on a distributed time-domain model*, WIAS Workshop “Dynamics of Semiconductor Lasers”, September 15–17, Berlin, September 17.

——, *Simulation of 40 GHz mode-locked multisection DBR lasers*, European Semiconductor Laser Workshop (ESLW’03), September 19–20, Torino, Italy, September 20.

——, *Thermodynamic designed energy model*, 3rd Topical meeting on Numerical Simulation of Semiconductor Optoelectronic Devices (NUSOD’03), October 14–16, University of Tokyo, Japan, October 14.

U. BANDELOW, M. RADZIUNAS, *Simulation of mode-locked lasers with LDSL-tool*, European Quantum Electronics Conference (EQEC 2003), June 23–27, München, June 26.

E. BÄNSCH, *Finite element methods for surface diffusion*, Otto-von-Guericke-Universität Magdeburg, Fakultät für Mathematik, January 14.

——, *Finite element methods for surface diffusion*, Technische Universität Dresden, Institut für Numerische Mathematik, January 21.

——, *Finite-Elemente-Verfahren für Phasengrenzphänomene*, Friedrich-Alexander-Universität Erlangen-Nürnberg, Institut für Angewandte Mathematik, February 5.

——, *Finite element methods for surface diffusion*, Forschungszentrum Caesar, Bonn, February 18.

——, *Finite element methods for surface diffusion*, INTERPHASE 2003 Numerical Methods for Free Boundary Problems, April 14–17, Isaac Newton Institute for Mathematical Sciences, Cambridge, UK, April 17.

——, *Finite element methods for curvature driven problems*, 15th International Conference on Domain Decomposition Methods, July 21–25, Freie Universität Berlin, July 24.

——, *Finite elements and incompressible flows*, Korean-German Seminar on Applied Physics and Mathematics, November 25 – December 2, Academy of Sciences of the DPR of Korea, Pyongyang, North Korea, November 28.

——, *Finite Elemente für die Oberflächendiffusion*, Georg-August-Universität Göttingen, Institut für Numerische und Angewandte Mathematik, December 9.

M. BARO, *Coupled Schrödinger drift-diffusion models and applications to RTD*, Université Paul Sabatier, Laboratoire de Mathématiques pour l'Industrie et la Physique, Toulouse, France, June 20.

M. BIRKNER, *A size-biased look at directed polymers, branching populations, and random environments*, The Erwin Schrödinger International Institute for Mathematical Physics (ESI), Vienna, Austria, December 16.

J. BORCHARDT, *Solution of linear systems with sparse matrices and its application within the process simulator BOP*, 5th International Congress on Industrial and Applied Mathematics (ICIAM 2003), July 7–11, Sydney, Australia, July 8.

A. BOVIER, *Activated dynamics in glassy systems*, Meeting "Probabilités et Mécanique Statistique", March 9–20, 3 talks, Centre International de Rencontres Mathématiques (CIRM), Marseille, France, March 10–14. March 10, 11, and 14.

——, *Spin glasses, Gaussian processes, and continuous state branching*, Abschlusskolloquium des DFG-Schwerpunktprogramms „Interagierende Stochastische Systeme von hoher Komplexität", April 7–11, Technische Universität Berlin, April 10.

——, *Mean field spin glasses and Neveu's branching process*, Université Paris VI "Pierre et Marie Curie", Laboratoire de Probabilités et Modèles Aléatoires, France, April 22.

——, *Spin glasses, genealogies of measures, and continuous state branching*, Workshop "Stochastic Processes and Random Media", July 7–9, Bielefeld, July 8.

——, *From spin glasses to continuous state branching*, XXIX Conference on Stochastic Processes and their Applications and VII Brasilian School on Probability Theory, August 3–9, Bernoulli Society for Mathematical Statistics and Probability, Angra dos Reis, Brazil, August 4.

——, *Metastability for Kawasaki dynamics*, Programme "Interaction and Growth in Complex Stochastic Systems", Isaac Newton Institute for Mathematical Sciences, Cambridge, UK, September 11.

——, *From spin glasses to continuous state branching*, Random Media, October 27–31, Mathematisches Forschungsinstitut Oberwolfach, October 27.

——, *Metastability and spectral theory*, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, November 21.

——, *Metastability in Markov processes*, Technische Universität Ilmenau, Institut für Mathematik, December 5.

J. CERNY, *Aging in Bouchaud's trap model*, Workshop "Mathematics of Random Spatial Models from Physics and Biology", October 13–14, Universität Bielefeld, October 13.

D. DAVIS, *Flow and thermal convection in full-zone liquid bridges*, 5th EUROMECH Fluid Mechanics Conference, August 24–28, Conference Centre of Toulouse, France, August 26.

A. DEMIRCAN, *Generation of ultrabroad spectra in optical fibers*, WIAS Workshop "Dynamics of Semiconductor Lasers", September 15–17, Berlin, September 17.

W. DREYER, *Unerwünschte Phasenübergänge in einkristallinem Galliumarsenid*, Mathematisches Kolloquium, Universität Stuttgart, Mathematisches Institut A, February 20.

——, *On the influence of mechanical fields on chemistry, diffusion and interface motion*, International Workshop on Phase Field Models with Stress/Strain Coupling, April 9–10, Access e. V., Aachen, April 10.

——, *On the influence of mechanical fields on chemistry, diffusion and interface motion*, Workshop "Partial Differential Equations and Computational Mathematical Sciences", May 13–14, Isaac Newton Institute for Mathematical Sciences, Cambridge, UK, May 14.

——, *On mechanics and thermodynamics of phase transitions involving disordered and ordered solids*, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, June 13.

——, *On the modeling of thermochemical processes in semi-insulating gallium arsenide*, 5th EUROMECH Solid Mechanics Conference (ESMC-5), August 17–22, Thessaloniki, Greece, August 18.

——, *On mechanics and thermodynamics of phase transitions involving disordered and ordered solids*, Seminar über Nichtlinearität und Unordnung in komplexen Systemen, Otto-von-Guericke-Universität Magdeburg, Institut für Theoretische Physik, October 20.

——, *Modellierung und Simulation thermo-chemischer Prozesse in semiisolierendem Galliumarsenid*, Kolloquium des Fachbereichs Mechanik, Technische Universität Darmstadt, November 12.

——, *A study of the Grinfeld instability in liquid-solid interfaces*, Oberseminar Analysis und Anwendungen, Universität Stuttgart, Institut für Analysis und Modellierung, November 14.

J. ELSCHNER, *Inverse problems for diffraction gratings: Uniqueness results*, Meeting "Inverse Problems in Wave Scattering and Impedance Tomography", April 20–25, Mathematisches Forschungsinstitut Oberwolfach, April 22.

——, *Inverse problems for periodic diffractive structures*, Meeting "Functional Analysis and Partial Differential Equations", June 2–3, Han-sur-Lesse, Belgium, June 3.

——, *On the numerical solution of inverse periodic transmission problems*, University of Tokyo, Department of Mathematical Sciences, Japan, August 5.

V. ESSAOULOVA, *Some properties of Adaptive Weights Smoothing*, Workshop on Nonlinear Analysis of Multidimensional Signals, February 25–28, Teistungenburg, February 27.

A. FAGGIONATO, *Spectral characterization of aging: Some results*, Workshop "Mathematics of Random Spatial Models from Physics and Biology", October 13–14, Universität Bielefeld, October 13.

K. FLEISCHMANN, *Competing species superprocesses with infinite variance*, University of Bath, Department of Mathematical Sciences, UK, February 24.

——, *Competing species superprocesses with infinite variance*, University of Oxford, Department of Statistics, UK, March 3.

——, *Competing species superprocesses with infinite variance*, London Joint Analysis & Probability Seminar (Imperial College, King's College London, Queen Mary and Westfield College, and University College), UK, March 17.

——, *Compact interface property for symbiotic branching*, University of Alberta, Department of Mathematical and Statistical Sciences, Edmonton, Canada, May 22.

J. FUHRMANN, *A detailed numerical model for DMFC: Discretization and solution methods*, BIRS Workshop "Computational Fuel Cell Dynamics II", April 19–24, Banff International Research Station, Canada, April 24.

——, *pdelib — eine Toolbox für die numerische Lösung von PDEs*, Annual Conference of Deutsche Mathematiker-Vereinigung, September 14–19, Universität Rostock, September 17.

——, *pdelib — a toolbox for the numerical solution of PDEs*, Workshop on Parallel Adaptive Computing, November 9–12, Hohenwart bei Pforzheim, November 12.

H. GAJEWSKI, *On parabolic equations with nonlocal drift term*, International Conference "Nonlinear Partial Differential Equations", September 15–21, National Academy of Sciences of Ukraine, Institute of Applied Mathematics and Mechanics, Alushta, September 15.

——, *On the drift-diffusion model of charge transport in semiconductor devices*, Conference on Nonlinear Analysis and Numerics, October 27–29, Rheinische Friedrich-Wilhelms-Universität Bonn, Sonderforschungsbereich 611, October 29.

K. GÄRTNER, *A detailed numerical model describing DMFC: Species transport, reaction kinetics and temperature feedback*, BIRS Workshop "Computational Fuel Cell Dynamics II", April 19–24, Banff International Research Station, Canada, April 22.

——, *"Schwache" finite Volumenformulierung für Delaunay-Simplex-Gitter, mit Anwendungen auf Bildsegmentierung und Halbleitergleichungen*, Gerhard-Mercator-Universität, Institut für Mathematik, Duisburg, June 26.

B. GENTZ, *The effect of noise on coupled oscillators*, Mini-Workshop DFG-Schwerpunktprogramm „Interagierende Stochastische Systeme von hoher Komplexität", February 16–19, Universität Köln, Mathematisches Institut, February 18.

——, *Geometric singular perturbation theory for stochastic differential equations*, WIAS Workshop "Multiscale Systems and Applications", April 3–5, Berlin, April 4.

——, *Large deviations and Wentzell–Freidlin theory*, Colloquium Equations Différentielles Stochastiques, Université de Toulon et du Var, Physique Mathématique, France, October 20.

——, *Noise-induced passage through an unstable periodic orbit*, Workshop Mathematics and Physics of Nonlinear Stochastic Systems, November 7–8, Universität Augsburg, Mathematisch-Naturwissenschaftliche Fakultät, November 7.

——, *The law of the first-passage time through an unstable periodic orbit*, Université Paris VI "Pierre et Marie Curie", Laboratoire de Probabilités et Modèles Aléatoires, France, December 16.

A. GLITZKY, R. HÜNLICH, *Stationary solutions of two-dimensional heterogeneous energy models with multiple species*, Nonlocal Elliptic and Parabolic Problems, September 9–11, Będlewo, Poland, September 10.

J.A. GRIEPENTROG, *On a nonlocal phase separation model for multicomponent systems*, Nonlocal Elliptic and Parabolic Problems, September 9–11, Będlewo, Poland, September 11.

G. HEBERMEHL, *Eigen mode computation for high dimensional problems of microwave and laser structures*, SIAM Conference on Computational Science and Engineering (CSE03), February 10–13, San Diego, California, USA, February 11.

R. HENRION, *Hölder and Lipschitz stability of solution sets in programs with probabilistic constraints*, Charles University, Institute of Mathematics, Prague, Czech Republic, April 24.

——, *Quantitative Lösungs-Stabilität in Optimierungsproblemen mit Wahrscheinlichkeitsrestriktionen*, Martin-Luther-Universität Halle, Institut für Optimierung und Stochastik, December 4.

R. HENRION, W. RÖMISCH, *Hölder and Lipschitz stability of solution sets in programs with probabilistic constraints*, 18th International Symposium on Mathematical Programming (ISMP 2003), August 18–22, Copenhagen, Denmark, August 18.

M. HERRMANN, *Micro-macro transitions in the atomic chain*, Fourth Colloquium DFG Priority Program on Analysis, Modeling and Simulation of Multiscale Problems, June 2–4, Andreas Hermes Akademie, Bonn-Röttgen, June 3.

M. HERRMANN, *Atomic chain with temperature*, WIAS Workshop “Discrete Atomistic Models and their Continuum Limits”, December 4–6, Berlin, December 5.

D. HÖMBERG, *The surface hardening of steel — Modeling, simulation and optimal control*, SIAM Conference on Computational Science and Engineering (CSE03), February 10–13, San Diego, California, USA, February 12.

——, *A thermo-viscoelastic model related to capacitor resistance welding*, California State University, Department of Mathematics, Northridge, USA, February 19.

——, *Optimal control of surface heat treatments*, 2th International Conference on Thermal Process Modelling and Computer Simulation, March 31 – April 2, Nancy, France, April 1.

——, *A mathematical model for capacitor resistance welding*, 5th International Congress on Industrial and Applied Mathematics (ICIAM 2003), July 7–11, Sydney, Australia, July 10.

——, *Optimal design of inductor coils*, 5th International Congress on Industrial and Applied Mathematics (ICIAM 2003), July 7–11, Sydney, Australia, July 10.

——, *Surface hardening of steel — Part I: Optimal design of inductor coils*, 9th IEEE International Conference on Methods and Models in Automation and Robotics, August 25–28, Miedzyzdroje, Poland, August 26.

