Weierstraß-Institut
für Angewandte Analysis und Stochastik
(WIAS)

im Forschungsverbund Berlin e. V.

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Contents

1 Vorwort / Foreword

Das Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS) legt hiermit Kollegen, Förderern und Kooperationspartnern des Instituts seinen Jahresforschungsbericht 2002 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) herewith presents its Annual Scientific Report 2002 to its colleagues, supporters, and cooperation partners. In its first part, the report informs about the progress made and the results obtained in 2002, 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 2002 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 2002 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 einerseits wider in der im Vergleich zum Vorjahr deutlich gesteigerten Drittmitteleinwerbung, wobei es dem Institut erfreulicherweise gelang, die Einwerbung von Drittmitteln aus der Wirtschaft erneut merklich zu erhöhen; andererseits war die Anzahl der in referierten Fachzeitschriften erschienenen Publikationen und der eingeladenen Vorträge auf internationalen Tagungen erfreulich.

The positive development is reflected, on the one hand, by the distinctly increased third-party funds that have been raised in 2002, compared to last year's funds, and, much to our satisfaction, the institute succeeded again in raising substantially more funds from industry. On the other hand, also the number of publications that appeared in refereed journals and the number of invited talks at international conferences were positive.

Besonders augenfällig wird der hohe Stellenwert, den die am WIAS geleistete Arbeit in der Scientific Community hat, wiederum im Bereich der Berufungen: Im Berichtsjahr 2002 ergingen drei Rufe an Mitarbeiter des Instituts auf Professuren, davon eine auf einen Lehrstuhl im Ausland, eine auf eine C3-Professur im Inland, und eine auf eine Juniorprofessur.

The high rank of WIAS' research work in the scientific community becomes again especially clear in the field of calls: in 2002, three calls to professorships were received by WIAS collaborators, including one to a full professorship abroad, one to a C3 (associate) professorship in Germany, and one to a Junior Professorship. We are very proud that for the first time two

Besonders erfreulich war dabei, dass erstmalig zwei Mitarbeiterinnen berufen wurden. Insgesamt sind nunmehr seit der Gründung des Instituts im Jahre 1992 schon 24 Rufe an Mitarbeiter/innen des Instituts auf Professuren erfolgt (davon zwölf auf C4-Professuren und sieben auf Professuren im Ausland), eine Bilanz, die sich bei einer Zahl von derzeit 54 etatisierten Wissenschaftlern wirklich sehen lassen kann.

female collaborators have received calls. Altogether, since the institute's foundation in 1992, 24 calls have been received by collaborators of WIAS (including twelve to C4 (full) professorships and seven 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 in die Wege geleitet: Sowohl für die Berufung des Leiters der Forschungsgruppe „Nichtlineare Optimierung und Inverse Probleme“ auf eine C4-S-Professur für „Numerische nichtlineare Optimierung“ als auch für die Berufung des Leiters der Forschungsgruppe „Stochastische Systeme mit Wechselwirkung“ auf eine C4-S-Professur „Vernetzte stochastische Systeme“ wurden Berufungslisten erarbeitet. Es steht zu erwarten, dass am Ende des Jahres 2003 insgesamt fünf gemeinsame Berufungen auf C4-S-Professuren mit den Berliner Universitäten realisiert sein werden. Für die Einrichtung einer weiteren C4-S-Professur für „Partielle Differentialgleichungen“ an der Humboldt-Universität zu Berlin zur gemeinsamen Berufung des Leiters der Forschungsgruppe „Partielle Differentialgleichungen und Variationsgleichungen“ wurden die Voraussetzungen geschaffen.

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 2002, two joint appointments with the Technical University of Berlin have been lined up: Suitable applicants have been chosen for the appointment of the head of the research group "Nonlinear Optimization and Inverse Problems" to a C4 special professorship for "Numerical Nonlinear Optimization" as well as for the appointment of the head of the research group "Interacting Random Systems" to a C4 special professorship for "Networked Stochastic Systems", and we hope that at the end of the year 2003 altogether five joint appointments to C4 special professorships with the Berlin universities will be concluded. The foundations have been laid for the establishment of one further C4 special professorship, this one for "Partial Differential Equations" at Humboldt University of Berlin for the head of the research group "Partial Differential Equations and Variational Equations".

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 das absolute wissenschaftliche Highlight des Jahres die erfolgreiche Einwerbung des DFG-Forschungszentrums FZT 86 „Mathematik für Schlüsseltechnologien“ an der Technischen Universität Berlin zusammen mit den

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 absolute scientific highlight of the year 2002 has been the successful proposal for the DFG Research Center "Mathematics for Key Technologies" at the Technical University of Berlin together with the three Berlin universities and the Konrad-Zuse-Zentrum für

drei Berliner Universitäten und dem Konrad-Zuse-Zentrum für Informationstechnik Berlin. Durch das Forschungszentrum werden für zunächst vier Jahre jährlich mehr als fünf Millionen Euro an DFG-Fördergeldern nach Berlin fließen, um in Berlin einen international sichtbaren „Leuchtturm“ der Forschung in angewandter Mathematik zu errichten.

Informationstechnik Berlin (Konrad Zuse Center for Scientific Computing Berlin). Through the Research Center, DFG funds of more than five million euros will flow to Berlin in each of the next four years, at first, to erect in Berlin a “beacon” of research in Applied Mathematics to be visible to the whole world.

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 weitere wissenschaftliche Mitarbeiter und mehrere studentische Hilfskräfte konnten aus Zentrumsmitteln am WIAS eingestellt werden.

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 more scientific collaborators and several student assistants could be employed by WIAS from Center funds.

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.

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.

Die Herausforderungen im Jahr 2003 werden für das WIAS erheblich sein. An allererster Stelle steht dabei die für Anfang Juli angesetzte Evaluierung durch den Senat der Leibniz-Gemeinschaft (WGL). Hier gilt es, die bei der letzten Evaluierung durch den Wissenschaftsrat im Jahre 1997 erzielte positive Bewertung zu bestätigen. Die Mitarbeiter des Instituts sehen diesem für die weitere Entwicklung entschei-

The challenges in 2003 will be considerable for WIAS. First of all, there is the evaluation by the Senate of Leibniz Association (WGL) in July 2003. We will strive to confirm the positive results obtained by us in the 1997’s evaluation by the German Science Council. WIAS’s collaborators are facing this event, that will be decisive for the institute’s future, in eager anticipation. It is our firm conviction

denden Event mit gespannter Erwartung und der festen Überzeugung entgegen, in den vergangenen Jahren hervorragende Arbeit geleistet zu haben.

that we did a very good job in the last years.

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

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

Berlin, im Januar 2003 / in January 2003

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 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 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. 261; 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 261; 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 2002 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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Stochastische Systeme mit Wechselwirkung / Interacting Random Systems
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Stochastische Algorithmen und Nichtparametrische Statistik / Stochastic Algorithms and Nonparametric Statistics
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☎ 594
BIBLIOTHEK / LIBRARY
Dr.
W. Höppner
☎ 296
RECHENTECHNIK / COMPUTER DEPARTMENT
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G. Telschow
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☎ 458
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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 2002 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 2002, 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,
- Zur Analysis von thermodynamischen Modellen des Stoff-, Ladungs- und Energietransports in heterogenen Halbleitern,
- 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 wurden die Projekte:

- Numerische Simulation von Temperaturfeldern bei der Bestrahlungshärtung von kompliziert geformten Bauteilen,
- Numerische Simulation und Optimierung von MQW-Lasern.

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;
- Analysis of thermodynamical models for the transport of mass, charge, and energy in heterogeneous semiconductors;
- 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 projects

- Numerical simulation of temperature fields during beam hardening of workpieces with complicated shapes;
- Numerical simulation and optimization of MQW lasers

have been supported by industrial funds.

4.1.2 Projects

Simulation of the modulation response of strained multi-quantum-well lasers

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

Cooperation with: F. Fidorra, M. Krieg (MergeOptics GmbH, Berlin)

Supported by: MergeOptics GmbH

In cooperation with the company MergeOptics GmbH the electrical, thermal, optical and dynamical behavior of strained multi-quantum-well (SMQW) lasers was simulated for improving their performance. The simulations were carried out using the device simulator `WIAS-TeSCA` based on a drift-diffusion model which is self-consistently coupled to a heat-flow equation (see [1]) and to equations for the optical field. The main goal was the optimization of the modulation response of such lasers. For this purpose details of the structure (e.g., number of quantum wells, thickness of waveguides) and the doping were varied.
Methods and results are demonstrated here for some fictive edge-emitting ridge waveguide (RW) laser. The most important part of its transverse cross section is shown in Figure 1, the simulated *P-I* characteristic in Figure 2. Besides RW lasers we investigated also buried heterostructure lasers in more detail.

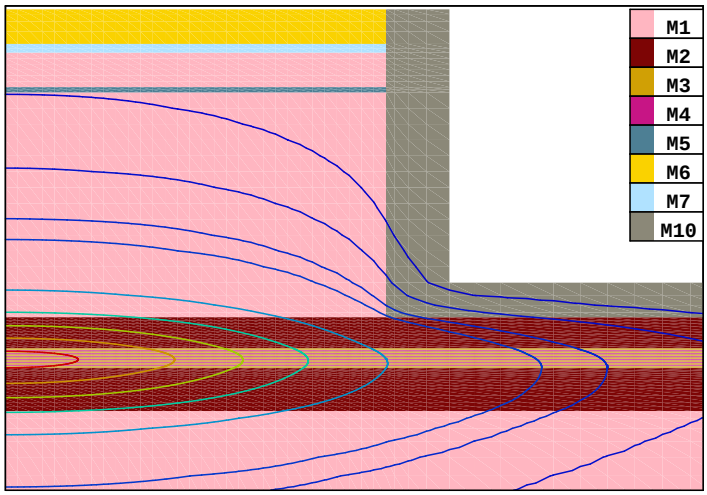

Fig. 1: Part of the transverse cross section of a RW-SMQW laser consisting of different materials M1, M2, and so on. There are also shown isolines of the power distribution of the fundamental optical mode.

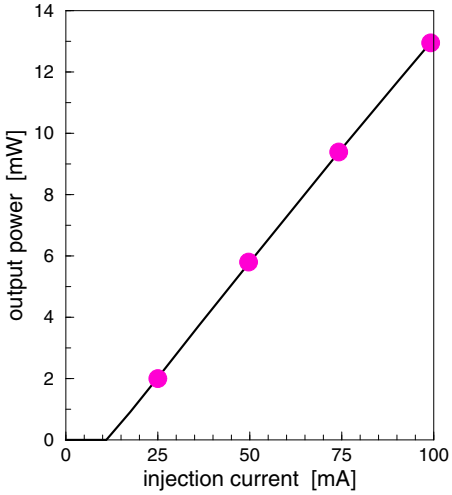

Fig. 2: *P-I* characteristic of the laser. The modulation response was computed in four operating points as marked in the figure.

We describe two methods for the calculation of the modulation response. The first one is the AC analysis (small signal analysis in the frequency domain). Here `WIAS-TeSCA` computes complex amplitudes $\widehat{I}(\omega)$, $\widehat{P}(\omega)$ corresponding to a small harmonic modulation of the bias voltage with angular frequency ω and amplitude ΔU ($\Delta U = 0.05$ mV). The complex response function is then given by $H(\omega) = \widehat{P}(\omega)/\widehat{I}(\omega)$, or in a normalized form by $H_n(\omega) = H(\omega)/H(0)$.

The squared modulus of H_n is seen in Figure 4. An excellent fit of H_n can be obtained according to the formula

$$H_n(\omega) = \mathrm{e}^{-\mathrm{j}\theta\omega} \frac{1}{1+\mathrm{j}\tau\omega} \frac{\omega_r^2}{\omega_r^2 - \omega^2 + \mathrm{j}\Gamma_r\omega}. \tag{1}$$

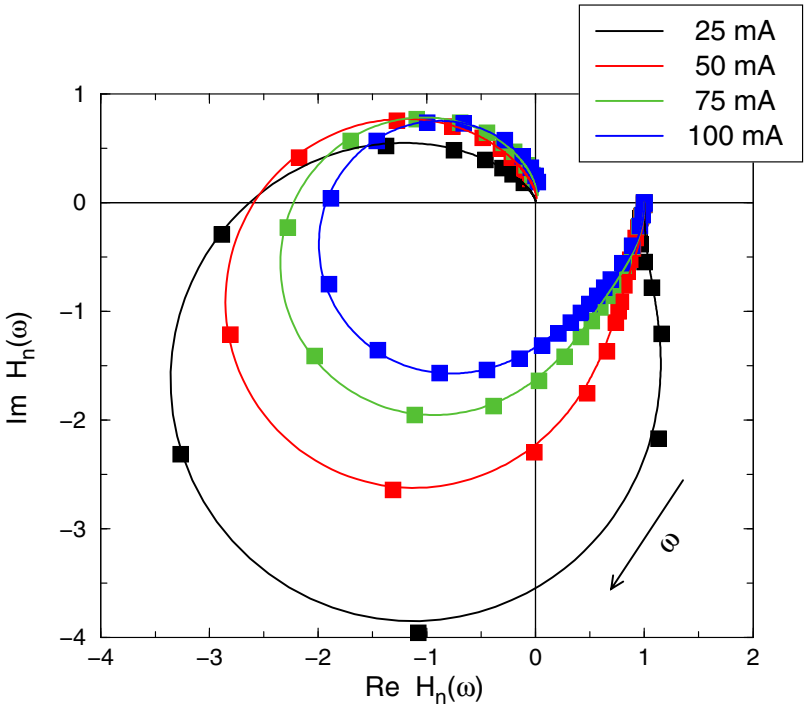

Fig. 3: Complex response functions $H_n(\omega)$. The symbols are results obtained by small-signal analysis while the lines are computed with (1) using extracted parameters as plotted in Fig. 5.

The last factor in (1) is well known from rate equation models (see [2]). The second factor is a low-pass filter while the first one describes some time delay. Both terms are due to parasitic effects, especially to the drift-diffusion transport through the device (see [3], too). The result of the fit is demonstrated in Figure 3. The extracted parameters $f_r = \omega_r/2\pi$, Γ_r, τ and θ are presented in a more suitable form in Figure 5. The frequency $f_{3\mathrm{dB}} = \omega_{3\mathrm{dB}}/2\pi$ is also shown there where $\omega_{3\mathrm{dB}}$ solves the equation $|H_n(\omega_{3\mathrm{dB}})|^2 = 1/2$. Let us note that a fit without using the parasitic terms gives insufficient results.

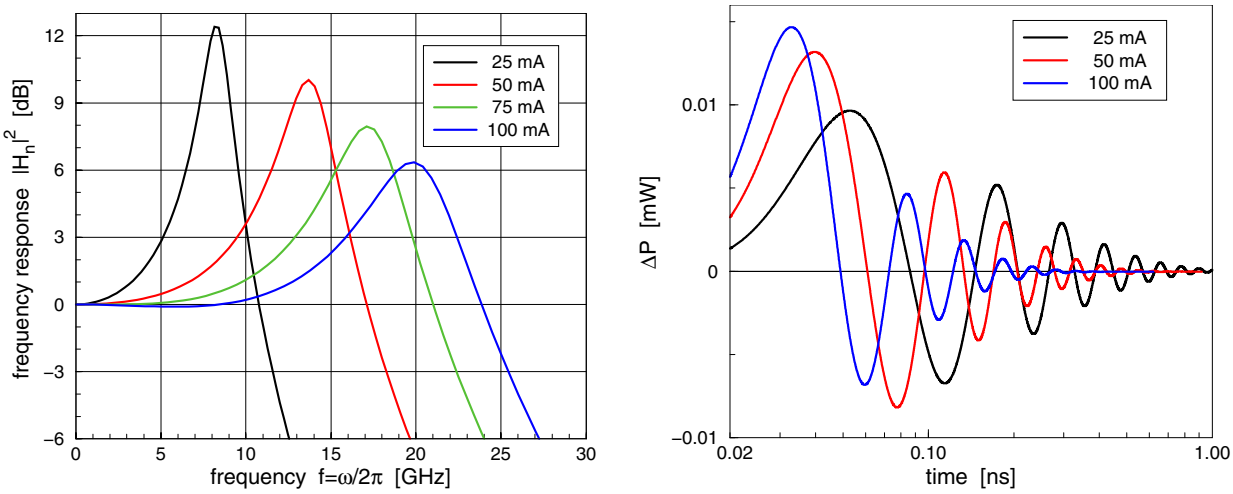

Fig. 4: Simulation results obtained by small-signal analysis in the frequency domain (left) and by pulse excitation in the time domain (right)

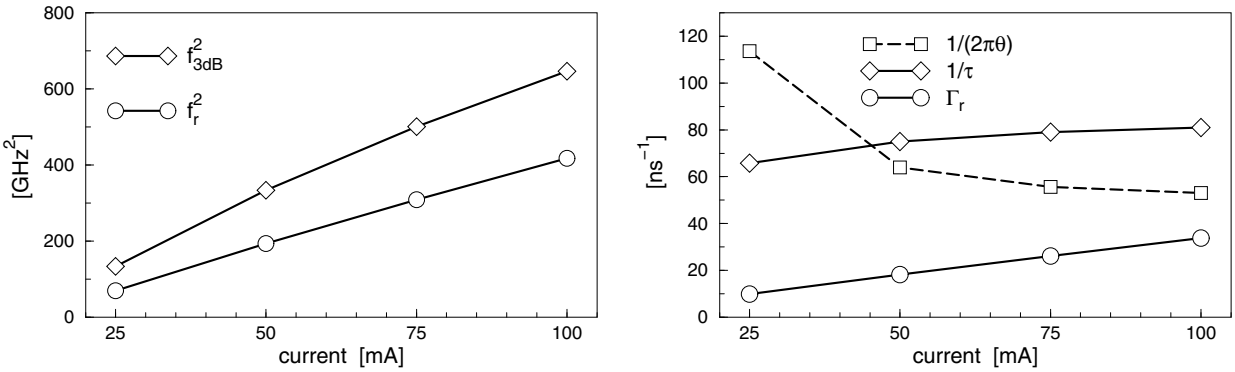

Fig. 5: Extracted parameters f_r^2, $f_{3\mathrm{dB}}^2$ (left) and Γ_r, τ^{-1}, $(2\pi\theta)^{-1}$ (right)

The second method is a current-driven transient simulation where a short rectangular pulse is added to the injection current ($\Delta I(t) = 0.1$ mA, $0 \le t \le 0.02$ ns). `WIAS-TeSCA` computes corresponding variations of the output power $\Delta P(t)$ which are seen in the right-hand side of Figure 4 for $t \ge 0.02$ ns (to enhance clearness the result for $I = 75$ mA was omitted here). Corresponding to (1) the functions ΔP were fitted according to the formula

$$\Delta P(t) = c_1\,\mathrm{e}^{-t/\tau} + c_2\cos(\omega_0 t + \delta)\,\mathrm{e}^{-\Gamma_r t/2}, \quad t \ge 0.02\ \text{ns}, \tag{2}$$

where $\omega_0^2 = \omega_r^2 - \Gamma_r^2/4$, and c_1, c_2, δ depend on ω_r, Γ_r,τ, θ. The parameters extracted in this manner coincide well with the values found by the first method, and with (1) nearly the same frequency response functions as on the left hand side of Figure 4 are obtained. But let us note that this method requires very small time steps in order to get correct results.

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Dissipative Schrödinger-Poisson systems

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

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

Supported by: DFG: "Kopplung von van Roosbroeck- und Schrödinger-Poisson-Systemen mit Ladungsträgeraustausch" (Coupling between van Roosbroeck and Schrödinger-Poisson systems with carrier exchange)

The description of semiconductor devices by drift-diffusion models (van Roosbroeck's system) has been widely accepted for a long time. Moreover, there are well-developed software packages for calculating semiconductors based on drift-diffusion models. However, with the developing miniaturization of semiconductor devices less and less atoms are involved in the processes inside many devices with the consequence that quantum effects become more and more important. Hence, one has to improve the classical drift-diffusion description taking quantum effects at least partially into account. It would be more correct to use a complete quantum mechanical description of semiconductors right from the beginning; however, at present it is not possible to handle such a description numerically. Therefore one has to look for a model which uses a drift-diffusion description in regions where this is recommended and a quantum mechanical one in regions where quantum effects are dominating, for instance, in the active zone of a laser. Both descriptions seem to be incompatible. From the physical point of view it would be desirable to have at least a continuity of the current densities at the interface between the two subregions. This leads to the necessity to consider open quantum systems which are, in contrast to closed quantum systems, not yet well developed.
Considering current coupled models one has at first to find open boundary conditions for the Schrödinger operator. In [6, 7], the proposal was made to use for this purpose the Schrödinger operators with non-selfadjoint boundary conditions which in application to a one-dimensional Schrödinger operator H

$$Hg = -\frac{\hbar^2}{2}\frac{d}{dx}\frac{1}{m}\frac{d}{dx}g + Vg \tag{1}$$

on the interval $\Omega := [a,b] \subseteq \mathbb{R}$, looks like

$$\frac{\hbar}{2m(a)}g'(a) = -\kappa_a g(a) \quad \text{and} \quad \frac{\hbar}{2m(b)}g'(b) = \kappa_b g(b) \tag{2}$$

$\kappa_a, \kappa_b \in \mathbb{C}_+$. Non-selfadjoint Schrödinger operators of the above type and for higher spatial dimensions have been investigated in [2]. In contrast to self-adjoint boundary conditions, which are used in case of closed Schrödinger-Poisson systems, one has to redefine the carrier and current densities. The best way to find suitable definitions is to close the open system since in this case the definitions are clear. In [5], the minimal self-adjoint dilation of H was chosen for the Hamiltonian of the covering closed system. The minimal self-adjoint dilation itself was explicitly constructed in [4] and investigated there in detail. It turned out that the obtained expression of the carrier density is a straightforward generalization of the

corresponding expression in the closed case. Indeed, if the carrier density in the closed case is given by

$$u_\rho(x) = \sum_{l=1}^{\infty} \rho_l |\psi(x,\lambda_l)|^2, \quad x \in [a,b], \tag{3}$$

where λ_l, $\rho(\lambda_l)$ and $\psi(x,\lambda_l)$ denote the eigenvalues, the occupation numbers at the eigenvalue λ_l and the eigenfunction corresponding to the eigenvalue λ_l, respectively, then in the open case one finds

$$u_\rho(x) = \int_{\mathbb{R}} d\lambda \left\langle \rho(\lambda)^T \begin{pmatrix} \psi(x,\lambda,b) \\ \psi(x,\lambda,a) \end{pmatrix}, \begin{pmatrix} \psi(x,\lambda,b) \\ \psi(x,\lambda,a) \end{pmatrix} \right\rangle \tag{4}$$

where $\rho^T(\lambda)$ is the transposed density matrix and $\psi(x,\lambda,b)$, $\psi(x,\lambda,a)$ are the generalized eigenfunctions of the dilation. Hence one has the following correspondence:

$$\begin{aligned} \lambda_l &\leftrightarrow \lambda \\ \psi(x,\lambda_l) &\leftrightarrow \begin{pmatrix} \psi(x,\lambda,b) \\ \psi(x,\lambda,a) \end{pmatrix} \\ \Sigma_{l=1}^{\infty} &\leftrightarrow \textstyle\int_{\mathbb{R}} d\lambda \\ \rho_l &\leftrightarrow \rho(\lambda). \end{aligned} \tag{5}$$

The current density j_ρ, which is always zero in the closed case, is now constant and is, in general, different from zero. Moreover, one gets the representation

$$j_\rho = \frac{1}{2\pi} \int_{\mathbb{R}} d\lambda \, \mathrm{tr}(\rho(\lambda) C(\lambda)) \tag{6}$$

where $C(\lambda)$ is related to the characteristic function of H. Using the redefined notion of carrier density, a dissipative Schrödinger-Poisson system was considered in [3] and we have shown that this system always has a solution. The electrostatic potential is always bounded by a constant which is determined by the data of the problem. The solution is in general not unique. In [1] an attempt was made to include generation and recombination effects into the dissipative Schrödinger-Poisson systems.

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Physical modeling and numerical simulation of heat and carrier transport for high-power semiconductor devices semiconductor devices

Collaborators: H. Gajewski, H. Stephan

Cooperation with: G. Wachutka, W. Kaindl (Technische Universität München)

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) [2]

In 2002 our model [1], describing heat and carrier transport for semiconductor devices, has been advanced to silicon carbide (SiC). SiC is used in different crystal configurations (6H-SiC, 4H-SiC, 3C-SiC). Each of these materials possesses promising properties as basic materials for high-power, high-temperature and high-frequency electronics. The reason for this are special physical characteristics, which distinguish SiC from conventional semiconductor materials such as silicon. Those are first of all:

- **Anisotropy:** For each crystal configuration it is typical that physical quantities, such as carrier mobilities or heat conductivity, depend on the crystal orientation. It follows that appropriate physical quantities are no longer scalars but tensors. For example, the electron mobility in the hexagonal plain of 4H-SiC is five times larger than in the perpendicular direction.
- **Wide band gap:** The band gap in SiC is up to 3.2 eV (for comparison, the band gaps in Si and GaAS are 1.1 eV and 1.42 eV, respectively). This makes the material interesting for optoelectronics (blue LEDs). However, numerical problems can arise, since the gap enters exponentially into the equations of state. Additionally, the wide gap may lead to an only incomplete ionization of the dopants (in particular boron). This means, dopants have to be considered as traps.
- **High temperature resistance:** This—very welcome characteristic—requires the consideration of a large parameter area for temperature dependence of material data for the simulation.

Deriving the system of nonlinear partial differential equations for the heat and carrier transport in semiconductor devices, we abided by the following physical principles:

1. postulation of the free energy density;
2. calculation of the equilibrium according to the entropy maximum principle;
3. definition of the thermodynamic potentials near the equilibrium state;
4. postulation of the evolution equations;
5. calculation of the currents and right-hand sides according to the second law of thermodynamics;
6. derivation of the heat equation.

The postulated system of equations

$$\begin{aligned}
-\nabla\cdot(\varepsilon\nabla\psi) &= D-n+p, \quad \text{(Poisson's equation)}\\
\frac{\partial n}{\partial t}-\nabla\cdot J_n &= G, \quad \text{(transport equation for electrons)}\\
\frac{\partial p}{\partial t}+\nabla\cdot J_p &= G, \quad \text{(transport equation for holes)}\\
\frac{\partial u}{\partial t}+\nabla\cdot J_u &= 0. \quad \text{(energy equation)}
\end{aligned}$$

describes electron, hole and energy transfer, which is nonlinearly coupled by the electrostatic potential ψ via Poisson's equation. Here, n, p and u are electron, hole and power density, J_n, J_p and J_u the appropriate currents, D the dopants and G the generation-recombination rate. (The ODEs describing the dynamics of electron/hole traps were described in detail in the WIAS Annual Research Report 1998.)
The determination of the equilibrium as state of maximal entropy by Lagrange's method suggests the Lagrange multipliers $\frac{\varphi_n}{T}$, $\frac{\varphi_p}{T}$ and $-\frac{1}{T}$ to be thermodynamic potentials. Their gradients are the driving forces for the currents. That leads to the following current, under consideration of Onsager's principle:

$$\begin{pmatrix} J_n \\ J_p \\ J_u \end{pmatrix} = \begin{pmatrix} -(\sigma_n+\sigma_{np}) & \sigma_{np} & a_{nu} \\ \sigma_{np} & -(\sigma_p+\sigma_{np}) & a_{pu} \\ a_{nu} & a_{pu} & a_u \end{pmatrix} \bullet \begin{pmatrix} \nabla\frac{\varphi_n}{T} \\ \nabla\frac{\varphi_p}{T} \\ -\nabla\frac{1}{T} \end{pmatrix}.$$

In the case of the anisotropic SiC, σ_p, σ_n and σ_{np}, and a_{nu}, a_{np} and a_u are 3×3 matrices. From the second law of thermodynamics (entropy S increasing in time)

$$\dot{S} = \int_\Omega \dot{s}\,dx = -\int_\Omega \nabla J_s\,dx + \int_\Omega d\,dx \geq 0$$

(here d denotes the dissipation rate) it follows for the currents

$$\begin{aligned}
J_n &= -\sigma_n z_n - \sigma_{np}(z_n - z_p),\\
J_p &= -\sigma_p z_p - \sigma_{pn}(z_p - z_n),\\
J_u &= -\psi\varepsilon\nabla\psi_t - \kappa_L\nabla T - (P_nT-\varphi_n)J_n + (P_pT+\varphi_p)J_p,
\end{aligned}$$

with

$$z_n = T\left(\nabla\frac{\varphi_n}{T} + (P_nT-\varphi_n)\nabla\frac{1}{T}\right), \quad z_p = T\left(\nabla\frac{\varphi_p}{T} - (P_pT+\varphi_p)\nabla\frac{1}{T}\right)$$

and the energy carrier interaction terms (κ_l is the heat conductivity)

$$\begin{aligned}
a_{nu} &= \sigma_n(\varphi_n - P_nT) + \sigma_{np}(\varphi_p + P_pT), \quad a_{pu} = \sigma_{np}(\varphi_n - P_nT) + \sigma_p(\varphi_p + P_pT)\\
a_u &= \sigma_n|\varphi_n - P_nT|^2 + \sigma_p|\varphi_p + P_pT|^2 + 2\sigma_{np}(\varphi_p + P_pT)(\varphi_n - P_nT) + \kappa_L T^2.
\end{aligned}$$

For this model, thermodynamically consistent algorithms were developed and implemented into our program system `WIAS-TeSCA`.

As an example we show a 6H-SiC DIMOS transistor—a typical high-power device ([4]). The crystal is oriented in such a way that the electron mobility in horizontal direction is five times higher than in the vertical direction. Figure 2 shows the electron flow for a gate voltage of 12 V and a drain voltage of 30 V. In comparison, Figure 3 shows the simulation result for isotropic mobility (e.g., in Si).

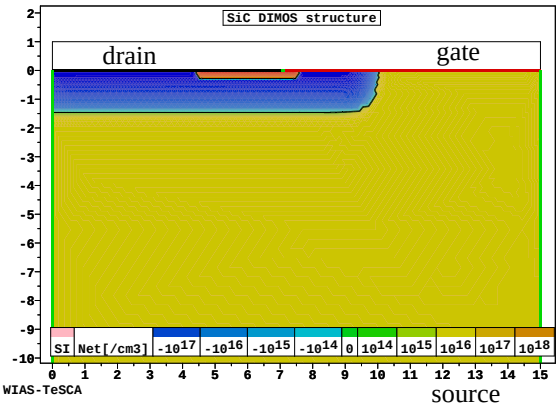

Fig. 1: Dopants

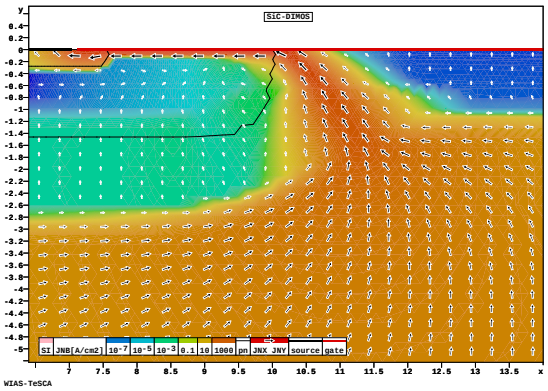

Fig. 2: Anisotropic case

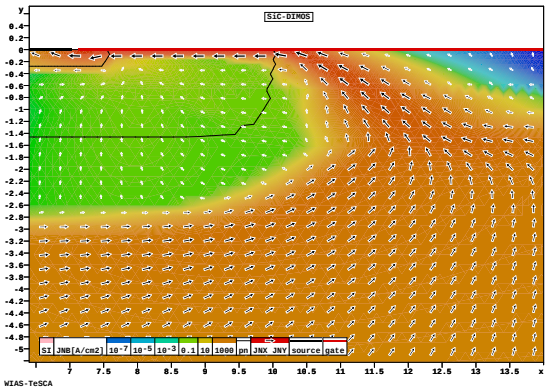

Fig. 3: Isotropic case

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Stationary solutions of two-dimensional heterogeneous energy models with multiple species near equilibrium

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Supported by: DFG: "Zur Analysis von thermodynamischen Modellen des Stoff-, Ladungs- und Energietransports in heterogenen Halbleitern" (Analysis of thermodynamic models for the transport of mass, charge and energy in heterogeneous semiconductors)

We consider a stationary energy model for reaction-diffusion processes of electrically charged species with non-local electrostatic interaction. Such problems arise in electrochemistry as well as in semiconductor device and technology modeling (see, e.g., [2]). But, in contrast to [2] we now additionally take thermal effects into account. We consider a finite number of species X_i, $i = 1,\dots,n$ (e.g., electrons, holes, dopants, interstitials, vacancies, dopant-defect pairs). Let φ and T be the electrostatic potential and the lattice temperature. We denote by u_i, ζ_i, q_i the particle density of the i-th species, its electrochemical potential and its charge number. The state equations are assumed to be given by the ansatz (see [1])

$$u_i = \bar{u}_i(x,T)\,\mathrm{e}^{(\zeta_i - q_i\varphi + E_i(x,T))/T}, \quad i = 1,\dots,n.$$

We consider a finite number of reversible reactions of the form

$$\alpha_1 X_1 + \dots + \alpha_n X_n \rightleftharpoons \beta_1 X_1 + \dots + \beta_n X_n.$$

The set of stoichiometric coefficients $(\alpha,\beta) = (\alpha_1,\dots,\alpha_n,\beta_1,\dots,\beta_n)$ belonging to all reactions is denoted by $\mathcal{R}$. According to the mass-action law the reaction rates $R_{\alpha\beta}$ are prescribed by

$$R_{\alpha\beta} = r_{\alpha\beta}(x,u,T)\Big(\mathrm{e}^{\sum_{i=1}^n \alpha_i\zeta_i/T} - \mathrm{e}^{\sum_{i=1}^n \beta_i\zeta_i/T}\Big), \quad (\alpha,\beta)\in\mathcal{R}.$$

Here u means the vector $(u_1,\dots,u_n)$. For the particle flux densities j_i and the total energy flux density j_e we make the ansatz (see [1])

$$j_i = -\sum_{j=1}^n \sigma_{ij}(x,u,T)\big(\nabla\zeta_j + P_j(x,u,T)\nabla T\big), \quad i = 1,\dots,n,$$

$$j_e = -\kappa(x,u,T)\nabla T + \sum_{i=1}^n (\zeta_i + P_i(x,u,T)T)\,j_i$$

with conductivities σ_{ij}, κ fulfilling

$$\sigma_{ij} = \sigma_{ji}, \quad \sum_{i,j=1}^n \sigma_{ij}(x,u,T)t_it_j \ge \sigma_0(u,T)\sum_{j=1}^n t_i^2 \quad \forall t\in\mathbb{R}^n, \quad \kappa(x,u,T)\ge\kappa_0(u,T)$$

where $\sigma_0(u,T)$, $\kappa_0(u,T) > 0$ for all non-degenerated states u, T. For the fluxes $(j_1,\dots,j_n,j_e)$ and the generalized forces $(\nabla[\zeta_1/T],\dots,\nabla[\zeta_n/T],-\nabla[1/T])$, the Onsager relations are fulfilled.

The basic equations of the energy model contain n continuity equations for the considered species, the conservation law of the total energy and the Poisson equation,

$$\left.\begin{aligned} \nabla \cdot j_i &= \sum_{(\alpha,\beta)\in\mathcal{R}} (\beta_i - \alpha_i) R_{\alpha\beta}, \quad i = 1,\dots,n, \\ \nabla \cdot j_e &= 0, \\ -\nabla \cdot (\varepsilon \nabla \varphi) &= f + \sum_{i=1}^{n} q_i u_i \end{aligned}\right\} \quad \text{in } \Omega \subset \mathbb{R}^2. \tag{1}$$

Here ε is the dielectric permittivity and f represents some fixed charge density. System (1) must be completed by suitable mixed boundary conditions. We introduce the new variables $\lambda = (\lambda_1,\dots,\lambda_{n+2}) = (\zeta_1/T,\dots,\zeta_n/T,-1/T,\varphi)$. With some functions H_i we can reformulate the state equations in the form

$$u_i(x) = H_i(x,\lambda), \quad i = 1,\dots,n.$$

Also the reaction rates $R_{\alpha\beta}$ are expressed in the new variables

$$R_{\alpha\beta}(x,\lambda) = r_{\alpha\beta}(x,H_1(\lambda),\dots,H_n(\lambda),-1/\lambda_{n+1}) \left(\mathrm{e}^{\sum_{i=1}^n \alpha_i\lambda_i} - \mathrm{e}^{\sum_{i=1}^n \beta_i\lambda_i} \right), \quad (\alpha,\beta) \in \mathcal{R}.$$

Then the stationary energy model can be written as a strongly coupled nonlinear elliptic system

$$-\nabla \cdot \begin{pmatrix} a_{11}(\lambda) & \cdots & a_{1,n+1}(\lambda) & 0 \\ \vdots & \ddots & \vdots & 0 \\ a_{n,1}(\lambda) & \cdots & a_{n,n+1}(\lambda) & 0 \\ a_{n+1,1}(\lambda) & \cdots & a_{n+1,n+1}(\lambda) & 0 \\ 0 & 0 & 0 & \varepsilon \end{pmatrix} \begin{pmatrix} \nabla\lambda_1 \\ \vdots \\ \nabla\lambda_n \\ \nabla\lambda_{n+1} \\ \nabla\lambda_{n+2} \end{pmatrix} = \begin{pmatrix} \sum_{(\alpha,\beta)\in\mathcal{R}} (\beta_1 - \alpha_1) R_{\alpha\beta}(\lambda) \\ \vdots \\ \sum_{(\alpha,\beta)\in\mathcal{R}} (\beta_n - \alpha_n) R_{\alpha\beta}(\lambda) \\ 0 \\ f + \sum_{k=1}^n q_k H_k(\lambda) \end{pmatrix}. \tag{2}$$

Here we have omitted the additional argument x of the coefficient functions. We assume that the Dirichlet parts Γ_D and the Neumann parts Γ_N of the boundary conditions coincide for all quantities. Then we can formulate the boundary conditions in terms of λ,

$$\begin{aligned} \lambda_i &= \lambda_i^D, \quad i = 1,\dots,n+2, \text{ on } \Gamma_D, \\ \nu \cdot \textstyle\sum_{j=1}^{n+1} a_{ij}(\lambda)\nabla\lambda_j &= g_i, \quad i = 1,\dots,n+1, \quad \nu \cdot (\varepsilon\nabla\lambda_{n+2}) = g_{n+2} \text{ on } \Gamma_N. \end{aligned} \tag{3}$$

We assume that $\Omega \cup \Gamma_N$ is regular in the sense of [4] and that the boundary values λ_i^D, $i = 1,\dots,n+2$, are traces of $W^{1,p}(\Omega)$ functions, $p > 2$. We are looking for solutions of (2), (3) in the form $\lambda = \Lambda + \lambda^D$. Under weak assumptions on the coefficient functions $a_{ij}(x,\lambda)$ and $\varepsilon(x)$ (such that heterostructures are allowed) we found $W^{1,q}$ formulations ($q \in (2,p]$) for that system of equations,

$$F(\Lambda,\lambda^D,f,g) = 0, \quad \Lambda \in W_0^{1,q}(\Omega \cup \Gamma_N)^{n+2}.$$

If the boundary values λ_i^{D*}, $i = 1,\dots,n+1$, are constants, $\lambda_{n+1}^{D*} < 0$ and λ_i^{D*}, $i = 1,\dots,n$, correspond to a simultaneous equilibrium of all reactions

$$\sum_{i=1}^n \alpha_i \lambda_i^{D*} = \sum_{i=1}^n \beta_i \lambda_i^{D*} \quad \forall (\alpha,\beta) \in \mathcal{R}\,,$$

and if λ_{n+2}^{D*}, $f^*, g^* = (0,\dots,0,g_{n+2}^*)$ are arbitrarily given, then there exists a unique solution Λ^* of $F(\Lambda^*,\lambda^{D*},f^*,g^*)=0$. $\lambda^* = \Lambda^* + \lambda^{D*}$ is a thermodynamic equilibrium of (2), (3). The operator F is continuously differentiable and the linearization $\frac{\partial F}{\partial \Lambda}(\Lambda^*,\lambda^{D*},f^*,g^*)$ turns out to be an injective Fredholm operator of index zero. This follows from results in [5] and from a regularity result of Gröger in [4] for systems of elliptic equations with mixed boundary conditions. Therefore we can apply the Implicit Function Theorem and obtain that for λ^D near λ^{D*}, f near f^* and g near g^* the equation $F(\Lambda,\lambda^D,f,g)=0$ has a unique solution Λ near Λ^*. Thus, near λ^* there is a locally unique Hölder continuous solution $\lambda = \Lambda + \lambda^D$ of (2), (3). For details and the precise assumptions of our investigations see [3].
Our local existence and uniqueness result for the stationary energy model (2), (3) works in two space dimensions. But let us note that in our model equations cross-terms with respect to all species and temperature are involved.

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Optimal control of surface heat treatments

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Supported by: Stiftung Industrieforschung, Köln

In most structural components in mechanical engineering, there are surface parts which are particularly stressed. The aim of surface hardening is to increase the hardness of the corresponding boundary layers by rapid heating and subsequent quenching. This heat treatment leads to a change in the microstructure, which produces the desired hardening effect.
Depending on the respective heat source one can distinguish between different surface hardening procedures, the most important ones being induction hardening and radiation treatments like laser- and electron-beam hardening.

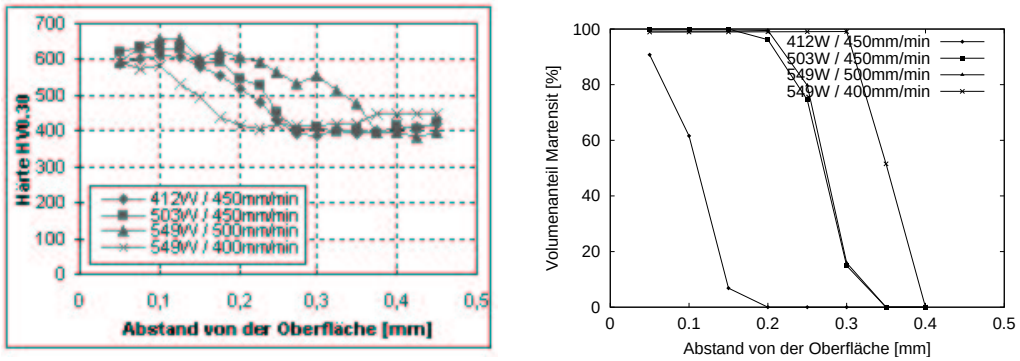

Fig. 1: Laser surface hardening of the steel X35CrMo17: Comparison of simulation (right) with experiment (left)

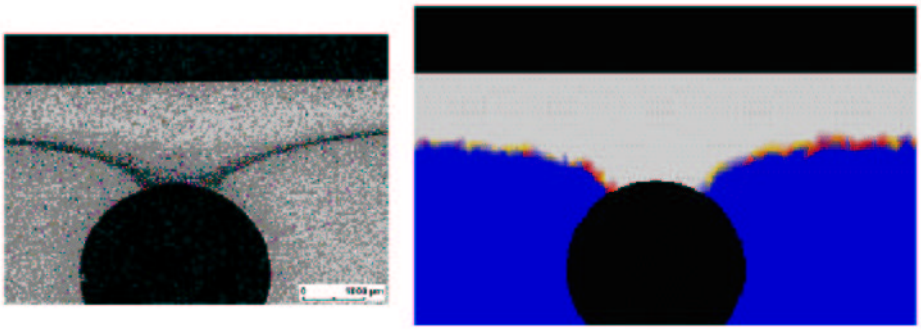

Fig. 2: Electron beam surface hardening of the steel C45: Comparison of simulation (right) with experiment (left)

To complete our industrial project on simulation and control of laser- and electron-beam hardening a Mathematica tool has been developed and used to identify the transformation parameters of our phase transition model for a number of relevant steels. These parameters have been added to the data base of `WIAS-SHarP`. Numerical simulations for all these steels,

with varying laser intensity and different workpiece geometries, have been carried out. The results, which are in good agreement with experiments (cf. Figures 1, 2), are documented in [1].
Another important control problem related to surface hardening is the optimal design of inductor coils for induction surface hardening. In [4] the speed method has been applied to investigate the sensitivity of solutions to the state equations with respect to perturbations of the inductor. In the case of inductors constructed from space curves it has been shown in [2] that one can relate the resulting shape gradient to a perturbation of the generating curve.

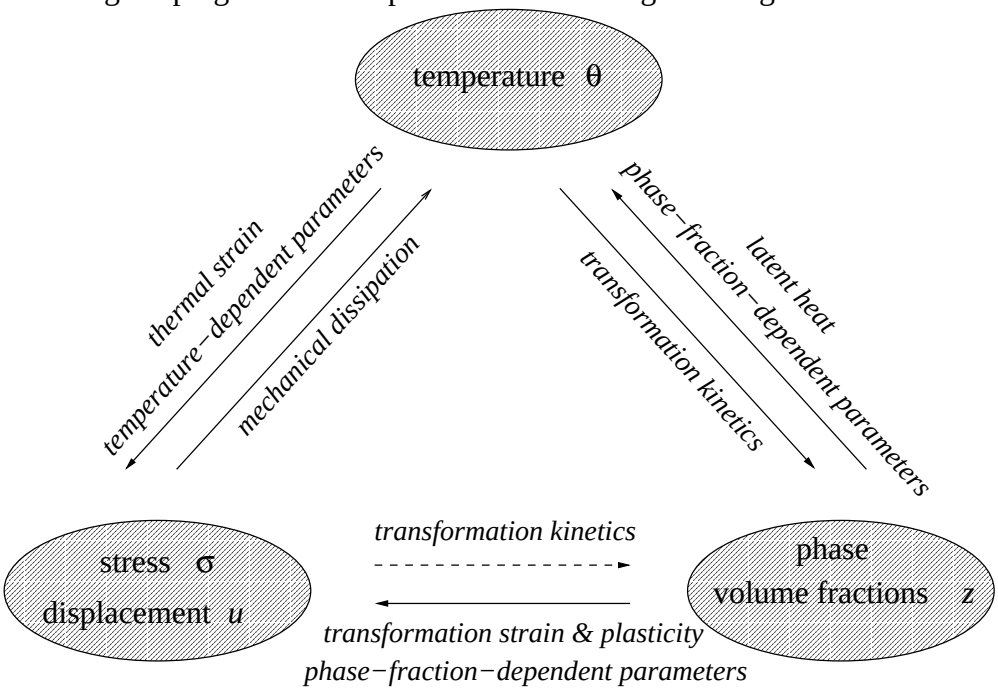

Fig. 3: Phase transitions with thermomechanics — interdependence of physical quantities

Figure 3 shows the complex interdependence of the relevant physical quantities for phase transitions in steel. The interplay between temperature θ and volume fraction z is well understood (cf., e.g., [1]). The metallurgical phases z_i have material parameters with different thermal characteristics, hence their effectice 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 [2], [3].

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Hysteresis phenomena

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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.

a) The modeling of uniaxial nonlinear thermo-visco-plastic developments leads to the system

$$\rho u_{tt} - \mu u_{xxt} = \sigma_x + f(x,t), \tag{1}$$

$$\sigma = \mathcal{H}_1[u_x, w] + \theta \mathcal{H}_2[u_x, w], \tag{2}$$

$$(C_V \theta + \mathcal{F}[u_x, w])_t - \kappa \theta_{xx} = \mu u_{xt}^2 + \sigma u_{xt} + g(x,t,\theta), \tag{3}$$

$$\nu w_t + \mathcal{H}_3[u_x, w] + \theta \mathcal{H}_4[u_x, w] = 0, \tag{4}$$

where u, θ, σ, and w are the unknowns displacement, absolute temperature, elastoplastic stress, and freezing index, respectively, ρ, μ, C_V, and ν are positive constants, f, g are given functions, and $\mathcal{H}_1, \ldots, \mathcal{H}_4$, and $\mathcal{F}$ are hysteresis operators. In [4], this system has been derived, its thermodynamic consistency has been proved, and the existence of a unique strong solution to an initial-boundary value problem for this system has been shown. In [1], this existence result has been generalized to the case of a more general boundary condition for u and a weaker assumption for $\mathcal{H}_2$ and $\mathcal{H}_4$. More precisely, the assumption that these operators are bounded has been replaced by the assumption that the clockwise admissible potential connected to these operators can be bounded from below by $-C\mathcal{F}$, with some positive constant C.

A large-time asymptotic result for this system has been derived in [2]. An approach used therein to derive uniform estimates for the solutions to partial differential equations involving hysteresis operators has been further investigated in [3], leading to the notion of "outward pointing hysteresis operators". Moreover, in [3], generalizations of scalar Prandtl-Ishlinskii operators have been introduced and investigated with respect to their thermodynamic consistency.

b) In [5], a control problem for an ordinary differential system with hysteresis has been investigated. For controls $u : [0,T] \to \mathbb{R}^m$, one considers the system

$$z' = f(t,z,y,u), \quad \text{in} \quad [0,T], \quad z(0) = z_0 \in \mathbb{R}^m, \tag{5}$$

$$y(t) = \mathcal{W}(g \circ z)(t) \qquad \text{in} \quad [0,T] \tag{6}$$

with $f : [0,T] \times \mathbb{R}^N \times \mathbb{R} \times \mathbb{R}^m \to \mathbb{R}^N$ and $g : \mathbb{R}^N \to \mathbb{R}$ being continuous functions, and $\mathcal{W} : C[0,T] \to C[0,T]$ being a hysteresis operator. Under appropriate conditions, the existence of at least one global solution has been proved. Moreover, $u(t) \in U$ for all $t \in [0,T]$, for a bounded, closed, convex set $U \subset \mathbb{R}^m$. For such controls u and the corresponding solutions (z,y) to (5), (6) we associate the cost functional

$$\int_0^T L(y(t), z(t), u(t))\,dt \tag{7}$$

with $L : \mathbb{R} \times \mathbb{R}^N \times U$ continuous in y,z, convex and lower semicontinuous with respect to u. It has been proved that the corresponding optimal control problem has at least one solution.

An approximation method and a conceptual algorithm are discussed as well.

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Quasilinear parabolic systems with discontinuous coefficients and mixed boundary conditions on two-dimensional space domains

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Supported by: DFG: "Kopplung von van Roosbroeck- und Schrödinger-Poisson-Systemen mit Ladungsträgeraustausch" (Coupling between van Roosbroeck and Schrödinger-Poisson systems including exchange of carriers)

The work of 2002 continued that reported in 2000; our aim was to prove a theorem on (local) existence for quasilinear parabolic systems on an L^p space which should enable the treatment of the van Roosbroeck system and similar reaction-diffusion systems in heterogeneous media in an L^p context. The motivation for this is the following: The natural formulation of balance laws is

$$\frac{\partial}{\partial t}\int_\Lambda u_k dx = \int_{\partial\Lambda} \langle \nu, j_k\rangle \, d\sigma + \int_\Lambda R_k(u_1,...,u_l)dx, \quad k=1,\dots,l. \tag{1}$$

Here u_k is the particle density of the k-th species, j_k is the corresponding flux, R_k a reaction term and Λ any (suitable) subdomain of the whole domain under consideration. However, generally such equations are treated by substituting the boundary integral of the normal component of the current by the volume integral of the divergence of the corresponding current. The problem whether the thus obtained solutions in fact also satisfy the original equations remains completely unsolved. The mathematical reason is that in the calculi used up to now indicator functions of sets are not admissible as test functions. Hence, Gauss' theorem, which underlies the above-mentioned reformulation, is not applicable. Even worse, the notion of the normal component of the flux cannot be strictly defined when operating in negatively indexed Sobolev spaces. With the aim of coupling van Roosbrock's system with an open quantum system (describing nanosubstructures within the device under consideration) it is unavoidable to have the normal component of the current through interfaces at hand because current coupling is the most natural way to combine both systems (cf. [5]).
Apart from that, space discretization of such systems is often performed using finite volume schemes, cf. [4]. In order to compare such a scheme with the original equations these equations have to be valid in the space of integrable functions on the simulation domain.
Mathematically, the main results are as follows:
Theorem 1 Spatially two-dimensional quasilinear systems of the type

$$\frac{\partial \mathbf{w}}{\partial t} + \begin{pmatrix} 1+Z_{1,1}(t,\mathbf{w}(t)) & \dots & Z_{1,l}(t,\mathbf{w}(t)) \\ \dots & \dots & \dots \\ Z_{l,1}(t,\mathbf{w}(t)) & \dots & 1+Z_{l,l}(t,\mathbf{w}(t)) \end{pmatrix} \begin{pmatrix} -J_1(t,\mathbf{w}(t))\nabla\mu_1\nabla w_1 \\ \dots \\ -J_l(t,\mathbf{w}(t))\nabla\mu_l\nabla w_l \end{pmatrix} = \mathbf{f}(t,\mathbf{w}(t)), \tag{2}$$

$\mathbf{w}(T_0)=\mathbf{w}_0$, admit exactly one (local) classical solution in a (suitably chosen) L^p space provided the data satisfy the following conditions:

i) Each J_k maps a suitable interpolation space between the domain of $(-\nabla\mu_1\nabla,...,-\nabla\mu_l\nabla)$ and $\left(L^p\right)^l$ into L^∞ and additionally satisfies some continuity conditions.

ii) The mappings $Z_{1,1},...,Z_{l,l}$ take their values in a set of compact operators on L^p and also satisfy some continuity conditions.

iii) The coefficients μ_k may be discontinuous and the operators $-\nabla\mu_k\nabla$ are complemented by mixed boundary conditions.

This theorem rests heavily on classical results for abstract quasilinear parabolic equations in a Banach space [7], [10], interpolation results for function spaces which carry a trace condition on part of the boundary [2] and resolvent estimates for elliptic operators in divergence form including discontinuous coefficients and mixed boundary conditions [1].
Having the above theorem at hand, one succeeds in proving:
Theorem 2 The spatially two-dimensional van Roosbroeck system admits (locally in time) a classical solution in L^p. Hereby a broad class of recombination terms, including nonlocal ones, are admissible.
This theorem is derived from the first one by reformulating van Roosbroeck's system in a rather cumbersome procedure: One expresses the densities in terms of the electrostatic potential and the quasi-Fermi levels, then eliminates the time derivative of the electrostatic potential and afterwards the electrostatic potential itself via the nonlinear Poisson equation. This way, one ends up with a quasilinear system as above for the quasi-Fermi levels. The authors believe that the consistent treatment of the equations in much more regular spaces as before is not accidental but caused by the physical expectation that the quasi-Fermi levels should be the most regular objects within a heterogeneous context.
Finally, we will give a short outlook on the 3D case, which in our opinion should also be treated in a concept which provides as much regularity as possible (strong differentiability of the solution, the divergence of the currents being L^p functions....). The cornerstone to carry out the same program for the 3D case would be a result that the operators $\nabla\mu_k\nabla$—including nonsmooth coefficients μ_k and mixed boundary conditions—provide isomorphisms between spaces $H^{1,q}_\Gamma$, $H^{-1,q}$ for a summability index q greater than 3. Unfortunately, this is known to be false in general (cf. [9]). In a forthcoming paper [8] it will be shown that it is true, however, in case of pure Dirichlet conditions and restrictions on the domain and the—discontinuous—coefficient functions. Further, it is expected that the same is true for smooth domains and the Laplace operator including mixed boundary conditions [3]. The task would be to prove that the latter assertion is really true, further to prove the analogous assertion in case of pure Neumann conditions and discontinuous coefficients and fit all these things together.

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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")

Owing to numerous technical applications in electronic and optoelectronic devices, such as lasers, diodes, and sensors, 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. It is the goal of this project to use mathematical modeling and numerical simulation to help optimizing the PVT method.
During PVT, a graphite crucible (see Figure 1) is placed in a low-pressure inert gas atmosphere consisting of argon. The crucible is then intensely heated, e.g., by induction heating, to temperatures up to 3000 K. Inside the crucible, polycrystalline SiC source powder sublimates, adding molecules made up of silicon and carbon to the gas phase. For the moment, we abuse notation to denote the total of the added species as the *SiC gas*, notwithstanding the fact that it consists predominantly of other molecules than SiC. The SiC gas diffuses 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, SiC gas crystallizes on the seed, which thereby grows into the reactor.

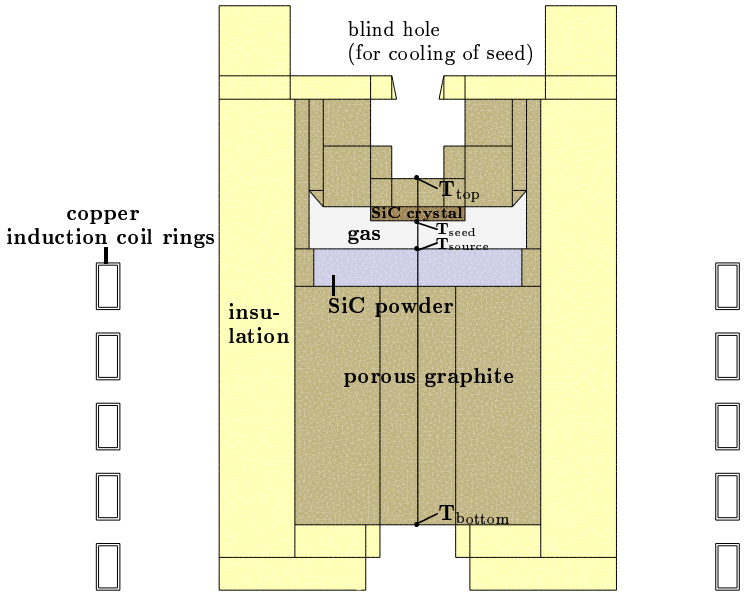

Fig. 1: Setup of growth apparatus according to [1]

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. Moreover, several free boundaries occur in the model, e.g., due to the growing crystal and due to the sublimating source powder. The main control parameters with respect to an optimization of the crystal growth process are the design of the growth apparatus, the position of the induction coil, the heating power, and the inert gas pressure.
Within the research year 2002, the conditions for the growth of the crystal have been further investigated. As a first approximation, one can assume that the pressure $p_{\text{SiC-gas}}$ of the SiC gas at the surface of the crystal is identical to the corresponding equilibrium pressure $p^{\text{eq}}_{\text{crystal}}$. At the powder surface, one would then make the corresponding assumption. However, this approach supposes that the growth process is limited by the transport through the gas phase and it omits the influence of the growth kinetics.
To take into account the influence of the growth kinetics, one can use a Hertz-Knudsen formula to determine the mass flux from the gas to the crystal:

$$j_{\text{gas}\,\rightarrow\,\text{crystal}} = \frac{s_{\text{crystal}}\, M_{\text{SiC}}^{1/2}}{(2\pi RT)^{1/2}} \left(p_{\text{SiC-gas}} - p^{\text{eq}}_{\text{crystal}} \right). \tag{1}$$

Here, $s_{\text{crystal}} \in [0,1]$ is a sticking coefficient. It denotes the probability for a molecule that collides with the surface to stick to that surface and be absorbed. Moreover, M_{SiC} is the molar mass of SiC (in kg/kmol), and R is the universal gas constant. On the powder surface, one would use a similar condition with some effective sticking coefficient, taking into account that the surface is jagged and porous.
If the model is to include the observed graphitization of the powder source, it becomes necessary to consider the different constituents of the "SiC gas", consisting of Si, SiC_2, Si_2C, Si_2, SiC, etc. Instead of simple sublimation, one has to consider several chemical reactions occurring at the surfaces. Then, instead of equilibrium pressures for the different components, one merely has relations between the different partial pressures in the equilibrium, resulting from the mass action laws of the considered chemical reactions. For example, from the reactions

$$2\text{SiC} \longrightarrow \text{Si} + \text{SiC}_2, \qquad \text{SiC} + \text{Si} \longrightarrow \text{Si}_2\text{C}, \qquad \text{SiC} + \text{Si}_2 \longrightarrow \text{Si}_2\text{C} + \text{Si}$$

involving solid SiC and some gas species, the mass action laws yield that there are temperature-dependent functions K_{I}, K_{II}, and K_{III} such that for the partial pressures of a gas mixture in equilibrium with the SiC crystal, it holds that

$$p_{\text{Si}}\, p_{\text{SiC}_2} = K_{\text{I}}(T), \qquad \frac{p_{\text{Si}_2\text{C}}}{p_{\text{Si}}} = K_{\text{II}}(T), \quad \frac{p_{\text{Si}_2\text{C}}\, p_{\text{Si}}}{p_{\text{Si}_2}} = K_{\text{III}}(T).$$

Further research is ongoing to formulate the corresponding mass action laws for reactions changing the composition of the surface, to model the kinetics of the chemical reactions, and to determine the involved material parameters.
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 [2, 3, 4].
The transient nonlinear and nonlocal heat transport equations are discretized using an implicit Euler scheme in time and a finite volume method in space. Within the period covered by this report, existence and uniqueness results for the solution to the resulting nonlinear and nonlocal

discrete scheme have been established. Moreover, discrete L^∞-L^1 a priori estimates have been proved [6].
Within the covered research period, the simulation software `WIAS-HiTNIHS` (see page 263) has been installed at the IKZ. Figure 2 depicts results of a numerical simulation of the heating process for the configuration of Figure 1 which we published in [5]. The angular frequency used for the induction heating is $\omega = 2\pi f$, where $f = 10$ kHz. The average total power P is prescribed according to the following linear ramp:

$$P(t) := \begin{cases} \frac{P_{\max}}{t_{\text{ramp}}} \cdot t & \text{for } 0 \le t \le t_{\text{ramp}}, \\ P_{\max} & \text{for } t \ge t_{\text{ramp}}, \end{cases} \tag{2}$$

where $t_{\text{ramp}} = 2$ h. Each simulation starts at $T_{\text{room}} = 293$ K.

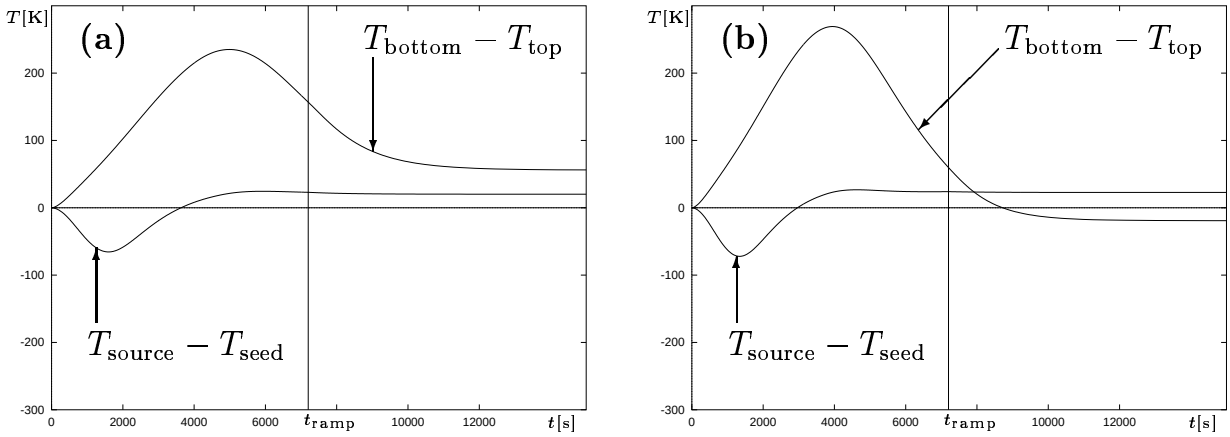

Fig. 2: The evolution of the temperature differences $T_{\text{bottom}} - T_{\text{top}}$ and $T_{\text{source}} - T_{\text{seed}}$ is compared for two different values of $P_{\max}$: $P_{\max} = 5.5$ kW in (a) and $P_{\max} = 8.5$ kW in (b). For the respective locations of T_{bottom}, T_{top}, T_{source}, and T_{seed}, it is referred to Figure 1.

We investigate the relation between the temperature differences $T_{\text{bt}} := T_{\text{bottom}} - T_{\text{top}}$ and $T_{\text{ss}} := T_{\text{source}} - T_{\text{seed}}$. The relation between T_{bt} and T_{ss} is of importance, as in physical growth experiments T_{bottom} and T_{top} are measured, and T_{bt} is often used as an indicator for T_{ss} which is not accessible to direct measurements, but crucial for the growth process. Figure 2 shows that in both cases, T_{bt} is no indicator for T_{ss} before T_{ss} has reached its quasi-stationary final state, but, more importantly, even in the stationary state at growth temperature, T_{bt} is almost three times as large as T_{ss} for $P_{\max} = 5.5$ kW, and T_{bt} and T_{ss} have different signs for $P_{\max} = 8.5$ kW. The numerical experiments show that for the considered configuration, there is generally no easy relation between T_{ss} and T_{bt}. Even though there might be configurations where the situation is better, for each real growth system, the validity of using T_{bt} as an indicator for T_{ss} needs to be verified by some other method (e.g., numerical simulation).

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Approximation and optimization of curved mechanical structures

Collaborators: J. Sprekels, D. Tiba

Cooperation with: V. Arnăutu ("Alexandru Ioan Cuza" University, Iasi, Romania)

The importance, and the many technical applications, of various curved mechanical structures like arches, curved rods, shells are well known. The scientific literature concerning their modeling is very rich, see [1], [2]. We only mention the classes of *polynomial models* and the *asymptotic models*.
The aim of this research project is the study of optimization problems naturally associated to such models. In the previous paper [3], the Kirchhoff-Love model for arches and its optimization have been discussed. In [4], we concentrate on the case of polynomial models for curved rods and shells. The model introduced for shells is of a generalized Naghdi type ([5]); it involves a system of six partial differential equations of elliptic type in two independent variables.
The minimization parameter is the shape of the curved rod or of the shell. The thickness is supposed to remain constant, which holds in many applications. Such problems are known in the literature as *shape optimization problems*. As the geometry of the curved rod or of the shell is parametrized by certain functions, we obtain control-by-the-coefficients problems.
The results obtained concern existence of minimizers, sensitivity analysis, and numerical experiments.
The existence question is intimately connected to the coercivity inequalities for the elliptic operator, uniformly with respect to the geometry. In the case of shells, an inequality of Korn's type was proved which is valid for the class of all the parametrized shells from some ball.
For the optimality conditions, the directional derivatives of the performance indices with respect to variations in the geometry have been investigated. The variations used for curved rods preserve the length of the rod, which is an important constraint for possible applications. This enables to use gradient algorithms for numerical experiments. The computed examples are curved rods.

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4.2 Research Group Laser Dynamics

4.2.1 Overview

Im Mittelpunkt der Forschungen stand 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,
- komplexe Dynamik und homokline Verzweigungen,
- verzögerter Stabilitätswechsel in Mehrskalensystemen.

Als Höhepunkte der Arbeit der Forschungsgruppe im Berichtszeitraum sollen genannt werden:

1. das Auffinden und die Analyse neuer dynamischer Effekte in verschiedenen Mehrsektions-Halbleiterlasern (z. B. Erregbarkeit, interne Feldreflektionen) unter Verwendung der Software `LDSL-tool`,
2. das Erscheinen des Forschungsreports „Singularly perturbed problems in case of exchange of stabilities“ (siehe S. 55) und
3. die Durchführung des internationalen Workshops „Dynamics and Control.“

Die Erfolge der Forschungsgruppe basierten auf enger nationaler und internationaler Kooperation, die finanziell durch die DFG, den DAAD und das BMBF gefördert wurde. Die Ergebnisse wurden in führenden internationalen Zeitschriften veröffentlicht.

The research of the group was focused on the development of analytic and numerical methods for the analysis, simulation, and control of dynamical systems and for 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;
- Complex dynamics and homoclinic bifurcations;
- Delayed exchange of stabilities in multi-scale systems.

As highlights of the work of the research group during the report period we mention

1. The detection and analysis of new dynamical effects in different multi-section lasers (e.g., excitability and internal field reflection) by means of the software `LDSL-tool`;
2. The appearance of the research report “Singularly perturbed problems in case of exchange of stabilities” (see page 55) and
3. The organization of the international workshop “Dynamics and Control”.

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

4.2.2 Projects

Dynamics of semiconductor lasers

Collaborators: M. Radziunas, K.R. Schneider, J. Sieber (until 9/02), D.V. Turaev, M. Wolfrum, S. Yanchuk (since 10/02)

Cooperation with: B. Sartorius, D. Hoffmann, H.-P. Nolting, O. Brox, S. Bauer (Heinrich-Hertz-Institut für Nachrichtentechnik, 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), U. Bandelow (WIAS: Research Group 1)

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: SFB 555 "Komplexe Nichtlineare Prozesse" (Collaborative Research Centre "Complex Non-linear Processes"), DFG-Forschungszentrum "Mathematik für Schlüsseltechnologien" (DFG Research Center "Mathematics for Key Technologies"),

Semiconductor laser devices play a key role in modern telecommunication systems for generating, transforming, and processing data at high speed. For optical networks they provide special components working in complicated nonlinear dynamical regimes (high frequency pulsations, synchronization, short pulses, fast switching).

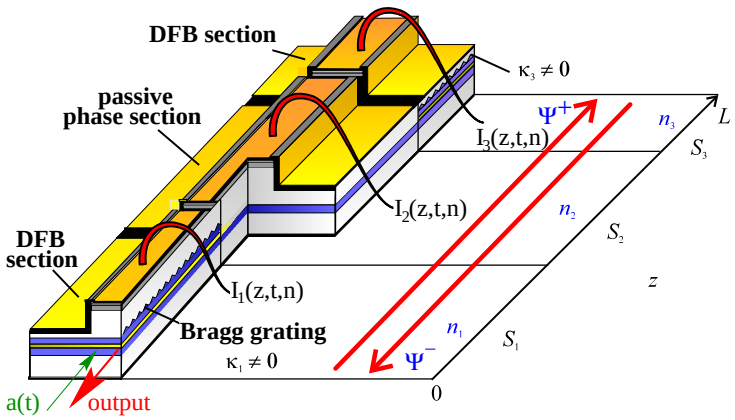

Fig. 1: 3-section DFB laser for all optical clock recovery (Heinrich Hertz Institute, Berlin).

The mathematical research performed in this project includes

- Efficient modeling of integrated devices and their components on different levels of complexity;
- Theoretical investigation of the models, their relations, and dynamical properties;
- Development of special numerical methods for simulation of system applications as well as bifurcation analysis.

Project 1: Lasers with delayed and amplified delayed feedback. Optical feedback is one of the main possibilities in a laser system to generate instabilities and complex dynamical phenomena. Based on the Lang-Kobayashi model

$$\frac{dE}{dT} = \frac{1}{2}(\mathcal{G}(N,|E(T)|^2) - \frac{1}{\tau_p}) \cdot E(T) + \kappa e^{-i\omega_0\tau_f} \cdot E(T-\tau_f),$$

$$\frac{dN}{dT} = I - \frac{N}{\tau_c} - \mathrm{Re}\left[\mathcal{G}(N,|E(T)|^2)\right] \cdot |E(T)|^2,$$

a system of delay differential equations, we studied in [16] analytically the instabilities of lasers under the influence of moderate delayed feedback. A local center-manifold theorem has been proved in [14]. Using scaling methods, analytic expressions for different types of Hopf instabilities have been derived, leading to different types of pulsations of the laser. Moreover, the dependence of the pulsation frequency on the feedback parameters has been analyzed.
Based on this theoretical insight, a new device concept has been developed at the HHI: An additional amplifying section allows higher and tunable feedback strength. This lead to a new optical microwave source, the Amplified Feedback Laser, which is tunable from 10 to 40 GHz ([18]).
The main tuning (or bifurcation) parameters of this device are the current injection I_A into the amplifier section and the current injection I_P into the phase tuning section which is equivalent to the phase ϕ of the feedback.
In order to understand the dependence of the dynamics of the Amplified Feedback Laser on I_A and ϕ, a complete bifurcation analysis of the two-mode approximation ([19]) of the traveling wave equations ([1]) has been performed. Figure 2 reveals the regions of self-pulsations of different types and their borders in the parameter plane ϕ–I_A. A point of particular interest for applications is the widening of the region of mode-beating pulsations compared to the setup with passive feedback ([19]).

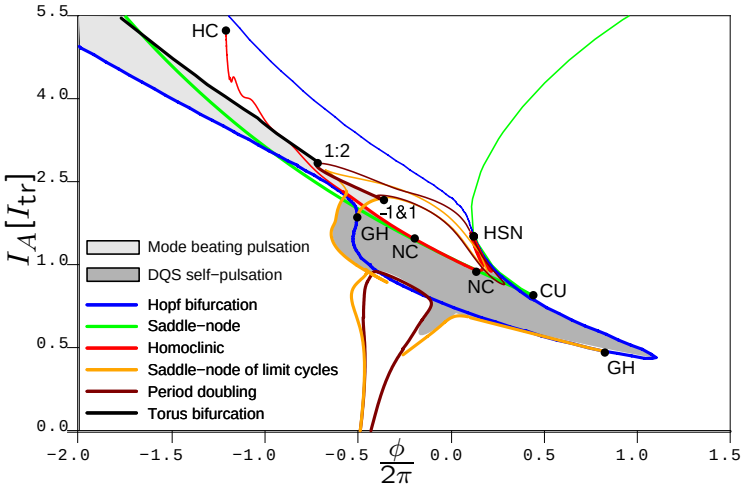

Fig. 2: Bifurcation diagram for the Amplified Feedback Laser in the parameter plane ϕ–I_A

A further important dynamical regime occurring in lasers with delayed optical feedback is excitability. The theoretical background in the context of homoclinic bifurcations for excitability in different laser systems has been studied in [17]. Corresponding experimental results for the case of lasers with delayed feedback and corresponding numerical simulation results have been presented in [6].

Project 2: Software `LDSL-tool`**.** The software `LDSL-tool` has been developed for the simulation and analysis of **l**ongitudinal **d**ynamics in multisection **s**emiconductor **l**asers. The underlying laser model is based on the traveling wave (TW) equations for the optical field propagating along the longitudinal axis of the laser ([1, 5]).
The agreement between simulations by `LDSL-tool` and experimental results is demonstrated in Figure 3 (see also [7, 8]), where the maximal field intensity of periodic solutions or stationary states in a 3-section DFB laser is represented in dependence on some parameter φ. Moreover, this figure can serve as an illustration of more advanced possibilities of `LDSL-tool` which are discussed below. Dashed brown and green lines show stable solutions observed in experiments (above) and in simulations of the TW model (below) for increasing and decreasing parameter φ. Solid red and blue lines show stable and unstable solutions of the system representing a two-mode approximation. Different bifurcations and regions where excitable behavior of a laser can be expected are indicated by thick symbols and yellow shading.

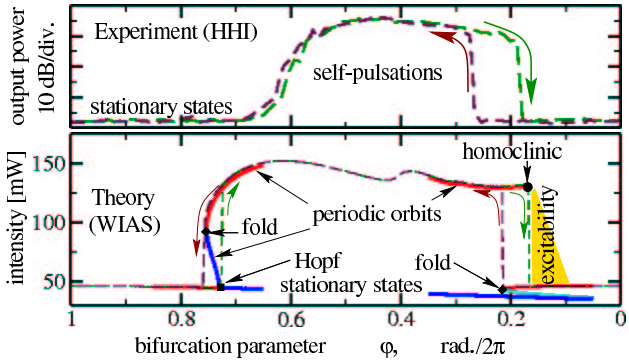

Fig. 3: Bifurcation diagrams

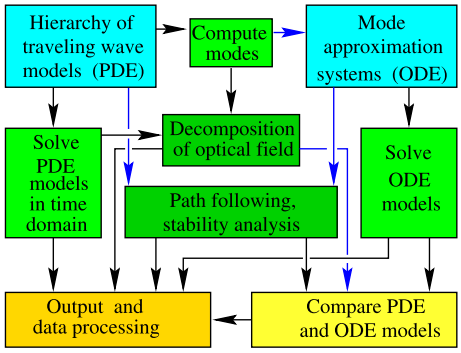

Fig. 4: A schema of `LDSL-tool`

The structure of `LDSL-tool` is discussed in [8, 10] and is represented by a brief schema in Figure 4. Here, blue, green and yellow boxes indicate the hierarchy of models, computational efforts and different data representation/processing procedures, respectively. Blue arrows show transitions which can be done only for some simplified models under some additional assumptions.
The potentialities of `LDSL-tool` are extended continuously. Besides of numerical integration of different TW models, `LDSL-tool` performs some post-processing procedures on the computed data stream ([5, 9]), solves spectral problems defining longitudinal modes of the optical field, and allows to study the dynamics of these modes ([3, 6]). Under some assumptions, the software can be used to perform model reductions, to integrate reduced mode approximation (MA) systems ([13]), and to compare their solutions with the solutions of the full TW model ([6, 8]). Moreover, a bifurcation analysis of MA systems allows to identify different types of the transition between dynamical regimes in the TW model [7]. After finding a good agreement between experiments and simulations by `LDSL-tool` (see [3, 5, 10] and comparing brown/green dashed lines in upper and lower diagrams of Figure 3), one is able not only to explain the origin of dynamics in the lasers (see bifurcations indicated in lower part of Figure 3), but also to predict some dynamical effects, such as excitable behavior of lasers (yellow shaded regions in Figure 3) realized later in experiments [4, 6].
At present, the software is successfully used by coworkers of the Department of Physics of the Humboldt University, of the Heinrich Hertz Institute, and of the Ferdinand Braun Institute to simulate and to analyze the behavior of different lasers. In particular, `LDSL-tool` is applied to study excitability in lasers with short external cavity ([4, 6]), self-pulsations in lasers with

amplified feedback ([11, 12]), in DFB lasers with dispersive feedback ([1, 5, 7]), in lasers with two active DFB sections ([3, 9, 10]), and high power pulse generation in DBR lasers ([15]).

Project 3: Research of effects degrading high-frequency self-pulsations. In the frame of the BMBF project *"Hochfrequente Selbstpulsationen in Mehrsektions-Halbleiterlasern: Analysis, Simulation und Optimierung" (High-frequency self-pulsations in multi-section semiconductor lasers: Analysis, simulations, and optimization)*, in cooperation with the Heinrich Hertz Institute, Berlin, and the company u^2t Photonics, Berlin, the behavior of a three-section laser with two active DFB sections (see Figure 1) has been investigated.
It was demonstrated experimentally and theoretically ([3]) that such a laser can operate at high frequency (∼20–160 GHz) self-pulsations (SP) due to mutual action of two modes. Nevertheless, only some of the produced nominally identical devices could operate at the required pair of modes. The identification of possible reasons for this failure is one of the most important tasks in this project. By extensive numerical simulations of the impact of several possible limiting effects it was possible to avoid a lot of time-consuming and expensive experiments and measurements.
Finally, in [10] we have suggested that such problems can arise due to non-vanishing reflectivities for the counter-propagating fields at the junctions of the laser sections S_1/S_2 and S_2/S_3. Since the phases of the complex reflectivity coefficients r_1 and r_2 can not be controlled during the production of the devices, it is important to estimate the reflectivity amplitudes $|r_{1,2}|$ permitting the same type of SP for any phase of reflectivity in order to find conditions which guarantee a robust behavior under the requirements of the production process.

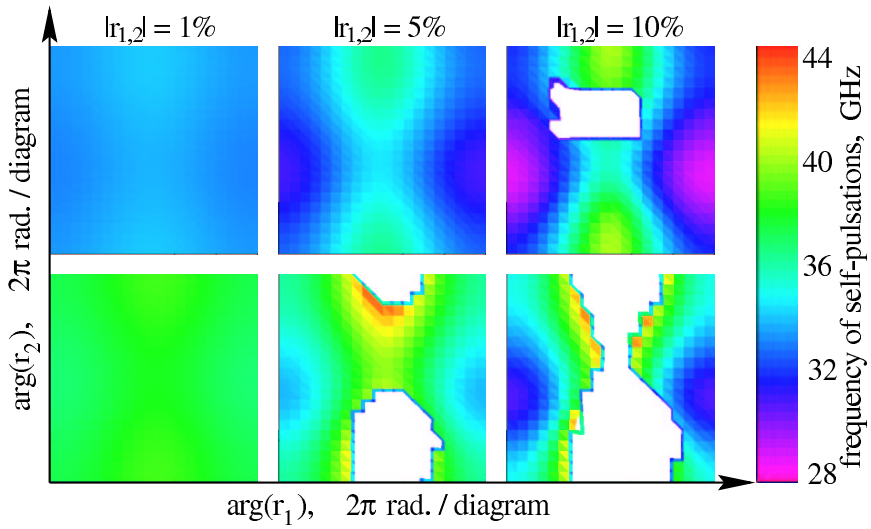

Fig. 5: Dependence of SP frequency on two internal reflectivity coefficients r_1 and r_2 at two slightly different operating conditions of self-pulsating laser

The diagrams in Figure 5 represent a study of the effect of internal reflectivity on two slightly different self-pulsations at 33.5 and 38 GHz frequency. The SP represented in the upper diagrams are chosen from the middle of the area of similar self-pulsations in the parameter space, while the lower diagrams indicate similar SP closer to the border of the same area. In both cases we have applied the same reflectivity amplitudes for both of the junctions (fixing them at 1, 5, and 10 % reflectivity) and have varied the reflectivity phases.
The white areas within the colored diagrams indicate totally different operational regimes. Therefore, 5 % amplitude reflectivity (which, actually, was present in the lasers made at the Heinrich Hertz Institute) do not degrade self-pulsations dramatically if we are in the middle of

the SP area in the parameter plane, but can cause trouble if we are operating close to the border of the same area.
These simulations have shown the importance of a control of internal reflectivities. Our partners now are producing a new generation of multi-section lasers with reduced level of reflectivities.

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Multiscale systems

Collaborators: K.R. Schneider, E.V. Shchetinina

Project 1: Exchange of stabilities in multiscale systems.

Cooperation with: V.F. Butuzov, 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

The problem of delayed exchange of stabilities for a scalar non-autonomous ordinary differential equation has been treated some time ago ([3]). Very recently, the same problem for the scalar singularly perturbed parabolic differential equation

$$\begin{aligned} &\varepsilon \left(\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} \right) = g(u,x,t,\varepsilon), \\ &(x,t) \in Q = \{(x,t) : 0 < x < 1,\ 0 < t \le T\},\ 0 < \varepsilon \ll 1 \end{aligned} \tag{1}$$

has been solved successfully by means of the method of asymptotic lower and upper solutions [2]. This result provides a first proof for the existence of canard solutions for partial differential equations.
Under the assumption that the degenerate equation

$$g(u,x,t,0) = 0$$

has exactly two roots $u \equiv 0$ and $u = \varphi(x,t)$ intersecting in some smooth curve $\mathcal{K}$ with the representation $t = t_c(x)$, $t_c \in C^1([0,1],(0,T))$, and that $g(0,x,t,\varepsilon) \equiv 0$ for all (x,t,ε) under consideration, we derive conditions on g and on u^0 such that the initial-boundary value problem to (1)

$$\begin{aligned} u(x,0,\varepsilon) &= u^0(x) && \text{for } x \in [0,1], \\ \frac{\partial u}{\partial x}(0,t,\varepsilon) &= \frac{\partial u}{\partial x}(1,t,\varepsilon) = 0 && \text{for } t \in [0,T] \end{aligned}$$

has for sufficiently small ε a unique solution satisfying

$$\begin{aligned} \lim_{\varepsilon \to 0} u(x,t,\varepsilon) &= 0 && \text{for } (x,t) \in [0,1] \times (0, t_{\min}), \\ \lim_{\varepsilon \to 0} u(x,t,\varepsilon) &= \varphi(x,t) && \text{for } (x,t) \in [0,1] \times (t_{\max}, T], \end{aligned}$$

that is, $t_{\min}$ and $t_{\max}$ are lower and upper bounds for the delay of exchange of stabilities.
The results of the research cooperation between WIAS and the Department of Mathematics of the Faculty of Physics of the Moscow State University in the field of exchange of stabilities in multiscale systems over the last five years have been represented as a report [1] which will appear as a research monography in Russia and in the USA.

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Project 2: Delayed loss of stability in non-autonomous delay-differential equations

Cooperation with: B. Lani-Wayda (Justus-Liebig-Universität Giessen)

Dynamical systems as mathematical models of real-life processes depend on several parameters which are assumed to be fixed within some time period. The influence of parameters on the behavior of a dynamical system is studied within the framework of bifurcation theory. This project aims to study the influence of some relevant system parameter λ changing slowly in time (for example, because of an aging process). For ordinary differential equations it is well known that a slowly changing parameter can lead to a special phenomenon known as *delayed loss of stability* [2]. Such phenomenon manifests in a jumping behavior of some state variables which can imply dramatic consequences (e.g., thermal explosion). The main goal of this project is to describe a similar effect for nonlinear differential-delay equations of the type

$$\frac{dx}{dt}(t) = g(t, x(t-1)). \tag{2}$$

For this purpose, we study the linear inhomogeneous equation

$$\frac{dx}{dt}(t) = a(t)x(t-1) + h(t) \tag{3}$$

assuming that the function a takes values in $[-3\pi/4, -\pi/4]$ and changes slowly. It is well known that for constant a and $h = 0$, the zero solution of the linear equation (3) is stable for $a \in (-\pi/2, 0)$, and unstable for $a < -\pi/2$. Contrary to the ODE case, the exponential rate of growth or decay is not directly given by a, but has to be estimated. We provide such estimates and derive a variation-of-constants formula for the case of nonconstant a and $h \neq 0$. This formula will be used to express solutions of (2) on successive time intervals I_i by solutions of the equation

$$\frac{dx}{dt}(t) = c_i\, x(t-1)$$

with constants c_i which are values of $\partial_2 g(\cdot, 0)$ on I_i. We establish estimates that express the phenomenon of delayed loss of stability for differential-delay equations of type (2). As an example we treat the equation

$$\frac{dx}{dt}(t) = (-\pi/4 - \varepsilon t)\arctan(x(t-1)).$$

Here, we study the initial value problem with the initial segment identically 1, and estimate the time until the solution is close enough to zero by a method that is not based on linearization. Figure 1 demonstrates this phenomenon numerically.

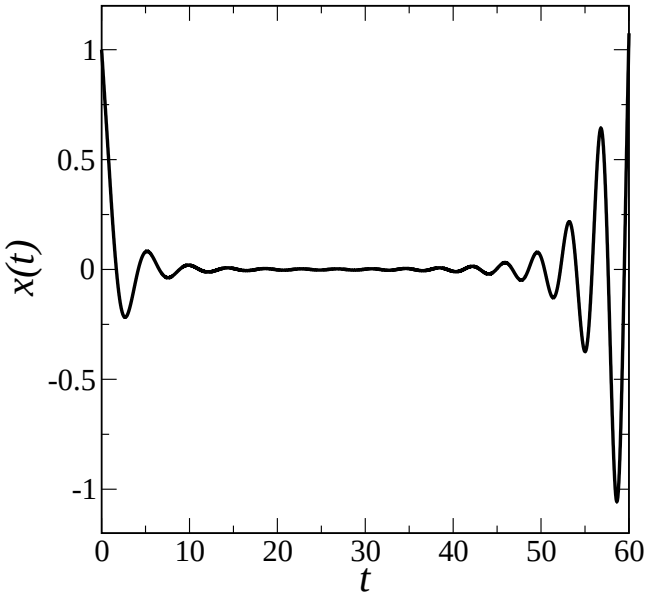

Fig. 1: Numerical solution of $\dot{x}(t) = (-\pi/4 - \varepsilon t)\arctan(x(t-1))$ with constant initial segment equal to 1 and $\varepsilon = 0.03$

Complementary to the results on delayed loss of stability, which express similar behavior of delay equations and ordinary differential equations (ODEs), we exhibit a substantial difference between both types of equations. Namely, the additive term $h(t)$ in the equation

$$\frac{dx}{dt}(t) = cx(t-1) + h(t)$$

inevitably has an influence on the development of all "components" of solutions (in terms of expansion into eigenfunctions of the homogeneous equation). Of course, for a linear constant coefficient system of ODEs, the perturbation h can be chosen such that it influences only specific components.

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Project 3: Integral manifolds of canard type for non-hyperbolic slow-fast systems

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

Slow-fast systems have been considered which can be transformed into the form

$$\begin{aligned} \frac{dy}{dt} &= \varepsilon Y(t,y,z,\varepsilon), \\ \frac{dz}{dt} &= B(t)z + Z(t,y,z,a(y,\varepsilon),\varepsilon) + a(y,\varepsilon) \end{aligned} \tag{4}$$

with $Z(t,y,0,0,0) \equiv 0,\ y \in R^n,\ z \in R^2$, ε is a small positive parameter, a is a 2-dimensional vector function, and $B(t)$ is the matrix

$$B(t) = \begin{pmatrix} 2t & 1 \\ -1 & 2t \end{pmatrix}.$$

Note that the eigenvalues of the matrix $B(t)$ are $2t \pm i$, that is, $B(0)$ has purely imaginary eigenvalues, and therefore (4) is a non-hyperbolic slow-fast system.
The aim of this project is to establish an integral manifold of the form $z = h(t,y,\varepsilon)$ to reduce the order of system (4) under non-hyperbolicity conditions. In the hyperbolic case the existence of such integral manifolds has been known for a long time (see, e.g., [3]).
As a result we derived conditions on Y and Z guaranteeing the existence of a function $a(y,\varepsilon)$ such that (4) has an integral manifold of the form $z = h(t,y,\varepsilon)$, where h is uniformly bounded, $||h||$ and $||a||$ tend to zero as $\varepsilon \to 0$. Moreover, we derived an algorithm to determine the coefficients in the asymptotic representation of the functions $a(y,\varepsilon)$ and $h(t,y,\varepsilon)$ as

$$a(y,\varepsilon) = \sum_{i=1}^{\infty} \varepsilon^i a_i(y),$$

$$h(t,y,\varepsilon) = \sum_{i=1}^{\infty} \varepsilon^i h_i(t,y).$$

The established manifold $z = h(t,y,\varepsilon)$ is of canard type, that is, it is attracting for $t < 0$ and repelling for $t > 0$.

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Project 4: Combustion wave of canard type

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

We consider the problem of thermal explosion in case of an autocatalytic combustion reaction. The goal of the project is to establish the existence of traveling wave solutions of the system

$$\begin{aligned} \gamma \frac{\partial \Theta}{\partial t} &= \eta(1-\eta)e^{\Theta} - \alpha\Theta + \delta \frac{\partial^2 \Theta}{\partial \xi^2}, \\ \gamma \frac{\partial \eta}{\partial t} &= \gamma\eta(1-\eta)e^{\Theta} + \mu \frac{\partial^2 \eta}{\partial \xi^2}, \end{aligned} \tag{5}$$

where Θ is the temperature, η the depth of conversion of the gas mixture, γ is a small parameter (case of highly exothermic reaction). The existence of a traveling wave $\Theta = \tilde{\Theta}(\xi + ct)$, $\eta = \tilde{\eta}(\xi + ct)$ to (5) is equivalent to the existence of a heteroclinic orbit of the system ($x = \xi + ct$)

$$\begin{aligned} \gamma c \frac{d\tilde{\Theta}}{dx} &= \tilde{\eta}(1-\tilde{\eta})e^{\tilde{\Theta}} - \alpha\tilde{\Theta} + \delta \frac{d^2\tilde{\Theta}}{dx^2}, \\ \gamma c \frac{d\tilde{\eta}}{dx} &= \gamma\tilde{\eta}(1-\tilde{\eta})e^{\tilde{\Theta}} + \mu \frac{d^2\tilde{\eta}}{dx^2} \end{aligned} \tag{6}$$

connecting two equilibria of the reaction system.
Basing on the fact that the reaction system has canard solutions separating the slow combustion regime from the explosive one [2], we prove by applying the geometric theory of singularly perturbed differential equations the existence of a new type of traveling wave solutions, the so-called canard traveling waves.

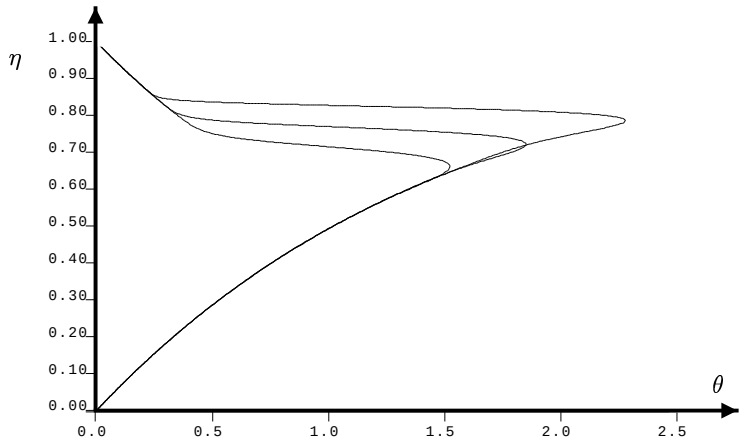

Fig. 2: Projection of canard trajectories of system (6) for $\gamma = 0.05$, $\delta = \mu = 1$, $\alpha = 0.66022803$, $\alpha = 0.66025281$, $\alpha = 0.66024835$

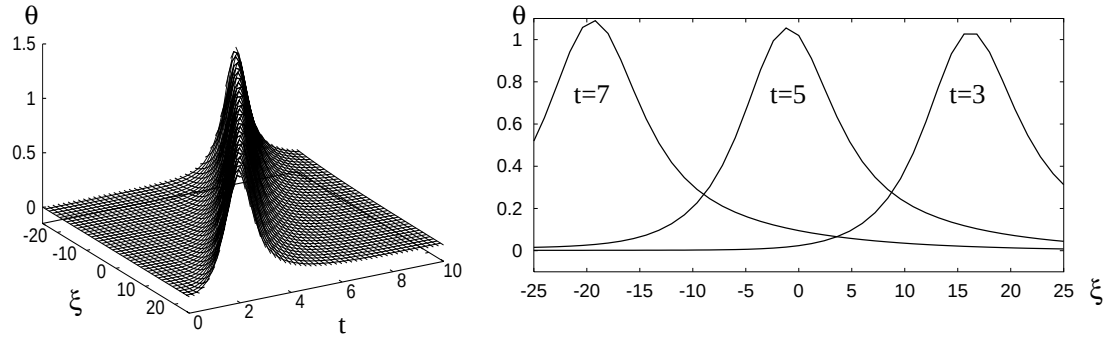

Fig. 3: Θ–profiles of the canard traveling wave solution of system (5) for $\gamma = 0.05$, $\alpha = 0.58443$, $\delta = \mu = 1$

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Homoclinic bifurcations

Collaborator: D.V. Turaev

Project 1: Dynamics near homoclinic tangencies

Cooperation with: S.V. Gonchenko, L.P. Shilnikov (Institute for Applied Mathematics and Cybernetics, Nizhny Novgorod, Russia)

Supported by: DFG grant no. 436 RUS, Prize of the Alexander von Humboldt Foundation

Since Poincaré's pioneering work, orbits which are homoclinic to saddle periodic ones have been one of the most attractive objects of study in the theory of dynamical systems. The main reason to study homoclinic orbits is that their presence implies complicated dynamics. It is well known that in any neighborhood of a transverse homoclinic orbit there exist infinitely many saddle periodic orbits and a continuum of non-trivial hyperbolic recurrent orbits. If the system has a non-transverse homoclinic orbit, that is, in the case of homoclinic tangency, then in any neighborhood of the given system there exist infinitely many *Newhouse regions* where systems with homoclinic tangencies are dense.

Since Newhouse regions exist near any system with a homoclinic tangency, it follows that they can be found in the space of parameters of any dynamical model demonstrating chaotic behavior in absence of uniform hyperbolicity, in particular in such popular examples as Hénon map, Chua circuit, Lorenz model, etc. Moreover, as numerics shows, the Newhouse regions can occupy quite large portions of the parameter space. Therefore, the problem of understanding the nature of the orbit structure for systems from Newhouse regions is quite challenging.

We have found that the dynamics of systems from the Newhouse regions is extremely rich and unusual (see Project 2). As it was shown in [2], a description of the dynamics of such systems requires an infinite set of invariants which means that any attempt to give a *complete* description of the dynamics and bifurcations in the Newhouse regions will fail. Therefore, we have to restrict the analysis to some particular details or to some most general features only.

As the most important of such general properties of systems in the Newhouse regions, we select *the coexistence of many periodic orbits of different stability types* (i.e., with different numbers of positive/negative Lyapunov exponents). It has been demonstrated in [1] that stable periodic orbits can coexist with saddle ones near a homoclinic tangency in three-dimensional systems. The questions which conditions provide the same phenomenon in the multidimensional case and which conditions could lead to the coexistence of saddles of different types within the regions of chaotic dynamics were raised by many authors. In the present work [4] we give a complete answer to these questions for systems from the Newhouse regions.

Consequently, following [3], we classify codimension-1 homoclinic tangencies by the value of the so-called *effective dimension* d_e. It is an integer which can be effectively computed for any given system with a homoclinic tangency. We have proven the following result.

Theorem 1. In the Newhouse regions the values of parameters are dense (and form a residual set) for which the system has infinitely many coexisting hyperbolic periodic orbits of (d_e+1) different stability types.

We describe exactly the types of these periodic orbits for different types of the Newhouse regions and show that orbits of other stability types cannot exist here. So, the question for the

maximal and minimal number of positive Lyapunov exponents of the orbits of systems under consideration, as well as the question for the coexistence of orbits with different numbers of positive Lyapunov exponents, has been solved completely. In particular, we obtain necessary and sufficient conditions for the denseness of systems with infinitely many stable periodic orbits in the Newhouse regions.

We also address the question for the coexistence of infinitely many *non-trivial attractors*. We have proven the following result.

Theorem 2. In the case $d_e \geq 2$, the values of parameters in the Newhouse regions are dense and form a residual set for which the system has infinitely many coexisting stable invariant tori.

The problem of the coexistence of infinitely many *strange attractors* in the case $d_e \geq 3$ was also discussed in [4].

Project 2: Richness of chaotic dynamics in non-hyperbolic systems

It has been proved in [2] that systems with homoclinic tangencies of arbitrarily high order are dense in the Newhouse regions, as well as systems having degenerate periodic orbits with all Lyapunov coefficients equal to zero. This implies that bifurcations of such systems are extremely involved and rich. Thus, the question arises: Can we estimate in exact terms how rich these bifurcations are? In [5] we give a definite answer for the example of two-dimensional area-preserving maps. It is shown that we deal here with the *ultimate* richness: Every possible dynamics can be obtained by a small perturbation of *any* system from a Newhouse region.

To be more precise, let f be a C^r-smooth area-preserving map of R^2. Define the *dynamical conjugacy class* of f as the set of all maps $f_{n,\psi}$ of a unit disc U_1 into R^2 obtained by the rule $f_{n,\psi} = \psi^{-1} \circ f^n \circ \psi$, where n is an integer, f^n is the n-th iteration of f, and ψ is an arbitrary C^r-smooth map of U_1 into R^2 with a constant Jacobian (hence, by construction, all the maps $f_{n,\psi}$ in the class are area preserving).

When we speak about the dynamics of a map, then we somehow describe its iterations, where the description should be independent of smooth coordinate transformations. Therefore, the class of maps f just introduced yields some representation of the dynamics of f. Note that the coordinate transformations ψ are not area preserving (they preserve the standard symplectic form up to a constant factor), i.e., the image $\psi(U_1)$ can be a disc of an arbitrarily small radius with its center located anywhere. Thus, the class of maps f contains information about the behavior of arbitrarily long iterations of f on arbitrarily fine spatial scales.

The general intuition here is that if the class of maps is large, then the dynamics is rich, while if the dynamics is sufficiently simple, then the class is somehow restricted. The following definition introduces maps whose dynamics is ultimately rich.

Definition. A C^r-smooth symplectic map f is called *universal* (or C^r-universal) if its dynamical class is dense in the C^r-topology among all C^r-smooth symplectic diffeomorphisms $U_1 \to R^2$.

By this definition, the detailed understanding of the dynamics of any single universal map is not simpler than the understanding of all other area-preserving maps *altogether*, i.e., it is beyond human abilities. What is astonishing, is that such universal maps are quite common. Namely, we show in [5] that the following statement is valid.

Theorem 3. *C^r-universal maps exist in any neighborhood (in the C^r-topology) of any area-preserving map with a homoclinic tangency, i.e., they are dense in the Newhouse regions.*

This theorem says that universal maps occur as often as homoclinic tangencies do. It is an empirical fact that if we have any explicitly given area-preserving map with chaotic behavior, then by slightly changing parameters we can quite often encounter a homoclinic tangency. Thus, according to the theorem above, if we have enough control parameters then we can tune our map as close as we want to any other area-preserving map in some carefully chosen coordinates.

Project 3: Problems of synchronization

Cooperation with: L.P. Shilnikov (Institute for Applied Mathematics and Cybernetics, Nizhny Novgorod, Russia)

Supported by: Prize of the Alexander von Humboldt Foundation

The problem of synchronization is one of the main problems of applied signal processing. It can be formulated as follows: Let a generator of periodic oscillations be forced by an external periodic signal. Under which conditions will the generator respond with the same frequency as the external signal? Can it respond to the signal with a fractional or multiple frequency? Which response should we expect in general?
When the amplitude of the external force is small, these questions are solved by the classical method of averaging: depending on the frequency detuning, either synchronization or beating regimes should be expected. In the case of finite amplitude, the situation becomes much more complicated: synchronization of different frequencies is possible for the same parameter values, as well as chaotic regimes. In [6] we study the problem of sudden transition from synchronization to chaos. This process can be modeled in geometrical terms as a bifurcation of a saddle-node periodic orbit with a *non-smooth* homoclinic loop (see Figure 1). We give criteria which allow to distinguish between two possible scenarios of what happens when the saddle-node has disappeared: either the dynamics is always chaotic, or zones of chaotic behavior interchange in the parameter space with zones of synchronization.
We also analyze in [6] the problem of coexistence of chaotic and synchronized behavior. The classical result of Cartwright and Littlewood from 1945 [7] (explaining earlier experiments by van der Pol) is that the coexistence of two synchronization regimes with different frequencies implies also the existence of a chaotic transient. We enhanced this by giving criteria for the coexistence of chaos with a single synchronized regime and for the existence of chaos in the absence of stable synchronized regimes.

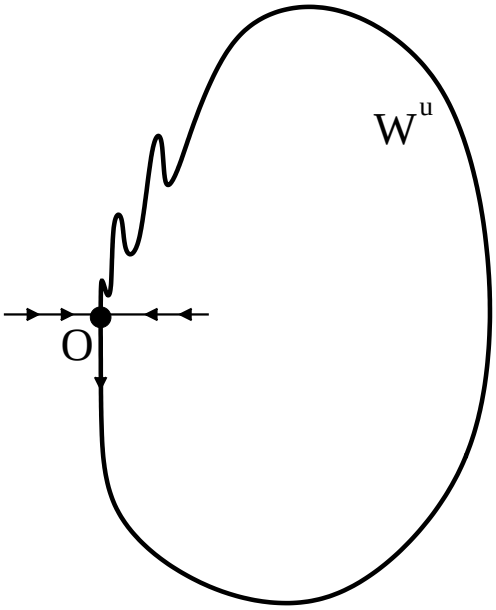

Fig. 1: The unstable manifold W^u of a saddle-node O may return to 0 making infinitely many wriggles

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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.

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.

Die thematischen Schwerpunkte waren:

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

Im September 2002 wurde der im Rahmen des DFG-Schwerpunktprogrammes 1095 „Analysis, Modellierung und Simulation von Mehrskalenproblemen“ veranstaltete Workshop *Multiscale Problems in Quantum and Classical Mechanics, Averaging Techniques and Young Measures* zusammen mit den Forschungsgruppen „Partielle Differentialgleichungen und Variationsgleichungen“ und „Kontinuumsmechanik“ durchgeführt (siehe Seite 239). Insbesondere die Vielzahl der Beiträge zu den beiden Schwerpunktthemen des Workshops, Halbleiter-Nanostrukturen und Probleme der

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.

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.

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.

In September 2002 the group organized in collaboration with the research groups “Partial Differential Equations and Variational Equations” and “Continuum Mechanics” the workshop *Multiscale Problems in Quantum and Classical Mechanics, Averaging Techniques and Young Measures* (see page 239) which was an event in the DFG Priority Program 1095 “Analysis, Modeling and Simulation of Multiscale Problems”. In particular the multitude of contributions to the main topics of the workshop, semiconductor nanostructures and problems of the atomic chain, have been proven

atomaren Kette, haben sich als hervorragende Grundlage zur intensiven wissenschaftlichen Diskussion und zum Knüpfen neuer Kontakte herausgestellt.

to be an excellent basis for intense scientific discussions and for the establishment and the fosterage of joined activities.

Im Oktober 2002 war die Forschungsgruppe Veranstalter der international ausgerichteten Tagung *Challenges in Scientific Computing* (siehe Seite 240). 54 Forscher aus vielfältigen Bereichen des Scientific Computing, Numerischer Analysis und Naturwissenschaften kamen zu einem intensiven wissenschaftlichen Austausch über aktuelle Probleme der Numerik von Reaktions-Diffusions-Transportsystemen zusammen.

In October 2002 the group organized the international conference *Challenges in Scientific Computing* (see page 240). This meeting provided a forum of intense scientific discussion for some 54 researchers from various fields of scientific computing, numerical analyzis and science on the state-of-the-art problems in the numerics of systems of reaction-diffusion-transport equations.

Die Forschungsgruppe hat an dem nachfolgend genannten forschungsgruppenübergreifenden Projekt mitgearbeitet:

- Hochskalierung mikroskopisch berechneter Daten und Kennlinien auf makroskopische Zustandsgleichungen (siehe S. 170) zusammen mit der FG „Partielle Differentialgleichungen und Variationsgleichungen“.

The group has collaborated on the following joint project with an other research group at WIAS:

- Upscaling of microscopic calculated characteristics to macroscopic state equations (see page 170) in cooperation with research group “Partial Differential Equations and Variational Equations”.

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. 43),
  - Spannungsanalyse in einer dünnen Wafer-Platte (siehe S. 164).
- Entwicklung spezieller Moduln und Features für `pdelib`, allgemeine Beratung in numerischen Fragen,
- Visualisierung.

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 43);
  - Stress analyzis of a thin wafer plate (see page 164).
- Development of special modules and features for `pdelib`, general advice for questions on numerical issues;
- Visualization.

4.3.2 Projects

Two-dimensional numerical simulation of a DMFC (Direct Methanol Fuel Cell)

Collaborators: J. Fuhrmann, K. Gärtner

Cooperation with: J. Divisek, H. Dohle (Forschungszentrum Jülich GmbH, IWV-3)

Supported by: IWV-3 Jülich

During the third year of this project (see Annual Research Report 2001[1]) we focused on:

1. The verification of the model and the calibration of some of its parameters with respect to experiments. This process was partially automated by the application of a least-squares fit of IV-curves or other parameter-dependent functionals.
2. The numerical study of the influence of geometry variations on the fuel cell performance;
3. A model taking into account the influence of contact plate designs on the fuel cell performance.

Summary of the status reached:
The essential problem is the precision, some of the model parameters are known. On the other hand one has a very limited amount of experimental data. The experimental setups aim on the normal working conditions of a fuel cell. Parameter verification would be supported much better by an enlarged range of parameter variations that clearly addresses different limiting conditions and special nonlinear effects.
The computations show a significant influence of the fuel cell geometry on the cathodic reaction rates, especially due to temperature feedback effects. This points to carefully designed experiments which could be verified by two-dimensional computations, and a possible need for further model improvements regarding the heat conduction model (boundary conditions, temperature coefficients of the oxygen kinetics), and the concurrency for free catalytic sites at the cathode (oxygen/H^+ versus the parasitic methanol oxidation).

Another topic of interest is to estimate the influence of contact plate designs on the fuel cell performance. Mechanical and production constraints limit the area exposed to oxygen and fuel while the contact plate material has to collect the electrons on the other hand. Due to the typical geometric situation (the height of the contact plate (z direction) is approximately two orders of magnitude smaller than the other dimensions (x, y)) the following simplified (height-integrated) model was solved numerically:

$$-\nabla \cdot \tilde{\sigma}_i(x)\nabla\phi_i = (-1)^{i+1}\tilde{\rho}(\phi_1 - \phi_2, x),$$

$i = 1,2$, 1: anode, 2: cathode, $\phi_i(x,y)$ electrostatic potential, $\tilde{\rho}(\phi_1 - \phi_2, x)$ IV-characteristics of the MEA (Membrane-Electrode Assembly, corrected with respect to horizontal losses in the graphite). The functions describing the effective conductivities are given for the metal-covered zone by $\tilde{\sigma} = h_{metal}\sigma_{metal} + h_{graphite}\sigma_{graphite}$, and the fuel or air region $\tilde{\sigma} = h_{graphite}\sigma_{graphite}$ respectively. The reaction rate (electron source/sink) in a region covered by metal was assumed to be zero. The following Figure 1 shows the basic features, a grid and a potential pattern. Due

[1] http://www.wias-berlin.de/publications/annual_reports/2001/node45.html

to the Dirichlet boundary conditions imposed on different segments of the anodic and cathodic contact plate the possibly existing symmetry is broken, and both plates have to be computed.

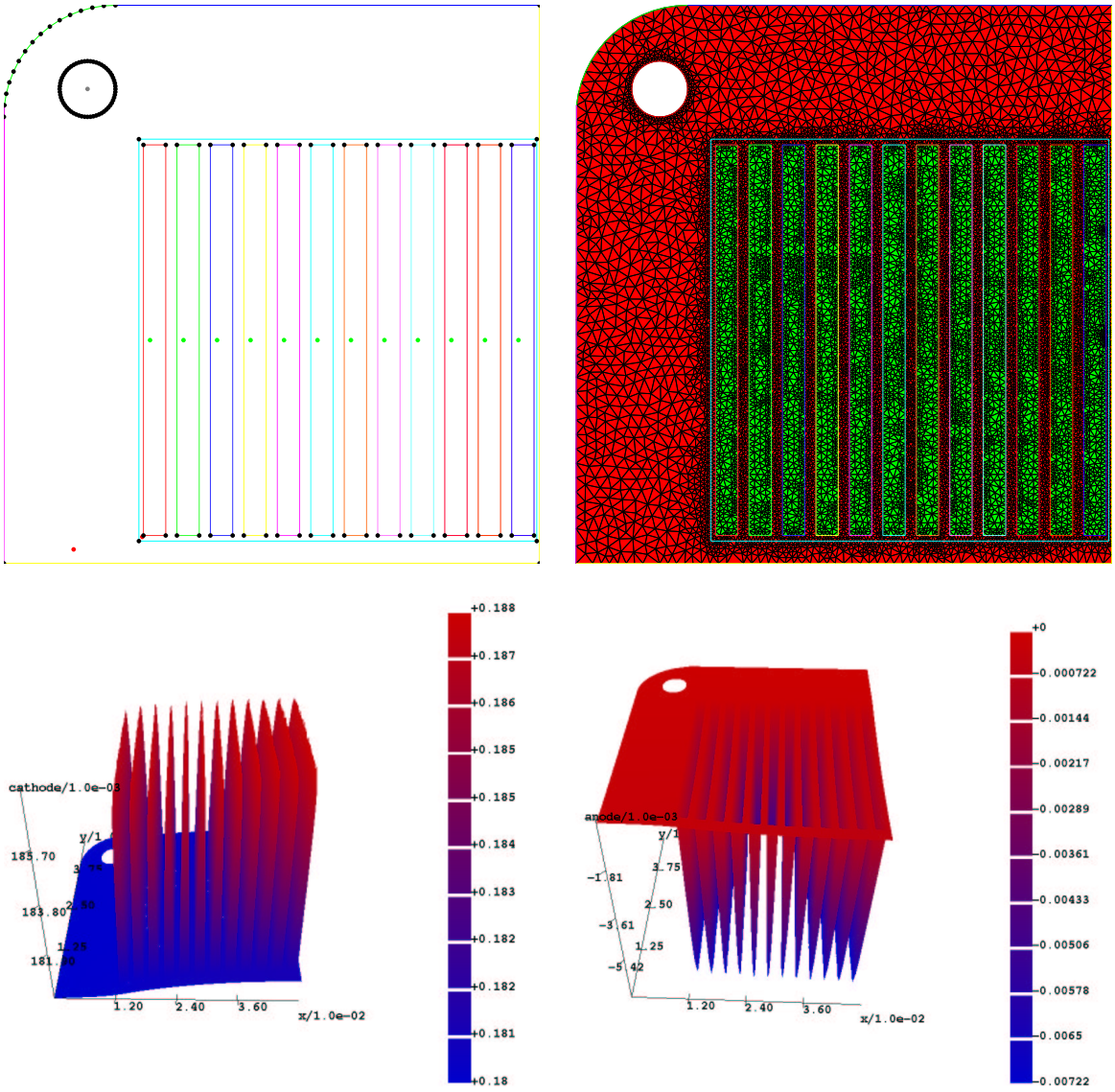

Fig. 1: Basic layout of a symmetry sector of a contact plate (UL), metal region (red), fuel and air zone (green) (UR), potential at the cathode (LL) and the anode (LR)

Thermal convection in sedimental basins

Collaborator: J. Fuhrmann

Cooperation with: U. Bayer (GeoForschungsZentrum Potsdam)

We regard the following model of thermal convection:

$$\partial_t(\varphi_s\rho_f) = \nabla\cdot(\rho_f\vec{v})$$
$$\vec{v} = \frac{k_s}{\mu_f}(\nabla p - \rho_f\vec{g})$$
$$\partial_t\left(((1-\varphi_s)\rho_s c_s + \varphi_s\rho_f c_f)T\right) = \nabla\cdot\left(\left((1-\varphi_s)\lambda_s + \varphi_s\lambda_f\right)\nabla T - T\rho_f c_f\vec{v}\right).$$

These equations describe fluid flow in a saturated porous medium, and energy transport driven by thermal diffusion in both the solid matrix and the fluid, and by convection based on the fluid flux.
The basic variables are the pressure p and the temperature T. $\rho_s, \rho_f(p,T)$, c_s, c_f, λ_s, λ_f are the densities, heat capacities and heat transfer coefficients for solid matrix and fluid, respectively. φ, k_s are the porosity and the hydraulic permeability of the solid. The remaining data are fluid viscosity $\mu_f(p,T)$, acceleration of gravity $\vec{g}$ and volumetric flux of water $\vec{v}$. The system is closed by standard boundary conditions. When applied to sedimental basins heated from below by the Earth core, heterogeneity is introduced by the strong variation of the solid matrix parameters between the sedimental layers.
Using a time implicit, Voronoi box based finite volume method, simulations for two-dimensional slices of the North-East German basin have been carried out. These suggest that a quasi-periodic, if not chaotic flow regime might be present in the basin region.

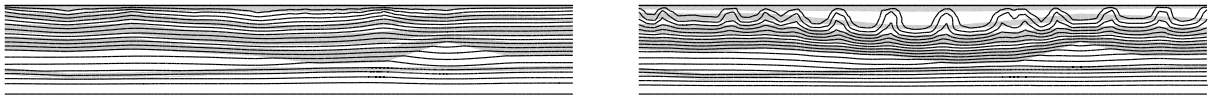

Fig. 1: Stationary and chaotic solutions after 10^7 years

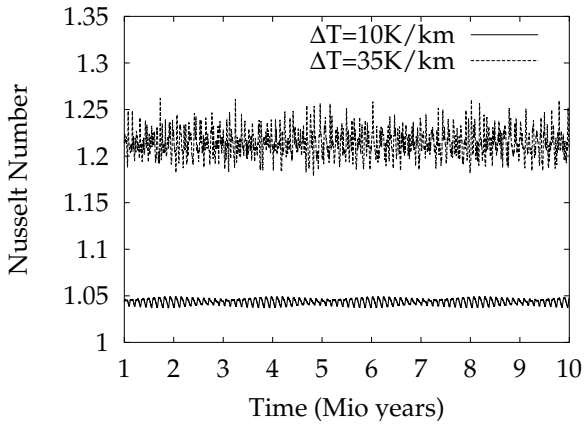

Fig. 2: Nusselt number time series of quasiperiodic and chaotic solutions, respectively, in a slice of the North-East German basin

From the viewpoint of the geosciences, the implications of a non-stationary flow behavior would be quite severe. Further investigation of this question, a more realistic model ansatz including

the dissolved salt, and the development of three-dimensional simulation tools are subject of further research.

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Finite element methods for surface diffusion

Collaborator: E. Bänsch

Cooperation with: P. Morin (Universidad Nacional del Litoral and Instituto de Matemática Aplicada del Litoral, Santa Fe, Argentina), R.H. Nochetto (University of Maryland, USA)

The overall goal of this work is to devise efficient numerical tools for simulating morphological changes in stressed epitaxial films and thereby study their complicated nonlinear dynamics. To model the misfit between the crystalline structure of the substrate and epitaxial film, the film may be thought of as subjected to mechanical stresses. This causes a plastic deformation of the free surface of the film. This morphological instability of the free surface may eventually lead to crack formation and fracture, an issue of paramount importance in Materials Science, [3] – [5].

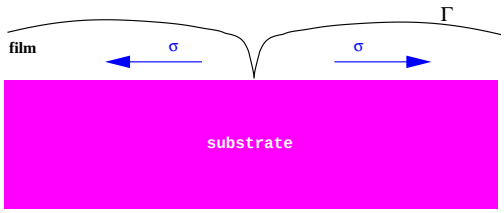

Fig. 1: Sketch of the physical situation: stressed epitaxial film situated on a substrate

The dynamics of the free surface Γ in $\mathbb{R}^d$ is governed by the highly nonlinear PDE

$$V = -\Delta_\Gamma(\kappa + \varepsilon), \tag{1}$$

where $d = 2$ or $d = 3$, V and κ are the (scalar) normal velocity and mean curvature of Γ, and ε is the elastic energy density of the bulk $\Omega(t)$ enclosed by $\Gamma(t)$. Solving the system of linear elasticity in $\Omega(t)$ provides indeed the trace of ε on $\Gamma(t)$. So far, we consider f as being given. The main mathematical and numerical problems arise from the 4th-order nonlinear Laplace-Beltrami operator and the fact that one cannot work directly with the curvature vector.
A variational finite element formulation of a semi-implicit time discretization which involves four unknowns, namely the vector normal velocity, (scalar) normal velocity, scalar curvature and curvature vector has been developed. A Schur complement form is used to reduce the system to the single unknown of scalar velocity. Under the assumption of non-degeneracy of the geometry unconditional stability of the scheme can be shown.
For the graph case an analogous formulation can be derived, resulting in a similar but simpler variational system consisting of 2 scalar unknows, namely the height u and the curvature κ. In this case, an optimal a priori error estimate could be proved, reading: let $e_u = u - u_h$ and $e_\kappa = \kappa - \kappa_h$, then

$$\sup_{t\in[0,T]} \left(\|e_u(t)\|_2^2 + \int_{\Gamma_h(t)} |\nabla_S e_u|^2 \right) + \int_0^T \left(\|e_\kappa(t)\|_2^2 + \int_{\Gamma_h(t)} |\nabla_S e_\kappa|^2 \right) dt \le C h^{2k}. \tag{2}$$

Here $C > 0$ depends on the regularity of u and κ, $k \ge 1$, is the polynomial degree. h is the mesh size.