R. HÜNLICH, *Simulation von Halbleiterbauelementen mit WIAS-TeSCA*, Institutskolloquium, Ferdinand-Braun-Institut für Höchstfrequenztechnik, Berlin, January 24.

A. HUTT, *Unbiased detection of quasi-stationary coherence in multivariate time series*, Workshop on Nonlinear Analysis of Multidimensional Signals, February 25–28, Teistungenburg, February 25.

——, *Methode zur Detektion von EKP/EKF-Komponenten*, 5th MindLab Workshop, April 28–29, DaimlerChrysler AG, Ulm, April 28.

——, *Detection of transients in phasic multivariate signals*, Universität Potsdam, Institut für Theoretische Physik, Gruppe Statistical Physics/Theory of Chaos, May 19.

——, *Analysis of nonlocal neuronal fields including propagation delay effects*, Technische Universität Berlin, Institut für Theoretische Physik, July 17.

——, *Analysis and modeling of spatio-temporal neurobiological activity*, Technische Universität Berlin, Institut für Neuronale Informationsverarbeitung, September 11.

——, *Pattern formation in intracortical neural fields*, Humboldt-Universität zu Berlin, Institut für Nichtlineare Dynamik und Stochastische Prozesse, November 18.

——, *Pattern formation in intracortical neural fields*, Universität Münster, Institut für Theoretische Physik, November 25.

H.-CHR. KAISER, *On space discretization of reaction-diffusion systems with discontinuous coefficients and mixed boundary conditions*, 2nd GAMM Seminar on Microstructures, January 10–11, Ruhr-Universität Bochum, Institut für Mechanik, January 10.

——, *Classical solutions of van Roosbroeck's equations with discontinuous coefficients and mixed boundary conditions on two-dimensional space domains*, 19th GAMM Seminar Leipzig on High-dimensional problems — Numerical treatment and applications, January 23–25, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, January 25.

O. KLEIN, *Asymptotic behaviour of evolution equations involving outwards pointing hysteresis operators*, 4th International Symposium on Hysteresis and Micromagnetic Modeling (HMM-2003), May 28–30, Universidad de Salamanca, Departamento de Física Aplicada, Spain, May 30.

A. KOLODKO, *Stochastic particle methods for Smoluchowski coagulation equation: Variance reduction and error estimation*, IV IMACS Seminar on Monte Carlo Methods (MCM 2003), September 15–19, Berlin, September 18.

——, *Upper bounds for Bermudan-style derivatives*, IV IMACS Seminar on Monte Carlo Methods (MCM 2003), September 15–19, Berlin, September 19.

——, *Estimation of the Bermudan-type option by Monte Carlo method*, Russian Academy of Sciences, Institute of Numerical Mathematics and Mathematical Geophysics, Novosibirsk, October 30.

D. KOLYUKHIN, *Stochastic Eulerian model for the flow simulation in the porous media*, IV IMACS Seminar on Monte Carlo Methods (MCM 2003), September 15–19, Berlin, September 15.

TH. KOPRUCKI, *Upscaling of microscopically calculated characteristics to macroscopic state equations*, Fourth Colloquium DFG Priority Program on Analysis, Modeling and Simulation of Multiscale Problems, June 2–4, Andreas Hermes Akademie, Bonn-Röttgen, June 2.

——, *Upscaling of microscopically calculated characteristics to macroscopic state equations*, Workshop on Multiscale problems in quantum mechanics and averaging techniques, December 11–12, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, December 11.

R. KRAHL, *Reorientation of a liquid surface — solving the Navier-Stokes equations in a time-dependent domain*, Tandem Workshop on Geometry, Numerics and Visualization, DFG Research Center "Mathematics for Key Technologies", May 26–28, Gutshof Sauen, May 27.

——, *An efficient finite element method for free surface flows*, 2nd International Berlin Workshop on Transport Phenomena with Moving Boundaries (IBW2), October 9–10, Technische Universität Berlin, Fluidsystemtechnik, October 10.

C. KÜLSKE, *Analogues of non-Gibbsianness in mean-field models*, Catholic University Leuven, Institute for Theoretical Physics, Belgium, June 2.

——, *Konzentrationsabschätzungen für Funktionen von abhängigen Zufallsvariablen*, Universität Bielefeld, Fakultät für Mathematik, July 21.

C. KÜLSKE, *Gibbs properties of the fuzzy Potts model in mean-field*, Workshop on "Gibbs vs. non-Gibbs" in statistical mechanics and related fields, December 8–10, EURANDOM, Eindhoven, The Netherlands, December 8.

P. MATHÉ, *Zur numerischen Analyse in variablen Hilbertskalen*, Universität Kaiserslautern, Fachbereich Mathematik, June 12.

——, *Towards numerical analysis in variable Hilbert scales*, Hong Kong Baptist University, Department of Mathematics, September 2.

——, *Orthogonal array based sampling for financial instruments*, Hong Kong Baptist University, Department of Mathematics, September 4.

——, *Using orthogonal arrays for high dimensional integration*, IV IMACS Seminar on Monte Carlo Methods (MCM 2003), September 15–19, Berlin, September 15.

——, *Linear ill-posed problems in variable Hilbert scales: Geometry and regularization*, University of California, Institute for Pure and Applied Mathematics, Los Angeles, USA, November 3.

——, *Linear statistically ill-posed problems under general source conditions*, Rencontres de statistiques mathématiques, December 15–19, Luminy, France, December 19.

G.N. MILSTEIN, *Estimation of transition density for SDEs by forward-reverse diffusion*, Seminar "Joint Applied Mathematics and Probability and Statistics", Wayne State University, Detroit, USA, February 4.

——, *Numerical analysis of Monte Carlo evaluation of Greeks by finite differences*, IV IMACS Seminar on Monte Carlo Methods (MCM 2003), September 15–19, Berlin, September 19.

H.J. MUCHA, *ClusCorr98 — Adaptive clustering, classification, multivariate visualisation and validation of results*, Annual Meeting of Gesellschaft für Klassifikation (GfKl), March 12–14, Cottbus, March 12.

——, *Improvement of cluster analysis by voting*, 54th World Congress of the International Statistical Institute (ISI), August 13–20, Berlin, August 19.

——, *Zur Stabilität von Ergebnissen hierarchischer Clusteranalysen*, Autumn Meeting of Gesellschaft für Klassifikation, November 14–15, Universität Düsseldorf, November 15.

H. NEIDHARDT, *Convexity of trace functionals and applications*, Université Paul Sabatier, Laboratoire de Mathématiques pour l'Industrie et la Physique, Toulouse, France, April 10.

——, *Coupling of drift-diffusion and dissipative Schrödinger-Poisson systems*, Nanolab Spring School, May 19–23, Université Paul Sabatier, Laboratoire de Mathématiques pour l'Industrie et la Physique, Toulouse, France, May 20.

——, *On the quantum transmitting Schrödinger-Poisson system*, Workshop "Spectral problems for Schrödinger-type operators II", November 11–14, Humboldt-Universität zu Berlin, Institut für Mathematik, November 14.

——, *Self-adjoint extensions with several gaps: Scalar-type Weyl functions*, 3rd Workshop Operator Theory in Krein Spaces and Nonlinear Eigenvalue Problems, December 12–14, Technische Universität Berlin, Institut für Mathematik, December 14.

P. PHILIP, *Towards optimal control of sublimation growth of SiC bulk single crystals*, Conference on Applied Inverse Problems: Theoretical and Computational Aspects, May 18–23, University of California, Institute for Pure and Applied Mathematics, Lake Arrowhed, USA, May 20.

J. POLZEHL, *Adaptive smoothing procedures for image processing*, Workshop on Nonlinear Analysis of Multidimensional Signals, February 25–28, Teistungenburg, February 25.

——, *Structural adaptive smoothing methods and applications in imaging*, Magnetic Resonance Seminar, Physikalisch-Technische Bundesanstalt, Berlin, March 13.

——, *Image processing using Adaptive Weights Smoothing*, Uppsala University, Department of Mathematics, Sweden, May 7.

——, *Standards needs & VAMAS role in modeling and simulation*, VAMAS Steering Committee and TWA Chairmen Meeting, May 12–14, Petten, The Netherlands, May 13.

——, *Local likelihood modeling by Adaptive Weights Smoothing*, Joint Statistical Meetings, August 3–7, San Francisco, USA, August 6.

——, *Local modeling by structural adaptation*, The Art of Semiparametrics, October 19–21, Humboldt-Universität zu Berlin, October 20.

S. QAMAR, *Kinetic solution of the Boltzmann-Peierls equation. Part II*, International Conference of Computational Methods in Sciences and Engineering 2003 (ICCMSE 2003), September 12–16, Kastoria, Greece, September 13.

M. RADZIUNAS, *Forced periodic frequency locking: Application of path-following tools*, WIAS Workshop "Dynamical Systems, Synchronization, Lasers", February 26–27, Berlin, February 27.

——, *Computation of the stationary states of traveling wave laser model and their analysis*, WIAS Workshop "Multiscale Systems and Applications", April 3–5, Berlin, April 5.

——, *Numerical bifurcation analysis of the PDE system describing dynamics in multi-section semiconductor laser*, The European Conference on Numerical Mathematics and Advanced Applications (ENUMATH 2003), August 18–22, Prague, Czech Republic, August 21.

——, *Dynamics of longitudinal modes in multisection semiconductor lasers*, WIAS Workshop "Dynamics of Semiconductor Lasers", September 15–17, Berlin, September 15.

J. REHBERG, *Solvability and regularity for parabolic equations with nonsmooth data*, International Conference "Nonlinear Partial Differential Equations", September 15–21, National Academy of Sciences of Ukraine, Institute of Applied Mathematics and Mechanics, Alushta, September 17.

——, *Makroskopische und quantenmechanische Modelle für Halbleiter*, Workshop "Classical and Quantum Mechanical Models of Many-Particle Systems", November 24–29, Mathematisches Forschungsinstitut Oberwolfach, November 28.

——, *A combined quantum mechanical and macroscopic model for semiconductors*, Workshop on Multiscale problems in quantum mechanics and averaging techniques, December 11–12, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, December 12.

O. REISS, *Mathematical methods for the efficient assessment of market and credit risk*, Universität Kaiserslautern, Fachbereich Mathematik, July 10.

——, *Mathematical methods for the efficient assessment of market and credit risk*, Universität Kaiserslautern, Fachbereich Mathematik, September 15.

——, *Fourier inversion algorithms for generalized CreditRisk+ models and an extension to incorporate market risk*, IV IMACS Seminar on Monte Carlo Methods (MCM 2003), September 15–19, Berlin, September 19.

——, *Fourier inversion algorithms for generalized CreditRisk+ models and an extension to incorporate market risk*, 10th Annual Meeting of Deutschen Gesellschaft für Finanzwirtschaft, October 10–11, Mainz, October 11.

——, *CreditRisk+: Numerische Methoden, Risikobeiträge und Verallgemeinerungen*, Mini-Workshop "Risikomaße und ihre Anwendungen", Humboldt-Universität zu Berlin, December 1.

K.K. SABELFELD, *Grid-free random walks for porous media*, Russian Academy of Sciences, Siberian Branch, Novosibirsk, May 24.

——, *A Lagrangian stochastic model for the transport in statistically homogeneous porous media*, IV IMACS Seminar on Monte Carlo Methods (MCM 2003), September 15–19, Berlin, September 15.

——, *Stochastic Eulerian model for the flow simulation in porous media*, IV IMACS Seminar on Monte Carlo Methods (MCM 2003), September 15–19, Berlin, September 15.

——, *Discrete random walk over large spherical grids generated by spherical means for PDEs*, IV IMACS Seminar on Monte Carlo Methods (MCM 2003), September 15–19, Berlin, September 16.

——, *Functional random walk on spheres method for the biharmonic equation: Optimization and error estimation*, IV IMACS Seminar on Monte Carlo Methods (MCM 2003), September 15–19, Berlin, September 16.

——, *Cost analysis of stochastic algorithms for solving Smoluchowski coagulation equation and a varinace reduction approach*, IV IMACS Seminar on Monte Carlo Methods (MCM 2003), September 15–19, Berlin, September 18.

——, *Stochastic Lagrangian footprint calculations over surfaces with changing roughness height*, IV IMACS Seminar on Monte Carlo Methods (MCM 2003), September 15–19, Berlin, September 18.

——, *Stochastic particle methods for Smoluchowski coagulation equation: Variance reduction and error estimation*, IV IMACS Seminar on Monte Carlo Methods (MCM 2003), September 15–19, Berlin, September 18.

——, *Stochastic models of flows in anisotropic porous media*, International Conference on Mathematical Methods in Geophysics, October 8–12, Russian Academy of Sciences, Institute for Computational Mathematics and Mathematical Geophysics, Novosibirsk, October 8.

——, *Stochastic approach for solving PDEs with random coefficients*, Russian Academy of Sciences, Institute of Computational Analysis and Stochastics, Novosibirsk, November 6.

G. SCHMIDT, *Approximate approximations and some of its applications*, University of Vienna, Department of Mathematics, Austria, November 4.

K.R. SCHNEIDER, *Complete synchronization of nearly identical systems*, WIAS Workshop "Dynamical Systems, Synchronization, Lasers", February 26–27, Berlin, February 26.

——, *Modeling of the longitudinal dynamics of semiconductor lasers*, 8th International Conference "Mathematical Modelling and Analysis 2003" (MMA), ECMI, May 28–31, Vilnius, Lithuania, May 29.

——, *Slow invariant manifold for a random dynamical system with two time-scales*, EQUADIFF 2003, July 21–26, Hasselt, Belgium, July 25.

——, *Canard solutions of finite and infinite-dimensional dynamical systems*, Moscow State University, Faculty of Physics, Russia, October 1.

——, *Qualitative theory of dynamical systems (in Russian)*, 12 talks, Grodno State University, Faculty of Mathematics, Belarus, November 17 – December 6.

——, *Immediate and delayed exchange of stabilities*, Belarussian State University, Institute for Mathematics, Minsk, November 18.

——, *Bifurcation in mode approximation models of semiconductor lasers*, Grodno State University, Faculty of Mathematics, Belarus, December 3.

J. SCHOENMAKERS, *Kreditrisiko Portfolio-Modelle*, Kreditanstalt für Wiederaufbau, Frankfurt, July 18.

——, *Transition density estimation for stochastic differential equations via forward reverse representations*, IV IMACS Seminar on Monte Carlo Methods (MCM 2003), September 15–19, Berlin, September 16.

——, *Monte Carlo methods for pricing and hedging American options*, IV IMACS Seminar on Monte Carlo Methods (MCM 2003), Workshop Financial Models and Simulation, September 15–19, Berlin, September 19.

——, *Robust calibration of LIBOR market models*, Petit Dejeuner de la Finace, November 4–5, Paris, November 5.

——, *Monte Carlo simulation of Bermudan derivatives by dual upper bounds*, Graduiertenkolleg Angewandte Algorithmische Mathematik, Workshop on the Interface of Numerical Analysis, Optimisation and Applications, November 13–14, Technische Universität München, November 14.

——, *Monte Carlo simulation of Bermudan derivatives by dual upper bounds*, Mini-Workshop "Risikomaße und ihre Anwendungen", Humboldt-Universität zu Berlin, December 1.

E. SHCHETININA, *Delayed exchange of stability*, Workshop on Multi-Scaled Systems and Hysteresis, January 17–18, University College Cork, Ireland, January 17.

——, *Different types of loss of stability in the Ziegler system*, WIAS Workshop "Multiscale Systems and Applications", April 3–5, Berlin, April 4.

——, *Different types of loss of stability in the Ziegler system*, EQUADIFF 2003, July 22–26, Hasselt, Belgium, July 22.

H. SI, *TetGen, a 3d tetrahedral mesh generator based on Delaunay method*, Tandem Workshop on Geometry, Numerics and Visualization, DFG Research Center "Mathematics for Key Technologies", May 26–28, Gutshof Sauen, May 27.

——, *TetGen, a 3d tetrahedral mesh generator based on Delaunay method*, Konrad-Zuse-Zentrum für Informationstechnik Berlin, Scientific Computing – Numerical Methods, October 28.

V. SPOKOINY, *Structural adaptive smoothing procedures and applications in imaging*, Kolloquium des DFG-SPP 1114 "Mathematische Methoden der Zeitreihenanalyse und digitalen Bildverarbeitung", April 29–30, Potsdam, April 29.

——, *Adaptive estimation of the tail index parameter*, Eidgenössische Technische Hochschule Zürich, Forschungsinstitut für Mathematik, Switzerland, June 12.

——, *Local likelihood modeling by Adaptive Weights Smoothing*, Universität Bern, Institut für mathematische Statistik und Versicherungslehre, Switzerland, June 13.

——, *Adaptive modeling for analysis of nonstationary time series*, Joint Statistical Meeting, August 2–9, San Fransicsco, USA, August 5.

——, *Wavelet thresholding: Adaptive Weights Approach*, Wavelet and Statistics, September 4–7, Grenoble, France, September 4.

——, *Pointwise adaptation via local change-point analysis*, Rencontres de statistiques mathématiques, December 15–19, Luminy, France, December 15.

J. SPREKELS, *Mathematical modelling of hysteresis phenomena*, 4 talks, Chiba University, Department of Mathematics, Japan, February 18–20.

——, *Modelling and simulation of the sublimation growth of SiC bulk single crystals*, INTERPHASE 2003 Numerical Methods for Free Boundary Problems, April 14–17, Isaac Newton Institute for Mathematical Sciences, Cambridge, UK, April 15.

——, *Modelling of curved mechanical structures*, 5th International Congress on Industrial and Applied Mathematics (ICIAM 2003), July 7–11, Sydney, Australia, July 8.

——, *Phase field models with hysteresis*, 5th International Congress on Industrial and Applied Mathematics (ICIAM 2003), July 7–11, Sydney, Australia, July 8.

——, *Analysis of curved structures: Models of rods and shells*, Conference on Nonlinear Partial Differential Equations and Their Applications, November 23–27, Fudan University, Shanghai, China, November 25.

H. STEPHAN, *An inequality for Radon measures and time asymptotics of evolution problems*, International Conference "Nonlinear Partial Differential Equations", September 15–21, National Academy of Sciences of Ukraine, Institute of Applied Mathematics and Mechanics, Alushta, September 17.

——, *Modellierung und 3D-Simulation von Bauelementen für Schaltkreise der Leistungselektronik*, Abschlusskolloquium zum DFG-Schwerpunktprogramm "Halbleiterbauelemente hoher Leistung", September 23–24, Aachen, September 24.

A. STURM, *A superprocess with infinite mean branching*, Mini–Workshop DFG–Schwerpunktprogramm „Interagierende Stochastische Systeme von hoher Komplexität", February 16–19, Universität Köln, Mathematisches Institut, February 17.

——, *A coalescent incorporating mutation and selection*, Mathematical Population Genetics and Statistical Physics, February 19–21, The Erwin Schrödinger International Institute for Mathematical Physics (ESI), Vienna, Austria, February 20.

G. TELSCHOW, *First experiences on GS1280*, Fall Meeting of the HP Consortium for Advanced Scientific and Technical Computing Users Group, September 21–24, Dallas, USA, September 22.

D. TIBA, *Optimal design of mechanical structures*, Conference on Control Theory of Partial Differential Equations, May 30 – June 1, Georgetown University, Department of Mathematics, Washington DC, USA, May 31.

D. TIBA, J. SPREKELS, *Optimization of curved mechanical structures*, 5th International Congress on Industrial and Applied Mathematics (ICIAM 2003), July 7–11, Sydney, Australia, July 8.

D. TURAEV, *Two modes dynamics of semiconductor laser*, WIAS Workshop "Multiscale Systems and Applications", April 3–5, Berlin, April 5.

——, *To the question on the genericity of the Newhouse phenomenon*, EQUADIFF 2003, July 22–26, Hasselt, Belgium, July 24.

V. VAKTHEL, *Wahrscheinlichkeiten großer Abweichungen für Galton-Watson-Prozesse*, Berliner Graduiertenkolleg "Stochastische Prozesse und probabilistische Analysis", Technische Universität Berlin, July 21.

A. VLADIMIROV, *Moving discrete solitons in multicore fibers and waveguide arrays*, Conference dedicated to the 60th birthday of Prof. Paul Mandel, April 11–12, Université Libre de Bruxelles, Optique Nonlinéaire Théorique, Belgium, April 11.

——, *Moving discrete solitons in multicore fibers and waveguide arrays*, European Quantum Electronics Conference, June 22–27, München, June 25.

——, *A new DDE model for passive mode-locking*, WIAS Workshop "Dynamics of Semiconductor Lasers", September 15–17, Berlin, September 17.

——, *Passive mode-locking in semiconductor lasers*, Institute for Laser Physics, St. Petersburg, Russia, December 25.

R. VODÁK, *Existence and asymptotic behaviour of solutions to compressible Navier-Stokes equations for isothermal fluids with a nonlinear stress tensor*, Mathematical Theory in Fluid Mechanics, Eight Paseky School, June 8–14, Charles University, Mathematical Institute and Department of Mathematical Analysis, Prague, Czech Republic, June 10.

B.A. WAGNER, *Sharp-interface model for eutectic alloys*, Access, International Workshop on Phase Field Models with Stress-Strain Coupling, April 9–10, Aachen, April 10.

——, *Destabilisation of dewetting fronts in the presence of slip*, BIRS Workshop "Nonlinear Dynamics of Thin Films and Fluid Interfaces", November 29 – December 4, Pacific Institute for the Mathematical Sciences, Banff, Canada, December 4.

W. WAGNER, *DSMC and the Boltzmann equation*, Workshop "Direct Simulation Monte Carlo: The Past 40 Years and the Future", June 2–5, Politecnico di Milano, Italy, June 2.

——, *A quasi-Monte Carlo simulation of cluster coagulation*, IV IMACS Seminar on Monte Carlo Methods (MCM 2003), September 15–19, Berlin, September 18.

——, *Gelation in stochastic models*, Workshop "Stochastic Methods in Coagulation and Fragmentation", December 8–12, Isaac Newton Institute for Mathematical Sciences, Cambridge, UK, December 10.

W. WEISS, *Surface hardening of steel — Part II: PID control of laser surface hardening*, 9th IEEE International Conference on Methods and Models in Automation and Robotics, August 25–28, Miedzyzdroje, Poland, August 26.

K. WILMANSKI, *On the thermodynamics of poroelastic media*, Seminar of the Seismics/Seismology Working Group, Freie Universität Berlin, Institut für Geologische Wissenschaften, January 13.

——, *Micro-macro transitions in two-component models of porous materials*, Universität Dortmund, Lehrstuhl für Mechanik, April 11.

——, *Bulk and surface waves in saturated poroelastic materials — low frequency approximation*, European School for Advanced Studies in Reduction of Seismic Risks, ROSE School, Collegio Alessandro Volta, Pavia, Italy, May 19.

——, *Micro-macro transitions in two-component models of porous materials — Gassmann relations*, Politecnico di Milano, Structural Engineering Department, Italy, May 21.

——, *Modeling of flows in porous media with mass exchange. Part I: Governing equations and thermodynamics*, Politecnico di Torino, Department of Geo-Resources and Land, Italy, May 23.

——, *Macroscopic modeling of porous and granular materials — Microstructure, thermodynamics and some boundary-initial value problems*, 19th Canadian Congress of Applied Mechanics (CANCAM03), June 1–6, The University of Calgary, Department of Mechanical & Manufacturing Engineering, Canada, June 3.

——, *Schallwellen in Böden und zerstörungsfreie Prüfverfahren in der Bodenmechanik: Modifiziertes Biot-Modell für poroelastische Körper und Parameterbestimmung*, Technische Universität Berlin, Institut für Bauingenieurwesen, July 10.

——, *Schallwellen in Böden und zerstörungsfreie Prüfverfahren in der Bodenmechanik: Schall- und Oberflächenwellen in gesättigten porösen Körpern*, Technische Universität Berlin, Institut für Bauingenieurwesen, July 17.

M. WOLFRUM, *Heteroclinic connections between rotating waves of scalar parabolic equations on the circle*, EQUADIFF 2003, July 22–26, Hasselt, Belgium, July 23.

——, *Instabilities of semiconductor lasers with delayed optical feedback*, Workshop “Delay Equations and Applications”, September 8–11, Bristol, UK, September 10.

——, *Attractors of semilinear parabolic equations on the circle*, Meeting “Dynamics of Structured Systems”, December 14–20, Mathematisches Forschungszentrum Oberwolfach, December 16.

S. YANCHUK, *Forced periodic frequency locking: Poincaré mapping approach*, WIAS Workshop “Dynamical Systems, Synchronization, Lasers”, February 26–27, Berlin, February 27.

——, *Synchronization of coupled autonomous systems*, National Academy of Sciences of Ukraine, Institute of Mathematics, Kiev, April 21.

——, *Synchronization of two coupled Lang-Kobayashi systems*, National Institute of Applied Optics, Florence, Italy, May 7.

——, *Synchronization problem in two-section semiconductor lasers*, Research Seminar “Angewandte Analysis”, Humboldt-Universität zu Berlin, Institut für Mathematik, July 7.

——, *Complete synchronization of symmetrically coupled autonomous systems*, EQUADIFF 2003, July 22–26, Hasselt, Belgium, July 25.

——, *Synchronization phenomena in semiconductor laser*, Sfb 555 Workshop "Complex Nonlinear Processes", September 11–13, Berlin, September 12.

——, *Synchronization of two mutually coupled semiconductor lasers: Instantaneous coupling limit*, WIAS Workshop "Dynamics of Semiconductor Lasers", September 15–17, Berlin, September 16.

6.4.2 Posters

M. BARO, H. GAJEWSKI, R. HÜNLICH, H.-CHR. KAISER, *Optoelektronische Bauelemente: mikroskopische & makroskopische Modelle*, MathInside — überall ist Mathematik, event of the DFG Research Center "Mathematics for Key Technologies" on the occasion of the Open Day of Urania, Berlin, September 13.

J. BORCHARDT, F. GRUND, D. HORN, *Block-Orientierter Prozesssimulator BOP*, ACHEMA 2003, Frankfurt am Main, May 19–24.

G. BRUCKNER, J. ELSCHNER, A. RATHSFELD, G. SCHMIDT, *Simulation, optimization and reconstruction of diffractive structures*, Conference "Diffractive Optics 2003", Oxford, UK, September 17–20.