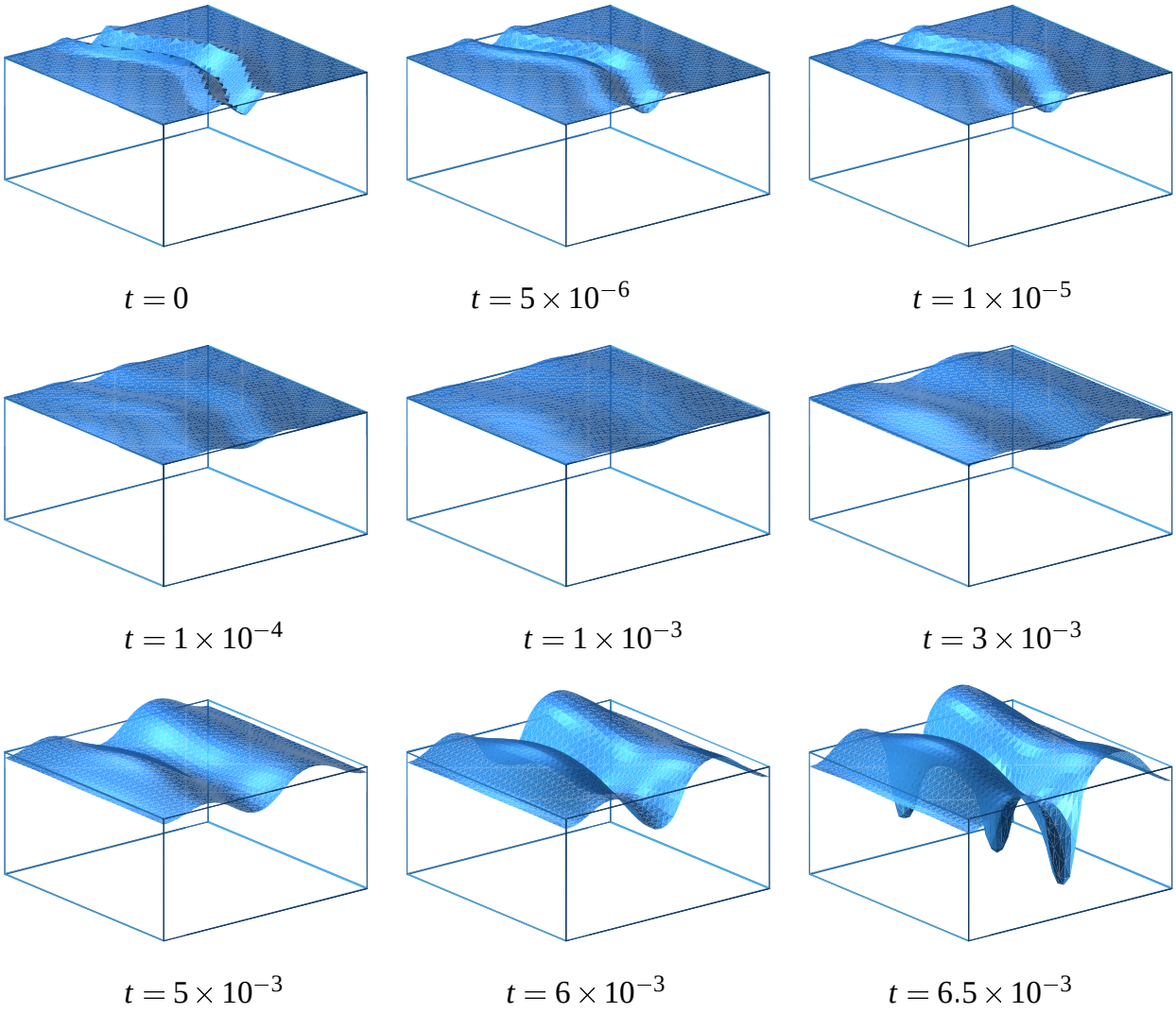

Fig. 2: Solutions for $\varepsilon = -50/u$ and $u_0(x) = 1 + \delta(x)$ at various time instants, with $\delta(x)$ a small perturbation across $y = \cos x$: crack formation

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

Collaborators: E. Bänsch, D. Davis, H. Langmach, G. Reinhardt, N. Scurtu, M. Uhle

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

Semiconductor single crystals and their properties are of central importance in the fields of computer technology and communication. An important application is the production of large crystals with homogeneous and low defect concentration. A well-established processing technique for this purpose is the vapor-pressure-controlled Czochralski method, which is used extensively at IKZ to grow gallium arsenide (GaAs) crystals. This method is characterized by crystal extraction from a crucible containing semiconductor (GaAs) melt, with a viscous encapsulant of relatively large Prandtl number surrounding the crystal and melt, and serving to minimize heat loss. The crucible is heated from the side and below, thereby provoking heat and mass transfer within the melt, and reducing the impurities therein. Furthermore, the crystal and the crucible are rotated since this can directly influence the shape of the liquid-solid interface at the crystal/melt surface, as has been demonstrated at IKZ; in particular, it has been shown that a desired convex interface is best achieved through iso-rotation, i.e. with the crystal and crucible rotated in the same direction.
The liquid mechanics are governed by the Navier-Stokes equations with Boussinesq approximation, together with equations for mass conservation and heat transport (and relevant boundary and initial conditions), i.e.

Navier-Stokes-Boussinesq equations

$$\partial_t \vec{u} + \vec{u}\cdot\nabla\vec{u} - \frac{1}{Re}\Delta\vec{u} + \nabla p = \frac{Gr}{Re^2} T \nabla x_3 \quad \text{in } \Omega\times[t_0,t_1];$$

continuity equation

$$\nabla\cdot\vec{u} = 0 \quad \text{in } \Omega\times[t_0,t_1];$$

heat transport equation

$$\partial_t T + \vec{u}\cdot\nabla T - \frac{1}{Re\,Pr}\Delta T = 0 \quad \text{in } \Omega\times[t_0,t_1].$$

Here, $\vec{u}$, p, T denote the dimensionless velocity, pressure and temperature (zeroed on the crystal melt temperature), while Re, Pr and Gr denote the (rotational) Reynolds, Prandtl and Grashof numbers, in turn. Also, Ω is the melt zone, while $[t_0,t_1]$ indicates an arbitrary time interval and x_3 is the axial coordinate.
There are three (disjoint) boundary sections: the crystal/melt interface (Γ_X), the encapsulant/melt interface (Γ_E) and the crucible surface (Γ_C) with $\partial\Omega = \Gamma_X \cup \Gamma_E \cup \Gamma_C$. The boundary conditions for the temperature play a pivotal rôle in determining the form of the flow and the thermal distribution within the melt. The simplest version of these is to impose a constant temperature on Γ_C (which naturally differs from the constant melt value imposed on Γ_X) together with an adiabatic condition on Γ_E. For the axisymmetric flow simulations, more realistic conditions for temperature, based on global temperature simulation results obtained at IKZ, have also been used, as described below. For the velocity, straightforward Dirichlet conditions, based on the rotational speeds of the crystal and crucible are used.

For this project, we have adapted our finite element code NAVIER for the simulation of the velocity field and the temperature distribution in the melt. This has been applied in a two-dimensional (2D) axisymmetric setting as well as for full three-dimensional (3D) flow simulations. The code uses Taylor-Hood elements (P^2, P^1) for the spatial discretization and a fractional-θ operator-splitting method for the temporal discretization. The numerical procedure, which favorably decouples the incompressibility condition from the treatment of the nonlinearity, is accurate and stable for a wide range of Reynolds numbers.

In simulating axisymmetric flows, we compared the time-averaged results of our unsteady simulations with results obtained at IKZ, where a commercial finite element program, simulating the quasi-stationary behavior of the flow, was employed. For moderate Reynolds numbers (up to 7500), excellent qualitative agreement has been obtained. Despite this, we generally observed the flow to be unsteady in nature, and hence, we believe that unsteady simulation is invaluable for a more precise understanding of the melt flow. Figure 1 shows a time-averaged result arising from the application of a linear temperature distribution on the crucible (with values 0.4, 1.0 and 0.9 at the lowest point, the junction of the curved and straight sections, and the highest point of the crucible, respectively, and interpolation with respect to the radial and axial coordinate on the curved and straight sections, in turn). Very similar qualitative solutions were obtained at critical locations in the melt zone (such as directly beneath the crystal) using constant temperature distributions on the crucible.

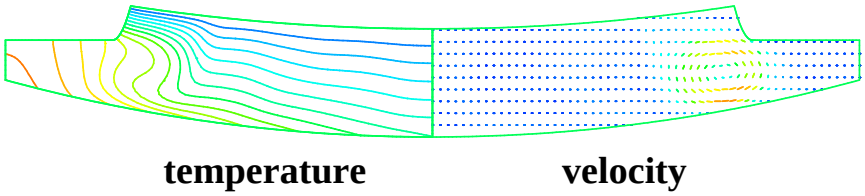

Fig. 1: Time-averaged results for axisymmetric flow simulation

In Figure 2, a time-history curve for the temperature at a given observation point (based on the linear temperature distribution) is shown. The given results were obtained using a rotation rate of 5 revolutions per minute, for both crystal and crucible, and furthermore the buoyancy parameter $Gr/Re^2 = 1.36$, $Pr = 0.068$ and $Re = 6365$.

For this given buoyancy parameter, axisymmetric computations performed in a cylindrical melt zone predict a switch from steady to unsteady motion at a critical Reynolds number $Re^* \approx 2200$. To allow for possible 3D flow structures beyond this critical value, the 3D version of NAVIER (applied to the same melt-zone geometry) has been implemented.

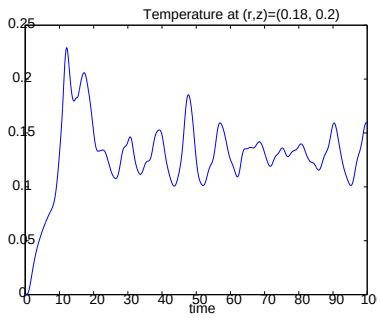

Fig. 2: Temperature time-history curve

For weakly supercritical cases, the flow is initially dominated by a linear instability mode with azimuthal wave number 4, but eventually the flow becomes fully asymmetric due, we believe, to weakly-nonlinear growth effects leading to a modified (and fully 3D) basic flow.

Figure 3 depicts an asymmetric 3D flow for Reynolds number $Re = 2500$ (with $Gr/Re^2 = 1.36$). The corresponding time-averaged values can be seen in Figure 4. They suggest that for moderate Reynolds numbers, 2D effects still dominate over larger time scales, and moreover, that only negligible distortions of the temperature field are observed beneath the crystal.

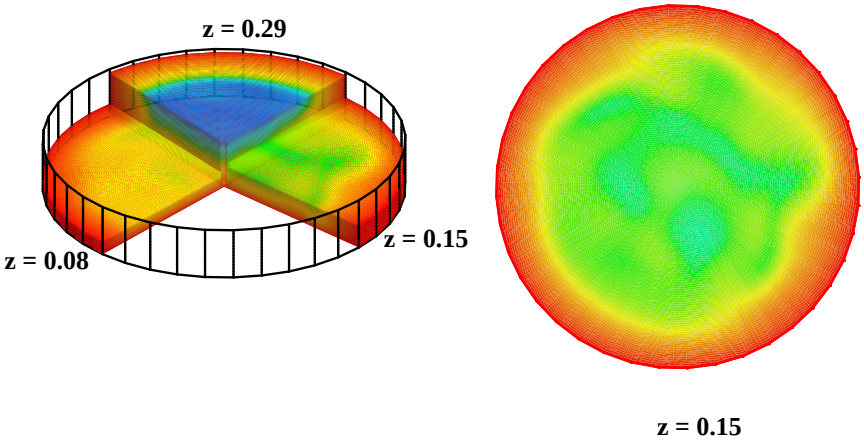

Fig. 3: Asymmetric temperature distribution

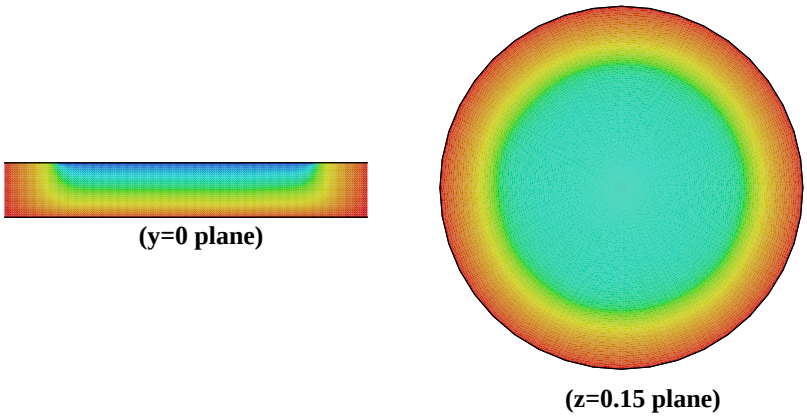

Fig. 4: Time-average temperature distribution

Planned future work in cooperation with IKZ:

- 3D simulations using realistic geometry plus the influence of variable aspect ratio;
- 3D and 2D simulations for several regimes of buoyancy and rotation, especially for larger Reynolds numbers, that is $O(10^4)$;
- 2D simulations incorporating a model for the phase transition at the crystal/melt interface.

Large-scale static and dynamic process simulation

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

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

Supported by: Alstom (Switzerland) Ltd., Baden

The more and more integrated modeling in process engineering leads to large-scale problems in static and dynamic process simulation. The complex real-world process models used in this field usually depend on numerous parameters, are in general highly nonlinear and often involve discontinuities. Using concentrated physical models, high-dimensional systems of nonlinear and differential-algebraic equations (DAEs) have to be solved in static and dynamic process simulation, respectively. For that purpose robust and efficient numerical simulation tools are needed. They are urgently necessary to improve process design, analysis, as well as operation in process industries.

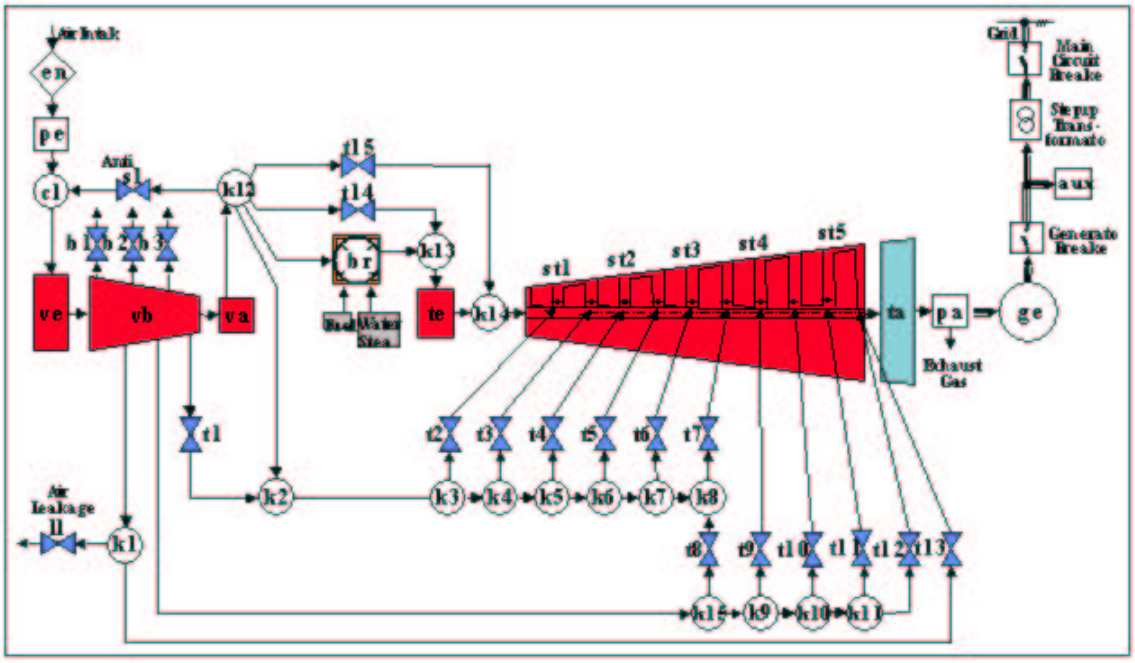

Fig. 1: Unit-oriented modular model of a gas turbine
(ALSTOM (Switzerland) Ltd.)

The simulation concept developed at WIAS is based on divide-and-conquer techniques and exploits the modular structure of the process, which in most cases is defined by the hierarchical unit structure of the underlying plant (see, e.g., Figure 1). With it the corresponding system of equations is structured into subsystems according to the units and can be partitioned into blocks, which can then be treated almost concurrently within appropriately modified numerical methods. The approach 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).
In the period under report, the homogeneous hierarchical simulation approach of BOP has been extended from chemical engineering to more general process engineering problems, and a

steady-state solver for static process simulation problems has been added. Within this approach a block-partitioned system of equations

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

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

has to be 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 [2] can be applied in both cases. While these methods have shown to be successful in the dynamic simulation mode [1], a completely new static simulation mode based on these methods has now been added to the simulator. It combines the well-known globalized Newton method with block-structured Newton-type techniques and some special features resulting from real-world process engineering. The new steady-state solver within BOP has shown first promising results in industrial applications of gas turbine process engineering.
The numerical methods realized within BOP require a repeated solution of linear systems with the same pattern structure of sparse, unsymmetric coefficient matrices. Our direct solver GSPAR solves these linear systems by using advanced direct methods based on Gaussian elimination. Within this approach a new dynamic column reordering algorithm is used to minimize the number of fill-ins, and a modified partial pivoting technique maintains the numerical stability of the method.

Table 4: CPU times (in seconds) for factorization: GSPAR2 compared with *WSMP V1.7*

				GSPAR2		*WSMP V1.7*	
Matrix	N	NNZ	Condition	First Factorization	Second Factorization	Analysis	Factorization
bayer01	57 735	277 774	$4.4 * 10^{15}$	0.840	0.160	2.640	0.460
lhr34c	35 152	764 014	$4.5 * 10^{9}$	6.260	1.460	2.710	0.470
circuit_4	80 209	307 604	$4.7 * 10^{9}$	1.430	0.050	1.980	0.300
shermanACb	18 510	145 149	$2.6 * 10^{6}$	3.020	0.730	0.460	0.110

This modified approach has been implemented in our new linear solver GSPAR2. It has been compared with the solver *WSMP (Watson Sparse Matrix Packages)* (Anshul Gupta, IBM Research Division, Yorktown Heights, New York, USA) concerning computing time. The results for linear systems with matrices arising from different real-world applications are given in Table 4. Here N denotes the order and NNZ the number of nonzeros of the matrices. The computations have been performed on an IBM 7040-681, pSeries 690 with 64-bit Power4 processors.
We have both ported the simulator BOP to PCs operating under Windows 2000 and realized some extensions in the process description. In particular, the process description language MLPE has been expanded with a so-called global section, which allows to identify variables of different units and to define global constraint equations. Additionally, the implementation of a subset of the language of the Aspen Custom Modeler^{TM} has been started.

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Simulation of microwave and semiconductor laser structures

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

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

Supported by: Ferdinand-Braun-Institut für Höchstfrequenztechnik (FBH)

The electric properties of circuits are described in terms of their scattering matrix using a three-dimensional boundary value problem for Maxwell's equations. The computational domain is truncated by electric or magnetic walls; open structures are treated using the Perfectly Matched Layer (PML) absorbing boundary condition.

The subject under investigation is about passive structures of arbitrary geometry. They are connected to the remaining circuit by transmission lines. Ports are defined on the waveguides. In order to characterize their electrical behavior the transmission lines are assumed to be infinitely long and longitudinally homogeneous.

The boundary value problem

$$\oint_{\partial\Omega} \vec{H}\cdot d\vec{s} = \int_{\Omega} j\omega[\varepsilon]\vec{E}\cdot d\vec{\Omega}, \qquad \oint_{\cup\Omega} ([\varepsilon]\vec{E})\cdot d\vec{\Omega} = 0,$$

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

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

is solved by means of a finite-volume scheme in the frequency domain. 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.

Due to the fact that only small fractions of a circuit can be simulated, the pressure for larger problem sizes and shorter computing times is evident. Thus, in the period under report, studies were continued in the following areas:

(1) Eigenmode problem [2]: Only a few modes of smallest attenuation are able to propagate and have to be taken into consideration. Using a conformal mapping between the plane of propagation constants and the plane of eigenvalues, the task is to compute all eigenmodes in a region, bounded by two parabolas. The region is covered by a number of overlapping circles. The eigenmodes in these circles are found solving a sequence of eigenvalue problems of modified matrices with the aid of the invert mode of the Arnoldi iteration using shifts. The method, developed initially for a reliable calculation of all complex eigenvalues from microwave structure computations [4], is expanded to meet the very special requirements of optoelectronic structure calculations. Relatively large cross sections and highest frequencies yield increased dimensions and numbers of eigenvalue problems. Using the results of a coarse grid calculation within the final fine grid calculation yields a remarkable reduced numerical effort. The use of the new linear sparse solver PARDISO [12] (see page 85) rather than UMFPACK [3], and two levels of parallelization result in an additional speed-up of computation time.

(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. The systems of linear equations are solved using a block Krylov subspace iterative method. Independent set orderings, Jacobi and SSOR preconditioning techniques are applied to reduce the dimension and the number of iterations [13]. In comparison to the simple lossy case the number of iterations of Krylov subspace methods increases significantly in the presence of Perfectly Matched Layers. This growth could be further reduced by applying suitable grids and PML. The speed of convergence depends on the relations of the edges in an elementary cell of the nonequidistant rectangular grid in this case. The best results can be obtained using nearly cubic cells grids. Moreover, overlapping PML conditions on the corners downgrade the properties of the coefficient matrix, and should be avoided.

(3) Consistent subgridding scheme: For the above-mentioned methods the geometry to be analyzed is subdivided into elementary rectangular cells using three-dimensional nonequidistant rectangular cells. Applying rectangular grids, a mesh refinement in one point results in an accumulation of elementary cells in all coordinate directions even though generally the refinement is needed only in certain regions. Due to the high spatial resolution required, CPU time and storage requirements are very high. A general approach to handle small structure details is to introduce local mesh refinement ([14]) with hanging nodes. Energy and divergence conservation have to be conserved throughout the discretization process for Maxwell's equations. Maxwell's grid equations have been derived for some kinds of submeshes.

(4) Tetrahedral grids [11]: Rectangular grids are not well suitable for the treatment of curved and non-rectangular boundaries. Thus, supported by FBH, the development of a finite-volume method was continued by using unstructured grids (tetrahedrals, see page 83) for the boundary value problem.

The new research results have been published in [5] – [10].

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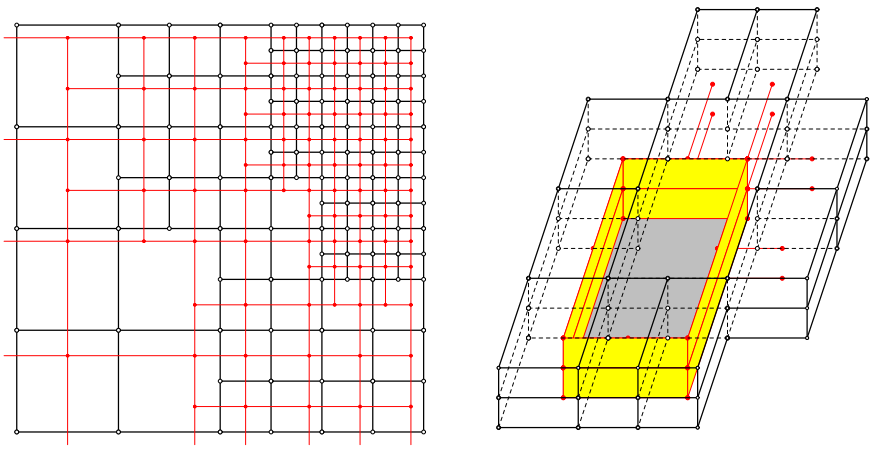

Fig. 1: Subgridding

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

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

The purpose of this project is the maintenance and further development of `pdelib`, a toolbox of software components for the numerical solution of partial differential equations. During the last year, efforts have been undertaken in order to develop a prototype of the new `pdelib2` kernel which is aimed at higher efficiency especially in the context of three-dimensional simulations while maintaining the modular structure of the existing version.
The present state is characterized by

- Shared memory parallelization of grid access and linear algebra. A parallelization layer has been developed which, depending on the available compilers, allows to work either with the pthreads library or OpenMP compiler directives.
- Equally efficient access of node-, edge-, facet- and cell-based degrees of freedom. This is facilitated by a mesh data structure based on adjacency matrices stored in index lists. On top of this, higher-order finite element functionality shall be implemented.
- Vectorizable element callback functions. In difference to the existing `pdelib` implementation, the atomic mesh item accessed by the user is a list of elements rather than a single element. In this way, superscalar optimizations and efficient cache re-use are organized. Furthermore, a modularization based on an element list level is connected with far less function call overhead.
- Efficient search functions on simplicial meshes;
- User input in the Lua language. The whole Lua user interface is restructured. The user can access mathematical objects like vectors, block vectors, and matrices in a mathematically motivated manner, similar to, e.g., matlab.
- Integration of TetGen (3D) and triangle (2D) boundary-conforming Delaunay mesh generation tools. A user of `pdelib2` will be able to describe the geometry in the Lua language. The corresponding data are directly fed to the mesh generators using the triangulateio resp. tetgenio data structures provided by them.
- Integration of `COG`;
- Support of complex numbers.

3D Delaunay mesh generation

Collaborators: I. Schmelzer, H. Si, K. Gärtner, H. Langmach

The generation of three-dimensional boundary conforming Delaunay meshes is an essential task in the development of simulation tools for many of the projects within and without WIAS. Project works include the further development of the mesh generator COG, and the development of the open source mesh generation tool TetGen.

COG In complex CAD and computer graphics applications, it happens that for some object a surface grid is already available but is too fine for a given application. The typical example is that a surface grid has been created for one application like computer-aided design, and we need a surface grid for another application like visualization where the rendering of a grid with too much detail would be too slow. During the year 2002, in a cooperation with I. Bremer (research group "Nonlinear Optimization and Inverse Problems"), based on the mesh generator COG, a fully automatical algorithm for such surface grid coarsening has been developed and implemented. The basic ansatz is to create a three-dimensional grid with COG and to extract the surface grid afterwards. Furthermore, an interface of COG to the IRIS Performer library has been created in order to be able to use this algorithm in a complex visualization context.

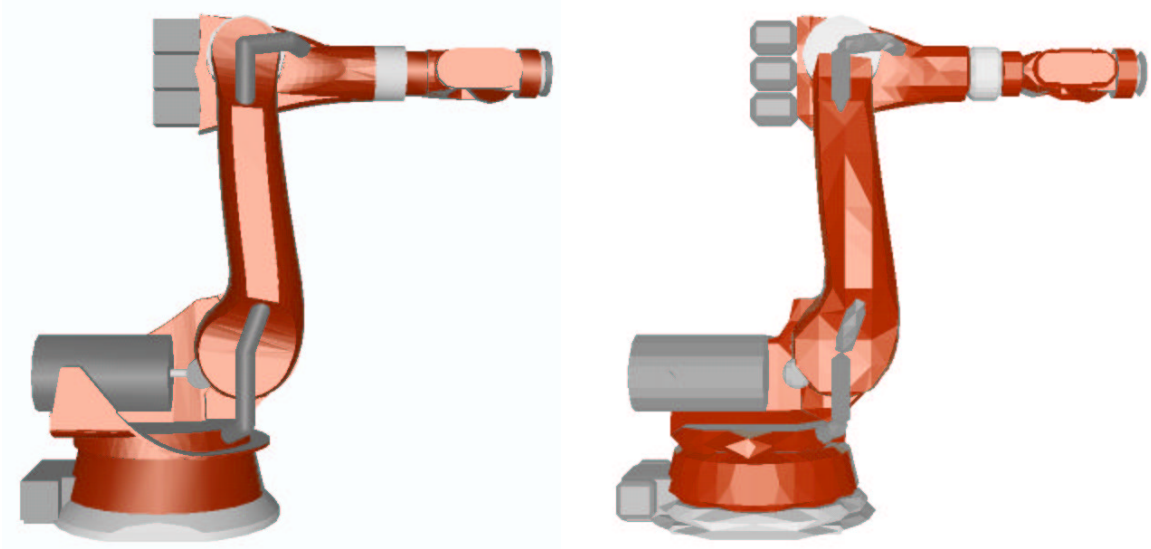

Fig. 1: COG: Full (left) and reduced (right) model of a robot. The number of triangles has been reduced to the half.

TetGen Starting with the year 2002, the Weierstrass Institute supports the development of the mesh generator TetGen developed by Hang Si. The source code is available from http://tetgen.berlios.de. This code is based on algorithms which essentially generalize the successful approach used in two space dimensions in the code triangle [1] to three space dimensions.
The aim of this project is twofold: There are several open problems in 3D mesh generation. Algorithm development based on a well-developed mathematical understanding of the problems shall provide a sound base for more robust tools. The support of a publicly available code (corresponding to the Open Source development paradigm) is an ideal vehicle for initiating communication between research groups interested in these developments.

At the other hand, there is considerable practical interest in having a robust tool just now. Correspondingly, TetGen is being improved within many respects of stability and user-friendliness. During 2002, project works focused on the following subjects:

- A new geometry library was added to TetGen which is based on numerically stable evaluation of geometric predicates. This library largely improved the stability and robustness of TetGen.
- A new structure “tetgenio” was added which allows input/output data directly from memory.
- A program (plcview) based on the `gltools` library can now be used to view the input geometry (.node, .poly, and .smesh) of TetGen.
- The code has been ported and debugged on several UNIX systems available at WIAS.

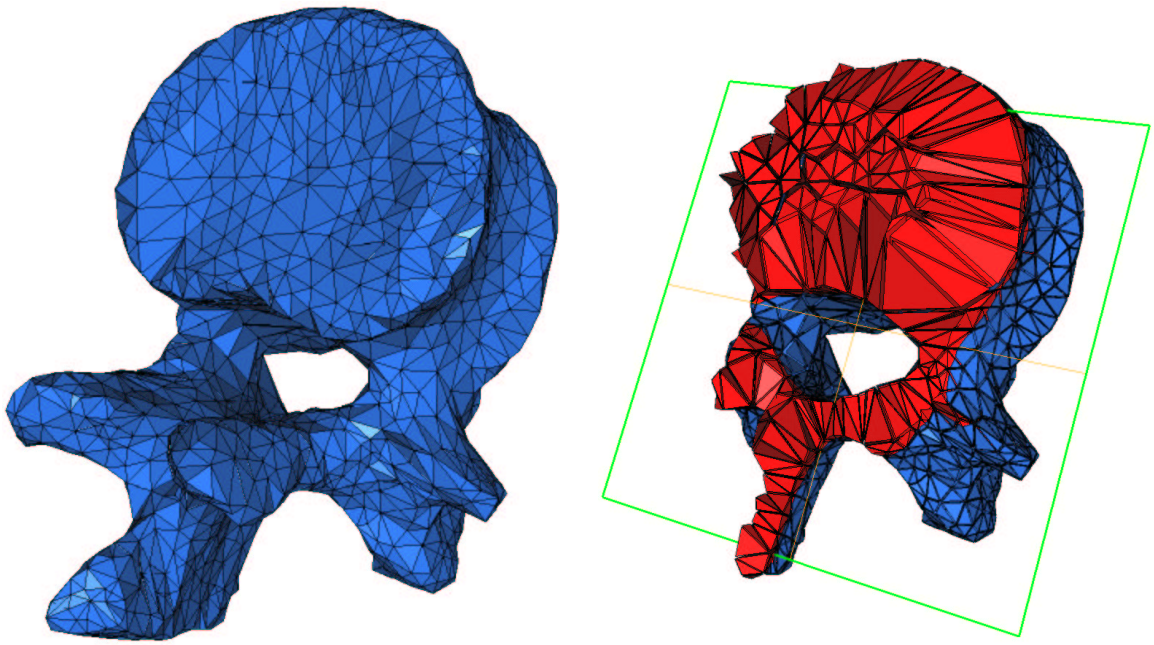

Fig. 2: TetGen: Constrained Delaunay tetrahedralization of the geometry of a human spine. Geometry courtesy by Hae Jung Yang, Department of Physics, Chosun University, South Korea

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PARDISO, improved parallel efficiency for direct sparse *LU*-factorization

Collaborator: K. Gärtner

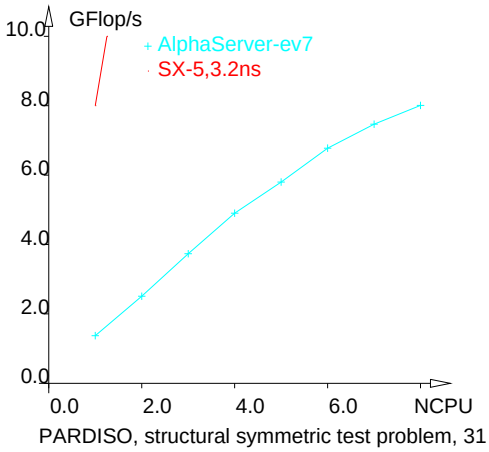
Cooperation with: O. Schenk (Universität Basel, IFI, Switzerland)

PARDISO is a SMP-parallel, direct solver for sparse linear systems with coefficient matrices close to structural symmetry. The development started within in the framework of the ETH-CRAY-SuperCluster collaboration and was continued over the years by both authors. PARDISO is well established in some application areas and distributed via computer vendor libraries (NEC, Compaq), too. The activities during the year 2002 focused on:

- Porting to IA-32/IA-64 SMPs using up-to-date versions of Intel's OpenMP Fortran compilers;
- Improvements for matrices far from structural symmetry (see [1]);
- Two-level scheduling to improve the parallel efficiency due to a reduced number of synchronization events without increasing the number of operations [2];
- Application to some special saddle-point problems to estimate the effort for a more general solution;
- Assistance for use in different IFI/WIAS applications.

The supported matrix types (complex and real, spd, Hermitian, complex symmetric), the low operation count, the BLAS3 performance reached during the factorization, and the fill-in close to $ln(n)n$ for 2D problems (n number of unknowns) make PARDISO a workhorse for solving many (especially 2D) partial differential equation problems.
An increased penetration speed of the code into WIAS application problems was observed during 2002. To name a few: diffractive optics (see page 90), eigenvalue problems for Maxwell's equations in microwave guides and lasers (see page 79), crystal growth modeling (see page 43).

Within an evaluation of the new ev7-based HP-AlphaServer generation, PARDISO was used, too. Typical (wall-clock) times are: a standard test problem (Laplace equation on a triangular unstructured grid with 151389 nodes) is factorized now in 0.9 sec on the 1.0 GHz single ev7 CPU, the 3D laser diode structural symmetric test problem (311819 unknowns) can be solved on the 8 CPU configuration in 6:13 min with parallel efficiency above 70 % without the two-level scheduling. On the other hand that last number is in the same range that could be reached on a single CPU SX-5 two years ago.



PARDISO, structural symmetric test problem, 31 preliminary test results ev7 1.0 GHz

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Visualization of numerical simulations and production of presentations

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

Cooperation with: U. Pirr (Humboldt-Universität zu Berlin)

In the period under review, the support for the graphical display of numerical results (for the whole institute) has been successfully continued. For the research groups “Numerical Mathematics and Scientific Computing” and “Stochastic Algorithms and Nonparametric Statistics”, videos were produced in MPEG and VHS formats.

We supplemented our software equipment with the visualization tool “AVS/Express” and the tool for digital video editing “Adobe Premiere”. The new visualization tool was required owing to the increase in visualization tasks in our institute. This is especially true in the field of computational fluid dynamics, where the simulation of unsteady, three-dimensional problems has produced large quantities of data, which required a modern and powerful visualization tool. Figure 1 shows several slices in a diagram of a simulation of melt flow during crystal growth; it was produced by the new visualization tool using data from one simulation step, and is 63 MBytes (360000 nodes, 265000 tetrahedra) in size.

The tool for digital video editing is applicable only for systems of personal computers. The change from the “workstation world” to the “PC world” was necessary, given the greater diversity of the PC tool. It has proven to be the case that tasks requiring digital video editing are better solved with software on PCs than with software on the operating system UNIX.

For the archiving of the visualization data and to ease the burden on our central file server, we have equipped one of our computers with a larger local harddisk capacity.

For the exhibition to celebrate the 10th anniversary of the “Forschungsverbund Berlin e.V.” in February 2002, we displayed and demonstrated our equipment used for visualizing simulation data to a wider public.

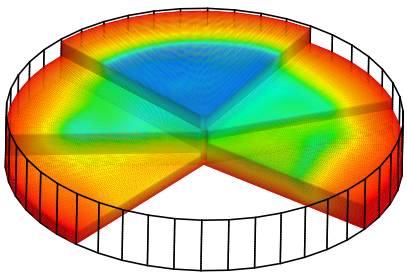

Fig. 1: Perspective view showing several slices in a melt-flow simulation

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, die EU, das BMBF und die DFG gefördert.

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, EU, BMBF, and DFG.

Die Forschungsschwerpunkte waren:

- Direkte und inverse Diffraktionsprobleme der Mikrooptik,
- Optimierungsprobleme mit zufälligen und nichtglatten Daten,
- Bahnplanung für Industrieroboter in der Automobilindustrie.

The main research topics were:

- Direct and inverse diffraction problems in microoptics;
- Optimization problems with random and nonsmooth data;
- Path planning for industrial robots in car industry.

Im Rahmen des DFG-Forschungszentrums „Mathematik für Schlüsseltechnologien“ wurde ein neues gemeinsames Projekt mit der Humboldt-Universität zu Berlin zur Kraftwerkseinsatzplanung initiiert.

Within the DFG Research Center “Mathematics for Key Technologies”, a new project on electricity portfolio management (jointly with Humboldt University of Berlin) was recently initiated.

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

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

- Optoelektronische Sensoren (zusammen mit der Forschungsgruppe „Partielle Differentialgleichungen und Variationsgleichungen“),
- Optimierung von 3D-Modellen (Visualisierungsperformance) (zusammen mit der Forschungsgruppe „Numerische Mathematik und Wissenschaftliches Rechnen“),

- Optoelectronic sensors (in cooperation with research group “Partial Differential Equations and Variational Equations”);
- Optimization of 3D models (visualization performance) (in cooperation with research group “Numerical Mathematics and Scientific Computing”);

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

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

4.4.2 Projects

Direct and inverse diffraction problems in microoptics

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)

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 simulation of diffraction by polygonal gratings (J. Elschner, A. Rathsfeld, G. Schmidt).
The diffraction of electromagnetic waves by optical gratings (surface structure consisting of periodically located "grooves", i.e. the structure is periodic in one surface direction and constant in the other) can be reduced to a plane wave diffraction problem for the two-dimensional cross section. Mathematically, a boundary value problem for the Helmholtz equation on a domain with the length of one period is to be solved by FEM-BEM coupling. For small wave numbers, this is easily done by standard FEM. In order to treat the highly oscillatory solutions for the case of larger wave numbers, a generalized FE method which employs piecewise approximate Helmholtz solutions for the trial space has been developed. The corresponding code GDPOGTR is able to compute gratings in the case of polygonal grating structures for different polarization types under classical and conical incidence. We have compared this code with the alternative partition of unity method (PUM) combined with mortar techniques. Contrary to the extremely ill-conditioned equations in case of the PUM, GDPOGTR turned out to work quite well. Table 6 and Figures 1 and 2 show the results of the computation for an echelle grating with superstrate air, with substrate aluminium, with MgF_2 coating of thickness 25 nm, with apex angle of 90° and blaze angle of 80° and with 166 grooves per mm. The grating is illuminated by a TE polarized wave of wavelength 155 nm under an incidence angle of 80°. Using classical FEM, no acceptable result can be obtained with less than 2 000 000 unknowns.

degrees of freedom	memory for solver	reflected efficiency of order -74
105 785	0.35 GB	37.931045
263 624	0.70 GB	67.384460
559 800	1.98 GB	68.390312

Table 6: Results of GDPOTR for echelle grid

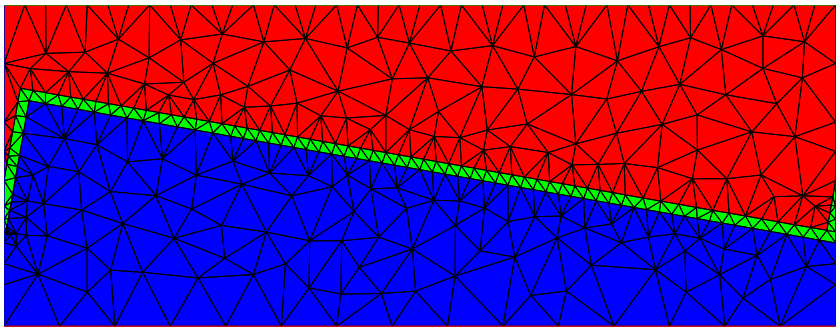

Fig. 1: Triangulation of coated echelle grating

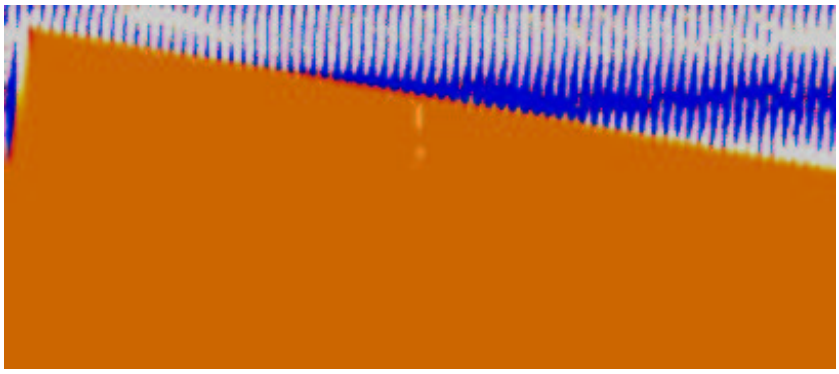

Fig. 2: Real part of transverse component of magnetic field for coated echelle grating

2. Modeling of 3D optical gratings (G. Schmidt).
In [9] the diffraction by biperiodic structures is considered which consist of in general anisotropic materials, are periodic in two not necessarily orthogonal directions and separate two regions with constant dielectric coefficients. The scattering of plane waves is modeled by time-harmonic Maxwell equations with special quasi-periodic radiation conditions.
The biperiodic diffraction problem is to find, for a given incident wave of arbitrary polarization, the scattered far-field pattern, i.e. the diffraction efficiencies and the states of polarization of all propagating diffracted waves. This problem is of considerable interest in different areas of modern optics, where such doubly periodic structures are called crossed anisotropic gratings. The numerical modeling of those devices has recently received considerable attention within the engineering community.
The analysis is based on a variational formulation for the magnetic field in a bounded biperiodic cell with nonlocal boundary conditions which is equivalent to Maxwell's system. Since the variational problem is strongly elliptic, quite complete results can be obtained concerning the solvability and uniqueness of the biperiodic diffraction problem. It is shown that the biperiodic diffraction problem for general structures is always solvable and that the solution is unique with the possibly exception of a discrete set of wavelengths converging to infinity. If the structure contains absorbing materials then the problem is uniquely solvable for all wavelengths. Moreover, the strong ellipticity of the variational formulation justifies the use of finite element methods to solve the biperiodic diffraction problem.

3. Reconstruction of grating profiles (G. Bruckner, J. Elschner, G. Schmidt).
The problem of recovering a periodic structure from knowledge of the scattered field occurs in many applications, e.g., in diffractive optics ([10]), radar imaging, and nondestructive testing. We studied the scattering of monochromatic plane waves by a perfectly reflecting diffraction grating in an isotropic lossless medium, which is modeled by the Dirichlet problem (transverse electric polarization) or the Neumann problem (transverse magnetic polarization) for the periodic Helmholtz equation.
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 the wave number k is a positive constant and $\theta \in (-\pi/2, \pi/2)$ is the incident angle. The *inverse problem* or the *profile reconstruction problem* can be formulated as follows.
(IP): Determine the profile function f from the knowledge of *one* wave number k, *one* incident direction θ and the total field $u|_{x_2=b}$ on a straight line $\{x \in \mathbb{R}^2 : x_2 = b\}$ with $b > \max(f)$.
Note that this problem also involves near-field measurements since the evanescent modes cannot be measured far away from the grating profile. The global uniqueness in problem (IP) is known if the wave number or the amplitude of the grating are sufficiently small ([8]). In general, global uniqueness may not be true. This can be seen from the simple counterexample of the scattering of $u^{in} = \exp(-ikx_2)$ when one moves the flat grating in certain multiples of the wavelength. Even if one excludes this flat case, the global uniqueness is not known with a single wave number.
We were able to solve this open problem in the practically important case of piecewise linear grating profiles [7]. A preliminary result for rectangular diffractive structures (e.g., for binary gratings) was established in [6]. The proof relies on the analyticity of solutions to the Helmholtz equation and the Rayleigh expansion of the scattered field.
Furthermore, in the case of the inverse Dirichlet problem, we continued to study the performance of reconstruction algorithms for grating profiles given by truncated Fourier series or piecewise linear profile functions. To this end, an unknown density function is computed from measured near-field data first, which allows us to represent the scattered field as a single layer potential. This is a severely ill-posed linear problem with a known singular value decomposition that helps to solve it at a low numerical expense. Then the computed density function is used as input to a nonlinear least squares problem which determines the unknown profile as the location of the zeros of the total field and is solved by the Gauss-Newton method. This approach, originally due to Kirsch and Kress in the case of acoustic obstacle scattering, avoids the solution of a direct problem in each iteration. Additionally, since only the grating parameters need be improved in each Gauss-Newton step, the linear system is of low dimension.
Numerical experiments with synthetic and noisy data have demonstrated the efficiency of the inversion algorithm [1]. The case when the minimization of the Tikhonov functional for the linear problem and the defect minimization of the Dirichlet condition is combined into one cost functional has been treated in [2]; see also [3] for its mathematical foundation in the general case of Lipschitz grating profiles.

4. Inverse medium problems (J. Elschner, A. Rathsfeld).
A more challenging inverse problem is the reconstruction from far-field measurements of gratings with unknown refractive index, i.e. the refractive index is to be determined as a function of the points in the cross-section domain. Again, we have reduced this task to an optimization problem. Now the electric field is included in the set of arguments and the residual of the Helmholtz equation is added as a penalty term into the objective functional. For a fixed regularization parameter, we proved the solvability of the optimization problem, and, for the parameter tending to zero, we showed the convergence to a minimizer. Using FE discretization and conjugate gradient or SQP, numerical experiments confirmed these results (cf. [5]). Of course, due to the large number of local minima for the high-dimensional problem, a good initial solution is required. The left picture of Figure 3 shows the refractive index function of a lamellar grating with substrate of index 1.5, with a small rectangle of index 1.5, and with a higher rectangle of index 1.3. Above the grating we assume air with index 1 and the period is 1 μm. For our reconstruction, we illuminated the grating by light with a wave length of 633 nm. The far-field data was chosen as the efficiencies and phase shifts corresponding to the reflected and transmitted modes for plane wave illumination incident from 25 different directions. The reconstructed function is shown in the right picture of Figure 3 and exhibits similar approximation properties like reconstructions in inverse scattering problems.

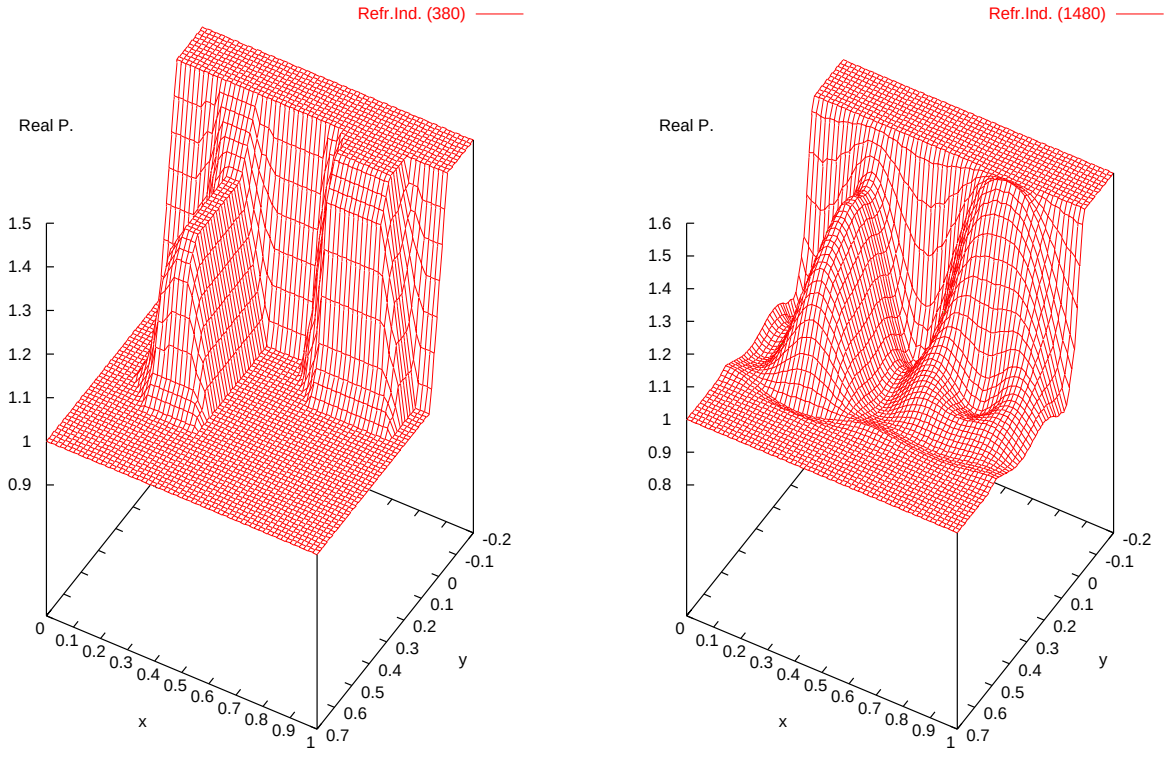

Fig. 3: Given and reconstructed two towers. CG method

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Optimization problems with random and nonsmooth data

Collaborator: R. Henrion

Cooperation with: W. Römisch (Humboldt-Universität (HU) zu Berlin), G. Wozny (Technische Universität (TU) Berlin), M. Steinbach (Konrad-Zuse-Zentrum für Informationstechnik Berlin (ZIB)), 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)

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

Many applied optimization problems are subject to random and/or nonsmooth parameters in the data. This research project deals with modeling, development of solution procedures and investigations on the structure and stability of such problems. It is embedded into a cooperation with other scientific institutions in Berlin via DFG research projects (with HU and TU), the joint organization of a yearly course for chemical engineers supported by DECHEMA (with TU and ZIB) and a joint research seminar (with HU and ZIB).
The focus of research is on optimization problems with probabilistic constraints. There are two major applications considered in this context:

- Optimization of a continuous distillation process under random inflow rate (previously supported DFG project);
- Mean risk models for electricity portfolio management and stochastic programming (recently supported joint DFG project with W. Römisch, HU Berlin).

The key problem in the first application was to cope with random inflow rates of a methanol/ water mixture to a feed tank 1. A basic control variable is given by the rate of directing the mixture from the tank to the distillation column such that the undesired violation of upper and lower filling levels in the tank are avoided at high probability. Figure 1 illustrates a part of results obtained for a column with 20 trays driven at TU Berlin. It opposes the extraction profile obtained by probabilistic constraints (red) to that obtained by simple averaging of the inflow process (blue). As can be seen from the filling level profiles in the tank (based on 100 simulated inflow profiles), the safety of meeting the upper and lower level constraints (lines) can be drastically increased while the objective function (heat consumption) could be kept at the same value. The solution of the overall control problem is illustrated by a selected control variable (heat profile) and a selected state variable (temperature profiles in the twenty trays).

The recently initiated second application (joint project with W. Römisch, HU Berlin) addresses the extension of traditional expected revenue maximization in power engineering to mean-risk models. The main task is to identify suitable risk measures (e.g., [3], [4]) that fit from the algorithmic and stability point of view to the framework of solution methods in power management (e.g., [2]). One aspect to be considered here is the formulation of risk in terms of probabilistic constraints. Preliminary work in this direction has focused on the implementation of an algorithm for solving programs with polyhedral chance constraints (joint work with J. Bukszar, University of Miskolc and T. Szántai, Technical University of Budapest).
Both applications gave rise to theoretical investigations such as suitable approximations of probability measures or the structure of the feasible set in stochastic programming ([5], [6],

[7]). The typically nonsmooth character of stochastic programs motivated to study the so-called calmness property of multifunctions which plays a fundamental role in the (nonsmooth) theory of first order necessary conditions, local error bounds, penalty methods, and weak sharp minima ([8], [9]).

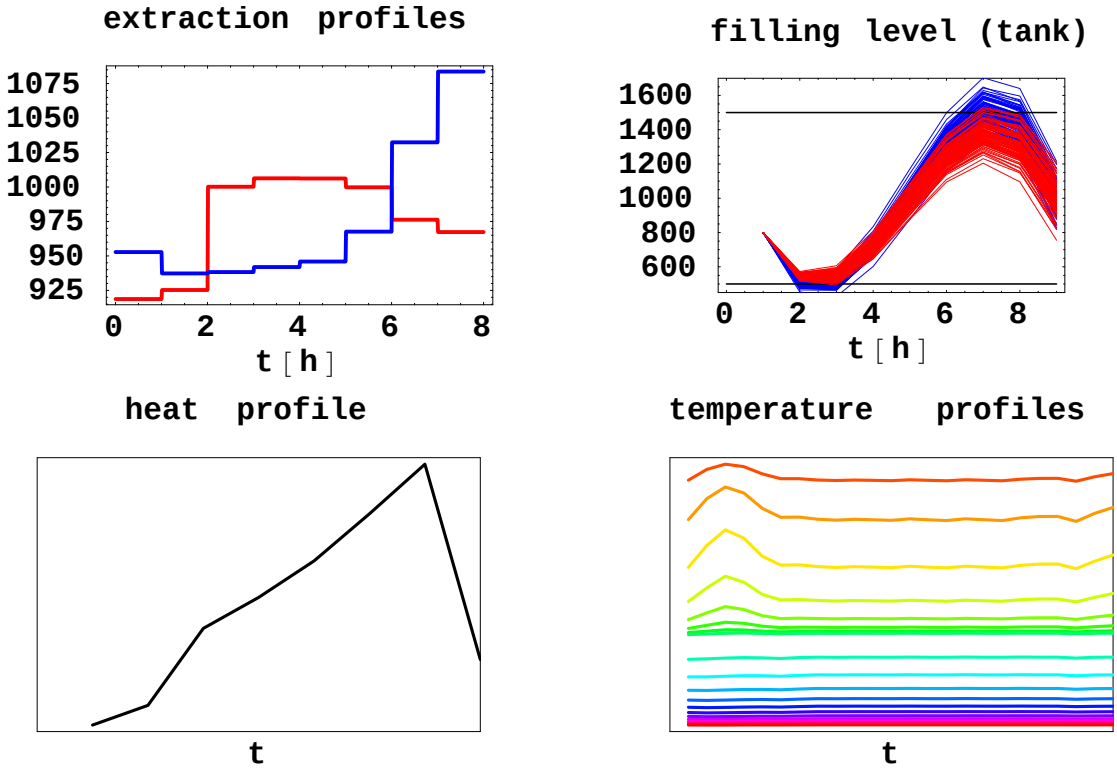

Fig. 1: Results for the optimal control of a distillation process

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Regularization of severely ill-posed problems and applications

Collaborator: G. Bruckner

Cooperation with: J. Cheng (Fudan University, Shanghai, China), S.V. Pereverzev (National Academy of Sciences of Ukraine, Kiev)

In the mathematical treatment of inverse problems ranging from tomography over non-destructive testing to satellite geodetic exploration, operator equations of the form

$$Ax = y \tag{1}$$

arise, where A is a linear operator, and the right-hand side y is given only approximately.
The problems (1) are ill-posed, in most cases even severely ill-posed, and have to be regularized for solution. Since the problems are usually given in infinite-dimensional spaces they must be additionally discretized. Therefore the well-known method of regularization by discretization seems to be natural and is frequently used. Moreover, because of the lack of information about the singular values of A and the smoothness of the solution x, for constructing regularization procedures, the a posteriori parameter choice by discrepancy principles has been proposed. Recently, T. Hohage [3] considered discrepancy principles with respect to Tikhonov's regularization, while the investigations of B. Kaltenbacher [4] referred to the moderately ill-posed case.
In the present project, the idea of regularization by discretization is continued with a new strategy of a posteriori parameter choice that assumes only estimates for the singular values and the smoothness of the solution (cf. [2]). The algorithm is not based on a discrepancy principle and selects a relevant discretized solution from a number of discretized solutions for subsequent discretization levels. The selected approximate solution has an optimal order of accuracy. Moreover, the algorithm is applied to a problem with a logarithmic convolution-type operator (cf. [1]), for which the assumptions can be verified. Further work is needed to apply this method to nondestructive testing, quality control of grating devices or other real-world problems.

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Integral equation methods for problems of mathematical physics

Collaborator: G. Schmidt

Cooperation with: V. Maz'ya, (Linköping University, Sweden), W. Wendland (Universität Stuttgart), V. Karlin, (University of Lancashire, Preston, UK)

Supported by: (EU) INTAS: "Development of constructive and numerical methods for solving nonlocal linear and nonlinear problems for partial differential equations"

The project "Development of constructive and numerical methods for solving nonlocal linear and nonlinear problems for partial differential equations", which was coordinated by the Weierstrass Institute, was supported by INTAS from 10/1999 till 10/2002. Groups from Germany, Sweden, Italy, Russia, Belorussia, Georgia, and Ukraine participated in this project.
Within the project in 2002 the following topics were studied:
In [1] a new cubature method for surface potentials via approximate approximations was developed. It is applied to the computation of multi-dimensional single layer harmonic potentials. Due to singularities under the integral sign, in the multivariate case usual cubature methods are very expensive if the potential has to be computed close to the surface.
Our approach uses the asymptotic expansion of surface integrals by integrals over the tangential plane, which can be transformed to one-dimensional ones for radial basis functions and provides therefore efficient high order cubature formulas for surface potentials.
In [2] we developed and implemented a new numerical method for solving the Sivashinsky equation, which models dynamics of the long wave flame instability. The discretization of this nonlocal nonlinear evolution equation is based on approximate approximations, which allows the exact computation of singular integrals.
Extended numerical experiments confirm theoretical results on the convergence of the method. They are used to study the sensitivity of flame fronts with respect to external perturbations.

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Path planning for industrial robots in car industry

Collaborator: I. Bremer

Cooperation with: Rücker Ges.m.b.H (Graz, Austria)

Industrial robots are used in a wide range of applications in car industry. In the planning phase, we use simulations of the production process based on a VR[2]-environment to get recommendations for the placement of the robots, the model choice for the time-behavior and other problems. In our project we treated a concrete, real-life problem: the path optimization for adhesive and sealant seams.
Last year's[3] results have been used for computing optimized speed profiles. The resulting seam depends on several parameters: the rotation number of the jet head, the flow rate, the speed of TCP (tool center point), the distance from TCP to the surface.
Data from measurements have been used to build an extrapolation table to get the width of the seam for given parameters. To simplify the mathematical model we replaced the rotating spray jet (or head) by a ring (as some kind of averaging).
The simulation for the seam creation in real-time was done by an appropriate time and space discretization in a 3D-VR-environment based on SGI performer for OpenGl.
The discretized model for the required seam was explicitly given to us or we extracted it from a CAD-made 3D graphical seam model.
We adjust the place, width and height of the computed seam to that of the required seam by an optimization step.
As a brief description of the algorithm we have

```
start speed profile
loop
 simulation of putting the material on the surface in realtime
 computing the difference between the resulting seam
  and the required seam
 correction of speed profile
endloop
```

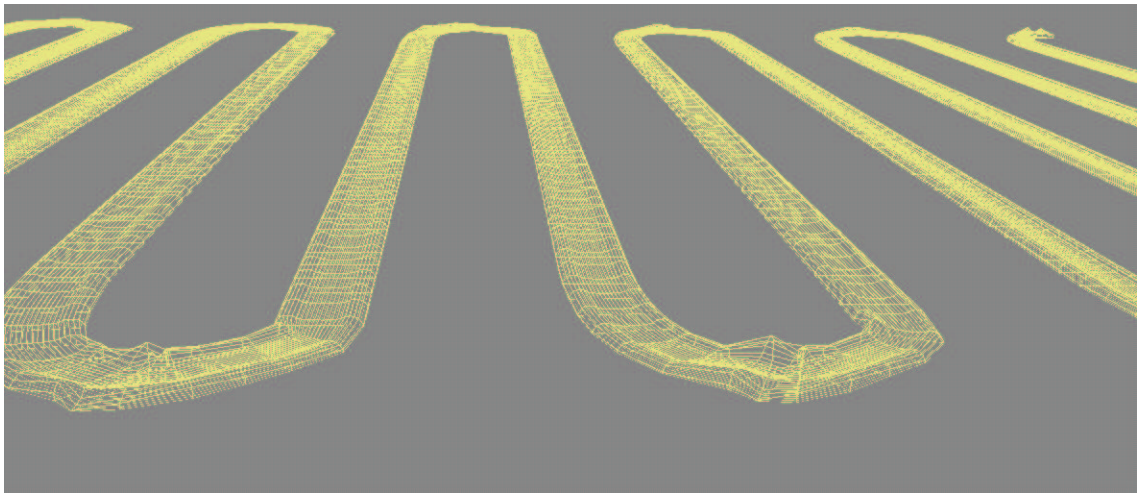

Fig. 1: Screen-shoot: grid of a resulting seam on a table with different given distances of TCP

[2]VR: Virtual Reality
[3]http://www.wias-berlin.de/publications/annual_reports/2001/node57.html

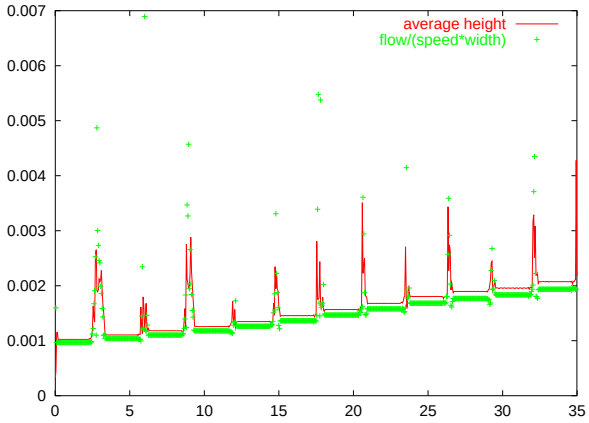

Fig. 2: Comparison of measured heights (thicknesses) of seams with simulated ones

4.5 Research Group Interacting Random Systems

4.5.1 Overview

Das Hauptinteresse der Forschung hat sich im vergangenen Jahr weiter auf stochastische dynamische Systeme konzentriert, wobei eine Anzahl bemerkenswerter Resultate erzielt werden konnte. Diese betreffen klassische Diffusionen in Driftfeldern, die von einem Potential herrühren, zufällige Störungen von schnell-langsamen dynamischen Systemen, unendlichdimensionale Diffusionsprozesse und wechselwirkende Verzweigungsprozesse. 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 stetige Verzweigungsprozesse eine wesentliche Rolle, eine Tatsache, die die vielfältigen Beziehungen zwischen den verschiedenen in der Gruppe untersuchten Fragestellungen illustriert.

The main focus of the research in the past year has further been on stochastic dynamical systems, where a number of remarkable results could be obtained. These concern classical diffusions in potential drift fields, stochastic perturbations of slow-fast dynamical systems, infinite-dimensional diffusion processes and interacting branching diffusion 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 branching processes play a crucial role, highlighting the mathematical coherence of the different areas of activity within the group.

Im Jahr 2002 haben zwei Doktoranden von S. Rœlly und ein Doktorand von W. Wagner ihre Dissertationen abgeschlossen. Mitglieder der Forschungsgruppe waren beteiligt an der Organisation des Workshops „Stochastic Methods from Statistical Physics III“ in Eindhoven, der im Rahmen des DFG-Schwerpunktprogramms „Interagierende Stochastische Systeme von hoher Komplexität“ stattfand, sowie an der Organisation des Workshops „Spatially Distributed and Hierarchically Structured Stochastic Systems“, der in Montreal abgehalten wurde. Das Programm „Random Dynamics in Spatially Extended Systems“ der European Science Foundation hat 2002 seine Arbeit aufgenommen. Es bietet eine Plattform für die Zusammenarbeit von Wissenschaftlern aus 13 europäischen Ländern zu Themen, die eng verwandt sind mit den Forschungsinteressen unserer Gruppe. Die Forschungsgruppe ist im Lenkungsausschuss des Programms vertreten.

In 2002, two students of S. Rœlly and one student of W. Wagner completed their Ph.D. thesis. Members of the group participated in the organization of the Workshop “Stochastic Methods from Statistical Physics III” in Eindhoven in the framework of the DFG Priority Program “Interacting Stochastic Systems of High Complexity” as well as of the Workshop “Spatially Distributed and Hierarchically Structured Stochastic Systems” that took place in Montreal. In 2002, the European Science Foundation Programme “Random Dynamics in Spatially Extended Systems” has become operative. It presents a platform for scientists from 13 European countries working on subjects related to the scientific interests of our research group to interact on the European level. The research group is represented in the Steering Committee of this program.

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

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

4.5.2 Projects

Stochastic dynamics

Collaborators: A. Bovier, B. Gentz

Cooperation with: G. Ben Arous (Courant Institute, New York, USA), N. Berglund (Centre de Physique Théorique, Marseille, and Université de Toulon, France), M. Eckhoff (University of Zürich, Switzerland), V. Gayrard (Centre de Physique Théorique, Marseille, France, and Ecole Polytechnique Fédérale, Lausanne, Switzerland), M. Klein (Universität Potsdam)

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 the past year, the results for discrete Markov chains obtained in [5] have been extended to diffusion processes in the continuum [6], [7]. The processes we consider have generators of the form

$$l_\varepsilon = -\varepsilon\Delta + \nabla F \cdot \nabla$$

where F is a real valued, smooth function on a regular subset of $\mathbb{R}^d$. Here $\varepsilon > 0$ is a small parameter. In this setting metastable behavior arises when F has several local minima. In this setting, we are able to again relate in a precise way *metastable mean exit times* to the small eigenvalues of the Markov generator. These eigenvalues are in turn related to the eigenvalues of a classical *capacity matrix*, associated to a capacitor made of small balls centered around the local minima of F. Using variational inequalities, it turns out that the relevant capacities can be computed in this case precisely up to multiplicative errors tending to one as $\varepsilon \downarrow 0$, under some non-degeneracy conditions on the function F. This allowed to give the first rigorous proof of some classical formulas attributed to Eyring [8] and Kramers [10]. A by-product of our proofs provides also very sharp estimates on the eigenfunctions corresponding to the exponentially small eigenvalues that allow to identify the "valley-structure" of the function F from the analysis of these eigenfunctions. We expect these results to be useful in the numerical domain decomposition methods initiated in [9].
On a second line, we continued our study of the combined effect of a slowly changing parameter and noise on dynamical systems. As already reported last year, we developed a new approach to one-dimensional systems with a slowly time-dependent parameter, [1], [2], [3]. This year,

we successfully extended the method to multi-dimensional systems where the parameter itself may evolve according to a stochastic differential equation. This leads to a general class of fully coupled stochastic slow-fast systems

$$\begin{aligned} dx_t &= \frac{1}{\varepsilon} f(x_t, y_t)\, dt + \frac{\sigma}{\sqrt{\varepsilon}} F(x_t, y_t)\, dW_t, \\ dy_t &= g(x_t, y_t)\, dt + \sigma' G(x_t, y_t)\, dW_t, \end{aligned}$$

where the fast variables x_t, the slow variables y_t, and the Brownian motion $(W_t)_t$ can be multi-dimensional. Such singularly perturbed stochastic differential equations are widely used in the sciences to model systems evolving on two well-separated time scales. Examples include systems containing heavy and light particles, predator-prey systems, and climate models like the Atlantic thermohaline circulation.

Under suitable assumptions on the associated deterministic system, we proved concentration results for the sample paths of the fast variables of the stochastic system. For small but finite values of the parameters $\varepsilon, \sigma, \sigma'$, the sample paths remain concentrated in a neighborhood of a so-called slow manifold at least up to a time of order one. Depending on the dynamics of the slow variables, such a result can hold considerably longer, up to exponentially long times, for instance when the slow variables of the deterministic system track an asymptotically stable periodic orbit. This allows to control the fluctuations of the fast variables due to noise and to study the (lower-dimensional) reduced dynamics on the slow manifold instead of the full system. In the important case when the slow manifold contains bifurcation points, we obtain similar concentration properties for the fast variables corresponding to non-bifurcating modes and conditions under which the system can be approximated by a lower-dimensional one, in which the fast variables contain only bifurcating modes [4].

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Low temperature phases in models with long-range interactions

Collaborators: A. Bovier, C. Külske

Cooperation with: A. Le Ny (EURANDOM, Eindhoven, The Netherlands), F. Redig (Technical University, Eindhoven, The Netherlands), M. Zahradník (Charles University, Prague, Czech Republic)

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

In this year the study of statistical mechanics models with long-range interactions (Kac models) was continued. The challenge of these models is their description not only on the level of thermodynamical potentials, but also on the level of their Gibbsian distributions. A crucial tool needed for the understanding of these models is a reformulation in terms of suitable contour models. Since uniformity of the estimates in the range of the interaction is desired, standard tools for short-range models can not be used. Contours need to be defined carefully. Due to the long-range nature of the model, interactions between those contours cannot be avoided and need to be treated appropriately by expansion methods.
In the past year the final formulation of a large class of Kac spin systems as contour models could be achieved for translation-invariant interactions in [1]. Once such a representation has been obtained, statements for the random Gibbs measures in the spirit of the Pirogov–Sinai theory for short-range models can be derived (see [2]), and control of the original Gibbs measures of the spin system is obtained.
The present aim is to go beyond translation invariant models and investigate the influence of frozen impurities. Here we focus on the specific example of the Kac–Ising model in a random magnetic field. Using the contour representation developed in [1] we could provide a proof [3] showing ferromagnetic order for sufficiently small randomness, in three dimensions. However, while it is hoped that there should be ferromagnetic order when the inverse temperature is large but uniform in the range of the interactions, we still need, at present, that the inverse temperature is large compared to the logarithm of the range of the interaction. In this regime the contour representation of [1] can be treated by renormalization group techniques developed by Bricmont and Kupiainen [4] for the nearest neighbor Ising model in a random magnetic field.
We are hoping for uniform estimates but these pose additional difficulties and we will need further refinements of the expansion techniques.
In a related but different line of research we investigated the mathematical foundations of the so-called grand-ensemble approach to equilibrium statistical mechanics of disordered systems with frozen disorder. Here the joint measures on the product of disorder space and spin space are interpreted in a formal way as equilibrium measures for the joint variables (the pair of spin variables and disorder variables), for a suitable non-trivial interaction. What are general properties of the joint measures in infinite volume and their corresponding interaction? We were able to show in earlier research [5] that these measures typically leave the realm of classical Gibbs measures with uniformly summable interactions, but are only Gibbs measures in a weak sense. A fundamental question arises, motivated also by various other earlier examples of generalized Gibbs measures: To what extent can the classical Gibbsian formalism be restored for generalized Gibbs measures? Does the variational characterization of Gibbs measures as minimizers of the free energy functional still hold? In this year we made some significant

progress in that direction [6], [7]: On the positive side, we were able to extend the variational principle to a certain class of generalized Gibbsian measures. On the other hand, it turned out that the joint measures of the random field Ising model (with short-range interaction) provide a concrete example for which the variational principle fails. This shows that the previously proposed class of so-called weakly Gibbsian measures is too broad for a variational principle to hold.

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Gibbs measures of highly disordered systems

Collaborator: A. Bovier

Cooperation with: I. Kourkova (Université Paris VI "Pierre et Marie Curie", France)

No materials in the history of solid state physics have been as intriguing and perplexing than certain alloys of ferromagnets and conductors, such as *AuFe* or *CuMg*, known as *spin glasses*. The attempts to model these systems have led to a class of *disordered spin systems* whose mathematical analysis has proven to be among the most fascinating fields of statistical mechanics over the last 25 years. Even the seemingly most simple model class, the *mean-field models* introduced by Sherrington and Kirkpatrick now known as SK models, haven proven to represent an amazingly rich structure that is mathematically extraordinarily hard to grasp. Theoretical physics has produced an astounding solution describing the thermodynamics properties of these models that is based on ad-hoc constructions (so-called "replica symmetry breaking" [8]) that so far have largely resisted attempts to be given a concrete mathematical sense. Rather than aiming at partial results in the SK model and its close relatives, we will start with the more accessible models generalizing the REM that were introduced by Derrida and Gardner [7], the Generalized Random Energy Models (GREM). They are characterized by the fact that the covariance of the Gaussian process X_σ on $\{-1,1\}^N$ is a function of the canonical ultrametric valuation $d_N(\sigma,\tau) \equiv N^{-1}(\min(i : \sigma_i \neq \tau_i) - 1)$ rather than of the overlap $R_N(\sigma,\tau) = N^{-1}\sum_i \sigma_i\tau_i$, i.e.

$$\mathrm{cov}(X_\sigma, X_\tau) = A(d_N(\sigma,\tau))$$

where A a continuous probability distribution on $[0,1]$ which can either be discrete (standard GREM) or have a continuous part ("CREM": GREM with "continuous hierarchies").
They form in fact a very rich class of models, in which all the phenomena expected in the SK models, such as continuous replica breaking occur. At the same time, they offer certain simplifying features that make a fully rigorous analysis feasible. In 1987, Ruelle [9] has suggested models based on so-called *Poisson cascades* that were suggested to represent the thermodynamic limits of Derrida's models. Two years ago, we have shown in the case of the simplest of these models, the REM, that the Gibbs measure converges indeed to the Gibbs measure associated to the corresponding Poisson model of Ruelle [1], [6]. This year we have extended this result to the full class of Derrida's models, including those with continuous hierarchies ([3], [4], [5]). This provides for the first time examples of models in which all of the rather "mysterious" features of Parisi's solution of mean-field spin glasses arise and can be understood in a precise mathematical way.
A major motivation for this work is that these results provide the basis for the analysis of the dynamics of these models. Such an analysis has already been carried out in the case of the REM [2], but we are now hopeful that similar results can be obtained for the far more complex models studied here.

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Interacting catalytic branching processes

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Pairs of interacting catalytic branching models describe the evolution of two materials which randomly move, split, and possibly disappear in space. The system is interactive in that the branching behavior of each material is dependent on the other one. This interaction destroys the usual independence assumption in branching theory, and requires new, different methods.
A major result this year is the construction of a *competing species model with infinite variance* [8]. This is a breakthrough since up to date exclusively interacting branching models with finite variance branching have been constructed. In this case a competing species model has been treated in dimensions $d < 4$ by Evans and Perkins [5], based on Barlow et al. [2]. Besides others, their key tools had been a Girsanov-type theorem of Dawson [4], and a Tanaka-type formula for collision local times of some interacting critical continuous super-Brownian motions in R^d, $d < 6$, from [2]. But both tools are not available anymore if the finite variance assumption is dropped. In fact, Girsanov's theorem requires continuity in time of the martingale component; this is true only under finite variance. Moreover, Barlow et al.'s proof of the Tanaka formula relies on some uniform bound of continuous super-Brownian motion's mass in small balls ([2]). This bound does not hold in our case, and validity of the Tanaka formula in the more general setup remains open. To prove convergence of approximating collision local times, we heavily apply a log-Laplace technique, originally used for collision local times in Mytnik [13]. In our interacting model, an application of log-Laplace tools is still possible since we can represent the collision local time for the pair of interacting superprocesses with killing as a linear combination of collision local times for independent and conditionally independent measure-valued processes. This representation (which also holds for approximating collision local times) is based on the domination of interacting pairs by a pair of independent superprocesses. The domination property is an extension of an analogous result proved in [2] for finite variance super-Brownian motions.
A related line of research has been concerned with convergence of population systems to the *heat equation with colored noise*. In [14] rescaled branching particle systems in a random environment and associated lattice systems (infinite systems of stochastic differential equations) are shown to converge to solutions of the aforementioned stochastic partial differential equation (SPDE). Due to the correlation in the random environment, the resulting SPDEs are driven by a colored noise term. The latter can be investigated in higher dimensions. This is in contrast to white noise SPDEs which are restricted to dimension one. Apart from establishing an SPDE description of a class of particle systems, the particle picture itself and the approximation by systems of related SDEs provide a representation of a general class of SPDEs that also arise in

other areas of application, for example in filtering theory. In our case, the approximation by a system of SDEs leads to a new existence result for the stochastic heat equation with colored noise and non-Lipschitz noise coefficients.

Motivated by investigations of Greven et al. [11] on linearly interacting Wright–Fisher diffusions on $\mathbb{Z}^d$ catalyzed by a voter model, in [9] we study the *extinction/explosion behavior in a supercritical super-Wright–Fisher diffusion* on $[0,1]$. In [11], the long-term behavior in their two-dimensional model was expressed in terms of a binary splitting Wright–Fisher diffusion with rate $\gamma = 1$ (see Figure 1).

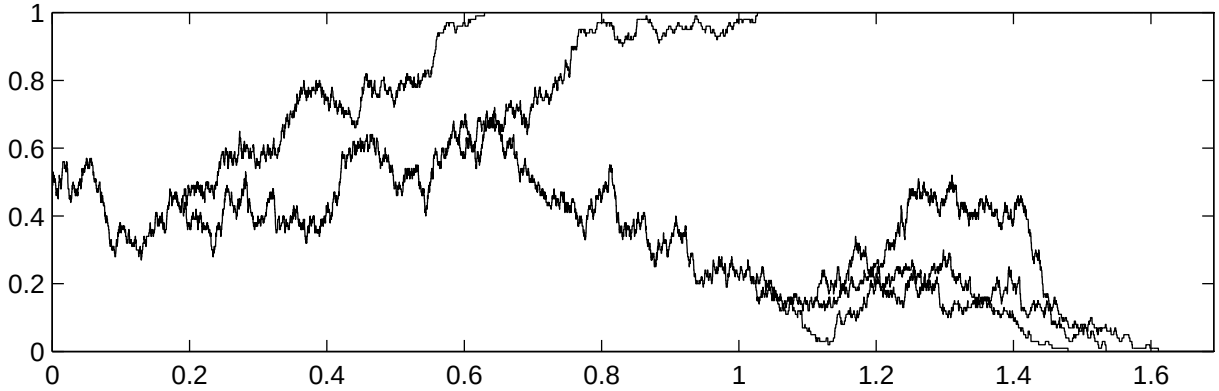

Fig. 1: Binary splitting Wright–Fisher diffusions with splitting rate $\gamma = 1$

We relate the latter model in a slightly more general case with the corresponding superprocess. Then the long-term behavior can be described completely: For rates $\gamma \leq 1$, mass in the interior $(0,1)$ dies out after a finite random time, while for $\gamma > 1$, the mass in $(0,1)$ explodes with positive probability. In the case of explosion, the mass in $(0,1)$ grows exponentially with rate $\gamma - 1$ and is approximately uniformly distributed over $(0,1)$. These results are applied to show that the related semi-linear Cauchy problem $u_t = \frac{1}{2}x(1-x)\,u_{xx} + \gamma u(1-u)$ on $\mathbb{R}_+ \times [0,1]$ has precisely four fixed points when $\gamma \leq 1$, and five when $\gamma > 1$, and we determine their domain of attraction. In a supercritical branching particle system, the *trimmed tree* consists of those particles which have descendants at all times. We develop this concept in the superprocess setting. For a class of continuous superprocesses, we identify the trimmed tree, which turns out to be a binary splitting particle system with a new underlying motion that is a compensated h-transform of the old one. We show how trimmed trees may be estimated from above by embedded binary branching particle systems [10].

By studying a *coalescent process in a random environment*, progress has been made in [3] towards understanding one of the key issues in population genetics: the influence of selection, mutation and linkage (probable joint inheritance) on the genealogy of several genes. In this work, the distribution of the diffusion limit of the ancestry of a sample of fixed size is derived when the overall population size tends to infinity. The simplest case of such a diffusion limit—generally referred to as a coalescent because of its inverted tree structure—has been treated by Kingman [12]. His coalescent and versions thereof have been used extensively in the analysis of population genetic data. Earlier work mostly considers a random sample from a population. This has made it difficult to model selection since the branching behavior of individuals depends on their genetic make-up, which hence has to be known. In order to incorporate general forms of selection we follow the genealogy of a sample conditioned on its genetic composition. For sample size two the limit is analyzed numerically. The analysis

confirms the intuition that selection and linkage have a significant influence on the distribution of biologically relevant quantities that more simplistic models failed to capture.
A super-Brownian motion in two and three dimensions is constructed where "particles" give birth at a higher rate, if they approach the origin [7]. This contradicts the intuition suggested by the fact that in more than one dimension Brownian particles do not hit a given point. Via a log-Laplace approach, the construction is based on Albeverio et al. [1] who calculated the fundamental solutions of the heat equation with *one-point potential* in dimensions less than four.
For a *super-Brownian catalyst reactant pair* in $\mathbb{R}$, a difficult tightness problem has been resolved this year ([6]) leading to a universal mass-time-space functional scaling limit theorem on path space.

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Probabilistic Cellular Automata

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Stochastic processes called *Probabilistic Cellular Automata*, and denoted by PCA, are discrete-time Markov chains with parallel updating (see, e.g., [1], [3], [6]). PCA models are useful in a large number of scientific areas, for example for parallel computing.
In [2], the authors present some links between the sets of reversible and stationary and Gibbs measures, respectively for general PCAs. They illustrate these results on the following particular class C of reversible PCAs with transition probability P:

$$P(d\sigma/\eta) = \otimes_{k\in\mathbb{Z}^d} p_k(d\sigma_k/\eta), \quad \sigma = (\sigma_k)_k \in \{-1,+1\}^{\mathbb{Z}^d}, \eta \in \{-1,+1\}^{\mathbb{Z}^d}$$

where

$$p_k(d\sigma_k/\eta) = \frac{1}{2}\Big(1 + \sigma_k \tanh\big(\beta \sum_{j\in\mathbb{Z}^d} \alpha(j-k)\eta_j + \beta h\big)\Big)$$

and the interaction α is of finite range.
In particular, they prove, using contour arguments that, for sufficiently small values of the temperature parameter $\frac{1}{\beta}$, *phase transition* occurs, that is, there are several Gibbs measures associated to the multibody potential ϕ defined by:

$$\phi_{\{k\}}(\sigma_k) = -\beta h\sigma_k, \quad \phi_{V_k}(\sigma_{V_k}) = -\log\cosh\big(\beta\sum_j \alpha(j-k)\eta_j + \beta h\big) \text{ where } V_k = \{j : \alpha(k-j) \neq 0\}.$$

Some of these Gibbs measures are stationary for P, which ensures the non-ergodicity of this PCA.
In [4], [5], the author studies ergodic properties of PCAs of the class C. In particular, he shows that in the attractive case (i.e. when $\alpha \geq 0$), if the set of Gibbs measures associated to the potential ϕ is reduced to one element μ which is moreover weak mixing, then the PCA is ergodic, its equilibrium measure is μ, and the convergence holds exponentially fast. The proof is based on a specific monotone coupling of PCAs. The domain of validity for this exponential ergodicity of attractive PCAs seems to be optimal, since it is known that, in the particular case $\alpha(k) = 1$ if $|k| = 1$ and $\alpha = 0$ otherwise, for all temperature larger than the critical one the unique Gibbs measure is weak mixing.

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Finite and infinite dimensional systems of diffusions with interaction

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In the following works, we are interested in the analysis of several types of interactive diffusions modeling phenomena coming either from Statistical Physics or from Population Dynamics. The underlying idea is to transpose important concepts and tools from Statistical Mechanics like Gibbs equilibrium measures, entropy, space-time limit, to mathematical objects like diffusions, or Brownian semi-martingales. Working on path space, we also obtain a better understanding of the behavior of such diffusions.
Together with M. Thieullen we study the class $\mathcal{R}(P_b)$ of all probabilities on the path space $C([0,T];\mathbb{R}^N)$ which have the same bridges as the following $\mathbb{R}^N$-valued reference Brownian diffusion denoted by P_b and law of the solution of the stochastic differential system:

$$dX_i(t) = b_i(t,X(t))\,dt + dB_i(t)\ , \quad t \in [0,T], \quad i \in \{1,\dots,N\},$$

where the drift $b = (b_i)_{i=1,\dots,N}$ is a regular function on $[0,T]\times\mathbb{R}^N$.
The class $\mathcal{R}(P_b)$ is called the *reciprocal class* of the reference diffusion P_b. The random processes in $\mathcal{R}(P_b)$ are Markovian fields with respect to time and therefore they are Gibbsian fields associated with a time parameter belonging to the compact interval $[0,T]$. We prove in [9] that, under the assumption of finite entropy, the set of probability measures in the reciprocal class of P_b is characterized as the set of probability measures Q under which the following system of functional equations holds:

$$\begin{aligned} Q(D_{g_i}\Phi) &= Q\Big(\Phi\,\delta(g_i)\Big) + Q\Big(\Phi\int_0^1 g_i(r)\int_r^1 (F_i + \frac{1}{2}\,div\,G_i)(t,X_t)\,dt\,dr\Big) \\ &\quad + Q\Big(\Phi\int_0^1 g_i(r)\int_r^1 G_i(t,X_t)dX_t\,dr\Big), \quad i \in \{1,\dots,d\}. \end{aligned} \tag{1}$$

Here, Φ is any regular test functional on $C([0,T];\mathbb{R}^N)$, g_i any step function on $[0,T]$ with vanishing integral, D_{g_i} denotes the Malliavin derivation operator in the direction g_i; $F \in C([0,T]\times\mathbb{R}^N;\mathbb{R}^N)$ and $G \in C([0,T]\times\mathbb{R}^N;\mathbb{R}^{N\times N})$ are functions called *reciprocal characteristics* associated to P_b, and defined as follows:

$$F_i(t,x) = \big(\partial_t b_i + \frac{1}{2}\partial_i(|b|^2 + div\,b)\big)(t,x), \quad G_{i,j}(t,x) = \big(\partial_j b_i - \partial_i b_j\big)(t,x).$$

Equation (1) is a perturbation of the duality equation satisfied by Brownian bridges, duality between the Malliavin derivation operator and the stochastic integral. The perturbation terms (second and third terms in the RHS of equation (1)) are to be compared with the Malliavin derivatives of the Hamiltonian function associated to Gibbs measures. The main difference from the one-dimensional situation studied before in [8] comes from the new last term in (1), the stochastic integral of the reciprocal characteristic G w.r.t. the coordinate process. This term vanishes if and only if the drift b of the reference Brownian diffusion is a gradient. In [8] this term was identically zero since each regular function is a gradient in dimension $N = 1$.
One finds in [9] several applications of this characterization of reciprocal processes. Among others, the authors prove a generalization of the famous Kolmogorov theorem about reversible diffusion: the existence of a reversible law in the reciprocal class of a Brownian diffusion with drift b can only occur if b is a gradient. In collaboration with L. Zambotti, they also study an application of the duality equation (1) in the singular case of δ-Bessel processes. There the difficulty consists in generalizing the reciprocal characteristics F and G associated to the degenerate drift function $b(x) = \frac{\delta-1}{2x}$.
The infinite-dimensional situation, when the index i gets continuous ($i \in [0,1]$) and the reference process is solution of a stochastic partial differential equation, is the next step in the study of such topics. It will be the subject of a forthcoming paper.
With D. Dereudre [3] we study Gibbsian properties on the path level of continuous systems of infinite-dimensional interactive Brownian diffusion. More precisely we consider the law of the solution of the following stochastic differential system with values in $(\mathbb{R}^d)^{\mathbb{N}}$:

$$dX_i(t) = -\frac{1}{2}\sum_{j\neq i}\nabla\varphi(X_i(t)-X_j(t))\,dt + dB_i(t)\ ,i \in \mathbb{N}, t \in [0,T], \tag{2}$$

where $(B_i)_i$ is a family of d-dimensional independent Brownian motions, and φ is a bounded regular symmetrical potential with finite range. Such systems were introduced and solved first by R. Lang in [6]. Since the coordinates of the process are indistinguishable, a solution of (2) can be represented by the point measure $\Gamma = \sum_i \delta_{X_i}$ on the path space $C([0,T];\mathbb{R}^d)$, and the law of Γ, denoted by Q, is then a point process—or a field—on $C([0,T];\mathbb{R}^d)$. We prove the equivalence between the following assertions: to be a Gibbsian field associated to an explicit Hamiltonian functional $\mathcal{H}$ on $C([0,T];\mathbb{R}^d)$, and to be solution of the infinite-dimensional system (2) with a fixed Gibbsian initial condition. To this aim, a new characterization (cf. [2]) of canonical Gibbs fields on $\mathbb{R}^d$ and $C([0,T];\mathbb{R}^d)$ as solutions of duality formulae is used. Several applications are deduced from the Gibbsian structure on the path level of Q, like, in particular, the behavior of Q under time reversal (reversible and non-reversible cases are treated).

In collaboration with P. Dai Pra and H. Zessin [5], we give a Gibbsian characterization for the stationary law of the interacting diffusion process $X = \{X_i(t), i \in \mathbb{Z}^\nu, t \in \mathbb{R}\}$ defined on the lattice $\mathbb{Z}^\nu$ and solution of the following type of stochastic differential system

$$dX_i(t) = \left(\mathbf{b}_{i,t}(X) - \frac{1}{2}\nabla\varphi(X_i(t))\right)dt + dB_i(t)\ ,i \in \mathbb{Z}^\nu, t \in \mathbb{R}. \tag{3}$$

The originality here is the fact that the interaction drift function $\mathbf{b}_{i,t}$ is a very general measurable bounded local functional on the path space, a priori non-Markovian. The authors could interpret the law Q of X as a space-time Gibbs distribution on $\Omega = C(\mathbb{R},\mathbb{R})^{\mathbb{Z}^\nu}$. The reference specification is given as the infinite product of the bridges of the Wiener measure drifted by $-\frac{1}{2}\nabla\varphi$, and the interaction potential is a certain Φ on Ω given in terms of $\mathbf{b}$.

In [4], based on the Gibbsian characterization shown in [5], a weak existence result for the solution of (3) is proved. The authors use a space-time cluster-expansion method, which is powerful when the coupling parameter **b** is sufficiently small. As conclusion, the Gibbsian approach to study infinite-dimensional processes seems to be very effective in situations where the stochastic calculus can not give an answer, like for example in the question of existence of solution for the non-Markovian equation (3).
Consider now the following model of Statistical Physics in random medium: Langevin dynamics for a ferromagnetic system submitted to a disordered external Bernoulli magnetic field: for $i \in \mathbb{Z}^\nu, t \in \mathbb{R}^+$,

$$dY_i^{(h)}(t) = dB_i(t) + \Big(\beta \sum_{j:|j-i|=1} Y_j^{(h)}(t) - \frac{1}{2}\nabla\varphi(Y_i^{(h)}(t))\Big)\,dt + \beta h_i\,dt \tag{4}$$

where the $(h_i)_i$ are Bernoulli i.i.d. variables. It is proved in [1] that such a system obeys a Strong Law of Large Numbers, in the sense that its empirical process converges towards a Dirac mass concentrated at some asymptotic dynamics Q, characterized as the law of the non-Markovian process $Y = (Y_i(t))_{i,t} \in C(\mathbb{R}^+,\mathbb{R})^{\mathbb{Z}^\nu}$ solution of the following stochastic differential system: for $i \in \mathbb{Z}^\nu, t \in \mathbb{R}^+$,

$$\begin{aligned} dY_i(t) &= dB_i(t) + \Big(\beta \sum_{j:|j-i|=1} Y_j(t) - \frac{1}{2}\nabla\varphi(Y_i(t)) \\ &+ \beta\tanh\Big(\beta\big(Y_i(t) - Y_i(0) + \int_0^t (\frac{1}{2}\nabla\varphi(Y_i(s)) - \beta \sum_{j:|j-i|=1} Y_j(s))ds\big)\Big)\,dt. \end{aligned} \tag{5}$$

In [7] the authors use the cluster-expansion method to show that the space-time correlation functions associated to Y decay exponentially fast in the high-temperature regime. In particular, they prove that for β small enough, the infinite-dimensional process $Y(t)$ is ergodic and the velocity of the convergence is exponential. The specific difficulty of this model (compared to the system (3)) comes from the fact that the non-Markovian interaction (last term in the RHS of (5)) is no more local in time: it depends on the values of Y on the full time interval $[0,t]$.
The process studied in [10] arises as diffusion limit of branching particle systems. It is called catalytic super-Brownian motion, in the sense that the branching procedure in the approximation depends strongly on a singular medium called catalyst. It is modeled as solution of the following stochastic partial differential equation:

$$dX_t(x) = \frac{1}{2}\Delta X_t(x)dt + M(dt,dx), \quad x \in \mathbb{R}, \quad t \in [0,T], \tag{6}$$

where M is a martingale measure with quadratic variation $X_t(x)\rho_t(dx)dt$, with ρ a given family of singular measures like Cantor measures. H. Zähle studies in [10] the regularity of the function-valued solution of (6). The case $\rho_t(dx) \equiv dx$ is well known and corresponds to the situation when the catalyst is not singular, like for the Dawson–Watanabe superprocess. The type of generalization presented in [10] is new. The modulus of continuity in time and space of the function-valued solution of (6) is expressed in terms of the Hausdorff dimension of the support of the measure $\rho_t(dx)$.

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Stochastic models and numerical algorithms for coagulation problems

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The phenomenon of coagulation occurs in a wide range of applications, e.g., in physics (aggregation of colloidal particles, growth of gas bubbles), meteorology (merging of drops in atmospheric clouds, aerosol transport), chemistry (reacting polymers, soot formation) and astrophysics (formation of stars and planets). The time evolution of the average concentration of particles of a given size in some spatially homogeneous physical system is described by Smoluchowski's coagulation equation

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

where $t \geq 0$ and $x = 1,2,\ldots$. The concentration of particles of size x increases as a result of the 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 purpose of the project is to study the relationship between stochastic interacting particle systems and solutions of equations of type (1). On the one hand, results on the asymptotic behavior of the particle system (when the number of particles increases) provide an insight into properties of the solution. On the other hand, appropriate stochastic particle systems are used for the numerical treatment of the macroscopic equation.

For sufficiently fast increasing coagulation kernels, there exists the phenomenon of gelation. At the level of the macroscopic equation (1), 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. In the standard direct simulation process gelation corresponds to the formation of a large particle (comparable in size to the size of the whole system) in finite time. An alternative stochastic particle system, called mass flow process, has been introduced in [1]. The corresponding algorithm shows better approximation properties (faster convergence) especially in the case of gelling kernels. Some conjectures based on detailed numerical observations have been stated in [2]. In particular, a new approach to the approximation of the gelation point

$$t_{\mathrm{gel}} = \inf\Big\{ t \geq 0 :\; m_1(t) < m_1(0) \Big\}, \quad \text{where} \quad m_1(t) = \sum_{x=1}^{\infty} x\, c(t,x)\,, \tag{2}$$

has been presented for a particular class of kernels.

The topic of studying coagulation processes by stochastic models has attracted much interest in recent years. An interesting direction of research is the consideration of more physical effect together with coagulation. In [3] 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 [4], [5].

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Efficient control of stochastic particle methods for rarefied gas flows

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Supported by: DFG: "Effektive Steuerung von stochastischen Partikelverfahren für Strömungen in verdünnten Gasen" (Effective control of stochastic particle methods for rarefied gas flow)

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.
Due to the high dimensionality of the problem (f is a function of 7 independent variables) stochastic algorithms are a commonly used tool for the numerical treatment of equation (1). Stochastic particle methods, like the standard DSMC (direct simulation Monte Carlo) technique, are based on the simulation of an appropriate large system of particles approximating the behavior of the real gas. Such methods provide results that are subject to random fluctuations. Thus, the construction of algorithms with reduced fluctuations is an important issue (variance reduction problem). The main purpose of the project is to contribute to this field of research.
In recent years a new approach to the variance reduction problem, called SWPM (stochastic weighted particle method), has been developed ([1]). It uses a system of weighted particles

$$\Big(g_i(t), x_i(t), v_i(t) \Big), \quad i = 1,\ldots,n, \quad t \geq 0,$$

where $g_i(t) \in (0,\infty)$, $x_i(t) \in D \subset \mathcal{R}^3$ and $v_i(t) \in \mathcal{R}^3$ denote the weight, position and velocity of the i-th particle at time t. The number of simulation particles is $n \sim 10^6 - 10^7$. The new method has been successfully applied to situations with strong density gradients. In [2] convergence of the stochastic weighted particle method for the Boltzmann equation 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 were performed illustrating both convergence and considerable variance reduction, for the specific problem of calculating tails of the velocity distribution.
The application of equation (1) is restricted to flows, where the mean free path between collisions of molecules is sufficiently large compared to the characteristic length scale of the problem. Some modification of the DSMC method, called Consistent Boltzmann Algorithm, has been developed in the literature, extending the field of application into the direction of moderately dense gases. In [3] the convergence behavior of this algorithm has been studied. The equation was found which is asymptotically solved by the particle system. This equation generalizes the classical Boltzmann equation (1). A further investigation of its relationship to the Enskog equation was the subject of [4]. First an H-theorem for the new equation was established. Then, following the classical derivation by Chapman and Cowling, approximations to the equations of continuity, momentum and energy were found. The first-order correction terms with respect to the particle diameter turned out to be the same as for the Enskog equation. A kinetic equation, related to quantum gases, was considered in [5]. In this paper a DSMC algorithm for the Uehling–Uhlenbeck–Boltzmann equation is described in terms of Markov processes. This provides a unifying framework for both the classical Boltzmann case as well as the Fermi–Dirac and Bose–Einstein cases. The foundation of the algorithm is established by demonstrating its link to the kinetic equation. By numerical experiments its sensitivity to the number of simulation particles and to the discretization of the velocity space is studied, when approximating the steady state distribution.

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4.6 Research Group Stochastic Algorithms and Nonparametric Statistics

4.6.1 Overview

Die Forschungsgruppe befasst sich mit Arbeiten zur angewandten, algorithmisch orientierten Wahrscheinlichkeitstheorie und zur 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.

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

- Nichtparametrische statistische Methoden der Bildverarbeitung, für Finanzmärkte, Ökonometrie, Cluster- und Diskriminanzanalyse,
- Angewandte Finanzmathematik, speziell Risikomessung und -steuerung, Bewertung und Simulation von Zinsderivaten sowie Portfolio-Optimierung unter Transaktionskosten,
- Stochastische Simulation komplexer hochdimensionaler Probleme (voll entwickelte Turbulenz, Partikelverhalten in turbulenten Regimen, dynamische stochastische Algorithmen).

The research of the 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.

For the last year the following main topics were set:

- Nonparametric statistical methods in imaging processing, for financial markets, econometrics, clustering and discriminant analysis;
- 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.

4.6.2 Projects

Statistical data analysis

Collaborators: V. Essaoulova, A. Hutt, S. Jaschke, P. Mathé, H.-J. Mucha, J. Polzehl, V. Spokoiny.

Cooperation with: F. Godtliebsen (University of Tromsø, Norway), G. Torheim (Amersham Health, Oslo, Norway), S. Sardy (Swiss Federal Institute of Technology (EPFL) Lausanne, Switzerland), A. Juditski (Université de Grenoble, France), M. Hristache (ENSAI, Rennes, France), W. Härdle (SFB 373, Humboldt-Universität zu Berlin), J. Horowitz (Northwestern University, Chicago, USA), S. Sperlich (University Carlos III, Madrid, Spain), D. Mercurio (Humboldt-Universität zu Berlin), I. Grama (Université de Bretagne-Sud, Vannes, France), C. Vial-Roget (ENSAI, Rennes, France), A. Goldenshluger (University of Haifa, Israel), Y. Xia (Cambridge University, UK), O. Bunke, B. Droge and H. Herwartz (SFB 373, Humboldt-Universität zu Berlin), H.-G. Bartel (Humboldt-Universität zu Berlin), R. Brüggemann (Institut für Gewässerökologie und Binnenfischerei, Berlin), J. Dolata (Johann Wolfgang Goethe-Universität Frankfurt am Main), U. Simon (Institut für Gewässerökologie und Binnenfischerei, Berlin), P. Thiesen (Universität der Bundeswehr Hamburg), O. Lepski and Yu. Golubev (Université de Marseille, France), A. Samarov (Massachusetts Institute of Technology, Cambridge, USA), S.V. Pereverzev (National Academy of Sciences of Ukraine, Kiev), R. von Sachs (Université Louvain-la-Neuve, Belgium), S. Zwanzig (Uppsala University, Sweden), B. Röhl-Kuhn (Bundesanstalt für Materialforschung und -prüfung (BAM) Berlin)

Supported by: BMBF: “Effiziente Methoden zur Bestimmung von Risikomaßen” (Efficient methods for the valuation of risk measures)
DFG: DFG-Forschungszentrum “Mathematik für Schlüsseltechnologien” (Research Center “Mathematics for Key Technologies”); 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 theoretical basis of the project *Statistical data analysis* are modern nonparametric statistical methods designed to model and analyze complex structures. WIAS has, with main mathematical contributions, become an authority in 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 (V. Essaoulova, A. Hutt, J. Polzehl, V. Spokoiny).

The studies of adaptive smoothing methods have mainly been motivated by applications to medical imaging, especially in the context of dynamic and functional Magnet Resonance Imaging (dMRI and fMRI), and the analysis of high-frequency financial time series. Research on imaging problems is carried out within the DFG Research Center “Mathematics for Key Technologies” and the DFG Priority Program 1114 “Mathematical methods for time series analysis and digital image processing”. Modeling of local stationary time series is based on cooperation within the SFB 373 “Quantification and simulation of economical processes” at

Humboldt University of Berlin and the BMBF project “Efficient methods for the valuation of risk measures”. Cooperation also exists with G. Torheim (Amersham Health, Oslo, Norway) and F. Godtliebsen (University of Tromsø, Norway) for the analysis of dMRI experiments.
Two main approaches have been proposed and investigated, a pointwise adaptive approach and adaptive weights smoothing. The *pointwise adaptive approach* was developed in [37] for estimation of regression functions with discontinuities. [29] extended this method to smoothing of 2D images. The procedure delivers an optimal (in rate) quality of edge recovering and demonstrates a reasonable numerical performance. Other interesting applications of this approach include the analysis of time-varying and local stationary time series and tail index estimation. [25] develop a pointwise adaptive approach for volatility modeling of financial time series. [9] extends this procedure to the case of multi-dimensional financial time series. Appropriate methods for local stationary time series are investigated in [6] and [7]. [5] propose a new method of adaptive estimation of the tail index of a distribution by reducing the original problem to the inhomogeneous exponential model and applying the pointwise adaptive estimation procedure. Although the pointwise adaptive procedure turns out to be asymptotically efficient, its computational complexity is high and results for finite sample sizes are less promising than for the other method called *adaptive weights smoothing* .

The adaptive weights smoothing approach has been proposed in [30] in the context of image denoising. The general idea behind the adaptive weights smoothing procedure is structural adaptation. The procedure attempts in an iterative way to recover the unknown local structure from the data and to utilize the obtained structural information for improving the quality of estimation. The procedure possesses a number of remarkable properties like preservation of edges and contrasts and nearly optimal noise reduction inside large homogeneous regions. It is also dimension-free and applies in high-dimensional situations. The original procedure designed for the local constant regression model has been thoroughly revised and generalized to a wide variety of models. Results have been presented at several conferences and are contained in [32, 33]. [32] describes how the AWS procedure can be used for estimation of piecewise smooth curves or manifolds by local polynomial approximation.

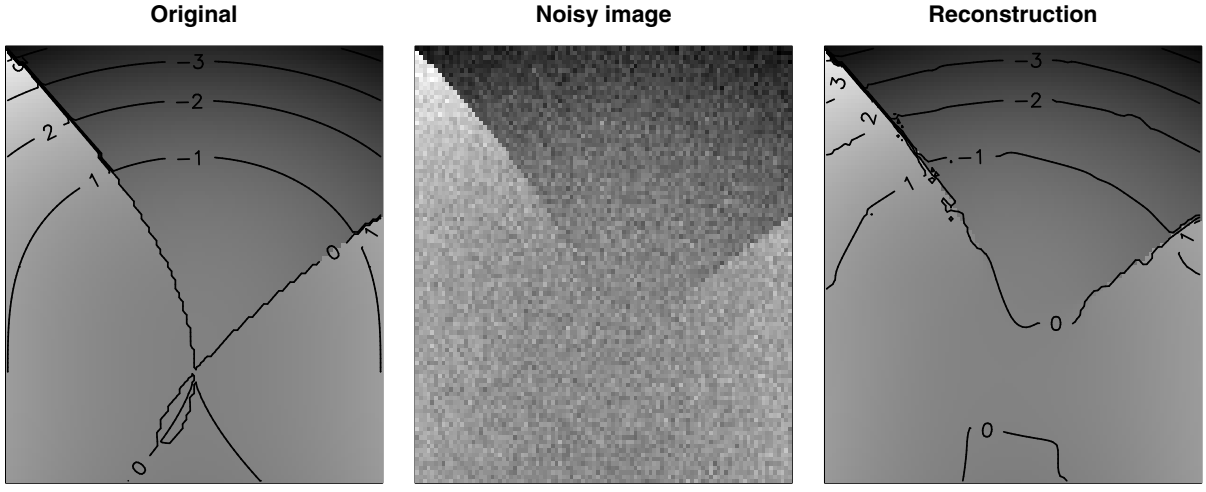

Fig. 1: Original (left), image with additive noise (central) and AWS reconstruction (right)

Figure 1 illustrates the result of a local quadratic fit of a discontinuous 2D regression surface. The left image gives the true function, the central image contains the noisy image while the right image provides the reconstruction.

[33] describes an extension of the AWS method to local likelihood estimation for exponential family models with varying parameters as well as applications to various particular problems. Important model classes include Poisson regression, binary response models, volatility models and exponential models. Applications are given for the following problems:

- Analysis of fMRI and dMRI experiments: Adaptive weights smoothing allows for the analysis of spatio-temporal structures. The methods proposed in [31] have been tested on dMRI datasets from cardiology. We are currently revising the vectorized procedures based on the generalizations described in [32, 33].
- Positron emission tomography data can be successfully described by the Poisson model with varying intensity. Figure 2 illustrates the results for a preliminary experiment using the Vard-Shepp-Kaufman phantom [42].

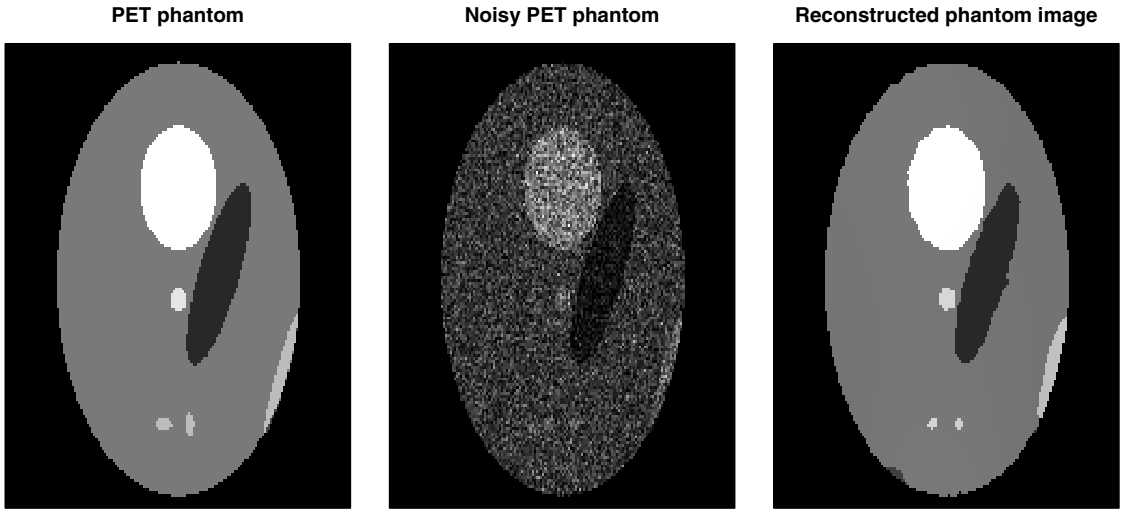

Fig. 2: Original phantom (left), image with Poisson noise (central) and AWS reconstruction from the noisy image (right)

- Density estimation: An adaptive weights procedure for density estimation has been obtained using the asymptotic equivalence of density estimation and Poisson regression.
- Classification: Nonparametric classification can be approached using the binary response model. The resulting method improves on nearest-neighbor rules and nonadaptive kernel smoothing.

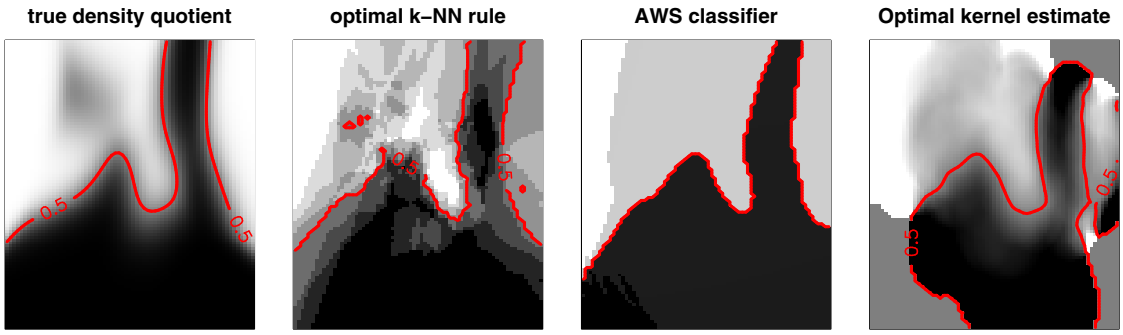

Fig. 3: Bayesian classification rule (left), and classification rules obtained by k-NN, AWS and kernel smoothing

Figure 3 illustrates the classification results obtained for an artificial discriminant analysis problem used in [10] for the adaptive weights, nearest-neighbor and kernel approach using optimal smoothing parameters in the last two methods.

- Time-inhomogeneous time series and volatility estimation: Time series models with varying coefficients are appropriate for a wide range of financial time series and biometric signals. An adaptive weights smoothing for AR- and ARCH-models with time-varying coefficients is under development.

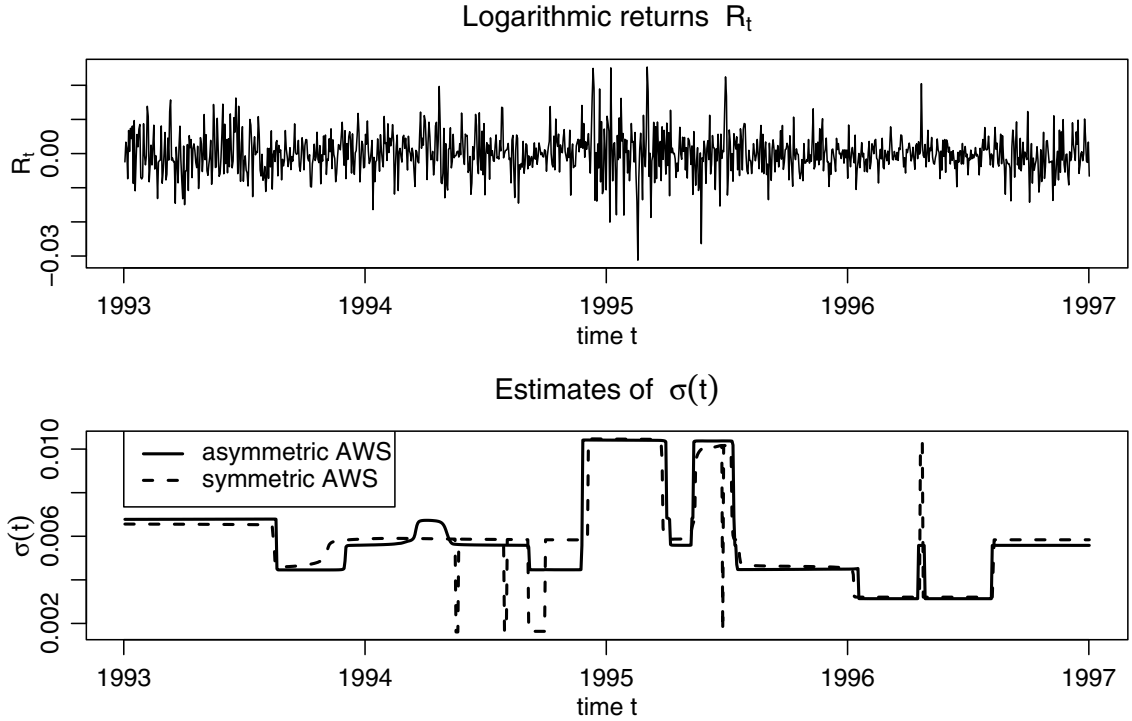

Fig. 4: Inhomogeneity of the volatility of the DM / US $ exchange rate

Figure 4 illustrates an analysis of the DM / US $ exchange rate (data are (C) 2001 by Prof. W. Antweiler University of British Columbia, Vancouver BC, Canada, and have been obtained from the Pacific Exchange Rate Service http://pacific.commerce.ubc.ca/xr/data.html). Displayed are the returns $|R_t|$ and estimates of the volatility σ_t obtained by the symmetric and asymmetric version of AWS for the time period from January 1993 to December 1997.

- 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. [33] use the idea employed in [5] to obtain an adaptive weights method. The resulting estimate can be viewed as a generalization of the Hill estimator with an adaptive choice of its smoothing parameter.

2. Dimension reduction (S. Jaschke, J. Polzehl, V. Spokoiny).

Many statistical applications are confronted with high-dimensional data. Typical examples are given by econometric or financial data. For instance, usual financial practice leads to monitoring about 1000 to 5000 different data processes. Single- and multi-index models are often used in multivariate analysis to avoid the so-called “curse of dimensionality” problem (high-dimensional

data are very sparse). 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 can be viewed as 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 calculation of these estimators leads to an optimization problem in a high-dimensional space, see [18]. In contrast, direct methods like the average derivative estimator, or sliced inverse regression are computationally straightforward, but the corresponding results are far from being optimal, again due to the "curse of dimensionality" problem. Their theory applies only under very restrictive model assumptions, see [2], [34] and [40].

[16] developed a structural adaptive approach to dimension reduction using the structural assumptions of a single-index and multi-index model. These models are frequently used in econometrics to overcome the curse of dimensionality when describing the dependencies between variables in high-dimensional regression problems. The new methods allow for a more efficient estimation of the effective dimension reduction space characterizing the model and of the link function. [39] 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.

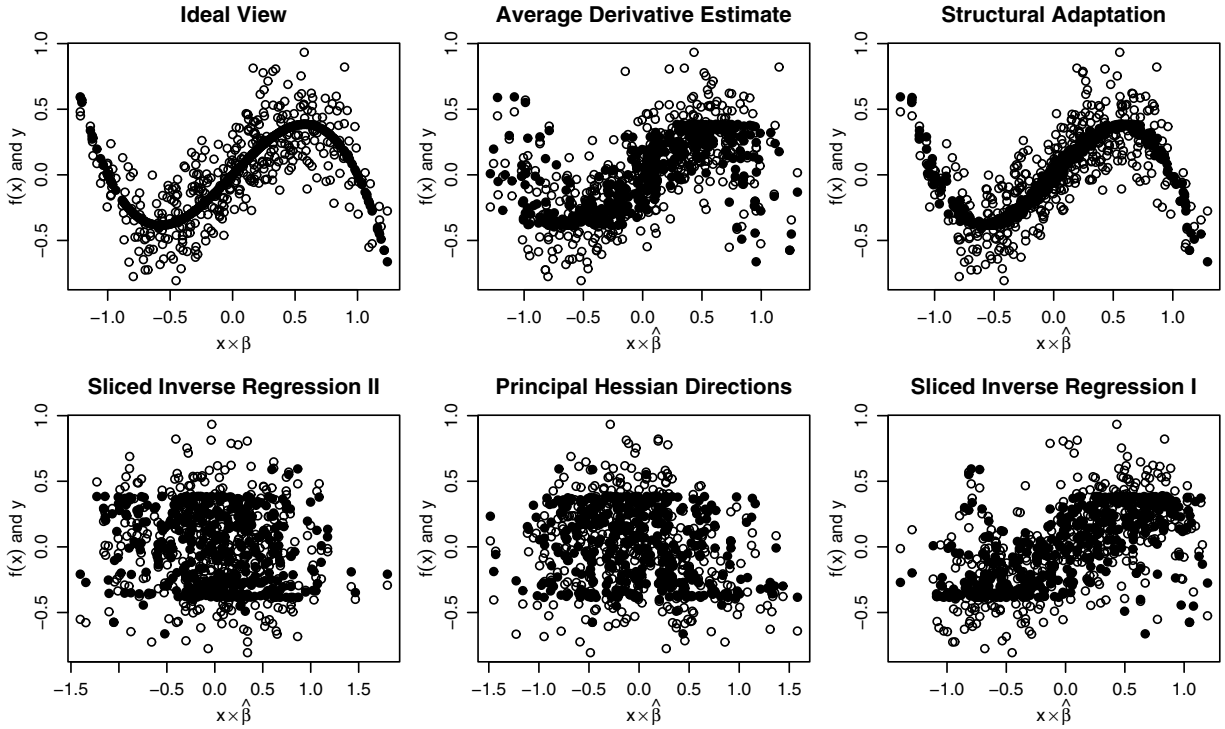

Fig. 5: Projections into the estimated index space obtained by structural adaptation and by established competitors. Data follow a single-index model in a 20-dimensional regressor space.