W. DREYER, M. HERRMANN, M. KUNIK, S. QAMAR, G. WARNECKE, *Kinetic schemes for the ultra-relativistic Euler equations*, Final Colloquium of the DFG Priority Program "Analysis und Numerik von Erhaltungsgleichungen", Magdeburg, September 3–5.

W. DREYER, M. HERRMANN, M. KUNIK, S. QAMAR, *Kinetic solutions of kinetic equations & hyperbolic systems*, Final Colloquium of the DFG Priority Program "Analysis und Numerik von Erhaltungsgleichungen", Magdeburg, September 3–5.

J. FUHRMANN, *Numerische Simulation von Direkt-Methanol-Brennstoffzellen*, H2Expo, Hamburg, October 9–11.

——, *pdelib — Werkzeug für Numerische Simulationen*, H2Expo, Hamburg, October 9–11.

A. HUTT, J. POLZEHL, *Spatial adaptive signal detection in fMRT*, Human Brain Mapping Conference, New York, USA, June 17–22.

C. MEYER, O. KLEIN, P. PHILIP, A. RÖSCH, J. SPREKELS, F. TRÖLTZSCH, *Optimalsteuerung bei der Herstellung von SiC-Einkristallen*, MathInside—überall ist Mathematik, event of the DFG Research Center "Mathematics for Key Technologies" on the occasion of the Open Day of Urania, Berlin, September 13.

S. BAUER, O. BROX, M. BILETZKE, J. KREISSL, M. RADZIUNAS, B. SARTORIUS, H.-J. WÜNSCHE, *Speed potential of active feedback lasers*, CLEO/Europe-EQEC 2003, München, July 22–27.

M. LICHTNER, M. RADZIUNAS, L. RECKE, J. REHBERG, K.R. SCHNEIDER, *D8 – Nichtlineare dynamische Effekte in integrierten optoelektronischen Strukturen*, MathInside—überall ist Mathematik, event of the DFG Research Center "Mathematics for Key Technologies" on the occasion of the Open Day of Urania, Berlin, September 13.

6.4.3 Contributions to Exhibitions

U. BANDELOW, *Darstellung des WIAS*, World of Photonics (LASER 2003), München, June 23–27.

J. BORCHARDT, F. GRUND, D. HORN, *Block-Orientierter Prozesssimulator BOP*, ACHEMA 2003, Frankfurt am Main, May 19–24.

J. FUHRMANN, *Numerische Simulation von Direkt-Methanol-Brennstoffzellen*, H2Expo, Hamburg, October 9–11.

6.5 Visits to other Institutions[6]

E. BÄNSCH, Forschungszentrum Caesar, Bonn, February 18–21.

M. BARO, Université Paul Sabatier, Laboratoire de Mathématiques pour l'Industrie et la Physique, Toulouse, France, February 1 – July 31.

M. BIRKNER, The Erwin Schrödinger International Institute for Mathematical Physics (ESI), Vienna, Austria, December 10–18.

A. BOVIER, The Erwin Schrödinger International Institute for Mathematical Physics (ESI), Vienna, Austria, December 22, 2002 – January 25, 2003.

——, Centre International de Rencontres Mathématiques (CIRM), Marseille, France, March 9–20.

——, Isaac Newton Institute for Mathematical Sciences, Cambridge, UK, July 22 – September 19, Programme "Interaction and Growth in Complex Stochastic Systems".

J. CERNÝ, Ecole Polytechnique Fédérale de Lausanne, Département de Mathématiques, Switzerland, July 14–18.

J. ELSCHNER, University of Tokyo, Department of Mathematical Sciences, Japan, July 28 – August 8, in the framework of the DFG project "Scientific cooperation with Japan: Inverse problems in electromagnetics and optics".

K. FLEISCHMANN, University of Bath, Department of Mathematical Sciences, UK, February 20–24.

——, University of Oxford, Mathematical Institute, UK, February 23 – March 15.

——, Imperial College London, Department of Mathematics, UK, March 15–18.

——, University of Alberta, Department of Mathematical and Statistical Sciences, Edmonton, Canada, May 6–29.

B. GENTZ, CNRS-Centre de Physique Théorique, Marseille, and Université de Toulon et du Var, Physique Mathématique, France, October 18–24.

——, CNRS-Centre de Physique Théorique, Marseille, and Université de Toulon et du Var, Physique Mathématique, France, November 28 – December 15.

R. HENRION, Universität Halle-Wittenberg, Institut für Optimierung und Stochastik, visiting professorship (C4), winter semester 2003/2004.

——, Institute of Information Theory and Automation, UTIA, Prague, Czech Republic, April 21–27.

A. HUTT, Leibniz-Institut für Neurobiologie, Magdeburg, July 21–25.

A. KOLODKO, Russian Academy of Sciences, Novosibirsk, October 18 – November 22.

[6]Only stays of more than three days are listed.

P. MATHÉ, Hong Kong Baptist University, Department of Mathematics, Hong Kong, August 15 – September 10.

——, University of California, Institute for Pure and Applied Mathematics, Los Angeles, USA, October 11 – November 21.

G.N. MILSTEIN, Wayne State University, Department of Mathematics, Detroit, USA, January 30 – February 17.

——, Ural State University, Department of Mathematics, Ekaterinburg, Russia, September 21 – October 21.

H. NEIDHARDT, Université Paul Sabatier, Laboratoire de Mathématiques pour l'Industrie et la Physique, Toulouse, France, April 7–13.

J. POLZEHL, Uppsala University, Department of Mathematics, Sweden, April 29 – May 9.

K.K. SABELFELD, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, April 24 – June 6.

——, Bonndata GmbH, Bonn, August 6–10.

——, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, October 5 – November 16.

——, Turkmen State University, Physics and Mathematics Research Center, Ashkhabad, November 17 – December 28.

G. SCHMIDT, University of Vienna, Department of Mathematics, and The Erwin Schrödinger Institute for Mathematical Physics, Vienna, Austria, November 3–8.

K.R. SCHNEIDER, Moscow State University, Faculty of Physics, Russia, September 23 – October 3.

——, Grodno State University, Faculty of Mathematics, Belarus, November 17 – December 5.

E. SHCHETININA, University College Cork, Department of Physics, Ireland, January 15 – February 11.

V. SPOKOINY, Institut d'Informatique et Mathématiques Appliquées de Grenoble (IMAG), France, August 31 – September 7.

J. SPREKELS, Chiba University, Department of Mathematics, Japan, February 16–23.

D. TIBA, University of Jyväskylä, Department of Mathematical Information Technology, Finland, February 26 – March 26.

——, University of Jyväskylä, Department of Mathematical Information Technology, Finland, November 18–28.

D. TURAEV, Weizmann Institute of Science, Department of Mathematics, Rehovot, Israel, August 22–30.

A.G. VLADIMIROV, Université Libre de Bruxelles, Optique Nonlinéaire Théorique, Belgium, March 20 – April 16.

W. WAGNER, Isaac Newton Institute for Mathematical Sciences, Cambridge, UK, September 23 – December 18, Programme “Interaction and Growth in Complex Stochastic Systems”.

S. YANCHUK, National Institute of Applied Optics, Florence, Italy, April 28 – May 9.

——, National Institute of Applied Optics, Florence, Italy, November 17–28.

6.6 Academic Teaching[1]

E. BÄNSCH, *Numerik II* (lecture), Freie Universität Berlin, 4 SWS, winter semester 2002/2003.

——, *Numerik II* (exercises), Freie Universität Berlin, 2 SWS, winter semester 2002/2003.

——, *Theorie und Numerik elliptischer und parabolischer Probleme (Numerik III)* (lecture), Freie Universität Berlin, 4 SWS, summer semester 2003.

——, *Theorie und Numerik elliptischer und parabolischer Probleme (Numerik III)* (exercises), Freie Universität Berlin, 2 SWS, summer semester 2003.

——, *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.

E. BÄNSCH, H. GAJEWSKI, J. SPREKELS, F. TRÖLTZSCH, R. KLEIN, C. SCHÜTTE, P. DEUFLHARD, R. KORNHUBER, AND OTHERS, *Numerische Mathematik/Scientific Computing* (senior seminar), Freie Universität Berlin, 2 SWS, winter semester 2002/2003.

——, *Numerische Mathematik/Scientific Computing* (senior seminar), Freie Universität Berlin, 2 SWS, summer semester 2003.

——, *Numerische Mathematik/Scientific Computing* (senior seminar), Freie Universität Berlin, 2 SWS, winter semester 2003/2004.

E. BÄNSCH, A. MÜNCH, B. WAGNER, *Dünne Filme: Modellierung, Analysis, Asymptotik und Numerik* (seminar), Technische Universität Berlin, 2 SWS, summer semester 2003.

A. BOVIER, *Markov Prozesse und Metastabilität* (lecture), Technische Universität Berlin, 2 SWS, summer semester 2003.

——, *Mathematische Physik I* (lecture), Technische Universität Berlin, 4 SWS, winter semester 2003/2004.

A. BOVIER, B. GENTZ, H. FÖLLMER, P. IMKELLER, U. KÜCHLER, J.-D. DEUSCHEL, J. GÄRTNER, M. SCHEUTZOW, *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), Technische Universität Berlin, 2 SWS, winter semester 2002/2003.

——, *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), Humboldt-Universität zu Berlin, 2 SWS, summer semester 2003.

——, *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2003/2004.

W. DREYER, *Analytische Methoden der Kontinuumsmechanik und Materialtheorie* (lecture), Technische Universität Berlin, 4 SWS, winter semester 2002/2003.

[1] SWS = semester periods per week

——, *Analytische Methoden der Kontinuumsmechanik und Materialtheorie* (exercises), Technische Universität Berlin, 2 SWS, winter semester 2002/2003.

——, *Analytische Methoden der Kontinuumsmechanik und Materialtheorie* (lecture), Technische Universität Berlin, 4 SWS, summer semester 2003.

W. DREYER, W.H. MÜLLER, *Grundlagen der Kontinuumsmechanik* (lecture), Technische Universität Berlin, 4 SWS, winter semester 2003/2004.

D. FERUS, J. FUHRMANN, J. RAMBAU, M. STEINBACH, *Analysis I für Ingenieure* (lecture), Technische Universität Berlin, 4 SWS, winter semester 2003/2004.

H. GAJEWSKI, *Analysis und Numerik von Drift-Diffusionsgleichungen* (lecture), Freie Universität Berlin, 2 SWS, winter semester 2002/2003.

——, *Analysis und Numerik von Drift-Diffusionsgleichungen* (lecture), Freie Universität Berlin, 2 SWS, summer semester 2003.

B. GENTZ, *Random perturbations of dynamical systems* (lecture), Universität Leipzig and Max-Planck-Institut für Mathematik in den Naturwissenschaften, 2 SWS, summer semester 2003.

A. GLITZKY, *Aspekte bei der Modellierung und mathematischen Behandlung von Reaktions-Diffusionsproblemen* (lecture), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2002/2003.

A. GLITZKY, *Optimale Steuerung bei parabolischen Differentialgleichungen* (lecture), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2003/2004.

J.A. GRIEPENTROG, *Nichtglatte elliptische Randwertprobleme* (lecture), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2002/2003.

R. HENRION, *Optimierungsprobleme mit Wahrscheinlichkeitsrestriktionen* (lecture), Humboldt-Universität zu Berlin, 2 SWS, summer semester 2003.

——, *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.

R. HENRION, W. RÖMISCH, M. STEINBACH, *Numerik stochastischer Modelle* (seminar), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2002/2003.

——, *Numerik stochastischer Modelle* (seminar), Humboldt-Universität zu Berlin, 2 SWS, summer semester 2003.

D. HÖMBERG, *Lineare Algebra für Ingenieure* (lecture), Technische Universität Berlin, 2 SWS, summer semester 2003.

——, *Nichtlineare Optimierung* (lecture), Technische Universität Berlin, 4 SWS, winter semester 2003/2004.

A. HUTT, *Physik II* (exercises), Humboldt-Universität zu Berlin, 8 SWS, winter semester 2003/2004.

O. KLEIN, *Nichtlineare partielle Differentialgleichungen* (lecture), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2002/2003.

——, *Mathematik für Chemiker I* (lecture), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2003/2004.

O. KLEIN, J. SPREKELS, *Partielle Differentialgleichungen* (seminar), Humboldt-Universität zu Berlin, 2 SWS, summer semester 2003.

C. KÜLSKE, *Stochastik von Mean-Field-Modellen* (lecture), Technische Universität Berlin, 2 SWS, winter semester 2002/2003.

C. KÜLSKE, *Zufallsgraphen* (lecture), Technische Universität Berlin, 2 SWS, winter semester 2003/2004.

H.-J. MUCHA, *Statistische Datenanalyse in der Archäologie* (exercises), Humboldt-Universität zu Berlin, 1 SWS, summer semester 2003.

K.R. SCHNEIDER, B. FIEDLER, *Nichtlineare Dynamik* (senior seminar), WIAS, Freie Universität Berlin, 2 SWS, winter semester 2002/2003.