Figure 5 illustrates the quality of the estimated index in comparison to other established methods, i.e. a generalized average derivative estimate (ADE), sliced inverse regression (SIR) and principal Hessian directions (PHD), for a single-index model in a 20-dimensional space. [35] propose a new method to analyze a partially linear model whose nonlinear component is completely unknown. The target here is variable selection, i.e. the identification of the set of

regressors which enter in a nonlinear way into the model. As a by-product the method allows to test the dimensionality of the nonlinear component.
Dimension reduction also turns out to be an essential component in the adaptive weights smoothing approaches to time-inhomogeneous time series in case of high dimensions of the parameter space. Methods to handle this problem are currently under investigation.

3. Goodness-of-fit and model check (V. Spokoiny).

In many statistical data analyses, the use of simple models described by a finite number of parameters would be preferable. However, an application of parametric modeling has to be combined with a careful goodness-of-fit test. In other words, a statistician has to check whether the data really follow (or, at least, do not contradict) the parametric assumption. This check can be naturally formulated as the problem of testing a simple or parametrically specified hypothesis. The modern statistical theory focuses on developing tests which are sensitive (powerful) for a possibly large class of alternatives. The classical Neyman-Pearson theory considers the very narrow class of parametric alternatives. The classical nonparametric procedures like von Mises, χ^2 or Kolmogorov-Smirnov have a serious drawback of being non-sensitive against a smooth wiggling alternative that typically arises in the goodness-of-fit problem. Optimal (in rate) nonparametric tests for such alternatives have been constructed by [17]. However, practical applications of such rate-optimal tests require to specify a smoothing parameter. A number of data-driven (adaptive) tests have been recently proposed in [3], [4], [19], among others. [36, 38] considered the problem of adaptive testing of a simple hypothesis for the “ideal” sequence space model against a smooth alternative and constructed an adaptive test which is optimal (in rate) in the class of such adaptive tests. [38] considered the case of a linear hypothesis for a regression model. [14] developed an adaptive rate-optimal test of a parametric hypothesis for a heterogeneous regression model. [15] extended the method and the results for the median regression model with an unknown possibly heterogeneous noise.

4. Cluster analysis, multivariate graphics, data mining (H.-J. Mucha).

Cluster analysis, in general, aims at finding interesting partitions or hierarchies directly from the data without using any background knowledge. Here a partition P(I,K) is an exhaustive subdivision of the set of I objects (observations) into K non-empty clusters (subsets, groups) C_k that are pairwise disjoint. On the other hand a hierarchy is a sequence of nested partitions. Having data mining applications and improvement of stability of results in mind some new model-based cluster analysis tools are under development. For example, clustering techniques based on cores can deal with both huge data sets and outliers, or, intelligent clustering based on voting can find usually much more stable solutions. A core is a dense region in the high-dimensional space that, for example, can be represented by its most typical observation, by its centroid or, more generally, by assigning weight functions to the observations. Almost all techniques of high-dimensional data visualization (multivariate graphics, projection techniques) can also take into account weighted observations. As an application in the field of water ecology, a result from model-based Gaussian clustering is presented in the figure below. The data under investigation comes from a snapshot of monitoring of phytoplankton.

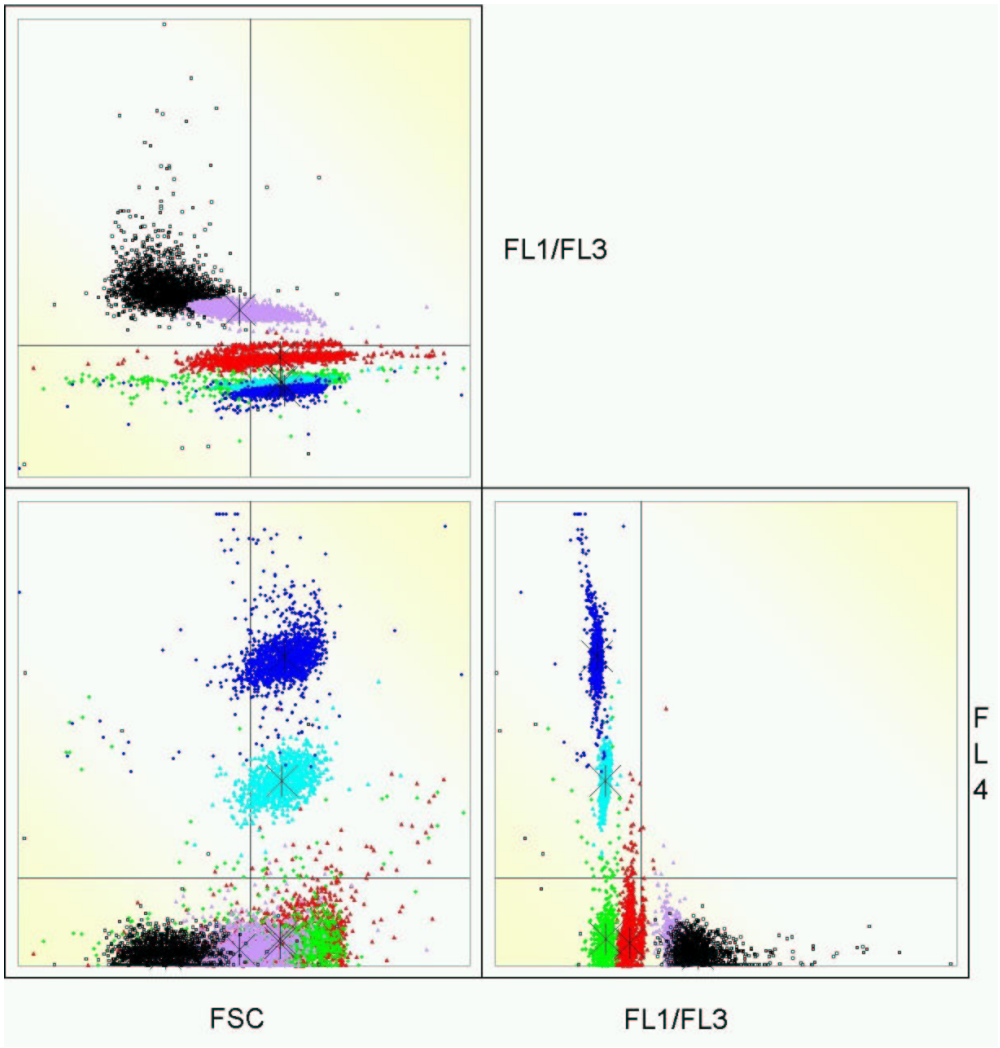

Fig. 6: Extract of a scatterplot matrix of cluster membership (data: flow cytometry measurements)

Model-based as well as heuristic clustering techniques are part of our statistical software `ClusCorr98`®. Moreover we offer multivariate visualization techniques like principal components analysis or correspondence analysis as well as other exploratory data analysis. `ClusCorr98`® uses the Excel spreadsheet environment and its database connectivity.

5. Ill-posed 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. Work in this direction is carried out in cooperation with the project *Numerical methods for inverse problems and nonlinear optimization* of the WIAS research group "Nonlinear Optimization and Inverse Problems" and with S.V. Pereverzev, Kiev.
We study problems

$$y_\delta = Ax + \delta\xi,$$

or their discretizations

$$y_{\delta,i} = \langle y_\delta, \varphi_i \rangle = \langle Ax, \varphi_i \rangle + \delta\xi_i, \quad i = 1, \ldots, n,$$

where A acts injectively and compact in some Hilbert space, and $\delta > 0$ describes the noise level of the data $y_{\delta,i}$.
Modern numerical analysis has developed a rich apparatus, which reflects different aspects of the sensitivity of ill-posed problems. In *Hilbert scales* such problems were systematically analyzed since Natterer [28]. Sometimes, this restriction does not give a flexible approach to estimating realistic convergence rates. Moreover, some important cases are not covered by the ordinary Hilbert scale theory. One interesting example is given in [1] which studies an inverse problem in optical diffraction.
For these reasons *variable Hilbert scales* were introduced by Hegland [11] and further developed in [12] and [41]. Within this framework the solution smoothness is expressed in terms of so-called general *source conditions*, given by some function over the modulus of the operator A involved in the ill-posed equation. These allow to describe local smoothness properties of the solution. Our research was carried out in the following directions.

- [22] presents the mathematical foundation of *regularization* of ill-posed problems in variable Hilbert scales.
- The other aspect concerns discretization. [23] extends the approach from [21] to projection methods in variable Hilbert scales.
- An adaptive strategy, which automatically provides the optimal order of accuracy for a wide range of source conditions is given in [22] and [23].
- The analysis was extended to *statistically ill-posed problems in variable Hilbert scales* in [24].

[8] studied one special statistical inverse problem of reconstructing a planar convex set from noisy observations of its moments. An estimation method based on pointwise recovering of the support function of the set has been developed. It is shown that the proposed estimator is near-optimal in the sense of the order of convergence. 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.

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Applied mathematical finance

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The project *Applied mathematical finance* of the research group "Stochastic Algorithms and Nonparametric Statistics" is concerned with the stochastic modeling of financial data, the valuation of derivative instruments (options), and risk management for banks. The implementation of the developed models and their application in practice is done in cooperation with financial institutions.
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 2002 in cooperation with and with support of 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.
The valuation of financial derivatives 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 American options and the valuation of financial derivatives involving the term structure of interest rates (LIBOR models) or volatility surfaces. By the continuing innovations in the financial industry new problems arise again and again. In the progressing research on interest rate (LIBOR) modeling and calibration [19, 32, 33] a crucial stability

problem has been uncovered with respect to direct least-squares calibration of LIBOR models. As a solution a stabilized procedure is proposed in [31] and was presented at Risk Europe 2002 (Paris) and at Risk Quantitative Finance 2002 (London). On this subject a consulting contract with Reuters Financial Software (Paris) has been set up.
The project "Applied mathematical finance" took part in the formation of the DFG Research Center "Mathematics for Key Technologies".

1. Mathematical methods for risk management (S. Jaschke, O. Reiß, J. Schoenmakers, V. Spokoiny, J.-H. Zacharias-Langhans).

Although the basic principles of the evaluation of market risks are now more or less settled, 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.
One of the problems that arose in the consulting with Bankgesellschaft Berlin led to a study of the Cornish-Fisher approximation in the context of delta-gamma normal approximations. This study was enhanced and completed [14]. The analysis shows a series of qualitative shortcomings of the method, while its quantitative behavior is satisfactory in specific situations. Regarding Bankgesellschaft's use of the Cornish-Fisher approximation, it is concluded that the method is a competitive technique if the portfolio distribution is relatively close to normal. It achieves a sufficient accuracy potentially faster than the other numerical techniques (mainly Fourier inversion, saddle-point methods, and partial Monte Carlo) over a certain range of practical cases. One should beware, however, of the many qualitative shortcomings and its bad worst-case behavior. If one takes the worst-case view and cares about the corner cases—as we believe one should in the field of risk management—the potential errors from the quadratic approximation are much larger than the errors from the Cornish-Fisher expansion. Hence a full-valuation Monte Carlo technique should be used anyway to frequently check the suitability of the quadratic approximation. This will also take care of the "bad" cases for the Cornish-Fisher approximation.

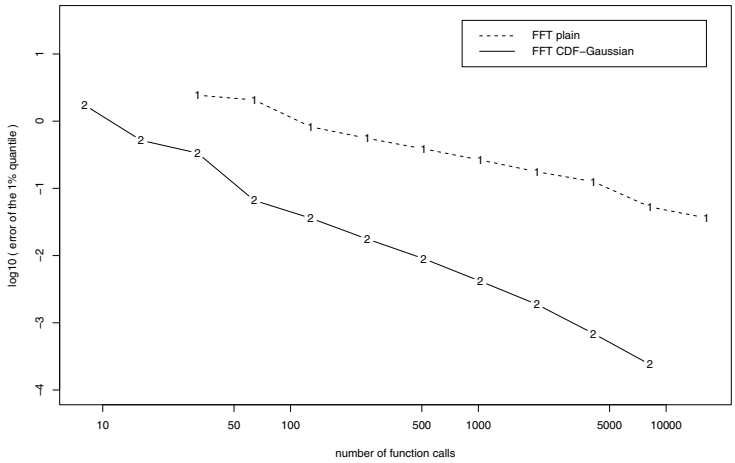

Fig. 1: A comparison of the improved FFT method and the plain FFT method

In the context of delta-gamma approximations, the study of Fourier inversion techniques was continued. [15] is a worst-case error analysis of non-adaptive, FFT-based approximations

to the Fourier inversion integral of the cumulative distribution function (minus the Gaussian CDF) in this context. The error analysis allows to optimize certain parameters to achieve the asymptotically optimal rate of convergence. Empirical evidence is presented to show how the results of the error analysis can improve the performance over a plain-vanilla FFT inversion. $K = 2^6$ evaluations of the characteristic function suffice to ensure an accuracy of one digit in the approximation of the 1% quantile over a sample of one- and two-factor cases. $K = 2^9$ function evaluations are needed for two digits accuracy. In comparison, a straightforward (non-optimized) FFT inversion of the probability density needs about 2^{13} function calls to achieve one digit accuracy (see Figure 1).
This error analysis required the characterization of the tail behavior of the probability distribution of quadratic forms of Gaussian vectors, which is the subject of [16]. It provides a complete analysis of the tail behavior of this class of distributions and solves a problem that remained open in [15].
An overview of the Fourier inversion, Monte Carlo simulation and Cornish-Fisher expansion in the context of delta-gamma normal models is given by [18].
In joint work with Gerhard Stahl (BAFin Bonn) and Richard Stehle (HU Berlin), an empirical analysis of the forecast quality of VaR models of the 13 German banks that use internal models for regulatory market risk capital is performed. The goal of the analysis is to answer the following questions:

- Are the VaR forecasts of the banks conservative or fair (unbiased)?
- How good is the forecast quality of the banks' forecasts compared to simple univariate (reduced-form) models?
- How are the profits and losses related across banks? That is, do losses tend to occur together? This is one of the most prominent questions for supervisory authorities.

In preparation of the lecture "Risk Management for Financial Institutions" (Risikomanagement für Banken), given by S. Jaschke in the winter semester 2001/2002, an extensive review of the general literature on the subject was done. The practical implementation of an enterprise-wide risk management system needs an understanding of the economic, statistical, numerical, social, and information technology aspects of the problem. The insights gained from the study of the general literature allow to assess not only the inner-mathematical relevancy, but also the practical relevancy of new ideas and open problems. The lecture notes are available from `http://www.cofi.de/risk-lecture.html`.
In the context of the BMBF project "Efficient methods for the valuation of risk measures", which is treated in cooperation with the Bankgesellschaft Berlin AG, we focus on the problem of estimating the market risk of large portfolios by the Monte Carlo method. Our first goal is the efficient estimation of the above-mentioned quantile-VaR, which is from a practical point of view the most important risk measure. The results obtained for the VaR shall subsequently be used for estimating more complex risk measures, like the conditional Value at Risk and related quantities.
There are only two possibilities for accelerating the convergence of the Monte Carlo procedure. First, to reduce the number of steps (i.e. portfolio evaluations) necessary for reaching a given error level by variance reduction (important sampling, stratified sampling, etc.). Second, to reduce the time needed for a single step, by using fast algorithms for pricing the portfolio's components. The latter possibility is described below. Concerning the first point, a well-known ([9]) technique for variance reduction, which is based on the delta-gamma normal approximation

has been implemented. By construction, this method fails to reduce variance, if the portfolio is very different from its delta-gamma approximation, which may happen for example if the portfolio is hedged. Therefore, we develop an adaptive sampling algorithm, where a Markov chain of Metropolis-Hastings type is used to create scenarios according to any given profit and loss distribution. Because of intrinsic difficulties, like the lack of global information, it is not clear whether this procedure can be used as a method for variance reduction. On the other hand, it allows for a detailed analysis of critical scenarios, giving for example information about the implied correlation structure, and the risk, inherent in changes of the correlation structure, the underlying processes are originally supposed to follow. Even small fluctuations of the correlation can cause huge losses, as the 1998 crash of hedge fund LTCM has impressively shown. Part of our work was also the programming of a Java-based graphical interface, which allows to dynamically value “real-life” portfolios. It organizes dependent market data and supplies the mathematical structures for the developed numerical routines, and also monitors and exploits statically the outcome of the Monte Carlo scheme during its run. Most of the numerical routines developed in context with this project are used in this program, which is actually running on a test level in the bank.

In cooperation with and supported by the Bankgesellschaft Berlin AG we worked on the efficient valuation of complex financial instruments, for example American options and convertible bonds. By some modifications of the standard binomial tree model, we could significantly increase speed and accuracy of the algorithm by reducing the computational effort of order N^2 to $N^{1.5}$, where N is the number of time steps used. Especially in context with high-accuracy calculations, which are necessary at the trading level for a stable treatment of sensitivities, the effect of this improvement becomes significant. So the use of very large numbers of time steps is now allowed, which is far beyond typical numbers used in comparative studies [1, 4]. Another modification, concerning the position of the tree nodes and which is interesting, for example, in view of the applicability of Richardson extrapolation techniques, led to an interpolation problem which could partially be solved, resulting in a smoothed convergence behavior of the algorithm. For standard American options, this method gives results comparable to the BBSR model described in [4]. By further improving the interpolation procedure, it seems to be possible to get even better results. A completely different algorithm, based on the Fast Fourier Transform, was also developed and analyzed. It was shown to be useful for the valuation of Bermudan-type options, but also for the standard American call, on an underlying paying of a large number of dividends, as for example index options. Another problem tackled in this context was how to incorporate credit risk in the valuation of instruments like, e.g., convertible bonds or ASCOTs. We implemented three distinct models, enabling therefore our cooperation partner to switch to the most adapted model for the specific situation.

The analysis of the delta-gamma normal algorithm to determine the Value at Risk has made substantial progress. In order to deal with rank deficient or perturbed correlation matrices a generalized Cholesky decomposition algorithm was developed [26]. To obtain the distribution of the profit-and-loss distribution, adapted Fourier inversion algorithms have been designed, and the use of the double exponential integration has been analyzed. Error bounds concerning the decay properties of the involved functions in x-space as well as in Fourier space have been developed.

One industrial standard to handle credit risk is CreditRisk+, which was developed by Credit Suisse First Boston in 1997. Based on the improving techniques we developed in the context of the delta-gamma normal method, this model has been analyzed and it turned out that similar Fourier inversion techniques can improve this model, too. Furthermore, generalizations of

this model have been introduced, and an incorporation of credit risk and market risk within such a generalized framework has been established [27]. The research on this topic is related to the research topic E5 "Statistical and numerical methods in modeling and valuation of financial derivatives and portfolio risk" of the DFG Research Center "Mathematics for Key Technologies".

2. Interest rate (LIBOR) modeling, calibration and pricing of non-standard derivatives (A. Kolodko, G.N. Milstein, O. Reiß, J.G.M. Schoenmakers).

A very popular interest rate model is the LIBOR market model [3, 13, 24] which is given by

$$dL_i = -\sum_{j=i+1}^{n-1} \frac{\delta_j L_i L_j \gamma_i \cdot \gamma_j}{1+\delta_j L_j}\, dt + L_i \gamma_i \cdot dW^{(n)}, \tag{1}$$

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 $\gamma_i = (\gamma_{i,1}, \ldots, \gamma_{i,d})$ deterministic volatility functions. Further, $(W^{(n)}(t) \mid t_0 \le t \le T_{n-1})$ is a d-dimensional Wiener process under the so-called terminal measure $\mathbb{P}_n$.

Calibration of a LIBOR market model 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. Previously we derived, on a conceptual basis, a variety of parsimonious correlation structures suitable for implementation in the LIBOR/EurIBOR market model (1). Here is an example of a realistic two-parametric structure,

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

These correlation structures combined with suitable parametrizations of the volatility norms $|\gamma_i|$ form the corner-stones of our calibration procedure. However, we detected an intrinsic stability problem in joint calibration of a multi-factor LIBOR market model with time-dependent volatility norms using the standard least-squares approach. This has led to incorporation of a new concept, the so-called "Market Swaption Formula" which is an intuition-based approximation of swaptions, in the objective function of the calibration routine [31]. By the method described in [31] stable calibration of a LIBOR market model to a whole system of caplet and swaption volatilities turns out to be feasible with only four parameters volatilities. Most of all this calibration remains stable even if the quality of the market data is less. Further, a refined approximation procedure for swaption prices has been derived. This method takes into account the issue of differently settled caps and swaptions and improves upon the method of Jäckel and Rebonato (2001). The respective algorithms are implemented as Excel add-ins and are currently used for consulting purposes (Reuters Financial Software).

In a more economically motivated study we previously developed the concept of dealing with assets and interest rates in a unified model which is completely specified by the assets alone. This allowed for endogenous derivations of dynamic relations between assets and interest rates from global structural assumptions (homogeneity and some spherical symmetry) on the market. In particular, with respect to a rather general well-structured model we derived a relationship between the so-called *spherical index* and the short rate which may be regarded as an extension of earlier results and has the following interpretation:

- *If $R(t_0,T) > r_0$, hence the yield curve goes* **up** *(most usual), then the local correlation of short rate r and (spherical) index I is* **negative**.
- *If $R(t_0,T) < r_0$, hence the yield curve goes* **down,** *then the local correlation of short rate r and (spherical) index I is* **positive**.

Further, when the spherical index satisfied the assumptions of the *Capital Asset Pricing Model* we obtained that

$$\frac{c}{|b_0|} = \rho_{I,r}\left(\frac{\bar{\mu}-r}{|\bar{\sigma}|^2} - 1\right)|\bar{\sigma}|, \tag{2}$$

where c is the *objective* drift, and b_0 the volatility of the short rate, $\bar{\mu}$ the *objective* drift and $\bar{\sigma}$ the volatility of the stock index, and $\rho_{I,r}$ the correlation between short rate and index. As a consequence, with respect to the new economic pointer $q := (\bar{\mu}-r)/|\bar{\sigma}|^2$, the market can be found in the following states:

size of q	short yield	c (real drift)
> 1	down	$+$
> 1	up	$-$
$= 1$	?	0
< 1	down	$-$
< 1	up	$+$

Table 9: Effect of q and the short yield on the objective (real) short rate drift c

The above research is currently subject of empirical study and was presented at the Bachelier Congress 2002 [28].
For computing of option sensitivities we developed in [29] an analytical method and in [21] a Monte Carlo approach. The methods in [21] have been extended to determine the price and hedge of certain American options [20]. In this research we utilize more sophisticated algorithms for the simulation of stochastic differential equations in the neighborhood of a boundary [23].
The research on Bermudan-style interest rate derivatives has been placed in the context of the DFG Research Center “Mathematics for Key Technologies”. In particular, we are currently investigating a connection of these types of derivatives with a method proposed by Rogers [30].

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Numerical analysis of complex stochastic models

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Stochastic models serve as a powerful instrument for studying the dynamics of processes in natural and life sciences, in the broad spectrum, from simple models of financial mathematics in the form of systems of stochastic differential equations we studied in [15] and [19], to very complicated turbulence models involving PDEs. Parameters of such equations are random fields, governing the movement of energy spectrum from smallest viscous scales to large energy-containing vorteces in the boundary layer of atmosphere and rivers we simulated in [3], [11], [16], and [29]. The principal research efforts were directed to the development of new stochastic models and simulation techniques for solving elasticity problems, transport of pollutants, gases and aerosol particles in the turbulent atmosphere, porous media, rivers and soil, as well as for stochastic Hamiltonian systems and Langevin-type equations. As a basis research used in these applied studies, different inner problems of the intrinsic stochastic numerical methods are investigated.

1. Random Walk methods for elasticity problems (K.K. Sabelfeld).

In many interesting boundary value problems the geometry of the domain is extremely complicated, and this is one of the main motivations for the development of the grid-free methods, e.g., particle and smoothed-particle methods. In stochastic simulation, we deal with two popular techniques of this kind: (1) the Random Walk methods based on the probabilistic representation of the solutions in the form of an expectation over random diffusion processes, and (2) the Probability Density Function (PDF) method which exploits the fact that the joint pdf of the state of the system satisfies some PDEs. However both methods have strong restrictions: The first one is known only for classical scalar PDEs, and becomes unefficient near the boundary because it is forced to make the integration step smaller and smaller. The PDF method is applied to a much broader class of problems, including nonlinear problems for the Navier-Stokes equation, but it cannot be considered as a rigorous method because it describes the processes in the framework of one-particle-fixed time distributions and involves therefore some semi-empirical closure assumptions.

The Random Walk methods which are based on the Monte Carlo solution of the equivalent integral equations present another class of methods which provide rigorous (i.e., with estimation of the accuracy) numerical solution of linear and nonlinear equations [27], [32]. We develop two different classes of Random Walk methods: the Walk on Boundary methods, and the Walk inside the domain. The Random Walk on Boundary methods are in a sense stochastic

counterparts of the boundary element methods [33]. The method is grid free and uses random points on the boundary. We are developing such methods for different second-order parabolic and elliptic equations and systems of elliptic equations. What is very important, in this method, in contrast to the conventional probabilistic representations, is that all boundary conditions are possible, and the exterior problems are solved by the same Random Walk on Boundary process. In the class of Random Walk inside the domain, we develop new versions of the Walk on Spheres method which enables us to solve systems of elliptic equations, for instance, the Lamé equation governing the static elasticity processes. In some sense this is a stochastic version of the Schwarz alternative procedure, but the numerical efficiency is much higher for problems of high dimension. We constructed convergent stochastic algorithms for solving the Lamé equation for a broad class of two- and three-dimensional domains [28] [30], [34], [35].
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 [35]. In a cooperation with the Institute of Computational Mathematics and Mathematical Geophysics, Russian Academy of Sciences, Novosibirsk, an additional validation of the model based on the DRWS method is made by applying the Random Walk on Boundary process.

2. Footprint problem (K.K. Sabelfeld).

One field where the stochastic Lagrangian models are very efficiently applied is the footprint problem.
When carrying out micrometeorological measurements of various scalar surface fluxes, for instance, CO_2 flux from vegetation, evaporation of fertilizer volatilization, the following problems arise: Since the fluxes are given as a correlation between the velocity and concentration of the constituent considered, the sensor cannot be placed too close to the ground for many reasons, in particular, the wind speed there is very small and the size of the measurement instruments is comparable to the length scale of the small eddies near the ground. In addition, near the surface you are in the roughness layer, where you cannot use the typical atmospheric surface-layer parametrizations.
The higher the measurement point is placed, the weaker is the signal from the ground, since more of the vertical surface flux is converted into a mean horizontal flux by advection. Also as the measurement height is increased, the sensor “observes” more of the upwind area. Thus if the sensor is placed above a field which abuts on a forest (in the upwind direction), some part of the measurement flux might stem from the forest and not from the field. The analysis of the elevated measurements is also pertinent to inferring surface fluxes from aircraft measurement. The problem now is twofold: How much weaker is the signal in the measurement height and how does the upwind area contribute to the flux in the measurement point. Footprint analysis made for horizontally homogeneous areas give an estimate of how much homogeneous fetch is needed to make the assumption of horizontal homogeneity valid. The analysis can be used for quantifying the reliability of measurements. One might think also of a footprint analysis before the erection of a mast for several possible positions in order to find “the best” positioning for the mast.
We develop stochastic models and codes for the evaluation of concentration and flux footprint functions, see [10], [11], [12], [16], [26]. Parametrization of the surface layer of atmosphere and comparison with the experimental measurements are made in cooperation with Helsinki (Finland), Risoe (Denmark) and Bayreuth (Germany) universities.

3. Turbulence simulation of the river flow (K.K. Sabelfeld).

Unlike most existing stochastic Lagrangian models, in our model (suggested in [9]) the Eulerian pdf p_E may be non-Gaussian, as, for instance, in the forest canopy [5]. It is believed that the model proposed is well suited for the case of a neutrally (or close to neutrally) stratified surface layer, which is one of the interesting tasks. One example is the simulation of the turbulent flow in a river we have carried out in cooperation with the Leibniz Institute of Freshwater Ecology and Inland Fisheries, Berlin, [3].

The effect of turbulence on aquatic photosynthetic organisms transported by river flow is generally associated with two distinctive scales. On a river depth scale (large scale), the turbulence mixing determines the dynamics of light supply to the suspended algae. The algae cells experience a fluctuating intensity and spectral composition of light due to its exponential, wave-length-dependent decline with distance from the free surface of flow. At a given light dosage, the intensity of mixing in the vertical plane influences the rate of photosynthesis, the inhibitory effects of UV and algae growth rate. The algae size varies broadly from the size of an individual cell to the size of large colonies or aggregates. On a scale of aggregates (small scale), the shear stresses control the rate of aggregation for algae colonies and their disruption. The maximum size of aggregates is limited by a characteristic microscale of river turbulence, Kolmogorov's scale, the scale at which hydrodynamic stresses could tear aggregates to pieces. Thus, properties of environment represented by turbulent flow play a critical role in the development of biological processes.

The results of simulation are given in [36].

4. Transport of interacting particles in porous media (A. Kolodko, D. Kolyukhin, K.K. Sabelfeld).

The study, prediction, and computation of the transport of particles within a porous medium advected by laminar or turbulent flows is a very challenging problem with broad applicability in many environmental and industrial areas [2], [4]. In addition, understanding flows through porous media is crucial to the efficient and environmental recovery of petrochemicals and other mineral resources.

Physically, the problem of flow through porous media includes an enormously wide range of spatial and temporal scales. The extremely high spatial heterogeneity makes conventional deterministic numerical methods practically ineffective. If one considers, for example, only the deterministic computation of even slightly turbulent flow in a porous medium the computational resources required to perform a direct numerical simulation exceed those available on even the most powerful and advanced of today's parallel supercomputers.

Therefore, a probabilistic numerical approach, which requires fewer computational resources, is quite natural as many of the parameters of the porous medium including the permeability, porosity, and hydraulic conductivity can be effectively modeled as random space functions. The flow through such a stochastically parametrized medium is hence itself also a random velocity field.

Many of the problems of interest have, in addition, interacting particles moving within the flows. A good example are problems of colloid formation and related issues of colloid stability and transport in a porous medium. These advected particles can interact chemically or through coagulation (aggregation) and disaggregation, so that the particle sizes range from monomers to large polymer clusters. The nonlinear processes of aggregation/disaggregation are described by the Smoluchowski equation in the inhomogeneous case governing the coagulation of particles

dispersed by a velocity field $\mathbf{v}(t,x)$:

$$\frac{\partial n_l(\mathbf{x},t)}{\partial t} + \mathbf{v}(\mathbf{x},t)\cdot\nabla n_l(\mathbf{x},t) = \frac{1}{2}\sum_{i+j=l} k_{ij} n_i n_j - n_l \sum_{i=1}^{\infty} k_{li} n_i,$$

where $n_l(\mathbf{x},t)$ is the concentration of clusters of size l, $l = 1,2,\ldots$ at a point $\mathbf{x}$ at time t; $\mathbf{v}(\mathbf{x},t)$ is the velocity of the host gas, $k_{ij} = k_{ij}(\mathbf{x},t)$ is the coagulation coefficient. It is supposed that the initial size distribution is given: $n_l(\mathbf{x},0) = n_l^0(\mathbf{x})$.

Hence, it is natural to consider using probabilistic models for the particle transformation and transport thus further motivating the construction of unified Monte Carlo algorithms for both the particle-particle and particle-fluid interactions. We suggested new stochastic algorithms for the inhomogeneous case in [7], [13], [25] and developed them further in [31].

In the porous media transport, only one type of stochastic models was used, namely, the random displacement method (RDM) for hydrodynamic dispersion equations. It should be stressed that RDM can be applied only if the displacement covariance tensor is known (e.g., from measurements, or numerical simulations), and cannot be applied if the functionals of interest are evaluated at times comparable with the characteristic correlation scale of the flow. In contrast, the Lagrangian stochastic models based on the tracking particles in a random velocity field extracted from the numerical solution of the flow equation (for brevity, we will call this model DSM, the direct simulation method) are free of these limitations, but the computational resources required are vast. Therefore, it is quite suggestive to construct a Langevin-type stochastic model which is an approximation to DSM, and is written in the form of a stochastic differential equation for the position and velocity. The basis for the Langevin-type approach comes from the Kolmogorov similarity theory of fully developed turbulence saying that the velocity structure tensor is a linear function in time which is universal in the inertial subrange. The linearity is the necessary condition to derive a Langevin-type equation to mimic the behavior of the real Lagrangian trajectories. Therefore, the crucial point is here to see if in the porous media this kind of linear law can be observed. We studied this problem by using the DSM, and detailed numerical simulations and comparisons with the random displacement model were carried out before we have constructed this Langevin-type model as a powerful instrument for practical calculations. Special small perturbation analysis is made in the case of small velocity fluctuations when the Gaussian velocity field is simulated directly through randomized spectral representation [8].

The work is done in cooperation with Université Libre de Bruxelles and FZ Jülich, Institut für Chemie und Dynamik der Geosphäre. The results are presented in [14], [29], [31].

5. Numerical methods for stochastic Hamiltonian systems and Langevin-type equations based on symplectic integrators. Stability problems of stochastic dynamics (G.N. Milstein).

In general we face many difficulties when implementing numerical methods for stochastic differential equations. At the same time, methods adapted to specific systems can be more efficient than general methods. In [21], [23] and [24], specific methods for stochastic Hamiltonian systems and Langevin-type equations are proposed. Stochastic Hamiltonian systems, like deterministic Hamiltonian systems, possess the property of preserving the symplectic structure. For instance, Hamiltonian systems with additive noise are a rather wide and important class of equations having this property. A lot of attention has been paid to symplectic integration of deterministic Hamiltonian systems. This interest is motivated by the fact that symplectic integrators in comparison with usual numerical schemes allow to simulate Hamiltonian systems

on very long time intervals with high accuracy. Symplectic methods for stochastic Hamiltonian systems, as proposed in [23], [24], have significant advantages over standard schemes for stochastic differential equations as well. We construct symplectic methods for general stochastic Hamiltonian systems as well as higher-order symplectic schemes for Hamiltonian systems with separable Hamiltonians, Hamiltonian systems with additive and colored noise, Hamiltonian systems with small noise, etc.

It is natural to expect that numerical methods which, in a sense, are close to symplectic ones, also have advantages when applied to stochastic systems close to Hamiltonian ones. An important and large class of such systems is given by Langevin-type equations. The Langevin-type equations are met in models from physics, chemistry, and biology. In [21] we construct special numerical methods (called quasi-symplectic) which preserve certain properties of Langevin-type equations. These methods degenerate to symplectic ones when the system degenerates to a Hamiltonian one, and their law of phase volume contractivity is close to the exact one. Numerical tests of both symplectic and quasi-symplectic methods clearly demonstrate superiority of the proposed methods over standard ones on very long time intervals.

Stability properties of stochastic systems are studied in [6], [17]. Much effort has been devoted to the stability analysis of stationary points for linear autonomous systems of stochastic differential equations

In [17], we introduce the notions of Lyapunov exponent, moment Lyapunov exponent, and stability index for linear non-autonomous systems with periodic coefficients. We study these problems extensively for second-order conservative systems with small random and periodic excitations and obtain an asymptotic expansion of the moment Lyapunov exponent. As an application we consider the Hill and Mathieu equations with random excitations.

In [20], several random walks for the general Dirichlet problem for multi-dimensional linear elliptic and parabolic partial differential equations are proposed. They are constructed on the basis of weak approximations for the characteristic system of stochastic differential equations due to the corresponding probabilistic representations of the solution to a corresponding boundary value problem. The methods of [20] are the simplest among methods of order $O(h)$, because inside the domain we use the Euler weak approximations and near the boundary we exploit linear interpolation. In addition, these methods have a layer structure, and, in particular, the one-step method of numerical integration can be used. Therefore it is possible to apply extrapolation methods. As a result we suggest a number of efficient Monte Carlo algorithms.

For evaluating a hedging strategy against a multi-asset European claim we have to know at every moment the solution of the Cauchy problem for the corresponding linear parabolic equation (the value of the hedging portfolio) and its derivatives (the deltas). In [19], we suggest to find these quantities by Monte Carlo simulation of the corresponding system of stochastic differential equations using weak solution schemes.

Nonlinear PDEs usually do not have analytic solutions and are mostly investigated by numerical methods, which are traditionally based on deterministic approaches. A probabilistic approach to constructing new numerical methods for solving the Cauchy problem for nonlinear parabolic partial differential equations is developed in [18]. The approach is based on making use of the well-known probabilistic representations of solutions to linear partial differential equations and ideas of numerical integration of stochastic differential equations in the weak sense. Despite their probabilistic nature these methods are nevertheless deterministic. The probabilistic approach takes into account a coefficient dependence on the space variables and a relationship between diffusion and advection terms in an intrinsic manner. In particular, the derived layer methods allow to avoid difficulties stemming from essentially changing coefficients and strong

advection. The numerical algorithms are tested using computer experiments, among them tests on the Burgers equation with small viscosity and the Kolmogorov–Petrovskij–Piskunov (KPP) equation. Results are in good agreement with theory. We also present a comparison analysis of the layer methods and the well-known finite-difference schemes, demonstrating some of the advantages of the proposed methods. The approach is also applied to the numerical solution of the Neumann problem for nonlinear parabolic equations in [22] and to Navier-Stokes equations in [1].

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4.7 Research Group Continuum Mechanics

4.7.1 Overview

Die Forschung der Forschungsgruppe Kontinuumsmechanik ist in der Berichtsperiode in zwei großen thematischen Gruppen fortgesetzt worden:

- Modellierung von verzerrbaren porösen Körpern,
- Mikro-Makro- und Phasenübergänge.

Auf dem Gebiet der Modellierung von porösen Körpern wurden Probleme in drei Bereichen untersucht:

1. Lineare Stabilität von stationären Strömungen in poroelastischen Materialien. Es wurde bewiesen, dass nur eine 2D-Störung mit Massenaustausch eine Instabilität der 1D-Strömung erzeugen kann. Der Bereich der Stabilität ist von drei Materialparametern abhängig: Durchlässigkeit des Körpers, Durchlässigkeit des Randes und innere Fläche der Kanäle des Körpers.
2. Ausbreitung von linearen Schallwellen in gesättigten porösen Körpern. Schwerpunktmäßig wurde der Bereich niedriger Frequenzen und langer Wellen untersucht. Für Oberflächenwellen wurden Körper mit undurchlässigen Rändern erforscht. Es wurde bewiesen, dass für Anfangswertaufgaben (d. h. Wellenzahl k ist reell) der Bereich langer Wellen mit $k < k_{cr}$, k_{cr} – eine kritische Wellenzahl, für die Ausbreitung von P2-Wellen verboten ist. Gleichzeitig wurde bewiesen, dass in Randwertaufgaben (d. h. Frequenz ω ist reell) die Wellenausbreitung sich im gesamten Frequenzbereich $(0,\infty)$ regulär verhält. Diese Eigenschaften beeinflussen die Ausbreitungsbedingungen für Oberflächenwellen, die auch untersucht wurden.

Research in the research group “Continuum Mechanics” in the period of this report has been a continuation of work on two big groups of problems:

- Modeling of deformable porous media;
- Micro-macro and phase transitions.

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

1. Linear stability of stationary flows in poroelastic materials. It was proven that solely a 2D disturbance with mass exchange can yield an instability in 1D flow. The range of stability depends on three material parameters: bulk permeability, surface permeability and internal surface of channels of the medium.
2. Propagation of linear acoustic waves in saturated porous bodies. Primarily the range of low frequencies and long waves was investigated. For the case of surface waves bodies with impermeable boundaries were considered. It has been proven that for initial value problems (i.e. the wave number k is real) a range of long waves, $k < k_{cr}$, limited by a critical value of the wave number k_{cr} is forbidden for P2 waves. Simultaneously it has been proven that for boundary value problems (i.e. the frequency ω is real) the propagation of waves is regular in the whole range of frequencies $(0,\infty)$. These properties influence the propagation conditions for surface waves, which have been investigated as well.

3. Thermodynamische Grundlagen der Modellbildung für gesättigte thermoporoelastische Körper. Es wurde gezeigt, dass die klassische Biot'sche Theorie als ein Grenzfall des Modells mit konstitutiver Abhängigkeit vom Gradienten der Porosität folgt. Für diese makroskopische Modellbildung wurde auch eine systematische Mikro-Makro-Methode zur Berechnung mancher Materialparameter (Kompressibilitäten) entwickelt, die als Sonderfall die klassischen Gassmann-Formeln ergibt.

3. Thermodynamic foundations of modeling of saturated poroelastic bodies. It has been shown that the classical Biot theory is a limit case of a general model which contains a constitutive dependence on the gradient of porosity. For this macroscopic modeling a systematic micro-macro method of evaluation of some material parameters (compressibilities) has been developed. The classical Gassmann relations become a special case of this method.

Auf dem Gebiet der Mikro-Makro-Übergänge wurden die folgenden vier Problemstellungen behandelt:

Within the area of *micro-macro transitions*, the research group "Continuum Mechanics" has considered four different fields of problems.

- Phasenübergänge, zum Teil gefördert im BMBF-Programm *Neue Mathematische Verfahren in Industrie und Dienstleistungen* unter 03DRM3B5

  Zurzeit werden hier zwei unterschiedliche Phänomene behandelt: Morphologieänderungen auf der μm-Skala von Lotmaterialien der Mikroelektronik und Phasenübergänge mit Tropfenbildung auf der *mm*-Skala in Wafermaterialien für optoelektronische Anwendungen.

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

  Currently, two different phenomena are studied: morphological changes on the μm scale of solder materials that are used in microelectronic devices and phase transitions including the formation of droplets on the *mm* scale of wafer material that is used in optoelectronic applications.

- *Mehrskalenmodellierung von thermoelastischen Körpern* und *Mikro-Makro-Übergänge in der atomaren Kette für verschiedene Skalierungen*, gefördert im DFG-Schwerpunktprogramm SPP 1095 „Analysis, Modellbildung und Simulation von Mehrskalenproblemen"

- *Multi-scale modeling of thermoelastic bodies* and *Micro-macro transitions of the atomic chain for various scalings*, funded within the DFG Priority Program SPP 1095 "Analysis, Modeling and Simulation of Multiscale Problems"

- *Kinetische Behandlung von ausgewählten Anfangs- und Randwertproblemen* für hyperbolische Systeme und kinetische Gleichungen, gefördert im DFG-Schwerpunktprogramm „ANumE — Analysis und Numerik von Erhaltungsgleichungen"

- *Kinetic treatment of selected initial and boundary value problems* of hyperbolic systems and kinetic equations, funded within the DFG Priority Program "ANumE — Analysis and Numerics of Conservation Laws"

- Die Spannungsanalyse von dünnen einkristallinen Wafern wurde als rein industrielle Anwendung im Berichtszeitraum wieder aufgenommen.

- Stress analysis of thin single crystal wafers—a purely industrial study—was restarted.

Die Untersuchung von Phasenübergängen gliedert sich zurzeit in drei Unterprojekte: 1. Einführung von modernen atomaren Mehrkörperpotentialen zur realistischen Berechnung der konstitutiven Größen im Phasenfeldmodell nach Dreyer/Müller, insbesondere die Berechnung der höheren Gradientenkoeffizientenmatrix. 2. Mathematische Untersuchungen zum Limes mit Phasengrenzen als singuläre Flächen. 3. Modellierung von chemischen Reaktionen, deren Dynamik durch spannungsbeeinflusste Diffusion und das Auftreten von flüssigen Arsentropfen in Wafermaterialien bestimmt wird.

The study on phase transitions is currently divided into three subprojects: (1) Introduction of modern atomic many-body potentials for a realistic calculation of the constitutive quantities, which appear in the phase-field model according to Dreyer/Müller, in particular, the calculation of the matrix of higher gradient coefficients. (2) Mathematical study on the sharp interface limit. (3) Modeling of chemical reactions, whose dynamics is controlled by stress-influenced diffusion and the appearance of liquid arsenic droplets in wafer materials.

Die Studie über Mehrskalenmodellierung ist ein Gemeinschaftsprojekt mit J. Sprekels und eine Kooperation mit A. Mielke (Universität Stuttgart). Am Beispiel der atomaren Kette wird für verschiedene Skalierungen die Möglichkeit rigoroser Mikro-Makro-Übergänge untersucht. Durch die Kooperation mit A. Mielke hat sich ein neuer Zugang ergeben, der die am WIAS gefundene mikroskopische Oszillatorbewegung zu allgemeinen mehrparametrigen *Traveling-Wave*-Lösungen der Newton'schen Bewegungsgleichungen in Beziehung setzt.

The study on multiscale modeling is a joint project with J. Sprekels and a collaboration with A. Mielke (Universität Stuttgart). The atomic chain serves as an example, where the possibility of rigorous micro-macro transitions for various scalings is discussed. Due to the collaboration with A. Mielke, a new aspect is introduced that relates the microscopic oscillator motion, which was previously observed at WIAS, to general multi-parametric traveling-wave solutions of Newton's equations of motion.

Die Studie über hyperbolische Anfangs- und Randwertprobleme wurde am Beispiel der Boltzmann-Peierls-Gleichung fortgeführt. Im Berichtszeitraum wurden insbesondere mathematische Resultate zur Existenz des Maximum-Entropie-Prinzips erhalten.

The study on hyperbolic initial and boundary value problems has been continued with the consideration of the Boltzmann-Peierls equation. During the period of this report mathematical results on the existence of the maximum entropy principle were obtained.

Aufgrund industrieller Nachfrage wurde das Projekt *Spannungsanalyse von dünnen Platten* wieder aufgenommen, um folgende Ziele zu erreichen: 1. Umwandlung des WIAS-Codes, welcher die von Kármán'schen Plattengleichungen implementiert, in kommerziell nutzbare Software. 2. Bestimmung der Zuverlässigkeit von Plattentheorien in Bezug auf das ursprüngliche 3D-Elastizitätsproblem.

Due to industrial request, the project on *Stress analysis of thin plates* is reconsidered in order to reach the following objectives: (1) Transformation of the WIAS code, that solves the von Kármán plate system, into a commercially usable software tool. (2) Determination of the reliability of plate theories with respect to the original 3D elasticity problem.

4.7.2 Projects

Stability and relaxation of flows in porous materials

Collaborator: B. Albers

Cooperation with: B. Straughan (University of Durham, UK)

The aim of the project is the linear stability analysis of flow processes without and with mass exchange in porous media, especially in soils. Last year we reported already about the relaxation properties of a 1D flow disturbed by longitudinal (1D) disturbances. We have shown that the 1D steady state flow through a porous material is stable with respect to a linear longitudinal disturbance without and with mass exchange in the whole range of control permeability parameters π and α. These parameters are two important model parameters: the bulk permeability coefficient π, and the surface permeability α. While the first one enters the field equations and describes the effective resistance of the skeleton to the flow of the fluid, the latter enters the model through the boundary conditions of the third type, and accounts for properties of the surface. It is one of the material parameters which determine the fluid velocity. Consequently the two important parameters control two competing mechanisms responsible for the stability of the flow.
This year we investigated another disturbance, namely a transversal (2D) disturbance of the 1D base flow following from the set of equations

$$\frac{\partial \rho^F}{\partial t}+\frac{\partial \rho^F v_x^F}{\partial x}=0, \quad \rho^F\left(\frac{\partial v_x^F}{\partial t}+v_x^F\frac{\partial v_x^F}{\partial x}\right)=-\frac{\partial p^F}{\partial x}-\pi v_x^F, \qquad 0<x<l,$$

which are the mass and momentum balances of the fluid. Here, ρ^F is the mass density of the fluid component and v_x^F is the fluid velocity in x-direction. The partial pressure in the fluid is denoted by p^F. We investigate solely steady-state processes. Consequently the base flow does not contain any influence from mass exchange.
For the stability analysis a regular perturbation method is employed, but restricted to zeroth and first-order contributions. This means that the fields are viewed as a superposition of the base solution (indicated by 0) and a small perturbation (indicated by 1):

$$\rho^F=\overset{0}{\rho}(x)+\varepsilon\overset{1}{\rho}(x,z,t), \quad v_x^F=\overset{0}{v}_x(x)+\varepsilon\overset{1}{v}_x(x,z,t),$$
$$c=\overset{0}{c}+\varepsilon\overset{1}{c}(x,z,t), \quad \xi=\overset{0}{\xi}(x)+\varepsilon\overset{1}{\xi}(x,z,t), \quad v_z^F=\varepsilon\overset{1}{v}_z(x,z,t).$$

Here, c denotes the concentration of the adsorbate in the fluid component, ξ is the fraction of occupied sites on the inner surface of the skeleton, and v_z^F is the velocity of the fluid/adsorbate mixture in z-direction. The disturbances follow in the first step of perturbation from the adsorption/diffusion model (see, e.g., [1])

$$\frac{\partial \rho^L}{\partial t}+\rho^L\left(\frac{\partial v_x^F}{\partial x}+\frac{\partial v_z^F}{\partial z}\right)+v_x^F\frac{\partial \rho^L}{\partial x}+v_z^F\frac{\partial \rho^L}{\partial z}=-\frac{\rho_{ad}^A}{\tau_{ad}}\left[\frac{cp^L}{p_0}(1-\xi)-\xi\right],$$
$$\rho^L\left[\frac{\partial c}{\partial t}+v_x^F\frac{\partial c}{\partial x}+v_z^F\frac{\partial c}{\partial z}\right]=-(1-c)\frac{\rho_{ad}^A}{\tau_{ad}}\left[\frac{cp^L}{p_0}(1-\xi)-\xi\right],$$
$$\frac{\partial \xi}{\partial t}=\left[\frac{cp^L}{p_0}(1-\xi)-\xi\right]\frac{1}{\tau_{ad}},$$

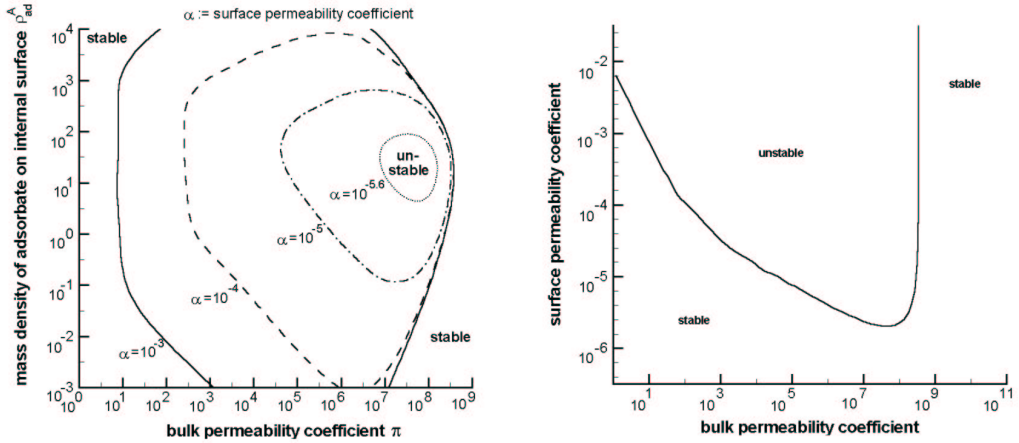
$$\rho^L\left[\frac{\partial v_x^F}{\partial t}+v_x^F\frac{\partial v_x^F}{\partial x}+v_z^F\frac{\partial v_x^F}{\partial z}\right] = -\frac{\partial p^L}{\partial x}-\pi v_x^F,$$
$$\rho^L\left[\frac{\partial v_z^F}{\partial t}+v_x^F\frac{\partial v_z^F}{\partial x}+v_z^F\frac{\partial v_z^F}{\partial z}\right] = -\frac{\partial p^L}{\partial z}-\pi v_z^F.$$

The following boundary conditions are assumed

$$-\rho^F v_x^F\big|_{x=0}=\alpha\left[p^F\big|_{x=0}-n_E p_l\right],$$
$$\rho^F v_x^F\big|_{x=l}=\alpha\left[p^F\big|_{x=l}-n_E p_r\right],$$
$$v_z^F\big|_{z=\pm b}=0.$$

After insertion of a wave ansatz for the disturbances, the eigenvalue problem for ω is numerically solved by using a second-order finite difference scheme in an equidistant mesh. Results show that with respect to a transverse disturbance without mass exchange similarly to the 1D disturbance an instability does not appear, but for transverse disturbances with mass exchange there appears a region of parameters π, α, and ρ_{ad}^A in which the base flow is unstable (see figure below). ρ_{ad}^A is an additional parameter entering the model through the mass source: the mass density of the adsorbate on the internal surface. It is proportional to the size of the internal surface which plays an enormous role for the global rate and amount of adsorption. For different soils it may vary a few orders of magnitude.

Not only the distinction in 1D and 2D disturbances plays an important role, but also the comparison of results for disturbances without and with mass exchange is an important result of this work. While already for 1D disturbances adsorption decreases the maximum values of the real parts of ω by orders of magnitude, for the 2D disturbances it even decides whether the base flow is stable or unstable. For small values of π the border of the instability region strongly varies with the surface permeability parameter α. On the side of large π, the unstable region is bounded from below by a single value of π. For sufficiently small α and ρ_{ad}^A, the base flow is unconditionally stable.



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Wave propagation in porous and granular materials

Collaborators: K. Wilmanski, B. Albers

Cooperation with: I. Edelman (Alexander von Humboldt fellow in WIAS, Russian Academy of Sciences, Moscow), S. Foti, R. Lancellotta (Università di Torino, Italy), C. Lai (Studio Geotecnico Italiano, Milano)

Aims and results of the project

The project is the continuation of the research devoted to a theoretical analysis of weak discontinuity waves on the basis of the own model (e.g., [1, 2]), as well as practical geotechnical applications particularly in a nondestructive testing of soils. Two main topics are in the process of investigation:

1. Long-wave and low-frequency approximations of surface waves on the interface: vacuum/porous body;
2. Gassmann relations and estimations of porosity by means of measurements of speeds of bulk waves.

It has been found out that results are different in the case when the problem of monochromatic waves is formulated in the space of real wave numbers, k (initial value problems), and in the case of real frequencies, ω (boundary value problems). For this reason a new asymptotic approximation has been developed by I. Edelman [3, 4, 5, 6]. She has shown that the P2 wave possesses a limit of the wave length beyond which this wave cannot propagate, i.e. the frequency becomes purely imaginary. The value of this limit depends on the bulk permeability coefficient. As the existence of Stoneley waves is coupled with the existence of P2 waves these waves possess a similar property. In the work [7] this property has been illustrated by a few numerical examples and compared with the properties of solutions for real ω.
In the subsequent works [8, 9] the properties of bulk and surface waves defined on the space of real ω have been investigated for the small frequency limit and it has been found out that the singularity discovered by Edelman does not exist in this formulation. The limits $\omega \to 0$ for P1 and S waves are regular and they give relations for the speeds of propagation:

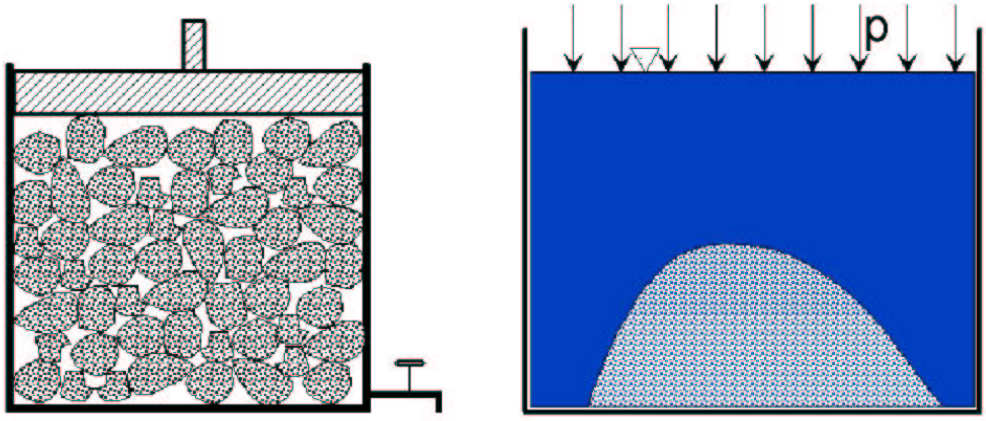
$$c_{oP1} = \sqrt{\frac{\lambda^S + 2\mu^S + \rho_0^F \kappa}{\rho_0^S + \rho_0^F}}, \quad c_{oS} = \sqrt{\frac{\mu^S}{\rho_0^S + \rho_0^F}},$$

where λ^S, μ^S, κ are Lamé constants and the compressibility of the fluid, respectively, while ρ_0^S, ρ_0^F are partial mass densities of the skeleton and of the fluid, respectively. These results agree with those of geophysicists. They show that the body reacts as if it was a composite of two elastic systems in a synchronized motion. Simultaneously, the limit for P2 waves is singular and it behaves as if the system were parabolic in connection with that mode which means that the speed limit of this wave goes to zero as $\sqrt{\omega}$.
Similar asymptotic analysis shows that the speed of the Stoneley wave becomes zero as ω goes to zero. The Rayleigh wave satisfies the following relation for the speed of propagation

$$\left(2 - \frac{c_{oRa}^2}{c_{oS}^2}\right) - 4\sqrt{1 - \frac{c_{oRa}^2}{c_{oS}^2}}\sqrt{1 - \frac{c_{oRa}^2}{c_{oP1}^2}} = 0,$$

which is identical with the classical Rayleigh equation except that speeds of bulk waves were replaced by the low-frequency limit counterparts.
The second topic arises in connection with a transition from microscopic to macroscopic relations for granular materials. As reported in the last year a nondestructive testing of soils by means of analysis of the field data for bulk and surface waves requires the transformation of microscopic compressibility properties into macroscopic parameters. This can be achieved by analysis of three simple tests:

- jacketed drained gedankenexperiment (left figure with open tap);
- jacketed undrained gedankenexperiment (left figure with closed tap);
- unjacketed gedankenexperiment (right figure).



All these tests must satisfy the following set of equations relating a macroscopic equilibrium state to a microscopic equilibrium state.

1. Geometric compatibility:
$$e = n_0 \varepsilon^R + (1 - n_0)\, e^R,$$
where e, ε^R, e^R denote macroscopic volume changes of the skeleton, microscopic volume changes of the fluid and of the grains, respectively, and n_0 is the porosity.

2. Dynamic compatibility:
$$p^F = n_0 p^{FR}, \quad p^S = (1 - n_0)\, p^{SR},$$
where p^F, p^S denote macroscopic partial pressures, p^{FR} is a pore pressure, and p^{SR} — pressure in the grains.

3. Constitutive relations:
$$\begin{aligned} p^F &= -\rho_0^F \kappa \varepsilon - Qe, \quad p^S = -\left(\lambda^S + \frac{2}{3}\mu^S\right) e - Q\varepsilon, \\ p^{FR} &= -K_f \varepsilon^R, \quad p^{SR} = -K_s e^R, \end{aligned}$$
where ε is the macroscopic volume change of the fluid, K_f, K_s denote microscopic (real) compressibilities, and Q is a coupling constant.