——, *Nichtlineare Dynamik* (senior seminar), WIAS, Freie Universität Berlin, 2 SWS, summer semester 2003.

——, *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 2002/2003.

——, *Mathematische Modelle der Photonik* (seminar), WIAS, Humboldt-Universität zu Berlin, 2 SWS, summer semester 2003.

——, *Mathematische Modelle der Photonik* (seminar), WIAS, Humboldt-Universität zu Berlin, 2 SWS, winter semester 2003/2004.

V. SPOKOINY, *Nichtparametrische Verfahren und ihre Anwendungen* (lecture), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2002/2003.

——, *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, summer semester 2003.

——, *Mathematische Statistik* (research seminar), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2003/2004.

V. SPOKOINY, H. LÄUTER, W. HÄRDLE, *Mathematische Statistik* (research seminar), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2002/2003.

J. SPREKELS, *Inkorrekt gestellte Probleme* (lecture), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2003/2004.

H. STEPHAN, *Anfänge der Analysis und euklidische Geometrie* (lecture), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2002/2003.

——, *Anfänge der Analysis und euklidische Geometrie* (lecture), Humboldt-Universität zu Berlin, 2 SWS, summer semester 2003.

——, *Arithmetische und rekursive Folgen* (lecture), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2003/2004.

G. TELSCHOW, *Einführung in die Datenverarbeitung I* (lecture), Technische Fachhochschule Berlin, 6 SWS, winter semester 2002/2003.

——, *Einführung in die Datenverarbeitung II* (lecture), Technische Fachhochschule Berlin, 6 SWS, summer semester 2003.

B.A. WAGNER, *Lie theory of differential equations* (lecture), Technische Universität Berlin, 2 SWS, summer semester 2003.

W. WEISS, *Mathematische Hilfsmittel zur Thermo- und Fluiddynamik* (lecture), Technische Universität Berlin, 2 SWS, winter semester 2002/2003.

——, *Mathematische Hilfsmittel zur Thermo- und Fluiddynamik* (exercises), Technische Universität Berlin, 2 SWS, winter semester 2002/2003.

K. WILMANSKI, *Dynamik von mehrkomponentigen Körpern* (lecture), Technische Universität Berlin, 2 SWS, winter semester 2002/2003.

——, *Nichtlineare Elastizitätstheorie* (lecture), Technische Universität Berlin, 2 SWS, summer semester 2003.

——, *Dynamik von mehrkomponentigen Körpern* (lecture), Technische Universität Berlin, 2 SWS, winter semester 2003/2004.

K. WILMANSKI, I. MÜLLER, *Thermodynamisches Seminar* (seminar), WIAS/Technische Universität Berlin, 2 SWS, winter semester 2002/2003.

——, *Thermodynamisches Seminar* (seminar), WIAS/Technische Universität Berlin, 2 SWS, summer semester 2003.

6.7 Calls, Awards and Distinctions, Habilitations, Ph.D. Theses, and Undergraduate-degree Supervision

Calls

E. BÄNSCH, C4 professorship, May 12, Universität Konstanz, Fachbereich Mathematik und Statistik.

A. BOVIER, C4 professorship, April 5, Technische Universität Berlin.

D. HÖMBERG, C4 professorship, April 15, Technische Universität Berlin.

D. TURAEV, C3 professorship, October 1, Ben-Gurion University of the Negev, Department of Mathematics.

Awards and Distinctions

J. POLZEHL, *Chairman Technical Working Area 18, Versailles Project on Advanced Materials and Standards (VAMAS).*

K.R. SCHNEIDER, *Badge of Honour "For merit in developing of sciences and economy of Russia", Russian Academy of Natural Sciences, Samara, Russia*, November 27, 2002, awarded in 2003.

J. SPREKELS, *member of the International Scientific Board of the Institute of Mathematics "Simion Stoilow" of the Romanian Academy, Bucharest.*

K. WILMANSKI, *Secretary and Treasurer of the International Society for the Interaction of Mechanics and Mathematics (ISIMM).*

Habilitations

B. GENTZ, *Fluctuations in the Hopfield model at the critical temperature and Stochastic slow-fast systems*, Technische Universität Berlin, March 5.

Ph.D. Theses

F. DUDERSTADT, *Anwendung der von Kármán'schen Plattentheorie und der Hertz'schen Pressung für die Spannungsanalyse zur Biegung von GaAs-Wafern im modifizierten Doppelringtest*, Technische Universität Berlin, supervisor: Priv.-Doz. Dr. W. Dreyer, November 27.

P. PHILIP, *Transient numerical simulation of sublimation growth of SiC bulk single crystals. Modeling, finite volume method, results*, Humboldt-Universität zu Berlin, supervisor: Prof. Dr. J. Sprekels, February 3.

S. QAMAR, *Kinetic schemes for the relativistic hydrodynamics*, Otto-von-Guericke-Universität Magdeburg, supervisor: Prof. Dr. G. Warnecke, September 26.

O. REISS, *Mathematical methods for the efficient assessment of market and credit risk*, Universität Kaiserslautern, supervisor: Dr. J.G.M. Schoenmakers, September 15.

Undergraduate-degree Supervision

R. SEEDORF, *Regelungsalgorithmen für die Laserhärtung von Stahl*, Technische Fachhochschule Berlin, Fachbereich II: Mathematik — Physik — Chemie, supervisor: W. Weiss, December 19.

6.8 WIAS Conferences, Colloquiums, and Workshops

WORKSHOP "DYNAMICAL SYSTEMS, SYNCHRONIZATION, LASERS"
Berlin, February 26–27
Organized by: WIAS (FG 2)

The international workshop was devoted to the following problems: Synchronization of nearly identical systems (K.R. Schneider, S. Yanchuk), forced frequency locking (M. Radziunas, L. Recke, S. Yanchuk), periodic, quasiperiodic, and chaotic regimes in lasers (S. Gonchenko, D. Rachinskii, L. Shilnikov, D. Turaev). About 20 participants from five countries attended the workshop. Seven talks were given.

WORKSHOP "MULTISCALE SYSTEMS AND APPLICATIONS"
Berlin, April 3–5
Organized by: WIAS (FG 2), Freie Universität Berlin
Sponsored by: WIAS, DFG Research Center "Mathematics for Key Technologies" (FZT 86)

The workshop has been attended by 43 participants, among them 16 from abroad. Twenty-six lectures have been delivered.
During the workshop, recent trends and new results for the study of multiscale systems have been presented and discussed.
The main foci of the workshop were: phase transitions, spikes, multiscale dynamics, including delayed exchange of stability (canard solutions), control of slow-fast systems.
From the viewpoint of applications, the emphasis was on the multiscale dynamics of semiconductor lasers, of oscillating systems in biology, and of liquid film, but also models for tin-lead alloys and for micro-macro transitions have been presented.
The mathematical approaches presented in the talks to treat multiscale systems ranged from asymptotic upper and lower solutions, methods of asymptotic expansions via invariant manifolds (basing on spectral gap conditions) to the method of desingularization in case of non-hyperbolicity in singularly perturbed systems.
In the frame of control theory of systems with different time scales, problems of robust control for uncertain systems and for systems with delay as well as optimal control problems have been considered.
Two different approaches to look for invariant manifolds in stochastic systems formed a special highlight of the workshop.

WORKSHOP "DYNAMICS OF SEMICONDUCTOR LASERS"
Berlin, September 15–17
Organized by: WIAS (FG 2), DFG Research Center "Mathematics for Key Technologies" (FZT 86), Ferdinand-Braun-Institut für Höchstfrequenztechnik Berlin, Fraunhofer-Institut für Nachrichtechnik Heinrich-Hertz-Institut Berlin, Humboldt-Universität zu Berlin
Sponsored by: WIAS, DFG (SFB 555, FZT 86)

During this workshop, new results have been presented from the fields of modeling, numerical simulation, and analysis of semiconductor devices, together with their applications in optical telecommunications.

Based on the financial support of the DFG Research Center "Mathematics for Key Technologies" (FZT 86) and the DFG Collaborative Research Center "SFB 555: Complex Nonlinear Processes", it was possible to invite leading experts from Europe and the USA, which made this workshop an event of high scientific significance.
Thematically, the workshop was focused on nonlinear dynamical effects in semiconductor devices. Following the tradition of preceeding workshops in 1999 and 2001, major attention was paid to an interdisciplinary approach, including the mathematical and physical background as well as technological applications, in particular optical telecommunication technologies. In the focus of interest were the subjects

- delayed coupling and feedback in lasers;
- mode-locked lasers and saturable absorbers;
- ultrafast effects in SOAs.

From a mathematical point of view, these topics are related to bifurcation theory and path-following techniques, in particular for delay differential equations, singular perturbations, synchronization, and waves in nonlinear, inhomogeneous media. Fifty-one participants attended the workshop. Twenty-six talks were given.

IVth IMACS Seminar on Monte Carlo Methods

Berlin, September 15–19
Organized by: WIAS (FG 6), Konrad-Zuse-Zentrum für Informationstechnik Berlin (ZIB)
Sponsored by: DFG, ZIB, WIAS

The research group "Stochastic Algorithms and Nonparametric Statistics" has organized (chairman: K.K. Sabelfeld) the IVth IMACS Seminar on Monte Carlo Methods. This Seminar is the world's largest international forum on stochastic simulation. In the IVth IMACS Seminar, 155 participants from more than 25 countries have made reports in 16 sessions on different basic research topics on stochastic simulation and applications in semiconductor structures, porous media, interacting particle systems, complex biological structures like ion channels, computer graphics, contaminant transport, finance models, and simulations, etc.
The selected papers will be published in a special issue of the journal *Monte Carlo Methods and Applications*.

Workshop "Discrete atomistic models and their continuum limits"

Berlin, December 4–6
Organized by: WIAS (FG 7), DFG Priority Program, Universität Stuttgart
Sponsored by: DFG, WIAS

Within the DFG Priority Program "Analysis, modelling and simulation of multiscale problems", W. Dreyer (FG 7), A. Mielke (Stuttgart), and J. Sprekels (FG 1) organized the workshop "Discrete atomistic models and their continuum limits". The central focus of the workshop was on multiscale problems of the atomic chain and various continuum limits of microscopic many-particle systems. However, there were also lectures and discussions on related topics as phase transitions, the Casimir effect, and the Boltzmann-Peierls equation.
All in all, 41 participants assembled to hear 19 talks.

6.9 Visiting Scientists[2]

6.9.1 Guests

M. ANTHONISSEN, Eindhoven University of Technology, Department of Mathematics and Computer Science, The Netherlands, November 9 – December 3.

V. ARNĂUTU, University "Al. I. Cuza", Department of Mathematics, Iaşi, Romania, October 15 – November 14.

——, November 15 – December 14.

E. BAUER, Technische Universität Graz, Institut für Allgemeine Mechanik, Austria, June 6–20.

D. BELOMESTNY, Universität Bonn, Institut für Angewandte Mathematik, September 25–30.

N. BERGLUND, CNRS-Centre de Physique Théorique, Marseille, and Université de Toulon et du Var, Physique Mathématique, France, January 20–24.

——, July 14 – August 15.

——, October 25 – November 2.

M. BIRKNER, Johann Wolfgang Goethe-Universität, Institut für Stochastik und Mathematische Informatik, Frankfurt am Main, May 8 – June 6.

J.C.R. BLOCH, DFG-Forschungszentrum "Mathematik für Schlüsseltechnologien" (FZT 86), Berlin, January 1 – October 30.

——, December 12–31.

M. BROKATE, Technische Universität München, Zentrum Mathematik, August 18–22.

C. BUTUCEA, Université Paris VI "Pierre et Marie Curie", Laboratoire de Probabilités et Modèles Aléatoires, France, January 27 – February 17.

V.F. BUTUZOV, Moscow State University, Faculty of Physics, Russia, April 1–30.

J. CERNÝ, Ecole Polytechnique Fédérale de Lausanne, Département de Mathématiques, Switzerland, February 3–28.

M.-Y. CHENG, National Taiwan University, Department of Mathematics, Taipei, August 22–30.

R. DAHLHAUS, Universität Heidelberg, Institut für Angewandte Mathematik, January 21–24.

A. DALALYAN, Université Paris VI "Pierre et Marie Curie", Laboratoire de Probabilités et Modèles Aléatoires, France, July 1–31.

D.A. DAWSON, Carleton University Ottawa, School of Mathematics and Statistics, Canada, August 12–20.

M. DELFOUR, Université de Montréal, Centre de Recherches Mathématiques, Canada, August 19–24.

[2]Only stays of more than three days are listed.

M. DELGADO, Universidad Carlos III de Madrid, Departamento de Economía, Spain, January 27–30.

M.A. EFENDIEV, Universität Stuttgart, Mathematisches Institut A, March 24–29.

——, July 28 – August 8.

M. ERMAKOV, Russian Academy of Sciences, Mechanical Engineering Problem Institute, St. Petersburg, November 1–30.

S.M. ERMAKOV, University of St. Petersburg, Faculty of Mathematics and Mechanics, Russia, August 23 – September 21.

R. EYMARD, Université de Marne-la-Vallée, Département de Mathématiques, Champs-sur-Marne, France, May 17–30.

——, October 25–29.