4. Equilibrium condition:
$$p = p^S + p^F,$$
where p is an external excess pressure.

The definitions of three gedankenexperiments lead to a system of equations which allows to determine the dependence of macroscopic parameters and microscopic parameters on porosity. These are the so-called Gassmann-type relations. Derivation of those relations shows that the method of micro-macro transition must be considerably improved in order to describe such properties of the porous material as a degree of saturation or capillarity effects. In spite of its flaws the above-described method yields results which agree quite well with the field experiments. This has been demonstrated in the works of the Italian partners of the project (e.g., [10]).

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Thermodynamic modeling of porous and granular materials

Collaborator: K. Wilmanski

Cooperation with: I. Müller (Technische Universität (TU) Berlin), R. Lancellotta (Università di Torino, Italy), C. Lai (Studio Geotecnico Italiano, Milano)

Aims and results of the project

The main task in this project is to establish a thermodynamic framework for multicomponent nonlinear thermomechanical models of porous materials. Due to the choice of the skeleton as the reference, the so-called Lagrangian description of motion [1] is used. Consequently, if we consider a porous medium whose channels are filled with a mixture of A fluid components, the model is constructed on a chosen reference configuration $\mathcal{B}_0$ of the solid component, i.e. all fields are functions of a spatial variable $\mathbf{X} \in \mathcal{B}_0$, and time $t \in \mathcal{T}$. In the work [5] we consider a thermomechanical model in which the governing fields are as follows:

1. ρ^S – mass density of the skeleton in the reference configuration;
2. $\rho^\alpha, \alpha = 1,\ldots,A$ – partial mass densities of fluid components referring to the unit volume of the reference configuration of the skeleton;
3. $\acute{\mathbf{x}}^S$ – velocity field of the skeleton;
4. $\mathbf{F}^S$ – deformation gradient of the skeleton;
5. $\acute{\mathbf{x}}^\alpha, \alpha = 1,\ldots,A$ – velocity fields of fluid components;
6. θ^S – absolute temperature of the skeleton;
7. $\theta^\alpha, \alpha = 1,\ldots,A$ – absolute temperatures of fluid components;
8. n – porosity (the volume fraction of voids).

Such a model was indicated in the work [2] (see as well [3, 4]), but the results were primarily related to the hierarchic structure of the so-called extended thermodynamics. In the present work we are primarily concerned with similarities and differences of the model with the classical Truesdell model of fluid mixtures. We show that the barycentric velocity of this classical theory must be replaced by the following relative Lagrangian velocity

$$\rho\dot{\mathbf{X}} := \sum_{\alpha=1}^{A} \rho^\alpha \acute{\mathbf{X}}^\alpha, \quad \acute{\mathbf{X}}^\alpha := \mathbf{F}^{S-1}(\mathbf{X},t)\left(\acute{\mathbf{x}}^\alpha(\mathbf{X},t) - \acute{\mathbf{x}}^S(\mathbf{X},t)\right), \quad \rho := \sum_{\alpha=1}^{A} \rho^\alpha.$$

With this relation in mind we obtain the following relation for the bulk Piola-Kirchhoff stress tensor

$$\mathbf{P} := \mathbf{P}^S + \sum_{\alpha=1}^{A} \mathbf{P}^\alpha - \mathbf{F}^S \left\{ \rho^S \dot{\mathbf{X}} \otimes \dot{\mathbf{X}} + \sum_{\alpha=1}^{A} \rho^\alpha \left(\acute{\mathbf{X}}^\alpha - \dot{\mathbf{X}}\right) \otimes \left(\acute{\mathbf{X}}^\alpha - \dot{\mathbf{X}}\right) \right\}.$$

This formula has a formal similarity to the classical Truesdell relations but it refers to the skeleton rather than to the center of gravity, and it is in the Lagrangian rather than Eulerian form.

Similarly we obtain for the bulk internal energy

$$\rho\varepsilon := \rho^S\varepsilon^S + \sum_{\alpha=1}^{A}\rho^\alpha\varepsilon^\alpha + \tfrac{1}{2}\left[\rho^S\mathbf{C}^S\cdot\left(\dot{\mathbf{X}}\otimes\dot{\mathbf{X}}\right) + \sum_{\alpha=1}^{A}\rho^\alpha\mathbf{C}^S\cdot\left(\acute{\mathbf{X}}^\alpha-\dot{\mathbf{X}}\right)\otimes\left(\acute{\mathbf{X}}^\alpha-\dot{\mathbf{X}}\right)\right],$$

where $\mathbf{C}^S = \mathbf{F}^{ST}\mathbf{F}^S$ is the Cauchy-Green deformation tensor for the skeleton, and for the bulk heat flux

$$\mathbf{Q}_I := \mathbf{Q}^S + \sum_{\alpha=1}^{A}\mathbf{Q}^\alpha - \rho^S\varepsilon^S\dot{\mathbf{X}} + \sum_{\alpha=1}^{A}\rho^\alpha\varepsilon^\alpha\left(\acute{\mathbf{X}}^\alpha-\dot{\mathbf{X}}\right) + \mathbf{P}^{ST}\mathbf{F}^S\dot{\mathbf{X}} - \sum_{\alpha=1}^{A}\mathbf{P}^{\alpha T}\mathbf{F}^S\left(\acute{\mathbf{X}}^\alpha-\dot{\mathbf{X}}\right)$$

$$+\tfrac{1}{2}\left[-\rho^S\dot{\mathbf{X}}\otimes\dot{\mathbf{X}}\otimes\dot{\mathbf{X}} + \sum_{\alpha=1}^{A}\rho^\alpha\left(\acute{\mathbf{X}}^\alpha-\dot{\mathbf{X}}\right)\otimes\left(\acute{\mathbf{X}}^\alpha-\dot{\mathbf{X}}\right)\otimes\left(\acute{\mathbf{X}}^\alpha-\dot{\mathbf{X}}\right)\right]\mathbf{C}^S.$$

These relations possess again a formal similarity to the Truesdell relations with the difference described above for the stress tensor.

By means of these relations one can evaluate the second law of thermodynamics which is assumed to have the form proposed by I. Müller (TU Berlin) for mixtures of fluids. In the Lagrangian form it is as follows. The entropy inequality

$$\frac{\partial(\rho\eta)}{\partial t} + \mathrm{Div}\left(\rho\eta\dot{\mathbf{X}} + \mathbf{H}\right) \geq 0, \quad \eta = \eta(C), \quad \mathbf{H} = \mathbf{H}(C),$$

where η is the entropy density in the reference configuration, $\mathbf{H}$ is the bulk entropy flux, and C denotes the set of constitutive variables, must hold for all solutions of field equations. An evaluation of this law has been done for fully nonlinear poroelastic isotropic materials with ideal fluid components. We discuss in detail the two-component case which has been investigated already in the projects of the previous years.

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Stress analysis of thin wafers

Collaborators: W. Dreyer, F. Duderstadt

Cooperation with: S. Eichler, M. Jurisch (Freiberger Compound Materials GmbH), M. Schaper (Technische Universität Dresden)

Supported by: Freiberger Compound Materials GmbH

In 2000 we have started a remittance study on the stress distribution in a thin wafer which is loaded by a steel sphere. This study is needed for industrial wafer manufacturers to form Weibull statistics in order to prove the resistance of wafers against fracture due to mechanical loading. The implemented WIAS FE code relies on the nonlinear von Kármán system in order to calculate stresses and strains in thin plates. There is a growing interest to transform this code into a commercial form that can be used by technicians. In the period of this report, the WIAS code has been used to point out serious experimental errors.
Furthermore, the WIAS team started a new study on the question how thin must a *real-life* wafer be, so that a plate theory which establishes the zero thickness limit of 3D elasticity can be used at all. This question has arised because wafer manufacturers use applied force against the measured maximal displacement graphs to test the reliability of plate theories. In an explicit example, the WIAS team could give the necessary conditions for this test of reliability to be appropriate.
Because the posed problem already appears within the Kirchhoff plate theory, which is the linearized version of the von Kármán system, the Kirchhoff solution is compared to its 3D counterpart. It could be proven that for a sufficiently large contact area of the external loading, the plate theory approximates the 3D theory with sufficient accuracy. On the other hand, if the contact area is of the order of the plate thickness, plate theory produces errors in the maximal stresses up to 5 %. However, if the contact area is significantly smaller than the thickness, errors up to 20 % may appear. This statement is exhibited in the following plot.

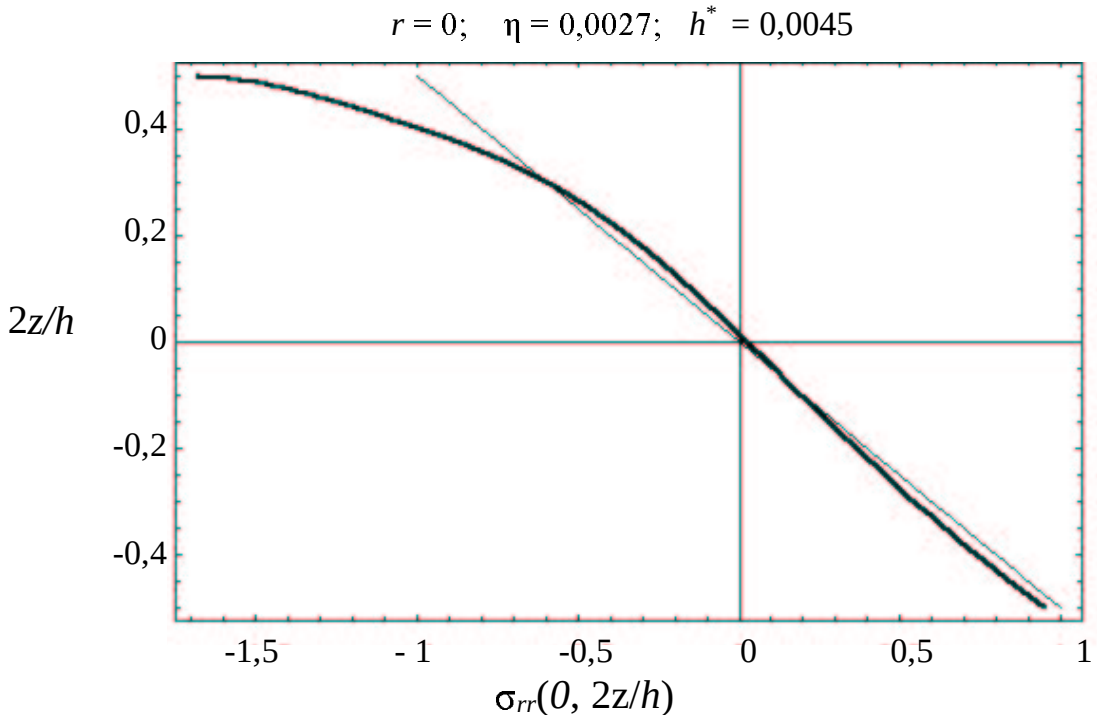

Fig. 1: Radial tension along the cylinder axis of the circle plate. Bold: 3D theory; fine: Kirchhoff theory; h: plate thickness; z: thickness coordinate; h^*: thickness per plate diameter; η: surface load diameter per plate diameter.

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Kinetic solution of sample initial and boundary value problems

Collaborators: W. Dreyer, M. Herrmann, Sh. Qamar

Cooperation with: M. Kunik (Otto-von-Guericke-Universität Magdeburg), M. Junk (Universität Kaiserslautern)

Supported by: DFG: "Kinetische Behandlung von ausgewählten Anfangs- und Randwertproblemen" (Kinetic solution of sample initial and boundary value problems), Priority Program "Analysis und Numerik von Erhaltungsgleichungen" (ANumE — Analysis and numerics for conservation laws)

At low temperatures the evolution of heat in crystalline solids is carried by phonons. In particular, the Fourier theory of heat fails to describe heat conduction at low temperatures. The evolution of a phonon gas is governed by the Boltzmann-Peierls equation which is a kinetic equation for the phase density φ of a phonon gas. For more details we refer to [6] and [4]. The Boltzmann-Peierls equation may be written as

$$\frac{\partial \varphi}{\partial t}(t,\mathbf{x},\mathbf{n}) + c_D n_i \frac{\partial \varphi}{\partial x_i}(t,\mathbf{x},\mathbf{n}) \quad = \quad (\Psi_R \varphi)(t,\mathbf{x},\mathbf{n}) + (\Psi_N \varphi)(t,\mathbf{x},\mathbf{n}). \tag{1}$$

Here t, $\mathbf{x}$ and $\mathbf{n}$ denote the time, the space and the normal wave vector, respectively. The collision operators Ψ_R and Ψ_N are relaxation operators and model the phonon-phonon interactions as well as the influence of the lattice.
The Boltzmann-Peierls equation implies a hierarchy of balance equations

$$\frac{\partial}{\partial t}\vec{u}(\varphi) + \frac{\partial}{\partial x_i}\vec{F}_i(\varphi) \quad = \quad \vec{P}(\varphi) \tag{2}$$

for densities $\vec{u}$, fluxes $\vec{F}_i$ and productions $\vec{P}$. The extended thermodynamics uses the kinetic entropy h, which here reads

$$h(\varphi) = \mu \int_{S^1} \varphi(\mathbf{n})^{\frac{2}{3}}\, d\mathbf{n}, \tag{3}$$

and the *Maximum Entropy Principle* (MEP) in order to close a finite system of balance equations. There result symmetric hyperbolic systems of PDEs.

The main problems we investigate in this project may be summarized as follows

1. Existence of MEP operators and properties of the corresponding moment systems;
2. Kinetic approximations for the MEP moment systems that have the form

$$\frac{\partial \varphi}{\partial t} + c_D n_i \frac{\partial \varphi}{\partial x_i} \quad = \quad \Psi_R \varphi + \Psi_N \varphi + \Psi_M \varphi \tag{4}$$

   with a suitable relaxation operator Ψ_M;
3. Kinetic schemes for the kinetic equations as well as for the moment systems;

4. Mathematical justification of the thermodynamical strategy to replace a kinetic equation by a hyperbolic moment system.

In the last year we concentrated on the mathematical properties of the above-mentioned nonlinear operators and equations. We obtained partial results concerning

1. Estimates that control L^p bounds for MEP phase densities;

2. Local existence and global uniqueness results for the Boltzmann-Peierls equation and for the kinetic approximations of MEP moment systems;

3. Modified collision and MEP operators leading to global existence results.

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4.8 Projects interconnecting research groups

On a nonlocal model of image segmentation

Collaborators: H. Gajewski (FG 1), K. Gärtner (FG 3)

Understanding an image as binary grey "alloy" of a black and a white component, we use a nonlocal phase separation model [1], [3], [4] to describe image segmentation and noise reduction.
The model consists in a degenerate nonlinear parabolic equation with a nonlocal drift term additionally to the familiar Perona-Malik model:

$$\frac{\partial u}{\partial t} - \nabla \cdot [f(|\nabla v|)\ (\nabla u + \frac{\nabla w}{\phi''(u)})] + \beta(u-g) = 0, \quad u(0,\cdot) = g(\cdot),$$

where

$$v = \phi'(u) + w, \quad w(t,x) = \int_\Omega \mathcal{K}(|x-y|)(1-2u(t,y))\,dy.$$

ϕ is a convex function, the kernel $\mathcal{K}$ represents nonlocal attracting forces, and v may be interpreted as chemical potential.
u has the meaning of a concentration/modified image, and g is the initial value/noisy image, respectively.
Relevant examples for ϕ and $\mathcal{K}$ are given by $\phi(u) = u\log u + (1-u)\log(1-u),\ 0 \le u \le 1$, $\mathcal{K}(s) = ke^{-s/\sigma}$.
The model parameters (β, k, σ in the example) can be adjusted by minimizing a functional evaluating smoothness and entropy of u and the distance between u and g.
We formulate conditions for the model parameters to guarantee global existence of a unique solution that tends exponentially in time to a unique steady state. This steady state is solution of a nonlocal nonlinear elliptic boundary value problem and allows a variational characterization.
The application of the model to noise reduction is related to model parameters guaranteeing a unique steady state. Image segmentation is related to parameters where a unique steady state may not exist.
Figure 1 demonstrates some properties of the model applied to the noise reduction problem.

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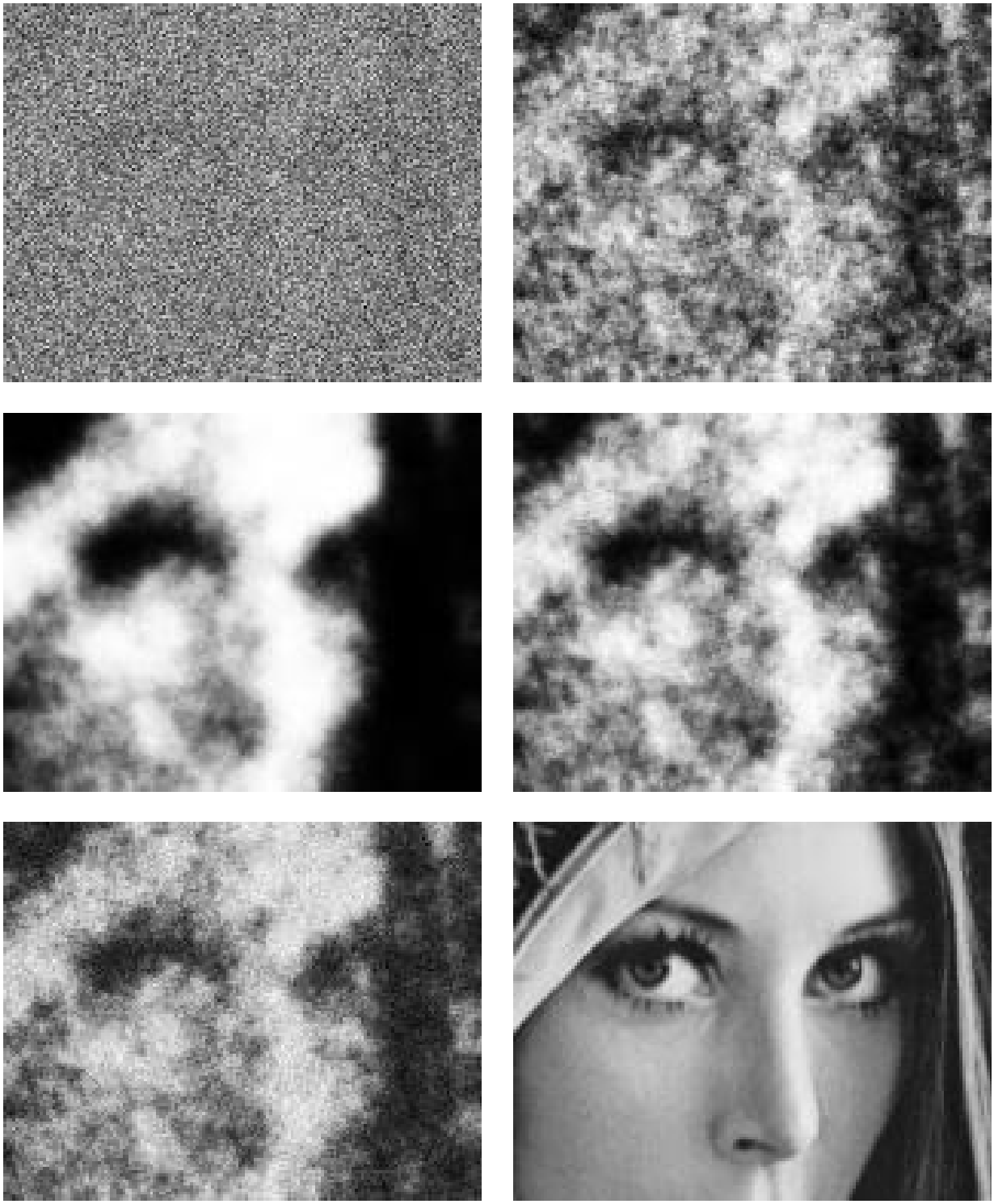

Fig. 1: Noisy picture (157 by 124 pixel section, UL), first optimization step (UR), intermediate optimization step (ML), final optimization result (MR), steady state (LL), original image (LR)

Upscaling of microscopically calculated characteristics to macroscopic state equations

Collaborators: U. Bandelow (FG 1), Th. Koprucki (FG 3)

Supported by: DFG: Priority Program „Analysis, Modellbildung und Simulation von Mehrskalenproblemen“ (Analysis, modeling and simulation of multiscale problems)

Eight-band kp-Hamiltonians [1] are detailed models for the calculation of quantum-confined states in semiconductor quantum-well structures, because they consistently include band mixing, spin-orbit interaction and strain effects. Quantities such as carrier densities or the optical response can be efficiently obtained in terms of the states ([2]). To utilize such microscopically calculated data for device simulation, e.g., with drift-diffusion-type models [2], [3], a suitable upscaling to macroscopic state equations is required. We have demonstrated upscaling schemes for the carrier densities, the peak gain characteristics and the spontaneous radiative recombination rate calculated with `WIAS-QW` for an example quantum-well structure [3].
The investigations have been carried out for an InGaAsP-based single quantum-well structure which is designed for emission at 1.55 μm consisting of a compressively strained quantum well of width $d_{QW} = 7$ nm sandwiched between tensile strained barriers.
As a first example for upscaling we consider the carrier densities. kp calculations [2] generically provide local carrier densities $n(z)$ and $p(z)$ depending on the Fermi levels F_e and F_h and the temperature T. Since the carriers localize very well in the quantum well [2] we can introduce an *average* carrier density per quantum well $\bar{n} = \int n(z)dz/d_{QW}$ as a natural quantity for upscaling. Thus we obtain from the microscopical model the relations $\bar{n}(F_e, k_BT)$ and $\bar{p}(F_h, k_BT)$ for the averaged carrier densities as depicted in Figure 1. The upscaling to a macroscopic level can then be performed by fitting the calculated relations $\bar{n}(F_e, k_BT)$ and $\bar{p}(F_h, k_BT)$ to macroscopic state equations such as the Fermi distribution used in drift-diffusion models. As shown in Figure 1 we observed that both quantities can be reasonably fitted to the relations

$$\bar{n} = N_c \mathcal{F}_{1/2}\Big(\frac{F_e - E_c}{k_BT}\Big), \quad \bar{p} = N_v \mathcal{F}_{1/2}\Big(\frac{E_v - F_h}{k_BT}\Big) \tag{1}$$

by adjusting the effective band edges E_c and E_v and the band-edge densities of state N_c and N_v. $\mathcal{F}_{1/2}$ is the Fermi integral of order $1/2$. The fit for the valence bands is very close to the calculated curve for a wide range of densities and temperatures whereas for the conduction bands the macroscopic state equation yields a good approximation only for a certain range of parameters. Thus, an upscaling of band-structure information by the dependence of the average density per quantum well on the Fermi level is possible. This allows us to treat the quantum well as a classical material with microscopically defined band-edge densities of state N_c and N_v and net band edges E_c and E_v which differ from the band-structure parameters of the well material and cannot be estimated elsewhere.

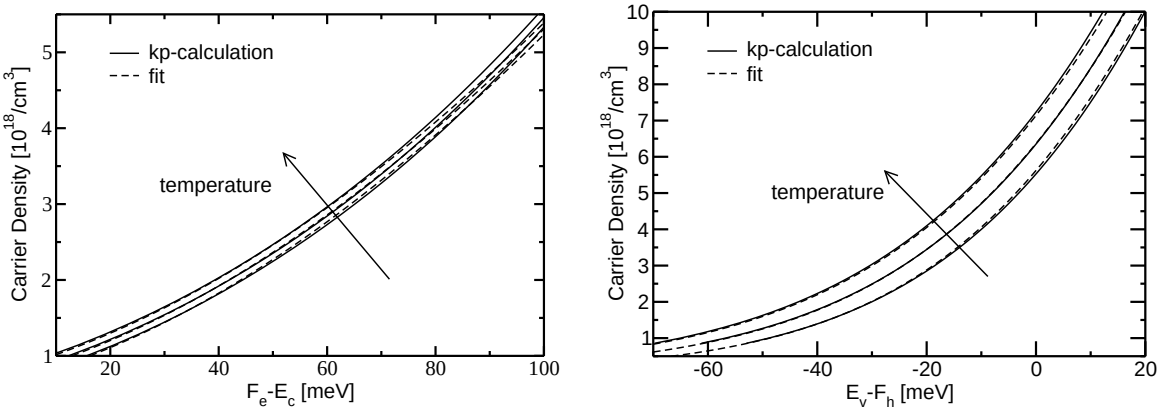

Fig. 1: Relation between the average carrier densities $\bar{n}, \bar{p}$ and the Fermi levels F_e, F_h relative to the net band edge E_c, E_v for the temperatures T=290 K, 315 K, 340 K. The dashed lines indicate the fit to the macroscopic state equation (1). Left: electrons occupying the conduction subbands, right: holes occupying the valence subbands.

Furthermore, the spectra of the optical material gain can be calculated in terms of the band-structure and transition matrix elements given by the wavefunctions [2], [3]. This defines a function $g(\hbar\omega, F_e, F_h, k_B T)$ depending on the transition energy $\hbar\omega$, the Fermi levels F_e and F_h and the temperature T. Most lasers are designed to emit at the spectral gain maximum. Therefore the peak gain g_p is an important quantity.

As a second example we have calculated the peak gain $g(\bar{n})$ (assuming charge neutrality $\bar{n}$=$\bar{p}$) as a function of the average carrier density introduced above. The result is depicted in Figure 2. For sufficiently high carrier densities (above $2.5 \cdot 10^{18} cm^{-3}$) this peak gain characteristics can be upscaled to a usually used state equation given by the logarithmic gain model

$$g_p(\bar{n}) = g_0 \ln(\bar{n}/n_{tr}) \qquad (2)$$

as shown in Figure 2. However, for low densities this way of upscaling completely fails. The constant g_0 appears to be nearly independent of the temperature whereas the transparency carrier density n_{tr} should roughly linearly increase with the temperature.

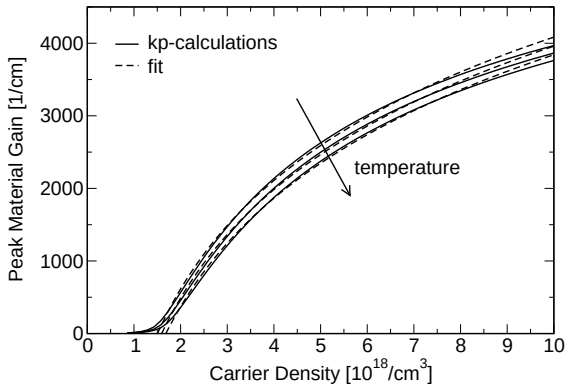

Fig. 2: Peak gain in dependence on the average carrier density $\bar{n}$ in the quantum well for 290 K, 300 K and 310 K. Dashed lines indicate the fit to the logarithmic gain model (2) with $g_0 = 2155\ cm^{-1}$.

As a third example we analyzed the upscaling of the spontaneous radiative recombination rate [3] which is a further important quantity for the analysis of semiconductor lasers, because it essentially determines the laser threshold. The spontaneous radiative recombination rate $R_{rad}(F_e, F_h, T)$ obtained by the kp calculations depends on the Fermi levels F_e and F_h and the temperature. Again, for local charge neutrality $\bar{n} = \bar{p}$ we found out that this relation can be suitably upscaled to the power law

$$R_{rad} = B \cdot \bar{n}^{\alpha}$$

as depicted in Figure 3. The exponent for the fit was approximately $\alpha = 1.5$, which differs from the commonly used models corresponding to $\alpha = 2$.

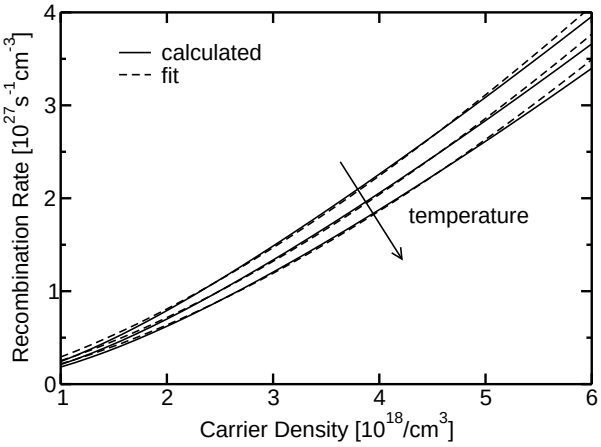

Fig. 3: Spontaneous radiative recombination rate for 290 K, 315 K, 340 K. Dashed: fit to $R_{rad} = B \cdot \bar{n}^{\alpha}$, with $\alpha = 1.47\ (290\ K), 1.51\ (315\ K), 1.55\ (340\ K)$.

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Sharp interface model for eutectic tin/lead alloy

Collaborators: B. Wagner (FG 1), W. Dreyer (FG 7)

Cooperation with: W.H. Müller (Technische Universität Berlin)

The reliability of solder joints plays a crucial role in the microelectronic packaging industry. In a real-life situation these solders, such as eutectic SnPb alloy, that consist of a fine mix of tin and lead, begin to form regions of high lead and tin concentration, see Figure 1. This coarsening process which is initiated by diffusion and enforced by the effects of surface tension as well as the exposure to thermo-mechanical stresses, has a drastic influence on the material properties of the solder.

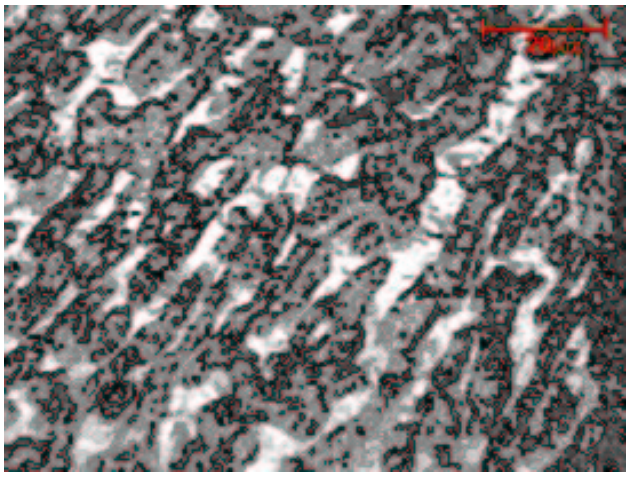

Fig. 1: Lead-rich lamellae after 20 hours of cooling (experiments by W.H. Müller)

We have investigated here specifically the influence of anisotropic surface tension on the shape of the precipitates formed in this process. For this purpose we derived in [4], on the basis of matched asymptotic analysis, a Sharp Interface Model (SIM) for the two-dimensional phase-field model for SnPb eutectic alloy, as developed and investigated by [1], [2] and [3].
The SIM considers the situation when the solution of the corresponding phase-field model has reached phase equilibrium and focuses on the slow (time scale $\tau = \varepsilon t$) evolution of the lead precipitates in a tin matrix. The resulting SIM is solved using a boundary integral method. In this setting it is also possible to derive the exact stationary solutions attained and to determine the dependence of their shape on anisotropy and mass. A linear stability analysis showed that, as in the isotropic case, the stationary solutions are stable.
For the numerical method we used a pseudo-spectral method for the spatial discretization of the boundary integral formulation for the precipitate-matrix interfaces. The parametrization of the boundary integral formulation is chosen such that it allows to isolate the stiffest terms in the evolution equation, which has to be treated implicitly, while the rest is updated explicitly.
Numerical simulations show strong dependence of the inter-precipitate mass flow on the shape of the precipitates.

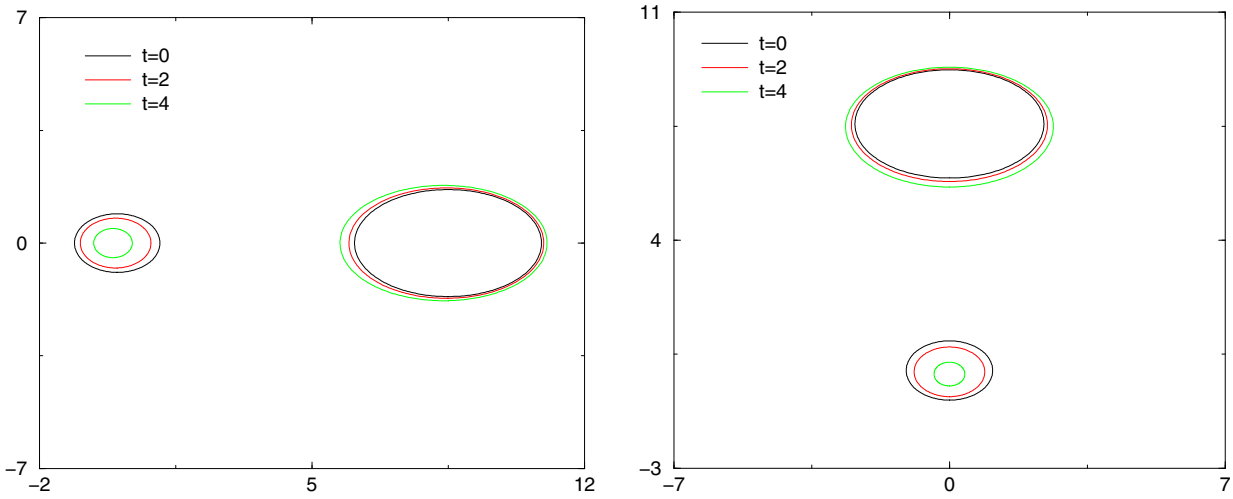

Fig. 2: Time evolution of two precipitates positioned side by side (left) and on top and bottom (right) with different mass

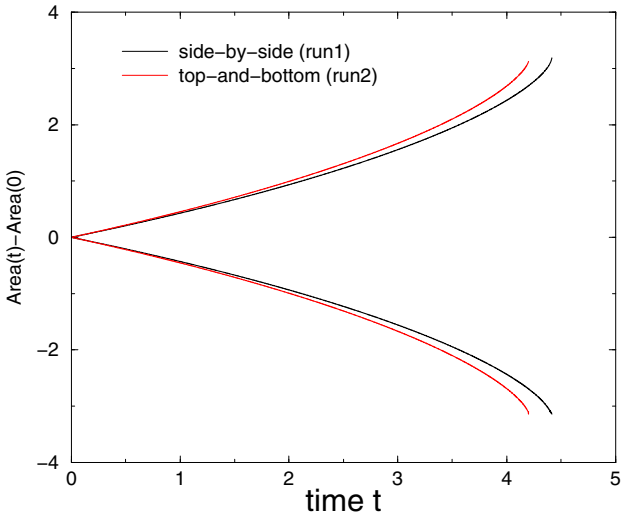

Fig. 3: Comparison of the change in area for the side-by-side (black) and top-and-bottom (red) case

In Figure 2 we start in both cases with precipitates which are stationary solutions by themselves. In both cases the closest distance to each other is the same. We observe that not high curvature but the length of the interfaces with smallest distance plays the dominant role for mass flux, see Figure 3. Moreover, interestingly, the shapes of the precipitates approach the form of elongated lamellae when they gain mass, while they become more circular when they loose mass.
We include the effects of the stress and strain and study their influence on the stability of our solutions.

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Micro-macro transitions of the atomic chain for various scalings

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Cooperation with: M. Kunik (Otto-von-Guericke Universität Magdeburg), A. Mielke (Universität Stuttgart)

Supported by: DFG: Priority Program "Analysis, Modellbildung und Simulation von Mehrskalenproblemen" (Analysis, modelling and simulation of multiscale problems)

In this project we study the initial value problem for an atomic chain consisting of a large number N of identical atoms. The dynamics of the chain is governed by Newton's equation

$$\ddot{x}_\alpha(t) \;=\; \Phi'\Big(x_{\alpha+1}(t)-x_\alpha(t)\Big)-\Phi'\Big(x_\alpha(t)-x_{\alpha-1}(t)\Big). \tag{1}$$

Here $x_\alpha(t)$ denotes the position of the atom α at time t. The interaction potential Φ is assumed to be nonlinear and convex.
Our main goal is to develop and to apply mathematical methods in order to pass to the *macroscopic* limit that results if the particle number N tends to infinity.
In the last report period we concentrated on the following setting for micro-macro transitions in the atomic chain.

1. We consider periodic boundary conditions.

2. In order to study macroscopic wave phenomena we use the hyperbolic scaling, i.e. time t, space x and particle index α will be scaled in the same way

$$\bar{t}=\varepsilon t, \quad \bar{x}=\varepsilon x, \quad \overline{\alpha}=\varepsilon\alpha, \quad \varepsilon=1/N. \tag{2}$$

3. In order to initialize the atomic distancies $r_\alpha=x_{\alpha+1}-x_\alpha$ we chose two macroscopic functions r_0^1, r_0^2 and define

$$r_\alpha(0)=\begin{cases} r_0^1(\varepsilon\alpha) & \text{if} \quad \alpha \text{ is odd,} \\ r_0^2(\varepsilon\alpha) & \text{if} \quad \alpha \text{ is even.} \end{cases} \tag{3}$$

   A similar procedure with two functions v_0^1 and v_0^2 determines the initial atomic velocities.

Next we discuss the special structure of the initial data. If the particle number is sufficiently large, there exist locally only two initial distancies r_0^1, r_0^2 and two initial velocities v_0^1, v_0^2 in the atomic chain. However, the values may vary on the macroscopic scale.
There are at least two reasons why these initial data are interesting for micro-macro transitions. Firstly, they pose an effective but simple possibility to create an initial temperature field in the chain. Secondly, in the case that r_0^1, r_0^2 and v_0^1, v_0^2 are constant, we can rigorously pass to the limit $N\to\infty$. All interesting thermodynamical quantities are then determined by a single ODE

$$\frac{d^2r}{d\tau^2}(\tau) \;=\; \Phi'\big(d-r(\tau)\big)-\Phi'\big(d+r(\tau)\big), \quad 2d=r_0^1+r_0^2. \tag{4}$$

In [1, 2] we start with the assumption that the special structure of our initial data is conserved for macroscopic times $\bar{t} > 0$. We show that if $N \to \infty$ there results the following system of PDEs

$$\begin{aligned} \partial_{\bar{t}}\ \tilde{r} \quad &- \quad \partial_{\bar{\alpha}}\ \tilde{v} \quad = \quad 0, \\ \partial_{\bar{t}}\ \tilde{v} \quad &+ \quad \partial_{\bar{\alpha}}\ \tilde{p} \quad = \quad 0, \\ \partial_{\bar{t}}\ (\frac{1}{2}\tilde{v}^2 + \tilde{u}) \quad &+ \quad \partial_{\bar{\alpha}}\ (\tilde{p}\,\tilde{v}) \quad = \quad 0. \end{aligned} \tag{5}$$

This system is the well-known Euler system for *specific length* $\tilde{r}$, *velocity* $\tilde{v}$, *pressure* $\tilde{p}$ and *specific internal energy* $\tilde{u}$. The Euler system is closed by the *equation of state*

$$\tilde{p} = \tilde{p}(\tilde{r}, \tilde{u}), \tag{6}$$

which can be derived from the ODE (4).
Furthermore, in [1] and [2] we predict the local distribution functions for the atomic velocities and atomic distancies and we derive the Gibbs equation for (5).
Numerical simulations indicate that the above-mentioned assumption leads to an appropriate description of the atomic chain for very large particle numbers. This fact is illustrated by the following figures.

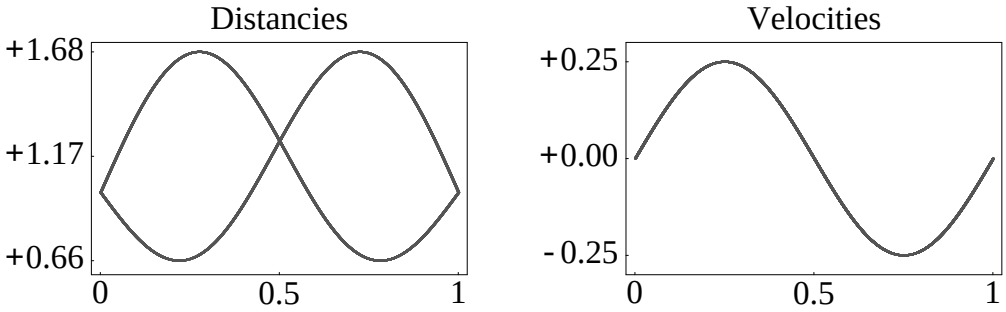


Fig. 1: The initial atomic distancies and velocities

Figure 1 shows the macroscopic initial configuration of a chain with 16000 atoms. The interaction potential is the well-known Toda potential.

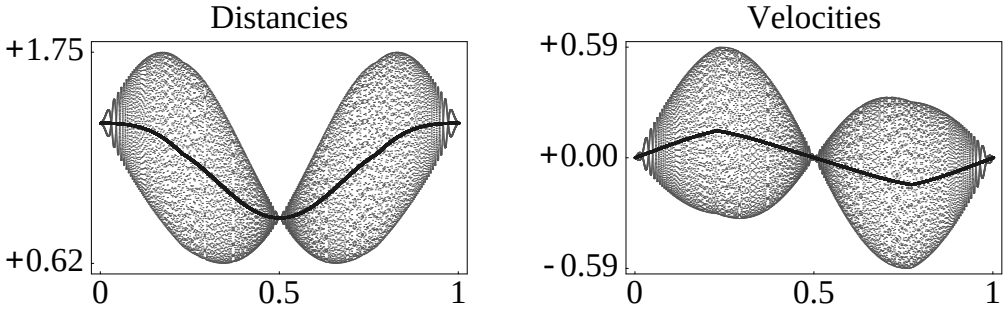


Fig. 2: The atomic distancies and velocities for fixed $\bar{t} > 0$

The resulting data for $\bar{t} = 0.5$ are depicted in Figure 2. The highly oscillating functions, which are not observable on the macroscopic scale correspond to atomic distancies and velocities. The dark-colored macroscopic curves are the mean values of the microscopic oscillations and represent the specific length $\tilde{r}$ and the macroscopic velocity $\tilde{v}$.
The last figure contains four examples of local distribution functions of the atomic distancies. The light-colored and continuous curves have been calculated by means of the macroscopic

fields. The dark-colored and dotted curves correspond to the distribution functions according to Newton's equations.

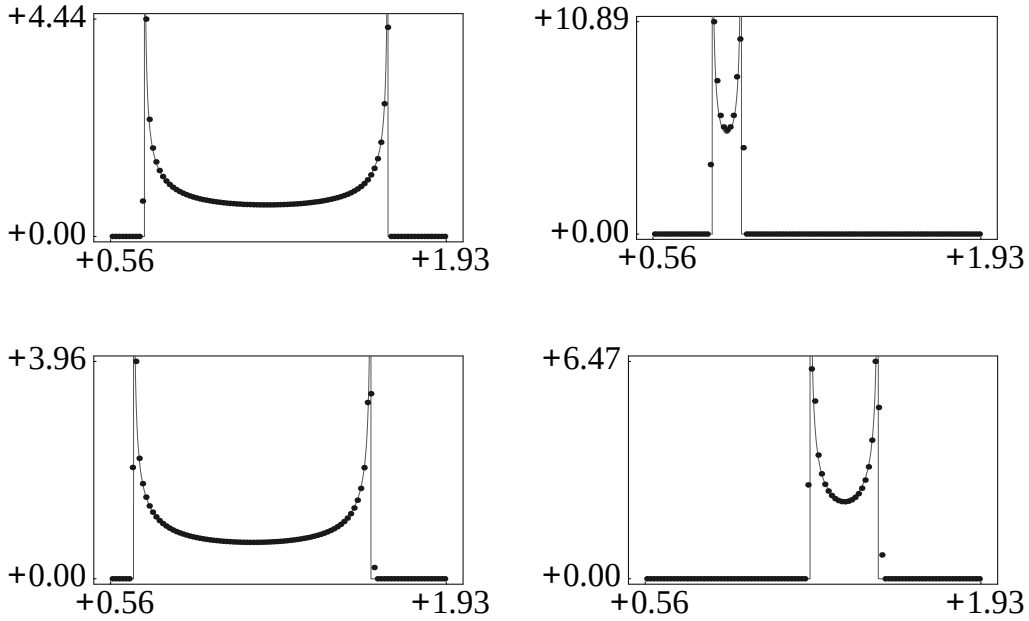
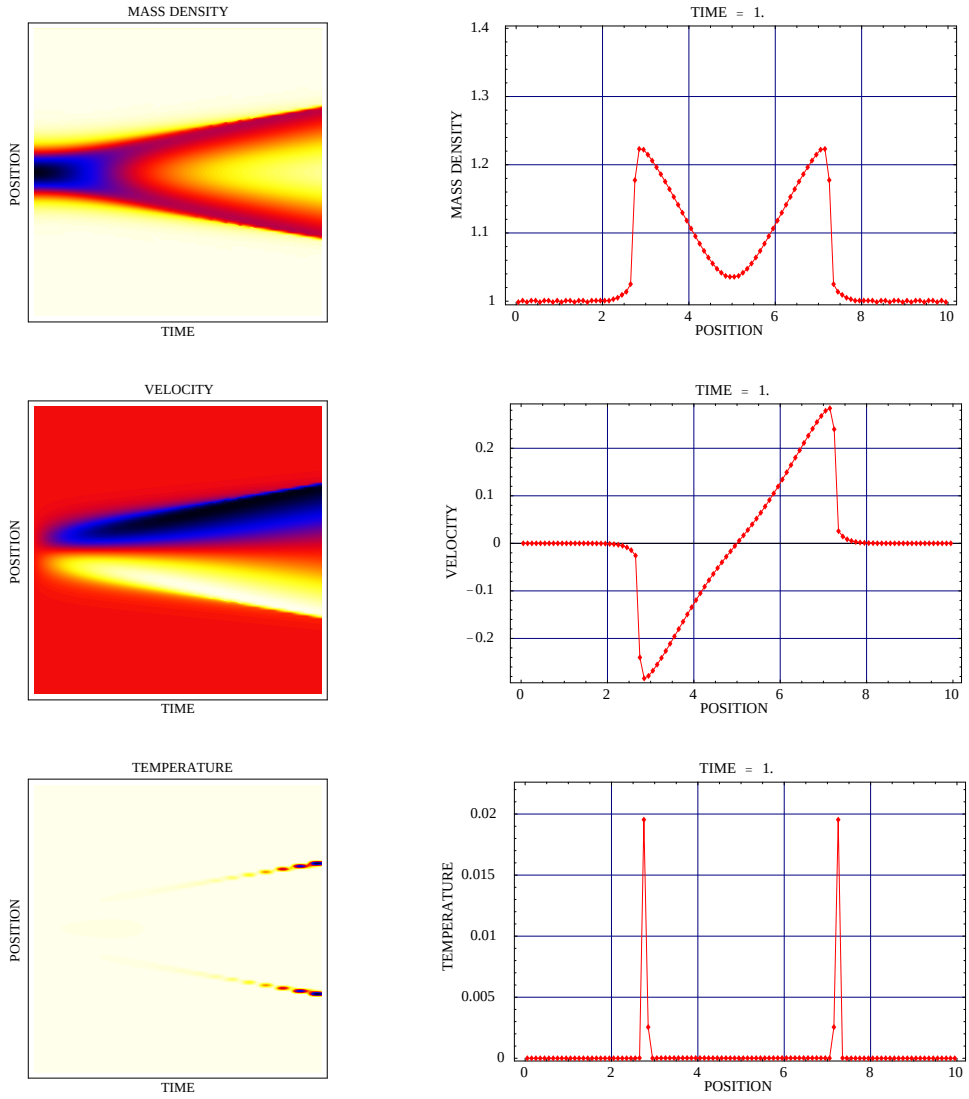


Fig. 3: The local distribution functions of the atomic distancies

Regarding the numerical solution of the microscopic equation of motion, the Verlet-Stoermer as well as the velocity-Verlet method are used. Both methods are applicable to molecular dynamics, however, the velocity-Verlet method tends to be more suitable to maintain the symplectic structure [3, 6] of the equation.
There follow two examples illustrating some of the numerical studies.

Continuous cold initial data with Gauss-distributed mass densities (in collaboration with N. Gröwe (Humboldt-Universität zu Berlin), R. Henrion (WIAS: research group "Nonlinear Optimization and Inverse Problems")).

For given values ρ^{min}, ρ^{max} and standard deviation s we define $w := (\rho^{max} - \rho^{min})/f_G(0.5, 0.5, s)$ and consider continuous cold initial data of the type $\rho(x) = \rho^{min} + w * f_G(x/L, 0.5, s)$, $v(x) \equiv 0$, $T(x) \equiv 0$. Here f_G denotes the Gaussian distribution density $f_G(z,m,s) := \frac{1}{\sqrt{2\pi}s} \exp\left(-\frac{(z-m)^2}{2s^2}\right)$. For a given atom index $\alpha \in \{0, \ldots, N-1\}$ the initial positions x_α of the atoms are iteratively computed by $\alpha := \int_0^{x_\alpha} \rho(x)dx = \int_0^{x_\alpha} \rho^{min} + w * f_G(x/L, 0.5, s)dx = w * L * 0.5 * \mathrm{Erf}(1/(2\sqrt{2}s)) + \rho^{min} * x_\alpha + w * L * 0.5 * \mathrm{Erf}((x_\alpha/L - 0.5)/(\sqrt{2}s))$. Here, an explicit representation of the required chainlength L is available from $N - 1 = \int_0^{x_{N-1}} \rho(x)dx = \int_0^L \rho(x)dx = \int_0^L \rho^{min} + w * f_G(x/L, 0.5, s)dx = \rho^{min} * L + 2 * w * L * 0.5 * \mathrm{Erf}(1/(2\sqrt{2}s))$. For a practial computation of the errorfunction see, e.g., [4]. The data are $N = 50001$, $\rho^{min} = 1.0$, $\rho^{max} = 1.4$, $s = 0.06$, $\lambda \approx 4716.3$. The numerical results depicted in the pictures below show that temperature may result from cold initial data.



An alternative approach for the generation of initial data for the thermal closure. In [1] thermal motion of the atomic chain is defined by the following assumptions:

1. The distributions of the atomic distances and velocities are completely uncorrelated.
2. The thermal velocities c are distributed by the Gaussian density with mean 0.0 and deviation $\sqrt{T}$
$$f(c) := \frac{1}{\sqrt{2\pi}\sqrt{T}} \exp\left(-\frac{c^2}{2T}\right).$$
3. The distances r are distributed by the density function
$$F(r) := \hat{F}(\alpha,\beta,r) := \frac{1}{\int_0^\infty \exp(-\alpha r - \beta\varphi(r))} \exp(-\alpha r - \beta\varphi(r)),$$
where φ is the potential, $\beta := 1/T$, and α is determined by the mean distance $1/\rho = \bar{r}(\alpha,\beta) := \int_0^\infty r\hat{F}(\alpha,\beta,r)dr$.

To prepare the atomic chain in thermal equilibrium, in [1] Section 9.2, the authors start with an equidistant distribution of the distances $r \equiv L/(N-1)$ and a distribution of the thermal velocities according to some auxiliary temperature T'. Solving the microscopic equation of motion after some iteration the distributions f(v) and F(r) will appear approximately.
To overcome the pre-iterations, the distribution of the velocities may be simulated by a random number generator for the Gaussian distribution as above using the initial temperature T instead of the auxiliary temperature T'. Since the cumulative distribution function of F is bijective, the distances may be generated by the inverse transform method [5]. For this purpose a sequence of random numbers $\{u_1,\ldots,u_N,\ldots\}$ will be generated which are uniformly distributed on $[0,1]$. Next the distances are initialized by $r_i := G^{-1}(u_i)$ where G denotes the distribution function of F. Then the resulting sequence $\{r_1,\ldots,r_N,\ldots\}$ will be distributed according to the density F.

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Phase transitions

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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)

There are two models for different aspects of phase transitions that were studied during the last report period.
(1) The standard model, which was designed by Dreyer/Müller, is able to describe morphological changes of binary alloys on the μm scale. In particular, a study of the coupling of mechanical stresses, diffusion and interface motion is of special interest for practical applications. An important difference between the Dreyer/Müller model and other similar models concerns the higher gradient part, which models surface energy of the interface boundary. That part is given by second derivatives of the concentration as $a_{ij}(c)\partial^2 c/\partial x_i \partial x_j$. The anisotropy and the concentration dependence of the matrix $a_{ij}(c)$ leads to quite new sharp interface limits that have not been studied before. While the numerical exploitation of the consequences was already done in former years, B. Wagner started a serious mathematical treatment of the problem. Moreover, the microscopic model to calculate the explicit structure of the matrix $a_{ij}(c)$ that was used up to now has been changed during the last report period. The atomic interactions were formerly described by central forces, however, their capability to describe properly atomic interaction in anisotropic crystals of, say, fcc or tetragonal lattice symmetry has become apparent. For this reason Dreyer/Müller started a rederivation of all atomic contributions to the free energy containing in particular the gradient matrix. This rederivation relies on microscopic embedded force potentials, where noncentral forces are modeled by the introduction of more than two body forces.
Regarding the applications of the model there are two aspects that were considered. The data basis for tin/lead alloys has been further extended and a collaboration with Bosch has been started to find out whether the Dreyer/Müller model can be described similarly to the formation of shear bands, the appearance of localized phase transitions that were observed in the Bosch labs and which might lead to the initiation of cracks. On the other hand, the collection of data for the intermetallic silver/tin is still of high importance, because due to environmental reasons silver/tin will probably substitute the tin/lead system as solder joint material in microelectronic devices in the very near future.
(2) The other model that was developed and extensively studied is designed to describe a process in semi-insulating gallium arsenide (GaAs), where a complex coupling between eigenstrain fields, due to dislocations and misfit, and diffusion, which is initiated by a heat treatment of GaAs, leads to the appearance of liquid arsenic droplets. Their inhomogeneous distribution on the *mm* scale means a serious problem regarding the use of GaAs as wafer material for optoelectronic devices.

The original mathematical model, which was developed at WIAS, contains a coupled system of partial differential equations for the variables strain, (As) concentration and a time- and space-dependent distribution indicating the size of the droplets. It has turned out during the last report period that a description of semi-insulating GaAs with only these variables is insufficient for its realistic thermodynamic description. There are further constituents which appear in semi-insulating GaAs. These are oxygen (O), silicon (Si), boron (B) and carbon (C) in very small quantities, but nevertheless these trace elements induce very important phenomena. Moreover, these elements as well as vacancies and the arsenic may carry charges and there are chemical reactions among these constituents and with electrons and holes, which must also be considered.
Several conferences with the wafer manufacturer FCM and with other experimenters have led to an extended description to simulate the evolution of arsenic droplets in GaAs. There are now 16 constituents included in the extended model that is designed as follows: Roughly speaking, there are two different time scales. Mechanical and chemical equilibrium is reached so much faster than diffusional and interfacial equilibrium that the mechanics and the chemistry are described by quasistatic equations whose time dependence is given by the evolution of diffusion and of interface motion. This leads to an elliptic second-order system to describe the strains and stresses and to 16 nonlinear algebraic equations to describe the chemistry. There is only a single diffusing constituent, which has turned out to be the uncharged arsenic interstitial, and there is thus (as before) a single diffusion equation. However, that equation is now of a quite complicated structure, because it couples to the solution of the chemical algebraic system and (as before) to the mechanical system.
Due to these new complexities, the evolution of droplets is currently described as a free boundary value problem for a single droplet. If all results of this simplification are fully exploited, the complete Becker/Döring model will be coupled again to the described model. To this end a multiscale transition is needed and will be carried out in collaboration with B. Niethammer (Bonn), who is the leading expert in Becker/Döring and related LSW models.

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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 100 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.

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 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 100 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.

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 2002 / Statistical information about the year 2002

Erwerbungen:	Acquisitions:
182 Bücher	182 books
284 gebundene Zeitschriftenbände	284 bound volumes of journals
894 Preprints und Reports	894 preprints and reports
54 Loseblattsammlungen	54 loose-leaf collections
Entleihungen aus der WIAS-Bibliothek:	Lent from the WIAS library:
3462 Bücher	3462 books
Aus anderen Bibliotheken beschaffte Literatur:	Literature provided from other libraries:
805 Bücher	805 books
645 Artikel	645 articles

5.2 Fachinformation / Science Information

Die Fachinformation des WIAS bietet unterschiedliche Recherchemöglichkeiten in bibliographischen Informations-Datenbanken und in Volltext-Datenbanken für alle Mitarbeiter des WIAS an:

- Die für die Mathematik wichtigsten Datenbanken „Zentralblatt MATH/Database“ und „MathSci“ (Mathematical Reviews),
- Zugangsmöglichkeiten zu natur- und ingenieurwissenschaftlichen Online-Datenbanken,
- Neben die bibliographischen Nachweis-Datenbanken treten zunehmend Volltext-Datenbanken im WWW, die mitunter (in ihren Anfangszeiten) noch frei zugänglich, meist aber lizenzpflichtig sind (Beispiel: Zeitschriftenartikel).

  Von der Fachinformation werden auf dem WIAS-Server in der Kollektion „Electronic journals“ (http://www.wias-berlin.de/service/fachinf/mathworld/ejournals) 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.

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 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/service/fachinf/mathworld/ejournals);
- Offline data-recall from CD-ROM databases on special PCs (e.g., in the library).

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.

- WIAS is a member of Math-Net and is represented there by a standardized "Secondary Homepage": http://www.wias-berlin.de/math-net.

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).

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).

Neben dem Einsatz immer leistungsfähigerer Workstations und PCs bestimmten folgende Projekte die Entwicklung der Rechentechnik des WIAS im Jahr 2002:

In addition to the purchase of more and more powerful workstations and PCs, the following projects have determined the development of the Computer Department in the year 2002:

1. Corporate Network, GWIN

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. Mit der Realisierung dieses Konzeptes wurde begonnen. Erste Teile werden bereit routinemäßig genutzt.

1. Corporate Network, GWIN

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 realization of the concept has been started and first parts are already routinely used.

2. LAN

Um einen einheitlichen Adressraum im Corporate Network des FVB zu erreichen, wurden alle IP-Adressen im Institut umgestellt. Dabei wurden viele Komponenten mit internen Adressen konfiguriert. Dadurch wurde die Sichtbarkeit potentiell unsicherer Netzkomponenten im Internet

2. LAN

All IP numbers in the institute have been changed in order to obtain a consistent address space in the Corporate Network of the FVB. In this process, many components have been configurated with internal addresses. Thus, the visibility of potentially insecure net components in the inter-

Die Namensdienste (DNS, NIS, Radius) des WIAS wurden auf neuen Rechnern (SUN Netra) installiert. Sie basieren nun auf einem iPlanet LDAP-Server. Zur Erhöhung der Zuverlässigkeit wurden sowohl die Hardware- als auch die Softwarekomponenten redundant ausgelegt.

3. Computeserver

Die Beschaffung des neuen Computeservers HP GS1280 mit acht Prozessoren und 32 GB Hauptspeicher wurde beschlossen. Die Lieferung wird Anfang 2003 erwartet.

4. Vortragsraum

Die Ausstattung des Vortragsraumes des WIAS wurde durch neue Möbel und neue Overhead-Projektoren weiter verbessert. Die neuen Projektoren verringern die Trapezverzerrung der dargestellten Bilder wesentlich.

5. SUNRays

Die im Jahre 2000/2001 beschafften Thin Clients SUNRay1 haben sich sehr bewährt. Es wurden zehn weitere Geräte beschafft und eingesetzt. An einigen Arbeitsplätzen wurden alte Workstations durch SUNRays ersetzt.