T. FATTLER, Universität Kaiserslautern, Institut für Mathematik, September 22 – October 5.

V. GAYRARD, Ecole Polytechnique Fédérale de Lausanne, Département de Mathématiques, Switzerland, June 1–30.

A. GOLDENSHLUGER, University of Haifa, Department of Statistics, Israel, January 19 – February 2.

——, September 7–16.

S. GONCHENKO, Institute for Applied Mathematics and Cybernetics, Nizhny Novgorod, Russia, February 6 – March 6.

I. GRAMA, Université de Bretagne Sud, Laboratoire SABRES, Vannes, France, April 1 – May 31.

P. GWIAZDA, University of Warsaw, Institute for Applied Mathematics, Poland, January 20 – February 16.

M. HAGEMANN, Universität Basel, Institut für Informatik, Switzerland, August 4–29.

O. HRYNIV, University of Cambridge, Statistical Laboratory, Centre for Mathematical Sciences, UK, February 23 – March 1.

——, December 14–23.

Y. INGSTER, St. Petersburg State Transport University, Department of Applied Mathematics, Russia, July 1 – August 31.

A. JOURANI, Université de Bourgogne, Département de Mathématiques, Dijon, France, June 1–14.

A. JUDITSKY, Université Joseph Fourier Grenoble I, Laboratoire de Modélisation et Calcul, France, April 16–30.

M. KAMENSKI, Université de Rouen, Département de Mathématiques, France, June 22–28.

J. KAMPEN, Universität Heidelberg, Institut für Angewandte Mathematik, September 18–25.

S. KASHENKO, Yaroslavl State University, Department of Mathematics, Russia, April 2–11.

S. KAVIANPOUR, University of Calgary, Department of Mechanical and Manufacturing Engineering, Canada, November 22 – December 8.

J. KEFI, Université Paul Sabatier, Laboratoire de Mathématiques pour l'Industrie et la Physique, Toulouse, France, November 29 – December 10.

A. KHLUDNEV, Russian Academy of Sciences, Lavrentyev Institute of Hydrodynamics, Novosibirsk, Russia, November 25 – December 24.

E.Y. KHRUSLOV, National Academy of Sciences of Ukraine, B. Verkin Institute for Low Temperature Physics and Engineering, Kharkov, May 22 – June 21.

A. KLENKE, Friedrich-Alexander-Universität Erlangen-Nürnberg, Mathematisches Institut, March 31 – April 6.

P. KNOBLOCH, Charles University, Institute of Numerical Mathematics, Prague, Czech Republic, September 10–30.

D. KOUROUNIS, University of Ioannina, Department of Material Science, Greece, August 5–15.

A. KRASNOSELSKIJ, Russian Academy of Sciences, Institute for Information Transmission Problems, Moscow, November 24 – December 21.

P. KREJČÍ, Academy of Sciences of the Czech Republic, Institute of Mathematics, Prague, October 13 – November 9.

O. KURBANMURADOV, Turkmen State University, Physics and Mathematics Research Center, Ashkhabat, September 2 – November 2.

S. LANGDON, Brunel University, Department of Mathematical Sciences, Uxbridge, UK, April 28 – May 16.

C. LECOT, Université de Savoie, Laboratoire de Mathématiques (LAMA), Le Bourget-du-Lac, France, September 13–20.

Z. LI, Beijing Normal University, Department of Mathematics, China, November 15 – December 13.

A. LINKE, DFG-Forschungszentrum "Mathematik für Schlüsseltechnologien" (FZT 86), Berlin, August 1 – December 31.

V.G. MAZ'YA, Linköping University, Department of Mathematics, Sweden, September 20–27.

P. MORIN, Universidad Nacional del Litoral, Departamento de Matemática, Santa Fe, Argentina, December 2–23.

P. MÖRTERS, University of Bath, Department of Mathematical Sciences, UK, January 8–22.

——, December 14–20.

L. MYTNIK, Technion Israel Institute of Technology, Faculty of Industrial Engineering and Management, Haifa, Israel, June 30 – August 10.

N.N. NEFEDOV, Moscow State University, Faculty of Physics, Russia, April 1–30.

J. OUTRATA, Academy of Sciences of the Czech Republic, Institute of Information Theory and Automation, Prague, November 2 – December 1.

S. PECERICENKO, Russian Academy of Sciences, Institute for Applied Mathematics and Mathematical Geophysics, Novosibirsk, September 1–30.

S.V. PEREVERZEV, National Academy of Sciences of Ukraine, Institute of Mathematics, Kiev, February 4–8.

S.V. PEREVERZEV, Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria, November 23 – December 7.

W. POLONIK, University of California, Department of Statistics, Davis, USA, May 10–17.

J.-H. PYO, Purdue University, Department of Mathematics, West Lafayette, Indiana, USA, May 15 – June 9.

A. QUARTERONI, Ecole Polytechnique Fédérale de Lausanne, Institute of Mathematics and Bernoulli Institute, Switzerland, September 22 – October 3.

D. RACHINSKII, Technische Universität München, Fakultät für Mathematik, February 24 – March 8.

S. RJASANOW, Universität des Saarlandes, Fachrichtung Mathematik, March 27 – April 17.

Y. ROGOVCHENKO, Eastern Mediterranean University, Department of Mathematics, Famagusta, Northern Cyprus, August 17–24.

A. SAMOILENKO, National Academy of Science of Ukraine, Institute of Mathematics, Kiev, May 17–24.

O. SCHENK, Universität Basel, Fachbereich Informatik, Switzerland, November 10–13.

I. SHALIMOVA, Russian Academy of Sciences, Institute for Applied Mathematics and Mathematical Geophysics, Novosibirsk, January 25 – February 25.

——, June 21 – July 21.

——, August 23 – September 23.

E. SHCHEPAKINA, Samara State University, Department of Differential Equations & Control Theory, Russia, November 1–30.

Z. SHI, Université Paris VI “Pierre et Marie Curie”, Laboratoire de Probabilités et Modèles Aléatoires, France, July 11–18.

J. SIEBER, University of Bristol, Department of Engineering Mathematics, UK, September 13 – October 4.

I.V. SKRYPNIK, National Academy of Sciences of Ukraine, Institute of Applied Mathematics and Mechanics, Donetsk, July 1–31.

V. SOBOLEV, Samara State University, Department of Differential Equations & Control Theory, Russia, November 1–30.

S. SPERLICH, Universidad Carlos III de Madrid, Departamento de Estadística y Econometría, Spain, January 17–24.

A. STEFANSKI, Technical University of Lodz, Division of Dynamics, Poland, October 26 – November 8.

J. SWART, Universität Erlangen-Nürnberg, Mathematisches Institut, June 16–27.

M. TRETJAKOV, University of Leicester, Department of Mathematics and Computer Science, UK, April 2 – May 1.

——, August 13–29.

A. TSYBAKOV, Université Paris VI "Pierre et Marie Curie", Laboratoire de Probabilités et Modèles Aléatoires, France, July 8–11.

D. TURAEV, Ben-Gurion University of the Negev, Department of Mathematics, Beer-Sheva, Israel, October 5–22.

A.B. VASILIEVA, Moscow State University, Faculty of Physics, Russia, October 11–31.

V.A. VATUTIN, Steklov Institute of Mathematics, Moscow, Russia, October 20 – November 20.

C. VIAL, Université de Rennes 1, Institut de Recherche Mathématiques de Rennes, France, September 21 – October 3.

P. VOGT, University of Bath, Department of Mathematical Sciences, UK, April 7–17.

S. WIECZOREK, Sandia National Laboratories, Semiconductor Device Sciences, Albuquerque, USA, September 9–20.

J.-J. XU, McGill University of Montreal, Department of Mathematics and Statistics, Canada, July 20 – August 20.

A.G. YAGOLA, Moscow State University, Department of Mathematics, Russia, September 7–11.

M. YAMAMOTO, University of Tokyo, Department of Mathematical Sciences, Japan, June 2–9.

——, September 6–30.

M. ZAHRADNÍK, Charles University, Faculty of Mathematics and Physics, Prague, Czech Republic, November 17–30.

H. ZORSKI, Polish Academy of Sciences, Institute of Fundamental Research, Warsaw, November 1–30.

S. ZWANZIG, Uppsala University, Department of Mathematics, Sweden, January 6–14.

6.9.2 Scholarship Holders

I. EDELMAN, Russian Academy of Sciences, Institute of Physics of the Earth, Moscow, Humboldt Research Fellowship, January 1 – August 31, 2003.

L. SHILNIKOV, Institute for Applied Mathematics and Cybernetics, Nizhny Novgorod, Russia, Humboldt Research Award, February 20 – March 27, 2003.

M. THIEULLEN, Université Paris VI "Pierre et Marie Curie", Laboratoire de Probabilités et Modèles Aléatoires, France, Humboldt Research Fellowship, September 1, 2002 – February 28, 2003.

V. VOLKOVA, Dnepropetrovsk State Technical University of the Railway Transport, Ukraine, EU INTAS Young NIS Scientist Fellowship Programme, May 1 – June 30, 2003.

J. XIONG, University of Tennessee, Department of Mathematics, Knoxville, USA, Humboldt Research Fellowship, July 1, 2003 – June 31, 2004.

6.9.3 Doctoral Candidates and Post-docs supervised by WIAS Collaborators

M. AN DER HEIDEN, Technische Universität Berlin, Graduate College "Stochastic Processes and Probabilistic Analysis", doctoral candidate, May 1, 2002 – April 30, 2004.

A. KLIMOVSKI, Technische Universität Berlin, Graduate College "Stochastic Processes and Probabilistic Analysis", doctoral candidate, June 1, 2003 – December 31, 2004.

6.10 Guest Talks

L. ADAMEK, MTU Aero Engines Friedrichshafen, *Brennstoffzellenaktivitäten der MTU Friedrichshafen*, April 7.

M. ANTHONISSEN, Eindhoven University of Technology, Department of Mathematics and Computer Science, The Netherlands, *Adaptive grid refinement using local defect correction applied to combustion*, November 27.

D. ARMBRUSTER, Arizona State University, USA, *Dynamics and control of supply chains*, April 29.

M. BAAKE, Universität Greifswald, Institut für Mathematik und Informatik, *Dynamics of recombination*, April 30.

G. BÄRWOLFF, Technische Universität Berlin, Institut für Mathematik, *Optimization of a thermal coupled fluid flow problem — algorithms and numerical results*, October 30.

E. BAUER, Technische Universität Graz, Institut für Allgemeine Mechanik, Austria, *Modellierung der Druck- und Dichteabhängigkeit granularer Medien im Rahmen der Hypoplastizität*, June 11.

S. BAUER, Fraunhofer-Institut für Nachrichtentechnik, Heinrich-Hertz-Institut, Berlin, *Synchronisation processes in lasers: Resonances on tori by optical feedback*, May 22.

J. BEHRNDT, Technische Universität Berlin, Institut für Mathematik, *Eine Klasse von Randwertproblemen, in denen die Randbedingungen vom Eigenwertparameter abhängen*, October 15.

D. BELOMESTNY, Universität Bonn, Institut für Angewandte Mathematik, *Constrained kernel deconvolution*, June 4.

N. BERGLUND, CNRS-Centre de Physique Théorique, Marseille, and Université de Toulon et du Var, Physique Mathématique, France, *On the noise-induced passage through an unstable periodic orbit*, October 29.

M. BIRKNER, Johann Wolfgang Goethe-Universität, Institut für Stochastik und Mathematische Informatik, Frankfurt/Main, *Longtime behaviour of spatial branching processes with local interaction*, May 14.

O. BROX, Fraunhofer-Institut für Nachrichtentechnik, Heinrich-Hertz-Institut, Berlin, *Controlled manipulation of laser dynamics by integrated feedback systems*, June 12.

M.V. BURNASHEV, Russian Academy of Sciences, Institute for Information Transmission Problems, Moscow, *On some singularities in parameter estimation problems*, March 26.

C. BUTUCEA, Université Paris VI "Pierre et Marie Curie", Laboratoire de Probabilités et Modèles Aléatoires, France, *Minimax estimation in the semiparametric convolution model*, February 5.

C. CARSTENSEN, Vienna University of Technology, Institute for Applied Mathematics and Numerical Analysis, Austria, *Adaptive finite elements for relaxed methods (FERM) in computational microstructures*, September 2.

K. CHELMINSKI, Technische Universität Darmstadt, Fachbereich Mathematik, *Thermoplastizität mit linearer kinematischer Verfestigung. Mathematische Analyse eines Modells*, April 9.

I. CHUECHOV, National University Kharkov, Ukraine, *Random monotone systems*, March 25.

R. DAHLHAUS, Universität Heidelberg, Institut für Angewandte Mathematik, *Graphical models for multivariate time series*, January 22.

K. DECKELNICK, Otto-von-Guericke-Universität Magdeburg, Institut für Analysis und Numerik, *An existence and uniqueness result for a phase-field model of diffusion-induced grain boundary motion*, July 10.

M. DELFOUR, Université de Montréal, Centre de Recherches Mathématiques, Canada, *Modelling of thin and asymptotic shells*, August 20.

M. DELGADO, Universidad Carlos III de Madrid, Departamento de Economía, Spain, *Distribution-free goodness-of-fit tests for time series models*, January 29.

M. DREYER, Universität Bremen, Zentrum für Angewandte Raumfahrttechnologie und Mikrogravitation, *Reorientierung freier Flüssigkeitsoberflächen bei Änderung der Beschleunigung*, April 28.

M.A. EFENDIEV, Universität Stuttgart, Mathematisches Institut A, *On the structure of invertible pseudo-differential operators and its applications*, March 25.

TH. ELSÄSSER, Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie, Berlin, *Nichtlineare Dynamik optischer Anregungen und Impulspropagation auf ultrakurzen Zeitskalen*, March 10.

H. EMMERICH, Universität Dortmund, Fachbereich Chemietechnik, *Phasenfeldsimulationen von Morphologien an verspannten epitaktischen Oberflächen*, February 6.

R. EYMARD, Université de Marne-la-Vallée, Département de Mathématiques, Champs-sur-Marne, France, *Some features of the convergence study of finite volume methods: I. Convergence/error estimate of finite volume methods for elliptic problems*, May 20.

——, *Some features of the convergence study of finite volume methods: II. Nonlinear parabolic/hyperbolic problems; the role of uniqueness theorems*, May 22.

——, *Some features of the convergence study of finite volume methods: III. Two coupled problems (two-phase flow in porous media, diffusion-reaction)*, May 23.

——, *Some features of the convergence study of finite volume methods: IV. Finite volume methods for incompressible Navier-Stokes equations*, May 27.

A. FEDOTOV, St. Petersburg State University, Faculty of Mathematics, Russia, *Renormalization method for almost periodic equation*, December 11.

S. FOREST, Ecole des Mines de Paris, Centre des Matériaux, France, *Notion of representative volume element for heterogeneous materials: Statistical and numerical approach*, July 2.

C. FRANZ, Universität Karlsruhe (TH), Institut für Werkstoffkunde I, *Simulation der Wärmebehandlung von Stahlbauteilen*, April 30.

M. GEORGI, N. JANGLE, Freie Universität Berlin, Institut für Mathematik, *Spiral waves in reaction-diffusion systems,* July 15.

I. GRAMA, Université de Bretagne Sud, Laboratoire SABRES, Vannes, France, *Estimation of the tail of a distribution by local exponential modeling*, April 16.

K. GRÖGER, Berlin, *Evolutionsgleichungen mit Konvektionsterm*, February 12.

P. GWIAZDA, University of Warsaw, Institute for Applied Mathematics, Poland, *Weak entropy solutions for balance laws with multifunction source term*, January 24.

——, *Existence via compactness for the Leray-Lions operators with discontinuous coefficients*, February 5.

K. HACK, GTT-Technologies, Herzogenrath, *Rechnergestützte Thermochemie — Eine Toolbox und ihre praktischen Anwendungen*, July 7.

S. HANDROCK-MEYER, Technische Universität Chemnitz, Fakultät für Mathematik, *Inverse Probleme für die Grad-Schafranov-Gleichung*, December 18.

L. HOFFMANN, Universität Kaiserslautern, Fachbereich Physik, *Application of field theoretical methods to phase transitions*, April 23.

O. HRYNIV, University of Cambridge, Statistical Laboratory, Centre for Mathematical Sciences, UK, *The opinion game: A microscopic stochastic model for share price evolution*, December 17.

B. HÜTTL, Fraunhofer-Institut für Nachrichtentechnik, Heinrich-Hertz-Institut, Berlin, *Amplitude fluctuations in mode-locked lasers*, November 27.

V. JOHN, Otto-von-Guericke-Universität Magdeburg, Institut für Analysis und Numerik, *Eddy Simulation turbulenter inkompressibler Strömungen*, July 10.

A. JOURANI, Université de Bourgogne, Département de Mathématiques, Dijon, France, *Hamiltonian necessary conditions for the generalized Bolza problem*, June 12.

A. JUDITSKY, Université Joseph Fourier Grenoble I, Laboratoire de Modélisation et Calcul, France, *Primal-dual stochastic approximation algorithms*, April 23.

M. JURISCH, Freiberger Compound Materials GmbH, *Thermochemische Aspekte der GaAs-Einkristallsynthese*, May 26.

M. KAMENSKI, Université de Rouen, Département de Mathématiques, France, *Averaging method via topological degree theory*, June 24.

J. KEFI, Université Paul Sabatier, Laboratoire de Mathématiques pour l'Industrie et la Physique, Toulouse, France, *Mathematical analysis of the two-band Schrödinger model*, December 3.

A. KHLUDNEV, Russian Academy of Sciences, Lavrentyev Institute of Hydrodynamics, Novosibirsk, *Crack problems for solids with nonlinear boundary conditions*, June 17.

——, *Fictitious domain method for the Signorini problem in a linear elasticity*, December 11.

E.Y. KHRUSLOV, National Academy of Sciences of Ukraine, B. Verkin Institute for Low Temperature Physics and Engineering, Kharkov, *Homogenized models of complex fluids,* June 4.

A. KIEU, University of Twente, Faculty of Mathematical Sciences, The Netherlands, *The forwards interest rate is driven by stochastic string*, May 6.

P. KNOBLOCH, Charles University, Institute of Numerical Mathematics, Prague, Czech Republic, *On Korn's first inequality for nonconforming finite elements*, September 18.

N. KORNEYEV, Humboldt-Universität zu Berlin, Institut für Physik, *Bifurcations of a laser by short-delay optical feedback: Simulation calculations with LDSL*, May 15.

YU.A. KRAVTSOV, Maritime University of Szczecin, Institute of Mathematics, Physics and Chemistry, Poland, *Concept of partial predictability: An inverse problem of chaotic dynamics*, February 20.

P. KREJČÍ, Academy of Sciences of the Czech Republic, Institute of Mathematics, Prague, *Evolutionsgleichungen mit nichtinvertierbaren Operatoren*, November 5.

A. KRENER, University of California, Department of Mathematics, Davis, USA, *Control bifurcations*, June 12.

S. LANGDON, Brunel University, Department of Mathematical Sciences, Uxbridge, UK, *A wavenumber independent boundary element method for an acoustic scattering problem*, May 13.

A. LINKE, DFG-Forschungszentrum "Mathematik für Schlüsseltechnologien" (FZT 86), Berlin, *3D-FEM-Simulation des Floating-Zone-Kristallzüchtungsverfahrens (Konvektion, freie Oberfläche), part 1*, September 18.

——, *3D-FEM-Simulation des Floating-Zone-Kristallzüchtungsverfahrens (Konvektion, freie Oberfläche), part 2*, September 25.

——, *Einführendes Tutorial: Templates und Scientific Computing*, December 11.

D. LUSS, University of Houston, Department of Chemical Engineering, USA, *Evolution and motion of hot zones in catalytic packed bed-reactors*, June 24.

N. MARKOVITCH, Russian Academy of Sciences, Institute of Control Sciences, Moscow, *Nonparametric estimation of the renewal function by empirical data*, December 3.

A. MATOUSSI, Université du Maine, Equipe Statistiques et Processus, Département de Mathématiques, Le Mans, France, *Maximum principle for parabolic SPDEs*, November 5.

G. MATTHIES, Otto-von-Guericke-Universität Magdeburg, Institut für Analysis und Numerik, *Numerische Simulation des Verhaltens von magnetischen Flüssigkeiten*, February 13.

K. MATTHIES, Freie Universität Berlin, Institut für Mathematik, *Atomic-scale localization of lattice waves*, July 8.

V.G. MAZ'YA, Linköping University, Department of Mathematics, Sweden, *New criteria in the spectral theory of the Schrödinger operator*, September 25.

J. MEHNERT, Universität Freiburg, Institut für Angewandte Mathematik, *Fehlerabschätzungen für die Navier-Stokes-Gleichungen mit freiem Kapillarrand*, July 17.

F. MEIER, Universität Stuttgart, Institut für Chemische Verfahrenstechnik, *Experimentelle Analyse des Betriebsverhaltens von Direktmethanol-Brennstoffzellen (DMFC)*, January 23.

P. MORIN, Universidad Nacional del Litoral, Departamento de Matemática, Santa Fe, Argentina, *Finite element methods for surface diffusion*, December 18.

T. MOUNTFORD, Ecole Polytechnique Fédérale de Lausanne, Département de Mathématiques, Switzerland, *The existence of a sharp interface for the one-dimensional voter model*, December 3.

L. MYTNIK, Technion Haifa, Israel, *Regularity and irregularity of the exit measure densities for (1+beta)-stable super-Brownian motions*, July 2.

N. NATARAJ, Indian Institute of Technology, Bombay, India, *On a mixed finite element method for IV order elliptic source/eigenvalue problems*, October 30.

N.N. NEFEDOV, Moscow State University, Faculty of Physics, Russia, *Multidimensional internal layers in singularly perturbed reaction diffusion systems*, October 21.

——, *Multidimensional internal layers of spike type*, October 28.

R. NOVA, Politecnico di Milano, Facoltà di Ingegneria di Milano — Leonardo, Italy, *The role of non-normality in soil mechanics*, May 5.

J. OSTROWSKI, ABB Baden, Switzerland, *FEM/BEM-gekoppelte Simulation des induktiven Härtens*, November 20.

J. OUTRATA, Academy of Sciences of the Czech Republic, Institute of Information Theory and Automation, Prague, *On modeling and optimization of delamination processes*, November 14.

C. PENSSEL, Universität Erlangen-Nürnberg, Mathematisches Institut, *Catalytic interacting Feller diffusion: Renormalisation and duality*, April 23.

S.V. PEREVERZEV, National Academy of Sciences of Ukraine, Institute of Mathematics, Kiev, *General approach to the regularization parameter choice*, February 4.

S.V. PEREVERZEV, Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria, *General approach to the regularization in Hilbert spaces*, December 1.

H.J. PESCH, Universität Bayreuth, Lehrstuhl für Ingenieurmathematik, *Numerische Simulation einer Schmelzkarbonat-Brennstoffzelle und ihre Steuerung*, March 13.

T. PFINGSTEN, Westfälische Wilhelms-Universität Münster, Institut für Festkörpertheorie, *Ladungsträgerdynamik in optisch angeregten Halbleitern: Relaxation und Transport*, May 7.

W. POLONIK, University of California, Department of Statistics, Davis, USA, *Nonparametric inference for multivariate volatility functions using concentration ideas and inverse regression*, May 14.

M. PRÄHOFER, Technische Universität München, Zentrum Mathematik, M5, *Fluctuations in one-dimensional stochastic growth*, November 12.

J.-H. PYO, Purdue University, Department of Mathematics, West Lafayette, Indiana, USA, *A finite element Gauge-Uzawa method for the evolution Navier-Stokes equations*, June 5.

A. QUARTERONI, Ecole Polytechnique Fédérale de Lausanne, Institute of Mathematics and Bernoulli Institute, Switzerland, *WIAS/FZT 86 SPECIAL GUEST LECTURE: Modelling cardiovascular flows: Mathematical and numerical aspects*, September 23.

——, *WIAS/FZT 86 SPECIAL GUEST LECTURE: Modelling cardiovascular flows: Numerical simulations and clinical applications*, September 24.

——, *WIAS/FZT 86 SPECIAL GUEST LECTURE: Domain decomposition methods for multiphysics*, October 1.

——, *WIAS/FZT 86 SPECIAL GUEST LECTURE: Numerical simulation for the America's cup*, October 2.

E. RADKEVICH, Moscow State University, Faculty of Mechanics and Mathematics, Russia, *On asymptotic stability of hyperbolic pencils*, February 19.

M. RASP, SiCrystal AG, Erlangen, *Siliziumkarbid-Einkristallzüchtung im industriellen Maßstab*, June 23.

L. RECKE, Humboldt-Universität zu Berlin, Institut für Mathematik, *Generic properties of initial boundary value problems with non-smooth data*, June 3.

W. REHBEIN, Fraunhofer-Institut für Nachrichtentechnik, Heinrich-Hertz-Institut, Berlin, *Experiments on 40 GHz mode-locked lasers*, June 12.

K. RICHAU, GKSS-Forschungszentrum, Institut für Chemie, Teltow-Seehof, *Conditioning, conductivity and permselectivity of free standing polymer membranes developed for DMFC applications*, January 23.

Y. ROGOVCHENKO, Eastern Mediterranean University, Department of Mathematics, Famagusta, Northern Cyprus, *Asymptotically linear solutions of nonlinear differential equations*, August 21.

A. SAMOILENKO, National Academy of Sciences of Ukraine, Institute of Mathematics, Kiev, *Some problems of the theory of differential-delay equations*, May 23.

E. SANGER, Freie Universität Berlin, Institut für Geologische Wissenschaften, *Numerical rock physics of 2d and 3d fractured media*, March 19.

A. SCHEEL, University of Minnesota, School of Mathematics, Minneapolis, USA, *Beyond the Gap Lemma — blowup in critical eigenvalue problems*, July 1.

R. SELLGER, ThyssenKrupp AG, Duisburg, *Modellierung der Phasenumwandlung in Kohlenstoffstählen*, February 24.

S. SHAPIRO, Freie Universität Berlin, Institut für Geologische Wissenschaften, *Seismic diffusion and propagating waves in rocks under stress*, March 19.