6. TFT-Displays

Es wurden weitere alte CRT-Farbmonitore durch TFT-Flachbildschirme ersetzt. Dadurch konnte die Qualität vieler Arbeitsplätze wesentlich verbessert werden.

WIAS' name services (DNS, NIS, Radius) have been implemented on new computers (SUN Netra). They are now based on an iPlanet LDAP server. Both the hardware and the software components have been redundantly designed in order to increase reliability.

3. Compute server

It was decided to purchase a new compute server HP GS1280 with eight processors and 32 GB main memory. The delivery is expected for the beginning of 2003.

4. Lecture room

The equipment of the lecture room of WIAS has been further improved by new furniture and new overhead projectors. The new projectors essentially reduce the trapezoid distortion of the projected pictures.

5. SUNRays

The Thin Clients SUNRay1s purchased in 2000/2001 have proved their worth. Ten more devices have been bought and connected. At some work-places, old workstations have been replaced by SUNRays.

6. TFT displays

More old CRT color monitors have been replaced by TFT flat screens. Thus the quality of many work-places was essentially improved.

6 Publications, Scientific Life[1]

6.1 Publications

6.1.1 Monographs

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R. HENRION, W. RÖMISCH, *Hölder and Lipschitz stability of solution sets in programs with probabilistic constraints*, Preprint no. 798, WIAS, Berlin, 2002.

D. HÖMBERG, *A mathematical model for induction hardening including mechanical effects*, Preprint no. 766, WIAS, Berlin, 2002.

D. HÖMBERG, A.M. KHLUDNEV, *On safe crack shapes in elastic bodies*, Preprint no. 716, WIAS, Berlin, 2002.

D. HÖMBERG, J. SOKOŁOWSKI, *Sensitivity analysis of an eddy current problem related to induction heating*, Preprint no. 776, WIAS, Berlin, 2002.

A. GOMBANI, S. JASCHKE, W. RUNGGALDIER, *A filtered no arbitrage model for term structures from noisy data*, Preprint no. 759, WIAS, Berlin, 2002.

H.-CHR. KAISER, H. NEIDHARDT, J. REHBERG, *Classical solutions of quasilinear parabolic systems on two-dimensional domains*, Preprint no. 765, WIAS, Berlin, 2002.

——, *Density and current of a dissipative Schrödinger operator*, Preprint no. 728, WIAS, Berlin, 2002.

O. KLEIN, *Asymptotic behaviour for a phase-field model with hysteresis in one-dimensional thermo-visco-plasticity*, Preprint no. 734, WIAS, Berlin, 2002.

O. KLEIN, P. KREJČÍ, *Outwards pointing hysteresis operators and asymptotic behaviour of evolution equations*, Preprint no. 748, WIAS, Berlin, 2002.

O. KLEIN, P. PHILIP, *Transient temperature phenomena during sublimation growth of silicon carbide single crystals*, Preprint no. 755, WIAS, Berlin, 2002.

H. LUO, D. KOLB, H.-J. FLAD, W. HACKBUSCH, TH. KOPRUCKI, *Wavelet approximation of correlated wavefunctions. II. Hyperbolic wavelets and adaptive approximation schemes*, Preprint no. 731, WIAS, Berlin, 2002.

C. KÜLSKE, *Analogues of non-Gibbsianness in joint measures of disordered mean-field models*, Preprint no. 800, WIAS, Berlin, 2002.

——, *Concentration inequalities for functions of Gibbs fields with application to diffraction and random Gibbs measures*, Preprint no. 742, WIAS, Berlin, 2002.

——, *Regularity properties of potentials for joint measures of random spin systems*, Preprint no. 781, WIAS, Berlin, 2002.

I. MATHEIS, W. WAGNER, *Convergence of the stochastic weighted particle method for the Boltzmann equation*, Preprint no. 739, WIAS, Berlin, 2002.

G.N. MILSTEIN, M.V. TRETYAKOV, *Numerical methods for Langevin type equations based on symplectic integrators*, Preprint no. 727, WIAS, Berlin, 2002.

Y. BELOPOLSKAYA, G.N. MILSTEIN, *An approximation method for Navier-Stokes equations based on probabilistic approach*, Preprint no. 733, WIAS, Berlin, 2002.

J. POLZEHL, V. SPOKOINY, *Local likelihood modeling by adaptive weights smoothing*, Preprint no. 787, WIAS, Berlin, 2002.

M. RADZIUNAS, H.-J. WÜNSCHE, *Dynamics of multi-section DFB semiconductor laser: Traveling wave and mode approximation models*, Preprint no. 713, WIAS, Berlin, 2002.

M. RADZIUNAS, H.-J. WÜNSCHE, O. BROX, F. HENNEBERGER, *Excitability of a DFB laser with short external cavity*, Preprint no. 712, WIAS, Berlin, 2002.

G. MASTROIANNI, C. FRAMMARTINO, A. RATHSFELD, *On polynomial collocation for second kind integral equations with fixed singularities of Mellin type*, Preprint no. 715, WIAS, Berlin, 2002.

O. REISS, *A generalized non-square Cholesky decomposition algorithm with applications to finance*, Preprint no. 760, WIAS, Berlin, 2002.

S. RŒLLY, M. SORTAIS, *Space-time asymptotics of an infinite-dimensional diffusion having a long-range memory*, Preprint no. 801, WIAS, Berlin, 2002.

S. RŒLLY, M. THIEULLEN, *Duality formula for the bridges of a Brownian diffusion. Application to gradient drifts*, Preprint no. 796, WIAS, Berlin, 2002.

P. DAI PRA, S. RŒLLY, *An existence result for infinite-dimensional Brownian diffusions with non-regular and non-Markovian drift*, Preprint no. 717, WIAS, Berlin, 2002.

O. KURBANMURADOV, K.K. SABELFELD, O.F. SMIDTS, H. VEREECKEN, *A Lagrangian stochastic model for the transport in statistically homogeneous porous media*, Preprint no. 786, WIAS, Berlin, 2002.

G. SCHMIDT, *On the diffraction by biperiodic anisotropic structures*, Preprint no. 751, WIAS, Berlin, 2002.

V. KARLIN, V. MAZ'YA, G. SCHMIDT, *Numerical algorithms to calculate periodic solutions of the Sivashinsky equation*, Preprint no. 771, WIAS, Berlin, 2002.

K.R. SCHNEIDER, V.A. SOBOLEV, *Existence and approximation of slow integral manifolds in some degenerate cases*, Preprint no. 782, WIAS, Berlin, 2002.

B. LANI-WAYDA, K.R. SCHNEIDER, *Delayed loss of stability and excitation of oscillations in nonautonomous differential equations with retarded argument*, Preprint no. 744, WIAS, Berlin, 2002.

N.N. NEFEDOV, K.R. SCHNEIDER, *Delayed exchange of stabilities in a class of singularly perturbed parabolic problems*, Preprint no. 778, WIAS, Berlin, 2002.

B. KRAUSKOPF, K.R. SCHNEIDER, J. SIEBER, S. WIECZOREK, M. WOLFRUM, *Excitability and self-pulsations near homoclinic bifurcations in semiconductor laser systems*, Preprint no. 750, WIAS, Berlin, 2002.

J. SCHOENMAKERS, *Calibration of LIBOR models to caps and swaptions: A way around intrinsic instabilities via parsimonious structures and a collateral market criterion*, Preprint no. 740, WIAS, Berlin, 2002.

J. SIEBER, *Longtime behavior of the traveling-wave model for semiconductor lasers*, Preprint no. 743, WIAS, Berlin, 2002.

M. GIURCANU, V. SPOKOINY, *Confidence estimation of the covariance function of stationary and locally stationary processes*, Preprint no. 726, WIAS, Berlin, 2002.

A. GOLDENSHLUGER, V. SPOKOINY, *On the shape-from-moments problem and recovering edges from noisy radon data*, Preprint no. 802, WIAS, Berlin, 2002.

J. SPREKELS, D. TIBA, *Optimization of ordinary differential systems with hysteresis*, Preprint no. 747, WIAS, Berlin, 2002.

A.K. STURM, *On convergence of population processes in random environments to the stochastic heat equation with colored noise*, Preprint no. 770, WIAS, Berlin, 2002.

N.H. BARTON, A.M. ETHERIDGE, A.K. STURM, *Coalescence in a random background*, Preprint no. 756, WIAS, Berlin, 2002.

D. TIBA, C. ZĂLINESCU, *On the necessity of some constraint qualification conditions in convex programming*, Preprint no. 710, WIAS, Berlin, 2002.

D. TURAEV, *Polynomial approximations of symplectic dynamics and richness of chaos in non-hyperbolic area-preserving maps*, Preprint no. 722, WIAS, Berlin, 2002.

D. TURAEV, V. ROM-KEDAR, *Soft billiards with corners*, Preprint no. 753, WIAS, Berlin, 2002.

D. TURAEV, S. ZELIK, *Homoclinic bifurcations and dimension of attractors for damped nonlinear hyperbolic equations*, Preprint no. 777, WIAS, Berlin, 2002.

S. GONCHENKO, L. SHILNIKOV, D. TURAEV, *Infinitely many elliptic periodic orbits in four-dimensional symplectic maps with a homoclinic tangency*, Preprint no. 791, WIAS, Berlin, 2002.

——, *On dynamical properties of diffeomorphisms with homoclinic tangencies*, Preprint no. 795, WIAS, Berlin, 2002.

A. KIRILLOV, D. TURAEV, *On modification of the Newton's law of gravity at very large distances*, Preprint no. 729, WIAS, Berlin, 2002.

B. WAGNER, *Second kind similarity solutions of the modified porous medium equation*, Preprint no. 779, WIAS, Berlin, 2002.

B. WAGNER, A. BERTOZZI, L. HOWLE, *Control of Rayleigh-Bénard convection*, Preprint no. 780, WIAS, Berlin, 2002.

A. EIBECK, W. WAGNER, *Stochastic interacting particle systems and nonlinear kinetic equations*, Preprint no. 732, WIAS, Berlin, 2002.

A.L. GARCIA, W. WAGNER, *A direct simulation Monte Carlo method for the Uehling-Uhlenbeck-Boltzmann equation*, Preprint no. 763, WIAS, Berlin, 2002.

K. WILMANSKI, *Note on weak discontinuity waves in linear poroelastic materials. Part I: Acoustic waves in saturated porous media*, Preprint no. 730, WIAS, Berlin, 2002.

——, *On thermodynamics of nonlinear poroelastic materials*, Preprint no. 792, WIAS, Berlin, 2002.

J. HÄRTERICH, M. WOLFRUM, *Describing a class of global attractors via symbol sequences*, Preprint no. 746, WIAS, Berlin, 2002.

M. WOLFRUM, D. TURAEV, *Instabilities of lasers with moderately delayed optical feedback*, Preprint no. 714, WIAS, Berlin, 2002.

S. YANCHUK, Y. MAISTRENKO, E. MOSEKILDE, *Identical synchronization of time-continuous chaotic oscillators*, Preprint no. 788, WIAS, Berlin, 2002.

6.2.2 WIAS Reports Series

Reports 2002[4]

V.F. BUTUZOV, N.N. NEFEDOV, K.R. SCHNEIDER, *Singularly Perturbed Problems in Case of Exchange of Stabilities*, Report no. 21, WIAS, 2002.

6.2.3 WIAS Technical Reports Series

Technical Reports 2002[5]

A. BUCHWALDER, D. HÖMBERG, T. JURKE, H.-J. SPIES, W. WEISS, *Simulation der Strahlhärtung von Stahl mit WIAS-SHarP*, Tech. rep. no. 3, WIAS, Berlin, 2002.

R. BRÜGGEMANN, H.-J. MUCHA, U. SIMON, *Model-based cluster analysis applied to flow cytometry data of phytoplankton*, Tech. rep. no. 5, WIAS, Berlin, 2002.

M. RADZIUNAS, *Sampling techniques applicable for the characterization of the quality of self pulsations in semiconductor lasers*, Tech. rep. no. 2, WIAS, Berlin, 2002.

H. SI, *TetGen. A 3D Delaunay tetrahedral mesh generator. v.1.2 Users manual*, Tech. rep. no. 4, WIAS, Berlin, 2002.

[4] http://www.wias-berlin.de/publications/index.pl?reports:2002
[5] http://www.wias-berlin.de/publications/index.pl?technicalreports:2002

6.2.4 Preprints/Reports in other Institutions

U. BANDELOW, R. HÜNLICH, TH. KOPRUCKI, *Simulation of static and dynamic properties of edge-emitting multi quantum well lasers*, Preprint no. 73, DFG Priority Program "Analysis, Modeling and Simulation of Multiscale Problems", Stuttgart, 2002.

M. BARO, M. DEMUTH, E. GIERE, *Stable continuous spectra for differential operators of arbitrary order*, Preprint no. 6, Technische Universität Clausthal, Institut für Mathematik, 2002.

A. BOVIER, *Metastability and ageing in stochastic dynamics*, Preprint, Universidad de Chile, Santiago, 2002.

A. BOVIER, I. KOURKOVA, *Derrida's generalized random energy models 1: Poisson cascades and extremal processes*, PMA-727, Université Paris VI "Pierre et Marie Curie", France, 2002.

——, *Derrida's generalized random energy models 2: Gibbs measures and probability cascades*, PMA-728, Université Paris VI "Pierre et Marie Curie", France, 2002.

——, *Derrida's generalized random energy models 3: Models with continuous hierarchies*, PMA-729, Université Paris VI "Pierre et Marie Curie", France, 2002.

W. DREYER, R. GUCKEL, *Micro-macro transitions by interpolation, smoothing, averaging and scaling of particle trajectories*, Preprint no. 52, DFG Priority Program "Analysis, Modeling and Simulation of Multiscale Problems", Stuttgart, 2002.

W. DREYER, M. HERRMANN, *A simple but rigorous micro-macro transition*, Preprint no. 50, DFG Priority Program "Analysis, Modeling and Simulation of Multiscale Problems", Stuttgart, 2002.

——, *Towards rigorous micro-macro transitions: The microscopic oscillator motion*, Preprint no. 51, DFG Priority Program "Analysis, Modeling and Simulation of Multiscale Problems", Stuttgart, 2002.

K. FLEISCHMANN, A. KLENKE, J. XIONG, *Pathwise convergence of a rescaled super-Brownian catalyst reactant process*, Preprint, Universität zu Köln, Mathematisches Institut, 2002.

D. HÖMBERG, J. SOKOLOWSKI, *Mathematical modelling of shape optimization problems for surface hardening*, Preprint no. 51, Université Nancy I, Institut Elie Cartan, 2002.

S. JASCHKE, C. KLÜPPELBERG, A. LINDNER, *Asymptotic behavior of tails and quantiles of quadratic forms of Gaussian vectors*, Disc. paper no. 280, Technische Universität München, 2002.

H.-J. FLAD, W. HACKBUSCH, D. KOLB, TH. KOPRUCKI, H. LUO, *Wavelet approximation of correlated wavefunctions. II. Hyperbolic wavelets and adaptive approximation schemes*, Preprint no. 53, DFG Priority Program "Analysis, Modeling and Simulation of Multiscale Problems", Stuttgart, 2002.

C. KÜLSKE, A. LE NY, F. REDIG, *Variational principle for generalized Gibbs measures*, Preprint no. 035, EURANDOM, Eindhoven, 2002.

V. MAZ'YA, G. SCHMIDT, W. WENDLAND, *On the computation of multi-dimensional single layer harmonic potentials via approximate approximations*, Preprint no. 10, Universität Stuttgart, Mathematisches Institut A, 2002.

D. TURAEV, S. ZELIK, *Homoclinic bifurcations and dimension of the attractors for damped nonlinear hyperbolic equations*, Preprint no. 170, Université de Poitiers, Laboratoire d'Applications des Mathématiques, 2002.

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.

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.

K.K. SABELFELD, (editor), Monte Carlo Methods and Applications, VSP, Zeist, The Netherlands.

——, Editorial Board, Mathematics and Computers in Simulation, Elsevier/North Holland, The Netherlands.

V. SPOKOINY, Editorial Board, Statistics and Decisions, Oldenbourg Wissenschaftsverlag, München.

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, *Zerstörungsfreie Prüfmethoden in der Geophysik, Teil II*, BTU Workshop „Geophysikalische Strömungen/Konvektion“, Brandenburgische Technische Universität (BTU) Cottbus, Internationales Begegnungszentrum, March 18.

——, *Linear stability of a 1d flow through a porous membrane*, International Conference on Multifield Problems, April 8–10, Universität Stuttgart, April 8.

——, *Relaxation properties of a 1d flow through a porous material without and with adsorption. Part I*, XXVIIth General Assembly of the European Geophysical Society, April 21–26, Nice, France, April 24.

——, *Mehrkomponentige Modellierung geophysikalischer Prozesse*, Universität Bremen, Fachbereich Geowissenschaften, May 24.

——, *Relaxations- und Stabilitätseigenschaften von Strömungen in porösen Körpern*, Colloquium Mechanics of Materials and Structures, Technische Universität Graz, Institut für Allgemeine Mechanik, Austria, June 20.

——, *Relaxation analysis and linear stability vs. adsorption in porous materials*, Symposium on Trends in Applications of Mathematics in Mechanics, September 29 – October 4, Maiori, Italy, October 3.

U. BANDELOW, *Quantum-classical coupling in multi quantum well lasers*, WIAS Workshop on Multiscale Problems in Quantum and Classical Mechanics, Averaging Techniques and Young Measures, September 19–21, Berlin, September 19.

——, *Towards a quasi-3d simulation of modulation properties of edge-emitting strained MQW lasers*, International Conference on Numerical Simulation of Semiconductor Optoelectronic Devices (NUSOD’02), September 25–27, Eidgenössische Technische Hochschule Zürich, Institut für Integrierte Systeme, Switzerland, September 25.

E. BÄNSCH, *Theory and numerics for parabolic problems*, 10 talks, Université de la Réunion, Faculté des Sciences et Technologies, Saint-Denis, France, April 2–29.

——, *Finite element discretization for “nonstandard” boundary conditions for the Navier-Stokes equations*, Seminar Analyse Numérique, Université de la Réunion, Faculté des Sciences et Technologies, Saint-Denis, France, April 18.

——, *Finite element methods for surface diffusion*, International Conference “Free Boundary Problems: Theory and Applications” (FBP2002), June 5–8, Università di Trento, Italy, June 6.

——, *Numerical methods for free surface flow*, Czech Technical University in Prague, Department of Mathematics, June 27.

——, *Finite element methods for surface diffusion*, Conference on Scientific Computing (ALGORITMY 2002), September 8–13, Slovak University of Technology, Department of Mathematics and Descriptive Geometry, Podbanské, September 9.

——, *Finite-Elemente-Verfahren für Phasengrenzphänomene*, Universität Konstanz, Fachbereich Mathematik und Statistik, October 24.

——, *Finite-Elemente-Verfahren für Phasengrenzphänomene*, Universität Karlsruhe, Fakultät für Mathematik, November 26.

——, *Finite element methods for some "interphase" problems*, University of Lisbon, Center of Mathematics and Fundamental Applications (CMAF), Portugal, December 5.

——, *Finite-Elemente-Verfahren für Surface Diffusion*, Oberseminar Analysis, Geometrie und Physik, Freie Universität Berlin, December 10.

M. BARO, *Dissipative Schrödinger-Poisson systems*, Conference on Operator Theory and its Applications in Mathematical Physics, May 11–18, Stefan Banach International Mathematical Center, Bedlewo, Poland, May 13.

——, *Kirkner-Lent-Poisson system*, WIAS Workshop on Multiscale Problems in Quantum and Classical Mechanics, Averaging Techniques and Young Measures, September 19–21, Berlin, September 19.

——, *Current coupling of drift-diffusion and Schrödinger-Poisson systems*, Université Paul Sabatier, Laboratoire de Mathématique pour l'Industrie et la Physique, Toulouse, France, October 17.

J. BORCHARDT, *Prozess-Simulation auf Parallelrechnern mit dem Simulator BOP*, 23. Norddeutsches Kolloquium über Angewandte Analysis und Numerische Mathematik, May 31 – June 1, Universität Bremen, June 1.

A. BOVIER, *From statics to dynamics in simple spin glass models*, "Journées de Physique Statistique", January 21–23, University de Cergy-Pontoise, Neuville-sur-Oise, France, January 22.

——, *Metastability, diffusion processes, and Eyring's formula*, University of Groningen, Institute of Mathematics and Computing Science, The Netherlands, February 5.

——, *Aging in the random energy model*, Tagung der Deutschen Physikalischen Gesellschaft, Leipzig, March 19.

——, *Aging in the random energy model*, Magdeburger Stochastik-Tage, German Open Conference on Probability and Statistics, Otto-von-Guericke-Universität Magdeburg, March 20.

——, *Metastability, diffusion processes, and Eyring's formula*, CNRS–Centre de Physique Théorique, Marseille, France, May 15.

——, *Metastability and diffusion processes I-III*, 3 talks, Université Paris VI "Pierre et Marie Curie", Laboratoire de Probabilités et Modèles Aléatoires, France, May 21–27.

——, *Rigorous results on a disordered system: Some efforts to understand the replica method*, Workshop "Phase Transitions and Algorithmic Complexity", June 3–5, University of California at Los Angeles, Institute for Pure and Applied Mathematics, USA, June 4.

——, *Metastability, diffusion processes, and Eyring's formula*, Seminar "Mathematische Physik", Technische Universität Berlin, Institut für Mathematik, June 24.

——, *Metastability and spectral theory for diffusion processes. Sharp asymptotics*, Workshop "Dynamics: Classical, Quantum and Stochastic", September 14–19, Cofin 2000, Theoretical and Mathematical Physics, Otranto, Italy, September 19.

——, *Asymptotik hochdimensionaler Zufallsprozesse: Gleichgewicht und Dynamik*, Kolloquium des Instituts für Mathematik, Technische Universität Berlin, October 22.

——, *Metastability, diffusion processes, and Eyring's formula*, Meeting "Stochastic Analysis", October 27 – November 2, Mathematisches Forschungsinstitut Oberwolfach, October 30.

——, *Metastability and ageing in stochastic dynamics*, IInd Workshop on Dynamics and Randomness, December 9–13, 3 talks, University of Chile, Center of Mathematical Modeling, Santiago, December 11–13.

G. BRUCKNER, *Regularization by projection of severely ill-posed problems with a posteriori parameter choice*, Fudan University, Department of Mathematics, Shanghai, China, November 7.

——, *Inverse problem of diffractive optics: Reconstruction by a two-step algorithm*, University of Tokyo, Department of Mathematical Sciences, Japan, November 12.

D. DAVIS, *Über die VCZ-Züchtung von GaAs-Kristallen*, 23. Norddeutsches Kolloquium über Angewandte Analysis und Numerische Mathematik, May 31 – June 1, Universität Bremen, May 31.

——, *Two- and three-dimensional melt-flow simulation in vapour-pressure-controlled Czochralski crystal growth*, Numerik-Seminar, Institut für Kristallzüchtung, Arbeitsgruppe Numerik-Modellierung, Berlin, December 2.

W. DREYER, *Auf dem Wege zu rigorosen Mikro-Makro-Übergängen. Teil I*, Forschungsseminar, Universität Stuttgart, Mathematisches Institut A, February 7.

——, *Über die Kopplung von Diffusion in mechanischen Spannungsfeldern und der Bildung von Tropfen in GaAs*, Kolloquium, Freiberger Compound Materials GmbH, March 4.

——, *On nucleation and growth of liquid droplets in single crystal GaAs*, International Workshop "Computational Physics of Transport and Interface Dynamics", Max-Planck-Institut für Physik komplexer Systeme, Dresden, March 5.

——, *On nucleation and growth of droplets in single crystals*, International Conference "Free Boundary Problems: Theory and Applications" (FBP2002), June 5–8, Università di Trento, Italy, June 5.

——, *Über die Bildung flüssiger Tropfen in einkristallinem Galliumarsenid*, Workshop "Angewandte Simulation in der Kristallzüchtung", October 10–11, Albert-Ludwigs-Universität Freiburg, Kristallographisches Institut, Memmelsdorf, October 10.

——, *Thermodynamic and atomistic modeling of evolving interfaces*, Kristall-Kolloquium, Martin-Luther-Universität Halle, Fachbereich Physik, November 11.

——, *Über die Bildung flüssiger Tröpfchen in einer kristallinen Matrix*, 15. Workshop "Composite Forschung in der Mechanik", November 18–20, WIAS, Berlin, November 19.

——, *Über die Bildung flüssiger Tropfen in GaAs*, Fachausschuss Computersimulation, November 20–22, VOEST-Alpine Industrieanlagen, Linz, Austria, November 22.

——, *On the formation and growth of liquid precipitates in crystalline gallium arsenide*, Workshop "Interfaces and Singularly Perturbed Interface Evolutions", Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, November 30.

——, *On the Becker-Doering theory of nucleation*, Workshop "Thermodynamische Materialtheorien", December 17–20, Mathematisches Forschungsinstitut Oberwolfach, December 18.

F. DUDERSTADT, *Anwendungen der von Kármán'schen Plattentheorie auf Waferplatten aus einkristallinem GaAs*, Mechanik-Seminar, Technische Universität Berlin, May 6.

——, *Beschreibung einkristalliner Waferplatten durch die von Kármán'sche Plattentheorie*, Forschungsseminar Festigkeitslehre, Otto-von-Guericke-Universität Magdeburg, May 30.

——, *Anwendung der von Kármán'schen Plattentheorie auf einkristalline Wafer*, Werkstoffseminar, GKSS Forschungszentrum Geesthacht, June 18.

——, *Spannungsanalyse dünner GaAs-Platten unter lokal begrenzten Lasten*, 15. Workshop "Composite Forschung in der Mechanik", November 18–20, WIAS, Berlin, November 19.

J. ELSCHNER, *Inverse scattering for periodic structures: Reconstruction of grating profiles*, European Symposium on Numerical Methods in Electromagnetics, March 6–8, Toulouse, France, March 7.

——, *Inverse problems for the periodic Helmholtz equation*, International Conference on Differential and Functional Differential Equations, Satellite Conference of the International Congress of Mathematicians (ICM) 2002 in Beijing, August 12–17, Moscow, Russia, August 14.

——, *Inverse problems for diffraction gratings*, BMBF Workshop "Boundary Element Methods — Modern Algorithms and Industrial Applications", September 30 – October 2, Saarbrücken, September 30.

——, *An inverse problem in periodic diffractive optics: Global uniqueness with a single wave number*, University of Tokyo, Department of Mathematical Sciences, Japan, November 25.

——, *On the numerical solution of periodic inverse diffraction problems*, Conference "New Trends in Boundary Elements", December 2–6, Mathematisches Forschungsinstitut Oberwolfach, December 2.

V. ESSAOULOVA, *Large deviations asymptotics for L_1 error of kernel density estimators and kernel regression function estimators*, Conference on Current Advances and Trends in Nonparametric Statistics, July 15–19, Crete, Greece, July 15.

——, *Large deviations of L_i-error of kernel and histogram density estimators*, University of the Free State, Department of Mathematical Statistics, Bloemfontein, South Africa, September 18.

——, *Large deviations of L_i-error of kernel and histogram density estimators*, Stellenbosch University, Department of Statistics and Actuarial Science, South Africa, September 27.

K. FLEISCHMANN, *Mutually catalytic branching in the plane*, DFG-Schwerpunktkolloquium „Interagierende Stochastische Systeme von hoher Komplexität“, January 6–9, WIAS, January 7.

——, *Gegenseitig katalysierende Verzweigungsprozesse in der Ebene*, Institutskolloquium, Friedrich-Alexander-Universität Erlangen-Nürnberg, Mathematisches Institut, January 15.

——, *Mutually catalytic branching in the plane*, University of Oxford, Mathematical Institute, UK, February 18.

——, *Mutually catalytic branching in the plane*, University of Bath, Department of Mathematical Sciences, UK, March 15.

——, *Recent progress in catalytic branching (I)*, Workshop on Spatially Distributed and Hierarchically Structured Stochastic Systems, April 4–10, Université de Montréal, Centre de Recherches Mathématiques, Canada, April 4.

——, *Recent progress in catalytic branching (II)*, Workshop on Spatially Distributed and Hierarchically Structured Stochastic Systems, Université de Montréal, Centre de Recherches Mathématiques, Canada, April 5.

——, *Pathwise convergence of a rescaled super-Brownian motion catalyst reactant pair*, Carleton University, School of Mathematics and Statistics, Laboratory for Research in Statistics and Probability, Ottawa, Canada, April 25.

——, *Mutually catalytic branching in the plane*, International Congress of Mathematicians 2002 (ICM), The First Sino-German Conference on Stochastic Analysis, August 29 – September 2, Beijing, China, August 29.

——, *Mutually catalytic and symbiotic branching*, Meeting “Stochastic Analysis”, October 27 – November 2, Mathematisches Forschungsinstitut Oberwolfach, October 27.

J. FUHRMANN, *Multiphysics systems solution by time-implicit Voronoi box finite volumes*, 3rd Symposium on Finite Volume for Complex Applications, June 24–28, Université de Provence, Aix-Marseille 1, Porquerolles, France, June 28.

——, *Implicit finite volume methods in complex applications*, Conference on Scientific Computing (ALGORITMY 2002), September 8–13, Slovak University of Technology, Department of Mathematics and Descriptive Geometry, Podbanské, September 10.

——, *Numerical simulation of thermal convection in the North-East-German basin*, WIAS Workshop “Challenges In Scientific Computing (CISC)”, October 2–5, Berlin, October 4.

H. GAJEWSKI, *On a nonlocal model of image segmentation*, Conference on Nonlinear Analysis, January 6–10, Universität Stuttgart, Institut für Mathematik, Kloster Irsee, January 10.

——, *On a nonlocal model of image segmentation*, WIAS Workshop “Challenges In Scientific Computing (CISC)”, October 2–5, Berlin, October 5.

——, *On a nonlocal phase-separation model*, Oberseminar Analysis, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, December 10.

K. GÄRTNER, *Introduction of Direct Methanol Fuel Cell models: Equations, numerical results, problems*, 9th Workshop on Numerical Methods for Free Boundary Problems (Interphase 2001), January 9–12, College Park, Maryland, USA, January 10.

——, *Numerical simulation of Direct Methanol Fuel Cells (DMFC)*, GKSS Forschungszentrum Geesthacht GmbH, Institut für Chemie, Teltow, May 27.

——, *Charge transport in semiconductors, properties of the Scharfetter-Gummel discretization on simplex grids*, Colloquium in honor of the 60th birthday of Prof. G. Stoyan, Szechenyi Istvan University, Department of Mathematics, Gyor, Hungary, June 14.

——, *Transport processes and electrochemistry in Direct Methanol Fuel Cells*, WIAS Workshop "Challenges In Scientific Computing (CISC)", October 2–5, Berlin, October 4.

——, *Application of recursive Schur complement approximations to the solution of the Newton linearized semiconductor device equations*, 2nd International Workshop on Parallel Matrix Algorithms and Applications, November 7–10, Faculté des Sciences, Neuchâtel, Switzerland, November 9.

B. GENTZ, *Concentration of sample paths in stochastic slow–fast systems*, Eidgenössische Technische Hochschule, Forschungsinstitut für Mathematik, Zürich, Switzerland, January 9.

——, *Stochastic slow–fast systems*, Workshop on Stochastic Systems with Interaction, February 18–20, DFG-Schwerpunktprogramm "Interagierende stochastische Systeme von hoher Komplexität", Universität Karlsruhe, Institut für Mathematische Stochastik, February 18.

——, *Stochastische Resonanz und Hysterese*, Ernst-Moritz-Arndt-Universität Greifswald, Institut für Mathematik und Informatik, March 5.

——, *Concentration of sample paths in stochastic slow–fast systems*, Magdeburger Stochastik-Tage, German Open Conference on Probability and Statistics, March 19–20, Otto-von-Guericke-Universität Magdeburg, March 19.

——, *Concentration of sample paths in stochastic slow–fast systems*, Ruhr-Universität Bochum, Fakultät und Institut für Mathematik, June 7.

——, *A sample-path approach to random dynamical systems*, Workshop "Stochastic Models from Statistical Physics III", October 7–11, EURANDOM, Eindhoven, The Netherlands, October 9.

——, *The effect of noise on slow–fast systems*, Universität Leipzig, Fakultät für Mathematik und Informatik, December 5.

F. GRUND, *Lösung von linearen Systemen mit schwachbesetzten Matrizen*, Leopold-Franzens-Universität Innsbruck, Institut für Technische Mathematik, Austria, October 25.

G. HEBERMEHL, *On the computation of propagating modes for microwave and optoelectronic devices*, GAMM Annual Conference 2002, March 25–28, Universität Augsburg, Institut für Mathematik, March 28.

——, *Eigen mode computation of microwave and laser structures including PML*, Scientific Computing in Electrical Engineering (SCEE-2002), June 23–28, University of Technology, Eindhoven, The Netherlands, June 24.

——, *Numerical simulation of microwave and semiconductor laser structures including absorbing boundary conditions*, WIAS Workshop "Challenges In Scientific Computing (CISC)", October 2–5, Berlin, October 2.

R. HENRION, *Optimierungsprobleme mit Wahrscheinlichkeitsrestriktionen*, Technische Universität Berlin, Institut für Mathematik, January 25.

——, *Polyhedral chance constraints: Computational and stability aspects*, IFIP/IIASA/GAMM Workshop "Dynamic Stochastic Optimization", March 11–14, International Institute for Applied Systems Analysis, Laxenburg, Austria, March 12.

——, *Structure and stability in programs with probabilistic constraints*, 7th SIAM Conference on Optimization, May 19–22, Toronto, Canada, May 21.

——, *Point conditions for local error bounds, calmness and linear conditioning*, 11th French-German-Polish Conference on Optimization, September 9–13, Brandenburgische Technische Universität Cottbus, September 10.

——, *Einführung in Methoden der Stochastischen Optimierung*, DECHEMA continuation course "Optimierung verfahrenstechnischer Prozesse", September 23–25, 3 talks, Technische Universität Berlin, September 25.

M. HERRMANN, *Kinetic solutions of the Boltzmann-Peierls equation and its moment systems*, Colloquium of the DFG Priority Program "Analysis and Numerics for Conservation Laws" (ANumE), Albert-Ludwigs-Universität Freiburg, Institut für Angewandte Mathematik, February 4.

——, *Auf dem Wege zu rigorosen Mikro-Makro-Übergängen. Teil II*, Forschungsseminar, Universität Stuttgart, Mathematisches Institut A, February 7.

——, *Micro-macro transitions in the atomic chain*, WIAS Workshop on Multiscale Problems in Quantum and Classical Mechanics, Averaging Techniques and Young Measures, September 19–21, Berlin, September 20.

D. HÖMBERG, *Optimierungsaufgaben bei der Oberflächenhärtung von Stahl*, Technische Universität Berlin, Fakultät II Mathematik und Naturwissenschaften, January 28.

——, *Ein elektro-thermoviskoelastisches Modell für das Widerstandsimpulsschweißen*, Oberseminar "Partielle Differentialgleichungen", Universität Konstanz, Fachbereich Mathematik und Statistik, January 29.

——, *The surface hardening of steel — Modeling, analysis and optimal control*, Technical University of Eindhoven, The Netherlands, October 23.

——, *Über ein elektro-thermoviskoelastisches Modell für das Widerstandsimpulsschweißen*, Technische Universität Darmstadt, Fachbereich Mathematik, November 14.

——, *Modellierung, Analysis und optimale Steuerung der Oberflächenhärtung von Stahl*, Technische Universität München, Zentrum Mathematik, November 19.

——, *Die Induktionshärtung von Stahl — Mathematische Modellierung und optimales Design von Induktoren*, Johannes Kepler Universität Linz, Institut für Numerische Mathematik, Austria, November 20.

——, *Modellierung, Simulation und optimale Steuerung von Phasenübergängen in Stahl*, Fachausschuss Computersimulation, November 21–22, VOEST-Alpine Industrieanlagen, Linz, Austria, November 21.

——, *On a thermoviscoelastic model related to resistance welding*, Université Henri Poincaré, Laboratoire de Mathématiques, Nancy, France, December 11.

S. JASCHKE, *Fourier inversion methods for Delta-Gamma Approximations*, Technische Universität München, Institut für Mathematik, January 16.

——, *Fourier inversion methods for Delta-Gamma Approximations*, Seminar Quantitative Finance, Humboldt-Universität zu Berlin, January 21.

——, *An overview of value-at-risk approximations*, GAMM Annual Conference 2002, March 25–28, Universität Augsburg, Institut für Mathematik, March 25.

——, *An overview of value-at-risk approximations*, Compstat 2002, August 24–28, Berlin, August 25.

——, *Algorithms and complexity for continuous problems, An overview of value-at-risk approximations*, Workshop on Algorithms and Complexity for Continuous Problems, September 29 – October 4, Schloß Dagstuhl, International Conference and Research Center for Computer Science, October 3.

TH. JURKE, *On cosmological consequences of the Einstein equation*, Universität Potsdam, Bereich Astrophysik, November 4.

——, *On future asymptotics in Gowdy spacetimes*, Seminar "Mathematical Relativity", November 10–16, Mathematisches Forschungsinstitut Oberwolfach, November 14.

H.-CHR. KAISER, *On the embedding of quantum mechanical models into the drift-diffusion model of semiconductor devices*, GAMM Annual Conference 2002, March 25–28, Universität Augsburg, Institut für Mathematik, March 25.

——, *Transversal modeling and simulation of edge-emitting semiconductor lasers*, International Conference on Numerical Simulation of Semiconductor Optoelectronic Devices (NUSOD'02), September 25–27, Eidgenössische Technische Hochschule Zürich, Institut für Integrierte Systeme, Switzerland, September 27.

——, *On finite volume methods for reaction-diffusion systems with discontinuous coefficients and mixed boundary conditions*, Workshop on Numerical Methods for Multiscale Problems, November 13–15, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, November 14.

O. KLEIN, *Surface movements during the sublimation growth of silicon carbide single crystals*, Workshop "Interfaces and Singularly Perturbed Interface Evolutions", November 29–30, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, November 29.

CHR. KÜLSKE, *Phase transitions in the Kac random field Ising model*, DFG-Schwerpunktkolloquium „Interagierende Stochastische Systeme von hoher Komplexität", January 6–9, WIAS, January 7.

——, *Can the usual Gibbs variational principle fail for WEAKLY Gibbsian measures?*, Workshop "Stochastic Systems with Interactions", February 18–20, Universität Karlsruhe, Institut für Mathematische Stochastik, February 19.

——, *Selbstmittelung bei der Diffraktion*, Ernst-Moritz-Arndt-Universität Greifswald, Institut für Mathematik und Informatik, March 5.

——, *Selfaveraging of random diffraction measures*, Magdeburger Stochastik-Tage, German Open Conference on Probability and Statistics, March 19–22, Otto-von-Guericke-Universität Magdeburg, March 20.

——, *Gitter-Spinmodelle mit zufälligen Potentialen: Gibbs-Maße und Phasenübergänge*, Universität Potsdam, Institut für Mathematik, April 26.

——, *Concentration inequalities for functions of Gibbs fields with application to diffraction*, Catholic University Leuven, Institute for Theoretical Physics, The Netherlands, June 6.

P. MATHÉ, *Optimal discretization of inverse problems*, Workshop on Inverse Problems and Applications, June 3–9, Istituto Nazionale di Alta Matematica, Cortona, Italy, June 6.

——, *Quasi-Monte Carlo integration over R^d*, Conference on Foundations of Computational Mathematics, Workshop "Approximation Theory", August 5–14, Minneapolis, USA, August 5.

——, *Moduli of continuity of operator-valued functions*, Conference on Foundations of Computational Mathematics, Workshop "Information based on complexity", August 5–14, Minneapolis, USA, August 10.

——, *Geometry of ill posed problems in variable Hilbert scales*, Workshop on Algorithms and Complexity for Continuous Problems, September 29 – October 4, Schloß Dagstuhl, International Conference and Research Center for Computer Science, Dagstuhl, September 30.

I. MATHEIS, *Stochastic weighted particle methods for the spatially homogeneous Boltzmann equation*, Herbstschule "Numerik und Stochastik", October 30 – November 3, Friedrich-Schiller-Universität Jena, Fakultät für Mathematik und Informatik, Siegmundsburg, October 31.

G. MILSTEIN, *Solving multi-dimensional linear partial differential equations by probabilistic approach*, Leicester University, Department of Mathematics and Computer Science, UK, September 19.

——, *Estimation of transition density for stochastic differential equations by forward-reverse diffusion*, University of Wales, Swansea, UK, October 8.

H.-J. MUCHA, *Intelligent clustering techniques*, International Conference on Modeling and Simulating Complex System, June 11–14, Business School of Sichuan University, Chengdu, China, June 11.

——, *Stabilised model-based clustering algorithms*, 8th Conference of the International Federation of Classification Societies, July 16–19, Krakow, Poland, July 18.

——, *Cluster analysis of bronzes from Luristan using their chemical composition*, 26th Annual Meeting of Gesellschaft für Klassifikation e. V., July 22–24, Universität Mannheim, July 22.

——, *Core-based clustering techniques: Methods, software, and applications*, 26th Annual Meeting of Gesellschaft für Klassifikation e. V., Universität Mannheim, July 23.

H. NEIDHARDT, *Recent results on the Trotter-Kato product formula: A survey*, Kanazawa University, Faculty of Science, Japan, January 30.

——, *Trotter-Kato product formula and operator norm convergence*, University of Groningen, Faculty of Mathematics and Natural Sciences, The Netherlands, March 28.

——, *Current coupling of drift-diffusion and Schrödinger-Poisson systems*, WIAS Workshop on Multiscale Problems in Quantum and Classical Mechanics, Averaging Techniques and Young Measures, September 19–21, Berlin, September 19.

——, *Current coupling of drift-diffusion and Schrödinger-Poisson systems*, Université Paul Sabatier, Laboratoire de Mathématique pour l'Industrie et la Physique, Toulouse, France, October 17.

——, *Kirkner-Lent-Poisson system*, CNRS-Centre de Physique Théorique, Marseille, France, October 23.

——, *Monotonicity for functions of operators*, Workshop on Operator Theory in Krein Spaces and Applications, December 6–7, Technische Universität Berlin, Fakultät II Mathematik und Naturwissenschaften, December 6.

P. PHILIP, *WIAS-HiTNIHS — Transient simulation with the high temperature numerical induction heating simulator*, DGKK Workshop "Angewandte Simulation in der Kristallzüchtung", Deutsche Gesellschaft für Kristallwachstum und Kristallzüchtung e.V., October 10–11, Albert-Ludwigs-Universität Freiburg, Kristallographisches Institut, Memmelsdorf, October 10.

J. POLZEHL, *Structural-adaptive smoothing methods*, French-German Seminar, Universität Potsdam, April 6.

——, *Structural adaptation I: Pointwise adaptive smoothing and imaging*, University of Tromsø, Department of Mathematics, Norway, April 11.

——, *Structural adaptation II: Time series and estimation of dimension reduction spaces*, University of Tromsø, Department of Mathematics, Norway, April 17.

——, *Structural adaptation I: Varying coefficient regression modeling by adaptive weights smoothing*, Workshop on Nonparametric Smoothing in Complex Statistical Models, April 27 – May 4, Ascona, Switzerland, April 30.

——, *Structural adaptive smoothing and its applications in imaging and time series*, Uppsala University, Department of Mathematics, Sweden, May 2.

——, *Varying coefficient modeling using structural adaptation*, Conference on Current Advances and Trends in Nonparametric Statistics, July 15–19, Crete, Greece, July 18.

——, *Structural adaptation methods in imaging*, Joint Statistical Meetings 2002, August 11–15, New York, USA, August 12.

——, *Statistische Grundlagen der Zertifizierung von Kurven*, Bundesanstalt für Materialforschung und -prüfung, Zertifizierungskomitee der Abteilung I, Berlin, December 12.

M. RADZIUNAS, *Dynamics of multi-section DFB semiconductor laser: Traveling wave and mode approximation models*, Physics and Simulation of Optoelectronics Devices X, January 21–25, San Jose, California, USA, January 21.

——, *Excitability of a DFB laser with short external cavity*, Physics and Simulation of Optoelectronics Devices X, San Jose, California, USA, January 24.

——, *Numerical bifurcation analysis of PDE system describing dynamics in multi-section semiconductor laser*, Dynamical Methods for Differential Equations, September 4–7, Medina del Campo, Spain, September 6.

——, *LDSL: A tool for simulation and analysis of longitudinal dynamics in multisection semiconductor lasers*, International Conference on Numerical Simulation of Semiconductor Optoelectronic Devices (NUSOD-02), September 25–27, Eidgenössische Technische Hochschule Zürich, Switzerland, September 25.

——, *Analysis and simulation of active feedback lasers*, Minisymposium “DFB Laser with Amplifying Feedback”, WIAS, Berlin, November 28.

A. RATHSFELD, *FEM and its generalization for the diffraction by polygonal profile gratings*, 9th International Conference on Mathematical Methods in Electromagnetic Theory (MMET*02), September 10–13, Kiev, Ukraine, September 11.

——, *FEM and its generalization for the diffraction by polygonal profile gratings*, BMBF Workshop “Boundary Element Methods — Modern Algorithms and Industrial Applications”, September 30 – October 2, Saarbrücken, October 2.

——, *Polynomial collocation for second kind integral equations with fixed singularities of Mellin type*, Conference “New Trends in Boundary Elements”, December 2–6, Mathematisches Forschungsinstitut Oberwolfach, December 3.

——, *Modellierung und Optimierung mikrooptischer Oberflächenstrukturen*, Carl Zeiss Oberkochen, December 9.

——, *Modellierung und Optimierung mikrooptischer Oberflächenstrukturen*, Statusseminar zum BMBF-Förderprogramm “Neue mathematische Verfahren in Industrie und Dienstleistungen”, December 16–17, Ludwigshafen, December 17.

J. REHBERG, *Existence and uniqueness for nonlinear evolution equations*, International Conference on Differential and Functional Differential Equations, Satellite Conference of the International Congress of Mathematicians (ICM) 2002 in Beijing, August 11–17, Moscow, Russia, August 15.

——, *Quasilinear parabolic systems including mixed boundary conditions in L^p*, Eidgenössische Technische Hochschule Zürich, Fachbereich Mathematik, Switzerland, October 31.

O. REISS, *Effiziente Methoden zur Bestimmung von Risikomaßen*, BMBF Workshop "Energie und Finanzwirtschaft", Bundesministerium für Bildung und Forschung, Berlin, March 4.

S. RŒLLY, *Equilibrium states for infinite dimensional diffusions*, 6th International Conference on Mathematical Problems of Statistical Physics, August 24–31, National Academy of Sciences of Armenia, Institute of Mathematics, Tsaghkadzor, Armenia, August 28.

——, *Diffusions en tant que mesures d'équilibre au sens de la mécanique statistique*, Journées de Probabilités, September 9–13, Université de la Rochelle, France, September 12.

——, *Infinite dimensional diffusions as equilibrium states in the spirit of Statistical Mechanics*, Johann Wolfgang Goethe-Universität Frankfurt, Mathematisches Seminar, October 16.

K.K. SABELFELD, *Recent developments in Random Walk Methods for 3D elasticity boundary value problems*, Seminar of the Institute of Computational Mathematics and Mathematical Geophysics, Russian Academy of Sciences, Novosibirsk, January 17.

——, *An explosion of the branching random walk on spheres for the Lamé equation*, St. Petersburg University, Department of Statistical Simulation, Russia, January 28.

——, *Stochastic Lagrangian models for simulation of particle transport in porous media*, International Conference on Numerical Mathematics, June 24–28, Russian Academy of Sciences, Novosibirsk, June 24.

——, *Stochastic models in porous medium*, Russian Academy of Sciences, Institute for Applied Mathematics and Mathematical Geophysics, Novosibirsk, August 27.

——, *Monte Carlo simulation of burning alumina particles*, Russian Academy of Sciences, Institute of Applied Mathematics and Mathematical Geophysics, Novosibirsk, September 5.

——, *Stochastic models of transport in porous media*, Russian Academy of Sciences, Institute of Applied Mathematics and Mathematical Geophysics, Novosibirsk, September 6.

——, *Monte Carlo simulation of random fields*, Keldysh Institute of Applied Mathematics, Moscow, Russia, September 18.

K.K. SABELFELD, I. SHALIMOVA, *Anisotropic Random Walk on spheres for static elasticity problems*, International Conference on Numerical Mathematics, Russian Academy of Sciences, Novosibirsk, June 25.

G. SCHMIDT, *Electromagnetic scattering by periodic structures*, International Conference on Differential and Functional Differential Equations, Satellite Conference of the International Congress of Mathematicians (ICM) 2002 in Beijing, August 12–17, Moscow, Russia, August 13.

——, *Diffraction by crossed anisotropic gratings*, BMBF Workshop "Boundary Element Methods — Modern Algorithms and Industrial Applications", September 30 – October 2, Saarbrücken, September 30.

——, *Electromagnetic scattering by biperiodic structures*, University of Tokyo, Department of Mathematical Sciences, Japan, November 25.

K.R. SCHNEIDER, *Modellreduktion und Verzweigungsverhalten*, Technische Universität Dresden, Institut für Lebensmitteltechnik und Bioverfahrenstechnik, January 7.

——, *Vibrational control of singularly perturbed systems*, Conference "Regelungstheorie", February 24 – March 2, Mathematisches Forschungsinstitut Oberwolfach, February 26.

——, *Einparametrige Canard-Zyklen*, GAMM Annual Conference 2002, March 25–28, Universität Augsburg, Institut für Mathematik, March 26.

——, *Forced canards*, International Workshop on Relaxation Oscillations & Hysteresis, April 1–6, Cork, Ireland, April 4.

——, *Hochfrequente Selbstpulsationen in Halbleiterlasern*, Meeting "Nichtlineare Dynamik", July 8–9, Verein Deutscher Ingenieure, Düsseldorf, July 9.

——, *Modeling of semiconductor lasers*, International Conference on Differential and Functional Differential Equations, Satellite Conference of the International Congress of Mathematicians (ICM) 2002 in Beijing, August 11–17, Moscow, Russia, August 12.

——, *Verzögerter Stabilitätsverlust in dynamischen Systemen*, Annual Conference of DMV, September 16–20, Universität Halle, September 17.

——, *Dynamics of semiconductor lasers*, Vth International Congress on Mathematical Modeling, September 30 – October 6, Dubna, Russia, September 30.

——, *Slow-fast systems in laser dynamics*, Moscow State University, Faculty of Physics, Russia, October 9.

J. SCHOENMAKERS, *Kalibrierung im LIBOR Modell*, Reuters AG, Düsseldorf, March 11.

——, *Accuracy and stability of LIBOR model calibration via parametric correlation structures and approximative swaption pricing*, Risk Conference 2002, April 23–24, Paris, France, April 23.

——, *Endogenous interest rates in asset markets*, 2nd World Congress of the Bachelier Finance Society, June 12–15, Crete, Greece, June 14.

——, *Calibration of LIBOR models to caps and swaptions: A way around intrinsic instabilities via parsimonious structures and a collateral market criterion*, Johann Wolfgang Goethe-Universität, MathFinance Institute, Frankfurt am Main, November 7.

——, *Calibration of LIBOR models to caps and swaptions: A way around intrinsic instabilities via parsimonious structures and a collateral market criterion*, Quantitative Finance 2002, Risk Waters Group, London, UK, November 26.

E. SHCHETININA, *Delay loss of stability in slow-fast systems*, International Workshop on Relaxation Oscillations & Hysteresis, April 1–6, Cork, Ireland, April 3.

——, *Integral manifolds of canard type in slow-fast systems*, Samara State University, Department of Mathematics, Russia, June 26.

H. SI, *3D quality Delaunay mesh generation methods and practical results*, WIAS Workshop "Challenges In Scientific Computing (CISC)", October 2–5, Berlin, October 2.

J. SIEBER, *High frequency oscillations in lasers subject to active optical feedback*, Spring School of the DFG Collaborative Research Centre "Complex Non-linear Processes", April 3–5, Wittenberg, April 4.

——, *Numerical bifurcation analysis of optical feedback effects in semiconductor lasers*, University of Bristol, Department of Engineering Mathematics, UK, May 3.

——, *Numerical bifurcation analysis of optical feedback effects in semiconductor lasers*, University College Cork, Department of Physics, Ireland, June 7.

——, *Semiconductor lasers subject to delayed optical feedback*, Summer School "Applied Analysis, KAM-Theory & Mathematical Optics", June 10–14, Twente, The Netherlands, June 10.

——, *Dynamics of semiconductor lasers*, Annual Conference of DMV, September 16–20, Universität Halle, September 17.

V. SPOKOINY, *Testing of the single-index hypothesis by structural adaption*, Conference on Current Advances and Trends in Nonparametric Statistics, Crete, Greece, February 17.

——, *Varying coefficient modelling by adaptive weights smoothing*, Université Paris VI "Pierre et Marie Curie", Laboratoire de Probabilité, France, March 7.

——, *Structural adaptation II: Identification and estimation of dimension reduction spaces*, Workshop on Nonparametric Smoothing in Complex Statistical Models, April 27 – May 4, Ascona, Switzerland, April 2.

——, *Robust coefficient modelling with applications to financial time series*, Annual workshop of Sfb 373, Motzen, May 2.

——, *Modeling of nonstationary time series by adaptive weights smoothing*, Conference on Current Advances and Trends in Nonparametric Statistics, July 15–19, Crete, Greece, July 17.

——, *An adaptive test of linearity for median regression model*, 24th European Meeting of Statisticians, August 19–23, Prague, Czech Republic, August 22.

J. SPREKELS, *On nonlocal models for non-isothermal phase transitions*, Academy of Sciences of the Czech Republic, Institute of Mathematics, Prague, February 19.

——, *Schlüsseltechnologie Angewandte Mathematik: Beiträge des Weierstraß-Instituts zu den Materialwissenschaften*, Adolf-Martens-Kolloquium, Bundesanstalt für Materialforschung und -prüfung, Berlin, February 27.

——, *On nonlocal models for nonisothermal phase transitions*, International Workshop and Seminar on Computational Physics of Transport Phenomena and Interface Dynamics, March 4–5, Max-Planck-Institut für Physik komplexer Systeme, Dresden, March 4.

——, *Modelling curved mechanical structures*, International Conference "Analysis and Optimization of Differential Systems", September 10–14, Ovidius University, Department of Mathematics and Informatics, Constanta, Romania, September 11.

——, *On nonlocal phase transition models for non-conserved order parameters*, Università degli Studi di Firenze, Dipartimento di Matematica "U. Dini", Italy, October 14.

——, *Phase-field models with hysteresis nonlinearities*, Memorial Seminar on the Occasion of the 50th Anniversary of the Mathematical Institute, Academy of Sciences of the Czech Republic, Institute of Mathematics, Prague, December 12.

H. STEPHAN, *Some properties of Fokker-Planck equations*, Seminar Stochastische Prozesse, Humboldt-Universität zu Berlin, Institut für Physik, July 9.

——, *Time asymptotics and inverse problems for Fokker-Planck equations*, International Conference "Inverse Problems and Nonlinear Equations" on the occasion of Prof. V.A. Marchenko's 80th anniversary, August 12–16, National Academy of Sciences of Ukraine, B. Verkin Institute for Low Temperature Physics and Engineering, Kharkov, August 15.

——, *Back front solitons of the KdV equation*, seminar of the Mathematical Department, National Academy of Sciences of Ukraine, B. Verkin Institute for Low Temperature Physics and Engineering, Kharkov, August 19.

——, *Modellierung und Simulation von Bauelementen für Schaltkreise der Leistungselektronik*, Colloquium of the DFG Priority Program "Semiconductor devices for high power applications", September 17–18, Ilmenau, September 18.

A. STURM, *On connections of spatially structured population processes to SPDEs in higher dimensions*, Probability Seminar Montréal, Université de Montréal, Centre de Recherches Mathématiques, Canada, February 8.

——, *On convergence of particle systems to SPDEs*, Ernst-Moritz-Arndt-Universität Greifswald, Institut für Mathematik und Informatik, March 5.

——, *A branching process in a random environment relating to SPDEs in higher dimensions*, Magdeburger Stochastik-Tage, German Open Conference on Probability and Statistics, March 19–22, Otto-von-Guericke-Universität Magdeburg, March 21.

——, *On limits of branching systems in a spatially correlated random media*, Workshop on Spatially Distributed and Hierarchically Structured Stochastic Systems, April 4–10, Université de Montréal, Centre de Recherches Mathématiques, Canada, April 8.

——, *The stochastic heat equation with coloured noise as limit of branching particle systems*, Johann Wolfgang Goethe-Universität Frankfurt, Fachbereich Mathematik, April 17.

——, *The genealogy of a given sample in the Moran model with mutation*, Johann Wolfgang Goethe-Universität Frankfurt, Fachbereich Mathematik, April 24.

——, *On branching particle systems in random environments — Diffusion limits and long-time behaviour*, Miniworkshop "Stochastische Prozesse in zufälligen Medien", May 19–25, Mathematisches Forschungsinstitut Oberwolfach, May 22.

——, *A coalescent in a random background*, Workshop "Stochastic Models from Statistical Physics III", October 7–11, EURANDOM, Eindhoven, The Netherlands, October 9.

——, *Branching processes and SPDE*, Universität Kaiserslautern, Fachbereich Mathematik, November 25.

——, *On SPDEs and branching processes*, DFG-Schwerpunktkolloquium „Interagierende Stochastische Systeme von hoher Komplexität", December 2–4, WIAS, December 3.

D. TIBA, *Analysis and optimization of nonsmooth mechanical structures*, Conference on Inverse Problems, Control and Shape Optimization, April 10–12, Université de Tunis El Manar, Laboratoire de Modélisation Mathématique et Numérique dans les Sciences de l'Ingénieur, Carthage, April 10.

——, *Sur l'optimisation des structures courbées*, Colloque Franco-Roumain de Mathématiques Appliquées, September 2–6, Université de Perpignan, Laboratoire de Théorie des Systèmes, France, September 2.

——, *Optimization of curved mechanical structures*, International Conference "Analysis and Optimization of Differential Systems", September 10–14, Ovidius University, Department of Mathematics and Informatics, Constanta, Romania, September 11.

——, *On the optimization of curved structures*, 3. Südosteuropa-Tagung "Wissenschaftsdialog in Südeuropa zum Thema Neue Technologien", October 18–20, Alexander von Humboldt-Stiftung, Zagreb, Croatia, October 18.

D. TURAEV, *Richness of chaos in area preserving two-dimensional maps*, University of Surrey, Department of Mathematics and Statistics, Guildford, UK, February 11.

——, *Richness of chaos in area preserving two-dimensional maps*, Workshop "Hamiltonian Dynamics", London, UK, February 15.

——, *Richness of chaos in area preserving two-dimensional maps*, University of Bristol, Department of Engineering Mathematics, UK, February 26.

——, *Richness of chaos in area preserving two-dimensional maps*, University of Groningen, Faculty of Mathematics and Natural Sciences, The Netherlands, May 27.

——, *Richness of chaos in area preserving two-dimensional maps*, EURANDOM, Eindhoven, The Netherlands, May 30.

——, *On superhomoclinic orbits in Hamiltonian systems*, Universitat de Barcelona, Departament de Matemàtica Aplicada i Anàlisi, Spain, September 25.

——, *Richness of chaos in area preserving two-dimensional maps*, Ben Gurion University of the Negev, Department of Mathematics and Computer Sciences, Beersheba, Israel, October 14.