E. SHCHEPAKINA, Samara State University, Department of Differential Equations & Control Theory, Russia, *Maximal temperature of save combustion in case of an autocatalytic reaction*, November 13.

Z. SHI, Université Paris VI "Pierre et Marie Curie", Laboratoire de Probabilités et Modèles Aléatoires, France, *The most visited sites of one-dimensional simple random walk*, July 16.

L. SHILNIKOV, Institute for Applied Mathematics and Cybernetics, Nizhny Novgorod, Russia, *Homokline Orbits zu Gleichgewichtspunkten vom Sattel-Fokus-Typ*, November 6.

J. SIEBER, University of Bristol, Department of Engineering Mathematics, UK, *Delay-differential equations: Basic theory for center manifold reduction*, September 25.

H. SILVA, GKSS-Forschungszentrum, Institut für Chemie, Geesthacht, *Membrane development for the DMFC—characterisation and modelling*, November 27.

D. SKRYABIN, University of Bath, Department of Physics, UK, *Radiation and scattering of linear waves and solitons in photonic crystal fibers*, December 4.

I.V. SKRYPNIK, National Academy of Sciences of Ukraine, Institute of Applied Mathematics and Mechanics, Donetsk, *Removable singularities of nonlinear elliptic equations*, July 16.

A.L. SKUBACHEWSKII, University of Aerospace Technology, Moscow Aviation Institute, Russia, *Multidimensional nonlocal elliptic problems and applications*, November 24.

D.M.J. SMEULDERS, Delft University of Technology, Department of Applied Earth Sciences, The Netherlands, *Shock-induced wave propagation in* (nn)*saturated poroelastic media*, February 21.

I. STEINBACH, Access e.V., Aachen, *Transientes Wachstum und Wechselwirkung äquiaxialer Dendriten: Ein Mehrskalenansatz*, February 10.

D. TASCHE, Deutsche Bundesbank, Banking Supervision/Research, Frankfurt am Main, *Kapitalallokation für Kreditportfolios*, March 31.

M. THIEULLEN, Université Paris VI "Pierre et Marie Curie", Laboratoire de Probabilités et Modèles Aléatoires, France, *An integration by parts formula for the bridges of diffusion processes*, January 29.

A. TSYBAKOV, Université Paris VI "Pierre et Marie Curie", Laboratoire de Probabilités et Modèles Aléatoires, France, *Optimal rates of aggregation*, July 9.

O. USHAKOV, Humboldt-Universität zu Berlin, Experimentelle Physik, *Bifurcations of a laser by short-delay optical feedback: Experimental investigations*, May 15.

V. VATUTIN, Steklov Mathematical Institute, Moscow, Russia, *Branching processes in a critical random environment*, November 19.

M. WEINERT, Fraunhofer-Institut für Nachrichtentechnik, Heinrich-Hertz-Institut, Berlin, *Pulse propagation in nonlinear fibers*, January 16.

S. WIELAND, Rheinische Friedrich-Wilhelms-Universität Bonn, Institut für Numerische Simulation, *Modellierung und mathematische Analyse kontaminierter dünner Flüssigkeitsfilme*, December 17.

T. WILHELM, Institut für molekulare Biotechnologie, Jena, *Statistische Analyse und dynamische Simulation zellulärer Netzwerke*, January 24.

A.G. YAGOLA, Moscow State University, Department of Mathematics, Russia, *Using a priori information for constructing regularizing algorithms*, September 9.

M. YAMAMOTO, University of Tokyo, Department of Mathematical Sciences, Japan, *Carleman estimate for hyperbolic equations with variable coefficients and its application to inverse problems*, June 5.

——, *Moment method for the Cauchy problem of the Laplace equation*, September 23.

E. ZIENICKE, Technische Universität Ilmenau, Fakultät Maschinenbau, *A shallow water model for the liquid metal pinch*, May 15.

H. ZORSKI, Polish Academy of Sciences, Institute of Fundamental Research, Warsaw, *Gibbs distributions with temperature dependent Hamiltonians*, November 19.

S. ZWANZIG, Uppsala University, Department of Mathematics, Sweden, *On saddlepoint approximations in regression models*, June 25.

6.11 Membership in Organizing Committees of non-WIAS Meetings

E. BÄNSCH, member of the Local Organizing Committee, *15th International Conference on Domain Decomposition Methods*, Freie Universität Berlin, July 21–25.

A. BOVIER, member of the Organizing Committee, *Workshop "Mathematics of Random Spatial Models from Physics and Biology"*, Universität Bielefeld, October 13–14.

H. GAJEWSKI, member of the Program Committee, *International Conference "Nonlinear Partial Differential Equations"*, Alushta, Ukraine, September 15–20.

——, member of the Scientific Committee, *Numerical Simulation of Semiconductor Optoelectronic Devices (NUSOD '03)*, Tokyo, Japan, October 13–16.

R. HENRION, organizer, *Mini-Workshop "Risikomaße und ihre Anwendungen"*, Humboldt-Universität zu Berlin, December 1.

D. HÖMBERG, organizer of a minisymposium, *5th International Congress on Industrial and Applied Mathematics (ICIAM 2003)*, Sydney, Australia, July 7–11.

D. MERCURIO, member of the Organizing Committee, *The Art of Semiparametrics*, Humboldt-Universität zu Berlin, October 18–20.

V. SPOKOINY, member of the Organizing Committee, *The Art of Semiparametrics*, Humboldt-Universität zu Berlin, October 18–20.

J. SPREKELS, member of the Local Organizing Committee, *15th International Conference on Domain Decomposition Methods*, Freie Universität Berlin, July 21–25.

——, member of the Scientific Committee, *Conference on Nonlinear Partial Differential Equations and Their Applications*, Fudan University, Shanghai, China, November 23–27.

W. WAGNER, member of the Organizing Committee, *Euroworkshop "Stochastic Methods in Coagulation and Fragmentation"*, Cambridge, UK, December 8–12.

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 that performs exploratory data analysis mainly by using adaptive methods of cluster analysis, classification, and multivariate visualization. Currently, there are two new main enhancements. Firstly, an automatic validation technique of cluster analysis results was developed that becomes 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. Secondly, clustering methods based on nonparametric density estimation are under development. This is a joint project with U. Simon and C. Duckhorn within the framework of an application to water ecology (monitoring of phytoplankton). The special

algorithms can find arbitrary-shaped clusters. Usually, they are used as a fast preclustering step for massive data sets or as stand-alone clustering methods that provide optimum solutions.
Up to now `ClusCorr98`® runs under the Excel spreadsheet environment taking advantage of both the data base connectivity and the object-oriented programming language Visual Basic for Applications (VBA). Now the upgrade of VBA to C# and VB.NET under the .NET framework is in progress.
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 and a comparison of the different models is 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: P. Philip, phone: +49 30/20372-480)
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, e.g., employing temperature-dependent laws of thermal and electrical conductivity. The simulator is designed to deal with complicated axisymmetric setups having a polygonal 2D projection. The induction coil is allowed to move during the simulation. 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. 40) supported by the BMBF and the DFG.
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 quite general radiation flux profiles and the implementation of two independent beam traces. 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

- **Neue Mathematische Verfahren in Industrie und Dienstleistungen (New mathematical methods in industry and services)**

  "Optoelektronische Sensoren" (Optoelectronic sensors, FG[1] 1)

  "Numerische Simulation und Optimierung der Züchtung von SiC-Einkristallen durch Sublimation aus der Gasphase" (Numerical simulation and optimization of SiC single crystal growth by sublimation from the gas phase, FG 1, 7)

  "Mathematische Modellierung und Simulation der Entstehung, des Wachstums und der Auflösung von Arsenausscheidungen in einkristallinem Galliumarsenid" (Mathematical modeling and simulation of the formation, growth, and dissolution of arsenic precipitation in single crystal gallium arsenide, FG 7)

  "Modellierung und Optimierung mikrooptischer Oberflächenstrukturen" (Modeling and optimization of microoptic surface structures, FG 4)

  "Effiziente Methoden zur Bestimmung von Risikomaßen" (Efficient methods for valuation of risk measures, FG 6)

- **Technische Anwendungen der Nichtlinearen Dynamik (Technical applications in nonlinear dynamics)**

  "Hochfrequente Selbstpulsation 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 association), Bonn

- **DFG-Forschungszentrum 86 "Mathematik für Schlüsseltechnologien" (DFG Research Center 86 "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)

  C11: "Modeling and optimization of phase transitions in steel" (FG 3, 4)

[1] research group

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 modelling of financial derivatives and valuation of portfolio risk” (FG 6)

- Collaborative Research Centre (Sfb) 373, Humboldt-Universität zu Berlin, “Quantifikation und Simulation ökonomischer Prozesse” (Quantification and simulation of economic processes)

  B1 “Kurvenschätzung und Resampling” (Curve estimation and resampling methods, FG 6)

  B2 “Stochastic models for financial markets and statistics of stochastic processes” (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 study of the spatial and temporal pattern formation in semiconductor lasers, FG 1, 2)

- Priority Program: “Halbleiterbauelemente hoher Leistung” (Semiconductor devices for high power applications)

  “Physikalische Modellierung und numerische Simulation von Strom- und Wärmetransport bei hoher Trägerinjektion und hohen Temperaturen” (Physical modeling and numerical simulation of current and heat transport at high carrier injection and high temperatures, FG 1)

- Priority Program: “Interagierende Stochastische Systeme von hoher Komplexität” (Interacting stochastic systems of high complexity)

  “Intermittenz und katalytische Medien” (Intermittency and catalytic media, FG 5)

  “Untersuchung von Tieftemperaturphasen ungeordneter Modelle mit langreichweitiger Wechselwirkung” (Study of low temperature phases of disordered models with long-range interaction, FG 5)

- Priority Program: “Analysis, Modellbildung und Simulation von Mehrskalenproblemen” (Analysis, modeling and simulation of multiscale problems)

  “Enveloppenfunktionsapproximation zur Beschreibung elektronischer Zustände in Halbleiter-Nanostrukturen” (Envelope function approximation 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)

  “Structural adaptive smoothing procedures with applications in imaging and functional MRI” (FG 6)

- Priority Program “Analysis und Numerik von Erhaltungsgleichungen” (ANumE — Analysis and numerics for conservation laws)

  “Kinetische Behandlung von ausgewählten Anfangs- und Randwertproblemen” (Kinetic treatment of selected hyperbolic initial and boundary value problems, FG 7)

- **Normalverfahren (Individual Grants)**

  “Hysterese-Operatoren in Phasenfeld-Gleichungen” (Hysteresis operators in phase-field equations, FG 1)

  “Kopplung von van Roosbroeck- und Schrödinger-Poisson-Systemen mit Ladungsträgeraustausch” (Coupling between van Roosbroek and Schrödinger-Poisson systems including exchange of carriers, FG 1)

  “Effektive Steuerung von stochastischen Partikelverfahren für Strömungen in verdünnten Gasen” (Effective control of stochastic particle methods for rarefied gas flows, FG 5)

  “Kinetische Lösungen für ausgewählte hyperbolische Anfangs- und Randwertprobleme” (Kinetic solutions for selected hyperbolic initial and boundary value problems, 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, 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

- Scientific cooperation with Japan: “Inverse problems in electromagnetics and optics” (FG 4)

- 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 3 scholarship holders (FG 5, 7), see page 245

Deutscher Akademischer Austauschdienst (German Academic Exchange Service), Bonn

- 1 short-term fellowship (FG 2)

- PROCOPE (FG 1)

International Projects

- **(EU) INTAS:** “Development of constructive and numerical methods for solving nonlocal linear and nonlinear problems for partial differential equations” (FG 4)
- **(EU) INTAS:** “Random walk models for the footprint problem in the turbulent atmosphere” (FG 5, 6)
- **(EU) INTAS:** “Young NIS Scientist Fellowship Programme” (FG 2)
- **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” (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))

Stiftung Industrieforschung (foundation for industrial research)

- “Numerische Simulation von Temperaturfeldern bei der Strahlbearbeitung von kompliziert geformten Bauteilen” (Numerical simulation of temperature fields during beam hardening of workpieces with complicated shapes, FG 1)

Verbundforschungsvorhaben (research network project): “Terabit Optics Berlin”

- B4: “Modellierung und Simulation von Pulsquellen” (Modeling and simulation of pulse sources, FG 1, 2)

Mission-oriented research

- ALSTOM (Switzerland) Ltd., Baden: “Prozesssimulation bei Kraftwerksanlagen” (Power plant process simulation, FG 3)
- Bundesanstalt für Materialforschung und -prüfung, Berlin: “Statistisch-methodische Verfahrensentwicklung zur Zertifizierung von Referenzmaterialien” (Statistical methods for certification of reference materials, 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)
- Freiberger Compound Materials GmbH: “Spannungs- und Dehnungsanalyse an GaAs-Waferplatten” (Stress and strain analysis of GaAs wafer plates, FG 7)
- LUMICS GMBH Berlin: “`WIAS-TeSCA` simulations of laser diodes” (FG 1)
- Reuters Financial Software Paris: Consulting contract (FG 6)
- Rücker Ges.m.b.H, Graz, Austria: “Bahnplanung für Industrieroboter und Menschmodelle” (Path planning for robots and human models, FG 4)

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