——, *Richness of chaos in area preserving two-dimensional maps*, The Weizmann Institute of Science, Department of Mathematical Sciences, Rehovot, Israel, October 15.

B. WAGNER, *Steuerung der Rayleigh-Bénard-Konvektion*, Universität Trier, Fachbereich Mathematik, January 24.

——, *Steuerung der Rayleigh-Bénard-Konvektion*, Universität-Gesamthochschule Siegen, Fachbereich 6 — Mathematik, July 4.

——, *Steuerung der Rayleigh-Bénard-Konvektion*, Universität Basel, Fachbereich Mathematik, Switzerland, November 15.

——, *Steuerung der Rayleigh-Bénard-Konvektion*, Universität des Saarlandes, Fakultät 6 — Mathematik, Saarbrücken, November 18.

——, *Exact solutions of a sharp interface model for eutectic tin/lead alloy*, Workshop "Interfaces and Singularly Perturbed Interface Evolutions", November 29–30, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, November 30.

W. WAGNER, *Stochastic algorithms for coagulation equations*, 5th ESMTB Tri-annual Conference "Mathematical Modelling and Computing in Biology and Medicine", Minisymposium "Stochastic Processes in Biology", July 2–6, European Society of Mathematical and Theoretical Biology (ESMTB), Milano, Italy, July 3.

——, *Stochastic models of coagulation*, Conference "Perspectives in Kinetic Theory", October 24–26, Italian Research Project "Mathematical Problems in Kinetic Theory", Sestri Levante, Italy, October 24.

——, *Stochastic models and Monte Carlo algorithms for Boltzmann type equations*, Fifth International Conference on Monte Carlo and Quasi-Monte Carlo Methods in Scientific Computing (MCQMC 2002), November 25–28, Singapore, November 28.

K. WILMANSKI, *Zerstörungsfreie Prüfmethoden in der Geophysik, Teil I*, BTU Workshop "Geophysikalische Strömungen/Konvektion", Brandenburgische Technische Universität (BTU) Cottbus, Internationales Begegnungszentrum, March 18.

——, *Surface waves on flat interfaces: Poroelastic medium/fluid*, International Conference on Multifield Problems, April 8–10, Universität Stuttgart, April 8.

——, *Waves in poroelastic materials*, XXVIIth General Assembly, April 21–26, European Geophysical Society, Nice, France, April 24.

——, *Schallwellen, Oberflächenwellen, zerstörungsfreie Prüfmethoden für poröse Körper*, Colloquium Mechanics of Materials and Structures, Technische Universität Graz, Institut für Allgemeine Mechanik, Austria, June 20.

——, *Modellbildung für granulare Stoffe*, 8 talks, Universität Innsbruck, Institut für Geotechnik und Tunnelbau, Austria, June 24–28.

——, *Microworld and macroworld — Multiscaling problems in modeling of geophysics*, 3rd Euroconference "Mathematical Foundations of Geomechanics", July 1–5, Horton, Greece, July 3.

——, *Acoustic waves and nondestructive testing of granular materials*, Symposium on Trends in Applications of Mathematics in Mechanics, September 29 – October 4, Maiori, Italy, October 2.

——, *Thermodynamic modeling of porous materials*, Université Paris VI "Pierre et Marie Curie", Laboratoire de Modélisation en Méchanique, France, November 15.

——, *Acoustic and surface waves in poroelastic materials — Theory, experiments and non-destructive testing*, Final Colloquium of Sfb 298, November 18–19, Technische Universität Darmstadt, Seeheim, November 18.

——, *Micro-macro transitions for granular materials. Estimations of porosity dependence*, Workshop "Thermodynamische Materialtheorien", December 15–19, Mathematisches Forschungsinstitut Oberwolfach, December 18.

M. WOLFRUM, *Heteroclinic connections and order structures for scalar parabolic PDE*, Instituto Superior Tecnico, Lisbon, Portugal, June 11.

J. ZACHARIAS-LANGHANS, *Fourier inversion methods for Delta-Gamma Approximations*, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, January 21.

——, *Effiziente Methoden zur Bestimmung von Risikomaßen*, BMBF Workshop „Energie und Finanzwirtschaft", Bundesministerium für Bildung und Forschung, Berlin, March 4.

6.4.2 Posters

U. BANDELOW, K. GÄRTNER, *Simulation tools for semiconductor lasers*, CeBIT Asia 2002, Shanghai, China, September 2–5.

W. DREYER, *Mathematische Modellierung und Simulation der Entstehung, des Wachstums und der Auflösung von Arsenausscheidungen in einkristallinem Galliumarsenid*, Statusseminar zum BMBF-Förderprogramm "Neue mathematische Verfahren in Industrie und Dienstleistungen", Ludwigshafen, December 16–17.

W. DREYER, M. HERRMANN, M. KUNIK, *Kinetic solutions of the Boltzmann-Peierls equation and its moment systems*, Colloquium of the DFG Priority Program "Analysis and Numerics of Conservation Laws" (ANumE), Freiburg, February 4–6.

W. DREYER, M. HERRMANN, A. MÖLLER, J. SPREKELS, *Micro-macro transitions of the atomic chain for various scalings*, Third Colloquium of the DFG Priority Program "Analysis, Modeling and Simulation of Multiscale Problems", Bad Honnef, June 10–12.

J. ELSCHNER, A. RATHSFELD, G. SCHMIDT, *FEM simulation and optimization for polygonal profile gratings*, Statusseminar zum BMBF-Förderprogramm "Neue mathematische Verfahren in Industrie und Dienstleistungen", Ludwigshafen, December 16–17.

J. FUHRMANN, *Simulation and mathematics of Direct Methanol Fuel Cells*, Presentation of the Leibniz Association (WGL) to the European Union, Brussels, Belgium, October 1.

J. FUHRMANN, TH. KOPRUCKI, H.-CHR. KAISER, G. SCHMIDT, *Multiscale modeling of electronic states in semiconductor nanostructures*, Third Colloquium of the DFG Priority Program "Analysis, Modeling and Simulation of Multiscale Problems", Bad Honnef, June 10–12.

K. GÄRTNER, *Electrochemistry and transport in porous media: Direct Methanol Fuel Cells (DMFC)*, Workshop "Brennstoffzellen generieren Zukunftsprodukte — Mikrosystemtechnik als Schlüsseltechnologie", Grand Hyatt Berlin, February 27.

G. HEBERMEHL, F.-K. HÜBNER, R. SCHLUNDT, TH. TISCHLER, H. ZSCHEILE, W. HEINRICH, *Numerical techniques in the simulation of microwave and laser structures including PML*, 10th International IGTE Symposium on Numerical Field Calculation in Electrical Engineering, Technische Universität Graz, Austria, September 16–18.

O. KLEIN, P. PHILIP, *Induction heating during SiC growth by PVT: Aspects of axisymmetric sinusoidal modeling*, International IGTE Symposium on Numerical Field Calculation in Electrical Engineering, Technische Universität Graz, Austria, September 16–18.

O. KLEIN, P. PHILIP, J. SCHEFTER, J. SPREKELS, *Numerical simulation and control of sublimation growth of SiC bulk single crystals*, Statusseminar zum BMBF-Förderprogramm "Neue mathematische Verfahren in Industrie und Dienstleistungen", Ludwigshafen, December 16–17.

H.-J. MUCHA, *Core based clustering*, Compstat 2002, Berlin, August 2.

R. NÜRNBERG, *Optoelektronische Sensoren*, Statusseminar zum BMBF-Förderprogramm "Neue mathematische Verfahren in Industrie und Dienstleistungen", Ludwigshafen, December 16–17.

O. REISS, J. ZACHARIAS-LANGHANS, *Effiziente Methoden zur Bestimmung von Risikomaßen*, Statusseminar zum BMBF-Förderprogramm "Neue mathematische Verfahren in Industrie und Dienstleistungen", Ludwigshafen, December 16–17.

6.4.3 Contributions to Exhibitions

U. BANDELOW, K. GÄRTNER, *Simulation tools for semiconductor lasers*, CeBIT Asia 2002, Shanghai, China, September 2–5.

6.5 Visits to other Institutions[6]

B. ALBERS, Technische Universität Graz, Institut für Allgemeine Mechanik, Austria, June 19–23.

E. BÄNSCH, University of Maryland, Department of Mathematics, College Park, USA, January 12–20.

——, Université de la Réunion, Faculté des Sciences et Technologies, Saint-Denis, France, April 2–29.

——, Czech Technical University in Prague, Department of Mathematics, June 25–28.

——, University of Maryland, Department of Mathematics, College Park, USA, August 19–30.

——, University of Lisbon, Center of Mathematics and Fundamental Applications (CMAF), Portugal, December 5–8.

M. BARO, Université Paul Sabatier, Laboratoire de Mathématique pour l'Industrie et la Physique, Toulouse, France, October 14–20.

A. BOVIER, Charles University Prague, Faculty of Mathematics and Physics, Czech Republic, January 25–30.

——, EURANDOM, Eindhoven, The Netherlands, February 23–26.

——, Charles University Prague, Faculty of Mathematics and Physics, Czech Republic, February 27 – March 3.

——, Université Paris VI "Pierre et Marie Curie", Laboratoire de Probabilités et Modèles Aléatoires, France, May 1–31.

——, Università degli Studi di Roma "La Sapienza", Dipartimento di Matematica, Italy, September 20–27.

——, Erwin Schrödinger International Institute for Mathematical Physics (ESI), Vienna, Austria, December 22, 2002 – January 25, 2003.

G. BRUCKNER, Fudan University, Department of Mathematics, Shanghai, China, November 5–9.

——, University of Tokyo, Department of Mathematical Sciences, Japan, November 9–15, in the framework of the DFG project "Scientific cooperation with Japan: Inverse problems in electromagnetics and optics".

J. ELSCHNER, University of Tokyo, Department of Mathematical Sciences, Japan, November 18–26, in the framework of the DFG project "Scientific cooperation with Japan: Inverse problems in electromagnetics and optics".

K. FLEISCHMANN, University of Oxford, Mathematical Institute, UK, February 18 – March 10.

[6]Only stays of more than three days are listed.

——, University of Bath, Department of Mathematical Sciences, UK, March 10–15.

——, Carleton University, School of Mathematics and Statistics, Ottawa, Canada, April 11–30.

——, Carleton University, School of Mathematics and Statistics, Ottawa, Canada, November 11–29.

K. GÄRTNER, Universität Basel, Institut für Informatik, Switzerland, January 28 – February 1.

——, Swiss Federal Institute of Technology Zurich, Integrated Systems Laboratory, Switzerland, February 2–5.

B. GENTZ, Eidgenössische Technische Hochschule Zürich, Forschungsinstitut für Mathematik, Switzerland, January 1–18.

——, CNRS-Centre de Physique Théorique, Marseille, and Université de Toulon et du Var, Physique Mathématique, PHYMAT, France, November 4–16.

R. HENRION, Universität Halle-Wittenberg, Institut für Optimierung und Stochastik, visiting professorship (C4), winter semester 2001/2002.

——, Université de Bourgogne, Département de Mathématiques, Dijon, France, April 12–27.

D. HÖMBERG, Université de Nancy I, Laboratoire de Mathématiques, Vandœuvre-les-Nancy, France, December 9–13.

S. JASCHKE, Italian National Research Council, Institute for System Science and Biomedical Engineering, Padova, Italy, February 3–8.

C. KÜLSKE, Catholic University Leuven, Institute for Theoretical Physics, The Netherlands, June 3–9.

I. MATHEIS, Universität des Saarlandes, Fachrichtung Mathematik, Saarbrücken, March 20–23.

G.N. MILSTEIN, Leicester University, Department of Mathematics and Computer Science, UK, September 9 – October 2.

H. NEIDHARDT, Kanazawa University, Faculty of Science, Japan, January 26 – February 9.

——, Université Paul Sabatier, Laboratoire de Mathématique pour l'Industrie et la Physique, Toulouse, France, October 14–19.

——, CNRS-Centre de Physique Théorique, Marseille, France, October 19–25.

J. POLZEHL, University of Tromsø, Department of Mathematics, Norway, April 8–21.

——, Uppsala University, Department of Mathematics, Sweden, May 20–27.

S. RŒLLY, Université Lille 1, Laboratoire de Statistique et Probabilités, France, February 2–8.

——, Université Lille 1, Laboratoire de Statistique et Probabilités, France, July 8–19.

K.K. SABELFELD, St. Petersburg University, Department of Statistical Simulation, Russia, January 23 – February 3.

——, Bonndata GmbH, Bonn, March 1–7.

——, Russian Academy of Sciences, Siberian Department, Novosibirsk, Russia, June 2 – August 5.

——, Florida State University, Tallahassee, USA, September 2–30.

——, Keldysh Institute of Applied Mathematics, Moscow, Russia, October 1–12.

G. SCHMIDT, University of Tokyo, Department of Mathematical Sciences, Japan, November 18–26, in the framework of the DFG project "Scientific cooperation with Japan: Inverse problems in electromagnetics and optics".

K.R. SCHNEIDER, Moscow State University, Department of Physics, Russia, October 6–10.

J. SCHOENMAKERS, Delft University of Technology, Information Technology and Systems, The Netherlands, October 3–6.

E. SHCHETININA, Samara State University, Department of Mathematics, Russia, May 3 – July 29.

J. SIEBER, University of Bristol, Department of Engineering Mathematics, UK, April 25 – May 5.

——, University of Bristol, Department of Engineering Mathematics, UK, June 28 – July 3.

V. SPOKOINY, Université Paris VI "Pierre et Marie Curie", Laboratoire de Probabilité, France, March 7–12.

——, Université de Bretagne-Sud, Laboratoire SABRES, Vannes, France, June 4–29.

J. SPREKELS, Academy of Sciences of the Czech Republic, Institute of Mathematics, Prague, February 18–22.

——, Università degli Studi di Firenze, Dipartimento di Matematica "U. Dini", Italy, October 12–18.

A. STURM, Université de Montréal, Centre de Recherches Mathématiques, Canada, January 29 – February 22.

——, Johann Wolfgang Goethe-Universität Frankfurt, Fachbereich Mathematik, April 12 – May 3.

D. TIBA, University of Jyväskylä, Department of Mathematical Information Technology, Finland, November 11–22.

D. TURAEV, Universitat de Barcelona, Departament de Matemàtica Aplicada i Anàlisi, Spain, September 22–28.

——, The Weizmann Institute of Science, Department of Mathematical Sciences, Rehovot, Israel, October 7–18.

W. WAGNER, Universität des Saarlandes, Fachrichtung Mathematik, Saarbrücken, April 3–7.

——, Universität des Saarlandes, Fachrichtung Mathematik, Saarbrücken, October 16–20.

K. WILMANSKI, Technische Universität Graz, Institut für Allgemeine Mechanik, Austria, June 19–23.

——, Universität Innsbruck, Institut für Geotechnik und Tunnelbau, Austria, June 24–28.

——, Université Paris VI “Pierre et Marie Curie”, Laboratoire de Modélisation en Méchanique, France, November 12–17.

M. WOLFRUM, Technical University Lisbon, Department of Mathematics, Portugal, June 3–13.

6.6 Academic Teaching[1]

E. BÄNSCH, *Numerik für die Navier-Stokes-Gleichungen mit Nicht-Standard-Randbedingungen* (lecture), Freie Universität Berlin, 2 SWS, summer semester 2002.

——, *Numerik für die Navier-Stokes-Gleichungen mit Nicht-Standard-Randbedingungen* (exercises), Freie Universität Berlin, 2 SWS, summer semester 2002.

——, *Numerik II* (lecture), Freie Universität Berlin, 4 SWS, winter semester 2002/2003.

——, *Numerik II* (exercises), Freie Universität Berlin, 2 SWS, winter semester 2002/2003.

E. BÄNSCH, R. KLEIN, *Mehrskalenprobleme der Strömungsmechanik* (seminar), Freie Universität Berlin, 2 SWS, winter semester 2001/2002.

E. BÄNSCH, R. KORNHUBER, *Softwarepraktikum zur Simulation hydrologischer Prozesse* (seminar), Freie Universität Berlin, 2 SWS, winter semester 2001/2002.

——, *Strömungs- und Transportprozesse im Boden* (seminar), Freie Universität Berlin, 2 SWS, winter semester 2001/2002.

——, *Numerik von Phasenübergängen* (seminar), Freie Universität Berlin, 2 SWS, summer semester 2002.

E. BÄNSCH, R. KORNHUBER, H.G. DIERSCH, *Simulation hydrologischer Prozesse* (practical training), Freie Universität Berlin, 2 SWS, winter semester 2001/2002.

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 2001/2002.

——, *Numerische Mathematik/Scientific Computing* (senior seminar), Freie Universität Berlin, 2 SWS, summer semester 2002.

——, *Numerische Mathematik/Scientific Computing* (senior seminar), Freie Universität Berlin, 2 SWS, winter semester 2002/2003.

A. BOVIER, *Extrema stochastischer Folgen und Prozesse* (lecture), Technische Universität Berlin, 2 SWS, winter semester 2001/2002.

A. BOVIER, B. GENTZ, H. FÖLLMER, P. IMKELLER, U. KÜCHLER, J.-D. DEUSCHEL, J. GÄRTNER, M. SCHEUTZOW, *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), WIAS, 2 SWS, winter semester 2001/2002.

——, *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), Humboldt-Universität zu Berlin, 2 SWS, summer semester 2002.

——, *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), Technische Universität Berlin, 2 SWS, winter semester 2002/2003.

[1] SWS = semester periods per week

W. DREYER, *Analytische Verfahren der Kontinuumsmechanik und Materialtheorie* (lecture), Technische Universität Berlin, 4 SWS, winter semester 2001/2002.

——, *Analytische Verfahren der Kontinuumsmechanik und Materialtheorie* (exercises), Technische Universität Berlin, 2 SWS, winter semester 2001/2002.

——, *Analytische Methoden der Kontinuumsmechanik und Materialtheorie* (lecture), Technische Universität Berlin, 4 SWS, summer semester 2002.

——, *Analytische Methoden der Kontinuumsmechanik und Materialtheorie* (exercises), Technische Universität Berlin, 2 SWS, summer semester 2002.

——, *Analytische Methoden der Kontinuumsmechanik und Materialtheorie* (lecture), Technische Universität Berlin, 4 SWS, winter semester 2002/2003.

——, *Analytische Methoden der Kontinuumsmechanik und Materialtheorie* (exercises), Technische Universität Berlin, 2 SWS, winter semester 2002/2003.

H. GAJEWSKI, *Analysis und Numerik von Drift-Diffusionsgleichungen* (lecture), Freie Universität Berlin, 2 SWS, winter semester 2002/2003.

B. GENTZ, *Lineare Algebra für Ingenieure* (lecture), Technische Universität Berlin, 2 SWS, winter semester 2001/2002.

——, *Singulär gestörte stochastische Differentialgleichungen* (lecture), Technische Universität Berlin, 2 SWS, summer semester 2002.

A. GLITZKY, *Aspekte bei der Modellierung und mathematischen Behandlung von Reaktions-Diffusionsproblemen* (lecture), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2002/2003.

J.A. GRIEPENTROG, *Lebesgue- und Sobolev-Räume* (lecture), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2001/2002.

——, *Geometrische Maßtheorie* (lecture), Humboldt-Universität zu Berlin, 2 SWS, summer semester 2002.

——, *Nichtglatte elliptische Randwertprobleme* (lecture), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2002/2003.

R. HENRION, W. RÖMISCH, M. STEINBACH, *Numerik stochastischer Modelle* (seminar), Humboldt-Universität zu Berlin, 2 SWS, summer semester 2002.

——, *Numerik stochastischer Modelle* (seminar), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2002/2003.

S. JASCHKE, *Risikomanagement für Banken* (lecture), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2001/2002.

O. KLEIN, *Mathematische Modellierung von Phasenübergängen* (lecture), Humboldt-Universität zu Berlin, 2 SWS, summer semester 2002.

——, *Nichtlineare partielle Differentialgleichungen* (lecture), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2002/2003.

C. KÜLSKE, *Stochastik von Mean-Field-Modellen* (lecture), Technische Universität Berlin, 2 SWS, winter semester 2002/2003.

J. POLZEHL, *Computerintensive Statistik* (lecture), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2002/2003.

K.R. SCHNEIDER, B. FIEDLER, *Nichtlineare Dynamik* (senior seminar), WIAS, Freie Universität Berlin, 2 SWS, winter semester 2001/2002.

——, *Nichtlineare Dynamik* (senior seminar), WIAS, Freie Universität Berlin, 2 SWS, summer semester 2002.

——, *Nichtlineare Dynamik* (senior seminar), WIAS, Freie Universität Berlin, 2 SWS, winter semester 2002/2003.

K.R. SCHNEIDER, L. RECKE, H.J. WÜNSCHE, *Mathematische Modelle der Photonik* (seminar), WIAS, Humboldt-Universität zu Berlin, 2 SWS, winter semester 2001/2002.

——, *Mathematische Modelle der Photonik* (seminar), WIAS, Humboldt-Universität zu Berlin, 2 SWS, summer semester 2002.

——, *Mathematische Modelle der Photonik* (seminar), WIAS, Humboldt-Universität zu Berlin, 2 SWS, winter semester 2002/2003.

V. SPOKOINY, *Nichtparametrische Verfahren und ihre Anwendungen* (lecture), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2002/2003.

V. SPOKOINY, O. BUNKE, W. HÄRDLE, *Mathematische Statistik* (research seminar), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2001/2002.

——, *Mathematische Statistik* (research seminar), Humboldt-Universität zu Berlin, 2 SWS, summer semester 2002.

——, *Mathematische Statistik* (research seminar), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2002/2003.

J. SPREKELS, *Funktionalanalysis* (lecture), Humboldt-Universität zu Berlin, 4 SWS, winter semester 2001/2002.

——, *Lineare partielle Differentialgleichungen* (lecture), Humboldt-Universität zu Berlin, 4 SWS, summer semester 2002.

H. STEPHAN, *Anfänge der Zahlentheorie* (lecture), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2001/2002.

——, *Anfänge der Analysis und euklidische Geometrie* (lecture), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2002/2003.

G. TELSCHOW, *Einführung in die Datenverarbeitung III* (lecture), Technische Fachhochschule Berlin, 4 SWS, winter semester 2001/2002.

——, *Einführung in die Datenverarbeitung III* (exercises), Technische Fachhochschule Berlin, 4 SWS, winter semester 2001/2002.

——, *Elektronische Datenverarbeitung II* (lecture), Technische Fachhochschule Berlin, 2 SWS, summer semester 2002.

——, *Elektronische Datenverarbeitung II* (exercises), Technische Fachhochschule Berlin, 4 SWS, summer semester 2002.

——, *Einführung in die Datenverarbeitung I* (lecture), Technische Fachhochschule Berlin, 6 SWS, winter semester 2002/2003.

W. WAGNER, *Grundlagen der Monte-Carlo-Methode* (lecture), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2001/2002.

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 2001/2002.

——, *Nichtlineare Elastizitätstheorie* (lecture), Technische Universität Berlin, 2 SWS, summer semester 2002.

——, *Dynamik von mehrkomponentigen Körpern* (lecture), Technische Universität Berlin, 2 SWS, winter semester 2002/2003.

K. WILMANSKI, I. MÜLLER, *Thermodynamisches Seminar* (seminar), WIAS/Technische Universität Berlin, 2 SWS, summer semester 2002.

——, *Thermodynamisches Seminar* (seminar), WIAS/Technische Universität Berlin, 2 SWS, winter semester 2002/2003.

6.7 Calls, Awards and Distinctions, Habilitations, Ph.D. Theses, and Undergraduate-degree Supervision

Calls

A. BOVIER, full professorship, Rijksuniversiteit Groningen, The Netherlands, Chair in Probability and Statistics, September 20 (refused).

S. ROELLY, C3 professorship, Universität Potsdam, December 2.

A. STURM, Junior professorship, Technische Universität Berlin, December 1.

Awards and Distinctions

J. POLZEHL, *Chairman Technical Working Area 18, Versailles Project on Advanced Materials and Standards (VAMAS).*

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

D. HÖMBERG, *Induction heat treatments — Modeling, analysis and optimal design of inductor coils*, Technische Universität Berlin, June 5.

Ph.D. Theses

D. DEREUDRE, *Diffusions infini-dimensionnelles et champs de Gibbs sur l'espace des trajectoires continues* $C([0,1];\mathbb{R}^d)$, Ecole Polytechnique, Paris, France, supervisor: Dr. S. Rœlly, December 11.

P.-Y. LOUIS, *Automates cellulaires probabilistes: Mesures stationnaires, mesures de Gibbs associées et ergodicité*, Université Lille 1, France, supervisor: Dr. S. Rœlly, September 23.

A. EIBECK, *Stochastische Teilchensysteme zur Approximation der Koagulationsgleichung*, Humboldt-Universität zu Berlin, supervisor: Dr. W. Wagner, May 24.

A. STURM, *On spatially structured population processes and relations to stochastic partial differential equations*, University of Oxford, UK, supervisor: Dr. A.M. Etheridge, May 27.

Undergraduate-degree Supervision

A. BECKER, *Entwicklung eines Kompressionsalgorithmus für beliebige Daten*, Technische Fachhochschule Berlin, supervisor: Dr. G. Telschow, September 18.

6.8 WIAS Conferences, Colloquiums, and Workshops

KOLLOQUIUM DES SCHWERPUNKTPROGRAMMS „INTERAGIERENDE STOCHASTISCHE SYSTEME VON HOHER KOMPLEXITÄT“ (Colloquium of the DFG Priority Program “Interacting stochastic systems of high complexity”)
Berlin, January 7–9
Organized by: WIAS (FG 5), DFG Priority Program, Technische Universität Berlin and Universität Erlangen
Sponsored by: DFG

At the beginning of the year, the annual colloquium of the DFG Priority Program “Interacting stochastic systems of high complexity” took place at WIAS with the aim to present, in 12 talks, selected results of the participating groups. The agenda was completed by three talks by foreign guests (E. Bolthausen, M. Keane and C. Maes). As in the past years, the colloquium was a success and contributed largely to the networking of the scientists collaborating on different subsections of stochastics in the program. High-quality talks of younger collaborators proved the program’s worth in the field of the promotion of young scientists.

WORKSHOP ON MULTISCALE PROBLEMS IN QUANTUM AND CLASSICAL MECHANICS, AVERAGING TECHNIQUES AND YOUNG MEASURES
Berlin, September 19–21
Organized by: WIAS (FG 1, FG 3, FG 7)
Sponsored by: WIAS, DFG

The workshop “Multiscale Problems in Quantum and Classical Mechanics, Averaging Techniques and Young Measures” has been organized by H.-Chr. Kaiser (FG 1) and Th. Koprucki (FG 3) in cooperation with W. Dreyer (FG 7) and A. Mielke (Stuttgart). It is the second event in a series of new workshops within the DFG Priority Program “Analysis, Modeling and Multiscale Problems”, initiated by the meeting “Multiscale Problems in Quantum Mechanics and Averaging Techniques” held in Konstanz on October 25–26, 2001 (organizers: A. Jüngel (Konstanz) and A. Arnold (Saarbrücken)).
The general aim of this workshop was to foster joint activities within the priority program. The topics were many-particle systems, electronic structure calculation, quantum-classical coupling, semiconductor device simulation, semiconductor nanostructures, quantum hydrodynamics, time averages and Young measures, adiabatic and scaling limits, surface nanostructures, multiscale problems of the atomic chain, evolution of Young measures, wavelets, homogenization and two-scale finite elements. The schedule was coordinated with that of another workshop within the priority program: “Efficient Algorithms for Multiscale Dynamics” which took place on September 23–25, 2002, at the Freie Universität Berlin (organizers: M. Dellnitz (Paderborn), W. Huisinga (Berlin), Ch. Lubich (Tübingen), Ch. Schütte (Berlin)). Five participants attended both workshops.

CONFERENCE ON CHALLENGES IN SCIENTIFIC COMPUTING 2002 (CISC 2002)
Berlin, October 2–5
Organized by: WIAS (FG 3)
Sponsored by: COMPAQ, DFG, WIAS

The main focus of this conference was on the problem class of nonlinear transport/diffusion/ reaction systems, chief amongst these being: the Navier-Stokes equations, porous media-flow problems.
The purpose of the conference was to draw together researchers working in the fields of scientific computing, numerical analysis and modeling with a common interest in the numerical treatment and the computational solution of systems of nonlinear partial differential equations arising from applications of physical problems in science and engineering.
Themes included: finite element methods, treatment of incompressible flow problems, numerical simulations of free surface flows, geometric and algebraic multigrid methods, transport processes in porous media, image processing.
Of particular interest were those contributions which emphasize unsolved problems, challenging open questions from applications and assessing the various numerical methods used to handle them, instead of concentrating on accurate results from "solved" problems.
There were 54 participants including 31 invited speakers.
Some of the contributions will be published in "Lecture Notes in Computational Sciences and Engineering".
Further details can be found at http://www.wias-berlin.de/∼CISC2002.

WORKSHOP "DYNAMICS AND CONTROL"
Berlin, November 18–19
Organized by: WIAS (FG 2), GAMM, SFB 555
Sponsored by: WIAS, DFG (SFB 555)

The workshop has been organized by GAMM (Gesellschaft für Angewandte Mathematik und Mechanik (society for applied mathematics and mechanics)) and SFB 555 (DFG Collaborative Research Center "Complex non-linear processes"). It met with a good response (54 participants from 5 countries). It focused on modern approaches for controling complex processes (pattern formation, synchronization) and its application (process engineering, robotics, vehicle dynamics).

WORKSHOP "COMPOSITE FORSCHUNG IN DER MECHANIK" (Composite research in mechanics)
Berlin, November 18–20
Organized by: WIAS (FG 7), Technische Universität (TU) Berlin
Sponsored by: WIAS, TU Berlin

The category of composite materials consists of classical composites, like fibre-reinforced substances, patched metallic contacts, silicon carbide laminates as well as nonclassical composites like multiphase bodies. Both composite classes have been discussed in this workshop, with the special focus on problems resulting from industrial purposes.
The talks stressed in particular problems within the areas of elasto-plasto mechanics, mechanisms for failure and lifetime calculations, energy release rates related to the evolution of cracks and phase transitions within the framework of phase-field models.

MINISYMPOSIUM "DFB LASER WITH AMPLIFYING FEEDBACK"
Berlin, November 28
Organized by: WIAS (FG 2), SFB 555
Sponsored by: WIAS, Humboldt University of Berlin

The minisymposium has been organized by SFB 555 (DFG Collaborative Research Center "Complex non-linear processes"). It attracted more than 20 people from different research institutes in Berlin. It focused on high frequency self-pulsations of multi-section semiconductor lasers: modeling, simulation, experiments. The talks initiated an intensive scientific discussion.

6.9 Visiting Scientists[2]

6.9.1 Guests

E. AVRUTIN, University of York, Department of Electronics, Heslington, UK, October 22–25.

N. BERGLUND, CNRS-Centre de Physique Théorique, Marseille, and Université de Toulon et du Var, Physique Mathématique, PHYMAT, France, June 24–28.

N. BERGLUND, Université de Marseille, CNRS-Centre de Physique Théorique, and Université de Toulon et du Var, Physique Mathématique, PHYMAT, France, July 15 – August 16.

——, October 28 – November 1.

G. BONNET, University of North Carolina at Chapel Hill, Department of Mathematics, USA, June 4–7.

M. BROKATE, Technische Universität München, Zentrum Mathematik, June 14–29.

——, July 7–13.

V.F. BUTUZOV, Moscow State University, Faculty of Physics, Russia, April 1–30.

P. COLLI, Università di Pavia, Dipartimento di Matematica, Italy, November 25 – December 7.

D. DEREUDRE, Université Lille 1, Laboratoire de Statistique et Probabilité, France, May 13–17.

M.A. EFENDIEV, Universität Stuttgart, Mathematisches Institut A, March 11 – April 5.

——, July 16–30.

——, December 16–20.

M. ERMAKOV, Russian Academy of Sciences, Mechanical Engineering Problem Institute, St. Petersburg, November 1 – December 1.

T. FÜLLENBACH, Fraunhofer-Institut für Algorithmen und Wissenschaftliches Rechnen, Sankt Augustin, October 2–5.

V. GAYRARD, Ecole Polytechnique Fédérale de Lausanne, Département de Mathématiques, Switzerland, July 26 – August 26.

——, November 2–16.

O. GILSON, Université de Liège, Département de Mathématiques, Belgium, April 17 – May 1.

——, November 6–15.

A. GOLDENSHLUGER, University of Haifa, Department of Statistics, Israel, September 4 – October 4.

L. GOLDENTAYER, Tel Aviv University, Department of System Engineering, Israel, September 17–26.

[2]Only stays of more than three days are listed.

Y. GOLUBEV, Université de Provence, Centre de Mathématiques et Informatique, Marseille, France, May 20–26.

A. GOMBANI, National Research Council, Institute for Dynamical Systems and Bioengineering, Padua, Italy, July 7–14.

S. GONCHENKO, Institute for Applied Mathematics and Cybernetics, Nizhny Novgorod, Russia, March 11 – June 10.

——, October 23 – November 25.

V. GONCHENKO, Nizhny Novgorod State University, Department of Differential Equations, Russia, October 23 – November 25.

I. GRAMA, Université de Bretagne-Sud, Laboratoire SABRES, Vannes, France, July 1–31.

L. GRAZIANO, Università degli Studi di Torino, Dipartimento di Matematica, Italy, March 6 – May 15.

M. HAGEMANN, Universität Basel, Institut für Informatik, Switzerland, August 5–30.

O. HANSEN, Universität Mainz, Fachbereich Mathematik, April 21–26.

H. HARBRECHT, Technische Universität Chemnitz, Fakultät für Mathematik, November 11–15.

M. HRISTACHE, Université de Rennes, Unité de Formation et de Recherches de Mathématique, France, April 1–14.

O. HRYNIV, University of Cambridge, Statistical Laboratory, Centre for Mathematical Sciences, UK, December 15–21.

G.C. HSIAO, University of Delaware, Department of Mathematical Sciences, Newark, USA, June 4 – July 1.

Y. INGSTER, St. Petersburg State Transport University, Department of Applied Mathematics, Russia, July 1 – August 30.

A. JUDITSKY, Institut National de Recherche en Informatique et en Automatique, Grenoble, France, May 22 – June 4.

L. KALACHEV, University of Montana, Department of Mathematical Sciences, Missoula, USA, October 7 – November 7.

V. KARLIN, University of Lancashire, Centre for Research in Fire and Explosion Studies, Preston, UK, September 8 – October 5.

D. KESSLER, University of Maryland, Department of Mathematics, College Park, USA, June 13–18.

A. KOLODKO, Russian Academy of Sciences, Institute for Applied Mathematics and Mathematical Geophysics, Novosibirsk, September 11 – December 10.

I. KOURKOVA, Université Paris VI “Pierre et Marie Curie”, Laboratoire de Probabilités et Modèles Aléatoires, France, November 22 – December 6.

A. KOVAC, Universität-Gesamthochschule Essen, Mathematisches Institut, January 21–24.

T. KOZOUBSKAIA, Keldysh Institute of Applied Mathematics, Moscow, Russia, December 17–22.

M. KRAFT, University of Cambridge, Department of Chemical Engineering, UK, August 10 – September 8.

R. KRAHL, Universität Bremen, Fachbereich Mathematik und Informatik, October 1–5.

P. KREJČÍ, Academy of Sciences of the Czech Republic, Institute of Mathematics, Prague, November 25 – December 7.

H.-R. KÜNSCH, Eidgenössische Technische Hochschule Zürich, Seminar für Statistik, Switzerland, November 9–13.

O. KURBANMURADOV, Turkmen State University, Physics and Mathematics Research Center, Ashkhabad, March 2 – April 29.

——, November 14 – December 14.

C. LAI, Studio Geotecnico Italiano, Milano, May 6 – June 6.

A. LE NY, EURANDOM, Eindhoven, The Netherlands, July 13–19.

G.A. LEONOV, St. Petersburg University, Department of Mathematics and Mechanics, Russia, November 17–24.

Y. LI, Florida State University, Tallahassee, USA, May 21–24.

R. LIPTSER, Tel Aviv University, Department of Electrical Engineering, Israel, February 9 – March 9.

P.-Y. LOUIS, Université Lille 1, Laboratoire de Statistique et Probabilités, France, April 8–13.

——, September 3–6.

——, September 25 – October 1.

S. MÉLÉARD, Université Paris X, UFR Segmi, Equipe Modal X, Nanterre, France, January 22–27.

J.M. MELENK, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, October 2–5.

I. MEROLA, Università degli Studi di Roma “Tor Vergata”, Dipartimento di Matematica, Italy, April 7–20.

K. MIKULA, Slovak Technical University, Department of Mathematics, Bratislava, Slovakia, October 1–5.

P. MÖRTERS, University of Bath, Department of Mathematical Sciences, UK, July 15 – August 15.

A. MÜNCH, Technische Universität München, Zentrum Mathematik, August 5–30.

O. MUSCATO, Università di Catania, Dipartimento di Matematica e Informatica, Italy, April 8–14.

L. MYTNIK, Technion Israel Institute of Technology, Faculty of Industrial Engineering and Management, Haifa, September 22 – October 5.

N.N. NEFEDOV, Moscow State University, Faculty of Physics, Russia, April 1–30.

——, November 3–30.

N. NEUSS, Ruprecht-Karls-Universität Heidelberg, Institut für Angewandte Mathematik, October 1–5.

A. OSTERMANN, Universität Innsbruck, Institut für Technische Mathematik, Austria, April 18–21.

J. OUTRATA, Academy of Sciences of the Czech Republic, Institute of Information Theory and Automation, Prague, October 20 – November 22.

S.V. PEREVERZEV, National Academy of Sciences of Ukraine, Institute of Mathematics, Kiev, April 1–30.

——, July 8 – October 7.

M. PICASSO, Ecole Polytechnique Fédérale de Lausanne, Département de Mathématiques, Switzerland, October 2–5.

S. PRIGARIN, Russian Academy of Sciences, Institute for Applied Mathematics and Mathematical Geophysics, Novosibirsk, February 28 – March 2.

K. PROMISLOW, Simon Fraser University, Department of Mathematics and Statistics, Burnaby, Canada, October 1–6.

F. REDIG, Eindhoven University of Technology, Department of Mathematics and Computer Sciences, The Netherlands, January 27 – February 2.

——, July 15–19.

A. REUSKEN, Rheinisch-Westfälische Technische Hochschule Aachen, Lehrstuhl für Numerische Mathematik, October 2–5.

S. RJASANOW, Universität des Saarlandes, Fachrichtung Mathematik, June 19–22.

H.-G. ROSS, Technische Universität Dresden, Institut für Numerische Mathematik, October 2–5.

M.B. RUBIN, Technion Israel Institute of Technology, Faculty of Mechanical Engineering, Haifa, May 2–5.

S. SARDY, Ecole Polytechnique Fédérale de Lausanne, Département de Mathématiques, Switzerland, November 25 – December 3.

A. SCHMIDT, Universität Bremen, Zentrum für Technomathematik, October 2–5.

R. SCHNEIDER, Technische Universität Chemnitz, Fakultät für Mathematik, September 3–29.

M. SEAÏD, Technische Universität Darmstadt, Fachbereich Mathematik, October 2–5.

I. SHALIMOVA, Russian Academy of Sciences, Institute for Applied Mathematics and Mathematical Geophysics, Novosibirsk, May 17 – June 17.

E. SHCHEPAKINA, Samara State University, Department of Differential Equations and Control Theory, Russia, October 14 – November 12.

M. SHEARER, North Carolina State University, Department of Mathematics, Raleigh, USA, October 9–12.

E. SHKARUPA, Russian Academy of Sciences, Institute for Applied Mathematics and Mathematical Geophysics, Novosibirsk, October 26 – November 26.

H. SI, Hangzhou, Zheijiang, China, March 17–24.

——, September 26–30.

D. SILVESTER, University of Manchester, Institute of Science and Technology, UK, October 1–5.

I.V. SKRYPNIK, National Academy of Sciences of Ukraine, Institute of Applied Mathematics and Mechanics, Donetsk, July 1–31.

O. SMIDTS, Université Libre de Bruxelles, Service de Métrologie Nucléaire, Belgium, May 2–8.

V. SOBOLEV, Samara State University, Department of Differential Equations and Control Theory, Russia, October 14 – November 12.

S. SPERLICH, Universidad Carlos III de Madrid, Department of Mathematics, Spain, December 20, 2001 – January 8, 2002.

O. STENKIN, Imperial College London, UK, May 5–12.

J. SWART, Universität Erlangen-Nürnberg, Mathematisches Institut, May 5–17.

T. SZÁNTAI, Technical University of Budapest, Department of Differential Equations, Hungary, October 14 – November 2.

M. THIEULLEN, Université Paris VI “Pierre et Marie Curie”, Laboratoire de Probabilités et Modèles Aléatoires, France, April 13–27.

——, June 16–30.

M. TRETIAKOV, University of Wales, Department of Mathematics, Swansea, UK, January 2–22.

——, April 1–10.

——, December 10–21.

S. UBAL, Universidad Nacional del Litoral, INTEC, Santa Fe, Argentina, November 11–17.

Z. UZELAC, University of Novi Sad, Faculty of Technical Sciences, Yugoslavia, October 2–5.

P. VASSILEVSKI, Lawrence Livermore National Laboratory, Center for Applied Scientific Computing, USA, October 2–5.

O. VASSILIEVA, Moscow State University, Faculty of Mechanics and Mathematics, Russia, May 1 – June 30.

A. VLADIMIROV, St. Petersburg University, Faculty of Physics, Russia, December 1–31.

P. VOGT, University of Bath, Department of Mathematical Sciences, UK, December 14–21.

ST. VOLKWEIN, Karl-Franzens Universität Graz, Institut für Mathematik, Austria, February 18 – March 3.

R. VON SACHS, Université Catholique de Louvain, Louvain-la-Neuve, Belgium, January 7–10.

——, March 18–23.

M. WABRO, Johannes Kepler Universität Linz, Institut für rechenbetonte Mathematik, Austria, October 1–5.

N. WALKINGTON, Carnegie Mellon University, Mathematical Sciences Department, Pittsburgh, USA, October 1–6.

D. WAN, Universität Dortmund, Institut für Angewandte Mathematik, October 2–5.

A. WATHEN, Oxford University Computing Laboratory, Department of Numerical Analysis, UK, October 2–5.

Y. XIA, University of Cambridge, Department of Zoology, USA, April 14–19.

J. XIONG, University of Tennessee, Department of Mathematics, Knoxville, USA, May 21 – July 2.

J. XU, Pennsylvania State University, Department of Mathematics, USA, October 1–6.

M. YAMAMOTO, University of Tokyo, Department of Mathematical Sciences, Japan, May 10–16.

——, September 12 – October 7.

S. YANCHUK, National Academy of Sciences of Ukraine, Institute of Mathematics, Kiev, February 4 – April 30.

——, August 26 – October 28.

P. ZUNINO, Ecole Polytechnique Fédérale de Lausanne, Département de Mathématiques, Switzerland, October 1–6.

6.9.2 Scholarship Holders

I. EDELMAN, Russian Academy of Sciences, Institute of Physics of the Earth, Moscow, Humboldt Research Fellowship, (stipendium), January 1 – December 31, 2002.

A. HRYN, University of Grodno, Department of Algebra, Geometry and Mathematics Teaching Methods, Belarus, Scholarship of the Deutscher Akademischer Austauschdienst (German Academic Exchange Service), October 8 – December 22, 2002.

A. KOLODKO, Russian Academy of Sciences, Institute for Applied Mathematics and Mathematical Geophysics, Novosibirsk, Fellowship of the Deutsche Forschungsgemeinschaft (German research association), September 11 – December 10, 2002.

L. SHILNIKOV, Institute for Applied Mathematics and Cybernetics, Nizhny Novgorod, Russia, Humboldt Research Award, (stipendium), October 1 – December 31, 2002.

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.

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 – December 31.

A. FAGGIONATO, Technische Universität Berlin, Graduate College "Stochastic Processes and Probabilistic Analysis", post-doc, August 1 – December 31.

P.-Y. LOUIS, Technische Universität Berlin, Graduate College "Stochastic Processes and Probabilistic Analysis", doctoral candidate, January 1 – September 30.

——, Graduate College "Stochastic Processes and Probabilistic Analysis", post-doc, October 1 – December 31.

H. ZÄHLE, Technische Universität Berlin, Graduate College "Stochastic Processes and Probabilistic Analysis", doctoral candidate, January 1 – December 31.

6.10 Guest Talks

N. ACKERMANN, Universität Giessen, Mathematisches Institut, *Multiple equilibria in superlinear parabolic problems*, June 11.

H.-D. ALBER, Technische Universität Darmstadt, Fachbereich Mathematik, *Wie sollte man Probleme der Metallplastizität formulieren? — Was kann man zur Analysis sagen?*, June 5.

A. AMANN, Technische Universität Berlin, Institut für Theoretische Physik, *Efficient time-delayed feedback control using spatio-temporal Floquet eigenmodes*, April 30.

E. AVRUTIN, University of York, Department of Electronics, Heslington, UK, *Modelling approaches for mode-locked laser diodes*, October 24.

E. BAAKE, Universität Greifswald, Institut für Mathematik und Informatik, *Mutation-selection models: Branching, ancestry, and maximum principle*, February 13.

P. BASTIAN, Ruprecht-Karls-Universität Heidelberg, Interdisziplinäres Zentrum für Wissenschaftliches Rechnen, *Numerical simulation of transport processes*, October 4.

S. BAUER, Fraunhofer-Institut für Nachrichtentechnik, Heinrich-Hertz-Institut, Berlin, *Lasers with active feedback*, May 16.

——, *Experimental bifurcation analysis*, November 28.

S. BAUER, O. BROX, Fraunhofer-Institut für Nachrichtentechnik, Heinrich-Hertz-Institut, Berlin, *Multisection semiconductor lasers: New experimental results*, January 31.

N. BERGLUND, CNRS-Centre de Physique Théorique, Marseille and Université de Toulon et du Var, Physique Mathématique, PHYMAT, France, *Geometric singular perturbation theory for stochastic differential equations*, June 26.

M. BERVEILLER, French Embassy, Scientific Department, Berlin, *A new class of micro-macro models for elastic-viscoplastic heterogeneous materials*, February 15.

A. BETKE, Humboldt-Universität zu Berlin, Institut für Physik, *Measurement of the refractory time of an excitable laser with active feedback*, May 16.

J. BEUTHAN, G. MÜLLER, O. MINET, Laser- und Medizin-Technologie GmbH, Berlin, *Laser in Life Science — Vom Experiment zur Anwendung*, May 13.

J. BLOCH, Eberhard-Karls-Universität Tübingen, Institut für Theoretische Physik, *Solving the integral equations describing the strong interaction*, November 28.

G. BONNET, University of North Carolina at Chapel Hill, Department of Mathematics, USA, *The Burgers superprocess*, June 5.

M. BRAACK, Ruprecht-Karls-Universität Heidelberg, Institut für Angewandte Mathematik, *A posteriori control of modeling errors and discretization errors*, October 5.

J. BRAUN, H.-J. SACK, Universitätsklinikum Benjamin Franklin, Berlin, *Elastizität als neuer Bildkontrast in der MR-Tomographie*, April 22.

O. BROX, Fraunhofer-Institut für Nachrichtentechnik, Heinrich-Hertz-Institut, Berlin, *Generation of high-frequency self-pulsations*, November 28.

C. CLASON, I. HANSEN, Technische Universität München, Zentrum Mathematik, *Mathematische Modelle für die Kieferchirurgie*, January 17.

R. DEO, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, *On issues pertaining to predicting realised volatility using high frequency returns*, November 20.

S.YU. DOBROKHOTOV, Institute for Problems in Mechanics, Moscow, Russia, *Why is the square root of the quadratic form better than other weak point singular solutions of hydrodynamic equations?*, February 27.

M.A. EFENDIEV, Universität Stuttgart, Fakultät Mathematik, *On nonautonomous attractors of evolution equations of mathematical physics*, March 11.

——, *On a doubly nonlinear equations arising in mathematical physics*, December 17.

D. EISERT, OSRAM Opto Semiconductors GmbH, Regensburg, *Entwicklung von blauen Halbleiterlasern bei OSRAM*, February 11.

Y.H. FENG, Universität Konstanz, Fachbereich Mathematik und Statistik, *Simultaneously modelling of different volatility components in high-frequency financial data*, November 6.

M. FENGLER, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, *Implied volatility string dynamics*, December 11.

F. FIDORRA, MergeOptics GmbH, Berlin, *Quantum-Well-Laser für den optischen Datentransfer*, May 6.

F.D. FISCHER, Montanuniversität Leoben, Institut für Mechanik, Austria, *Multikomponentendiffusion, was gibt es da noch Neues?*, May 23.

TH. FRANK, Technische Universität Chemnitz, Fakultät für Maschinenbau und Verfahrenstechnik, *Parallele Algorithmen (MIMD) für die numerische Simulation 3-dimensionaler Fluid-Partikel-Strömungen in der Verfahrenstechnik*, May 23.

T. FÜLLENBACH, Fraunhofer-Institut für Algorithmen und Wissenschaftliches Rechnen, Sankt Augustin, *Algebraic multigrid for semiconductor device simulation*, October 4.

M. GLICKSMAN, at that time Rheinisch-Westfälische Technische Hochschule Aachen, Institut für Metallkunde und Metallphysik, *Materials science in microgravity: Current needs for analysis*, June 24.

Y. GOLUBEV, Institut National de Recherche en Informatique et en Automatique, Grenoble, France, *Recovering of sparse vector*, May 22.

O. GONCHAROVA, Universität Kaiserslautern, Fachbereich Mathematik, *Convection under low gravity: Numerical modelling in domains with fixed and free boundaries*, February 28.

S. GONCHENKO, Institute for Applied Mathematics and Cybernetics, Nizhny Novgorod, Russia, *On dynamics of multidimensional diffeomorphisms in the Newhouse regions*, June 18.

——, *Homoclinic bifurcations*, November 14.

V. GONCHENKO, Nizhny Novgorod State University, Department of Differential Equations, Russia, *Local bifurcations of fixed points of non-orientable reversible maps*, November 7.

L. GOSSE, University of Bari, Institute for Applied Mathematics, Italy, *Well-balanced schemes for discrete kinetic models in the diffusive limit*, June 18.

TH. GÖTZ, Universität Kaiserslautern, Institut für Mathematik, *Modellierung und Analysis von Schmelzspinnprozessen*, March 11.

M. GRIEBEL, Rheinische Friedrich-Wilhelms-Universität Bonn, Institut für Angewandte Mathematik, *A parallel three-dimensional incompressible Navier-Stokes solver for two-phase flow problems with surface tension using a level-set approach*, October 3.

A. GRIN, University of Grodno, Belarus, *Dulac functions and estimate of the number of limit cycles*, December 12.

G. GRÜN, Rheinische Friedrich-Wilhelms-Universität Bonn, Institut für Angewandte Mathematik, *Simulation of complex dewetting scenarios by convergent schemes for thin film equations*, April 25.

M. GÜNTHER, Universität Karlsruhe, Institut für Wissenschaftliches Rechnen und Mathematische Modellbildung, *Effiziente numerische Verfahren für Multiskalenprobleme im Chip-Design*, June 6.

H. HAAF, Commerzbank AG, Frankfurt/M., *Praktische Aspekte der Kreditrisikomodellierung*, March 25.

C. HAFNER, Erasmus University Rotterdam, Econometric Institute, The Netherlands, *Nonparametric multi-step ahead prediction in time series analysis*, October 2.

O. HANSEN, Universität Mainz, Fachbereich Mathematik, *The radiosity equation in spaces of continuous functions*, April 23.

H. HARBRECHT, Technische Universität Chemnitz, Fakultät für Mathematik, *Numerical solution of elliptic shape optimization problems using wavelet-based BEM*, November 12.

J. HÄRTERICH, Freie Universität Berlin, Institut für Mathematik I, *Semidiscretization and exponential dichotomies*, July 2.

K.-H. HASLER, Ferdinand-Braun-Institut für Höchstfrequenztechnik, Berlin, *Application of the TWE model to DBR lasers: New results*, February 7.

T. HAUCK, Motorola, München, *Festigkeitsanalyse metallischer Durchkontaktierungen in Leiterplatten*, November 19.

I. HERLE, Universität Innsbruck, Institut für Geotechnik und Tunnelbau, Austria, *Hypoplasticity*, November 4.

G.C. HSIAO, University of Delaware, Department of Mathematical Sciences, Newark, USA, *Wavelet analysis: An overview*, June 14.

——, *Boundary integral equations: A 30-year collaboration*, June 25.

B. HÜTTL, Fraunhofer-Institut für Nachrichtentechnik, Heinrich-Hertz-Institut, Berlin, *Experimental characterization of monolithic 40 GHz mode-locked lasers on GaInAsP/InP*, October 24.

A. JANSSEN, Universität Düsseldorf, Mathematisches Institut, *Resamplingmethoden in der Testtheorie: Bootstrap- und Permutationstest*, October 23.

J. JURECKOVA, Charles-University Prague, Institute for Mathematical Statistics, Czech Republic, *Two-step regression quantile*, June 5.

L. KALACHEV, University of Montana, Department of Mathematical Sciences, Missoula, USA, *Modeling of attraction of semilinear parabolic equations*, October 31.

V. KARLIN, University of Central Lancashire, Centre for Research in Fire and Explosion Studies, Preston, UK, *Hydrodynamic flame instability within the framework of the Sivashinsky equation*, September 24.

M. KASHTALYAN, Imperial College of Science, Technology and Medicine, London, UK, *Damage-induced anisotropy in composite laminates with intra- and interlaminar cracks*, November 19.

D. KESSLER, University of Maryland, Department of Mathematics, College Park, USA, *Modelling and numerical analysis of phase-field models*, June 13.

J. KIENITZ, K. SUNDERMANN, Reuters AG/Deutsche Postbank AG, *Mathematische Probleme aus der Finanzmathematik*, April 29.

J. KNOBLOCH, Technische Universität Ilmenau, Fakultät für Mathematik und Naturwissenschaften, *Lin's method and application*, October 29.

N. KORNEYEV, Humboldt-Universität zu Berlin, Institut für Physik, *Theory of stochastic processes (Tutorial)*, May 23.

R. KORNHUBER, Freie Universität Berlin, Fachbereich Mathematik und Informatik, *Monotone multigrid methods for discretized phase field equations*, October 4.

R. KRAHL, Freie Universität Berlin, Fachbereich Mathematik, *Reorientierung einer Flüssigkeitsoberfläche nach plötzlicher Reduzierung der Schwerkraft*, October 12.

P. KREJČÍ, Academy of Sciences of the Czech Republic, Institute of Mathematics, Prague, *Singuläre Evolutionsprobleme und Regelfunktionen*, November 26.

A. KROMBHOLZ, Fraunhofer-Institut für Werkstoffmechanik, Halle/Saale, *Bestimmung der kritischen Energiefreisetzungsrate an C/SiC-Laminaten mittels eines Chevron-Tests*, November 19.

M. KUNIK, Otto-von-Guericke-Universität Magdeburg, Institut für Analysis und Numerik, *Kinetic approaches for the ultrarelativistic Euler equations*, April 14.

——, *Ein Minikurs zum Primzahlensatz*, December 11.

H.-R. KÜNSCH, Eidgenössische Technische Hochschule Zürich, Seminar für Statistik, Switzerland, *Large algorithms and convergence results for the particle filter in state space models*, November 13.

N. KUZNETSOV, St. Petersburg University, Department of Mathematics and Mechanics, Russia, *Stability by first approximation for discrete systems*, July 9.

B. LANI-WAYDA, Universität Giessen, Mathematisches Institut, *Dynamics of delay equations and visualization of attractors*, February 21.

F. LAURENT-POLZ, Institut Non-Linéaire de Nice, France, *Dynamics of N point vortices on a sphere*, November 26.

B. LEMMENS, EURANDOM, Eindhoven, The Netherlands, *Periods of periodic points of nonexpansive maps*, May 28.

M. LICHTNER, Humboldt-Universität zu Berlin, Institut für Mathematik, *Lineare elliptische Randwertprobleme mit nichtglatten Daten und unbeschränkten Koeffizienten*, December 4.

M. MALIOUTOV, Northeastern University, Mathematical Department, Boston, USA, *Estimating singular functional of nonparametric regression*, December 18.

H. MAURER, Universität Münster, Institut für Numerische Mathematik, *Methoden der optimalen Steuerung zur Minimierung der Einschwingzeit in Lasern*, June 17.

S. MÉLÉARD, Université Paris X, UFR Segmi, Equipe Modal X, Nanterre, France, *Convergence from Boltzmann to Landau processes with soft potential and particle approximations*, January 23.

S. MERTENS, Otto-von-Guericke-Universität Magdeburg, Institut für Theoretische Physik, *Gefrierende Algorithmen — Phasenübergänge in der kombinatorischen Optimierung*, November 27.

M. METZGER, Siemens AG, Erlangen, *Thermische Prozessmodelle zur Steuerung und Regelung in Warmwalzwerken*, November 18.

A. MEYER, Technische Universität Chemnitz, Fakultät für Mathematik, *Projection techniques embedded in the PCGM for handling hanging nodes and boundary restrictions*, October 4.

C. MITTELSTEDT, Universität Siegen, Institut für Mechanik und Regelungstechnik — Mechatron, *Geschlossen-analytische Untersuchung des Spannungsfeldes an kräftefreien Ecken ebener Laminate*, November 19.

P. MÖRTERS, University of Bath, Department of Mathematical Sciences, UK, *Thick and thin points of Brownian intersection local times*, July 17.

TH. MRZIGLOD, Bayer AG, Leverkusen, *Anwendung neuronaler Netze in der chemischen Industrie*, December 2.

A. MÜNCH, Technische Universität München, Zentrum Mathematik, *Non-classical shock waves in thin film flows*, May 15.

N.N. NEFEDOV, Moscow State University, Faculty of Physics, Russia, *On reaction-diffusion systems with balanced nonlinearities*, April 23.

A. NESTEROV, U. TROPPENZ, Fraunhofer-Institut für Nachrichtentechnik, Heinrich-Hertz-Institut, Berlin, *Laser, Filter und Wellenlängenkonverter auf der Basis aktiver GaInAsP Mikroringresonatoren: Ziel, Modelle, Zwischenergebnisse*, October 31.

N. NEUSS, Ruprecht-Karls-Universität Heidelberg, Institut für Angewandte Mathematik, *A Common Lisp framework for finite elements*, October 2.

V.S. NGUYEN, Universität Paderborn, Fakultät für Maschinenbau, *Zur Identifikation und Optimierung von Materialparametern inelastischer Lotwerkstoffe*, November 19.

A. OSTERMANN, Universität Innsbruck, Institut für Technische Mathematik, Austria, *Zeitdiskretisierung abstrakter Differentialgleichungen: Fehlerschranken und Langzeitverhalten*, April 18.

J. OUTRATA, Academy of Sciences of the Czech Republic, Institute of Information Theory and Automation, Prague, *Shape optimization in contact problems with Coulomb friction*, November 5.

K. PASCHKE, Ferdinand-Braun-Institut für Höchstfrequenztechnik, Berlin, *Alfa-DFB laser: Theory and experiment of stationary state*, June 20.

S.V. PEREVERZEV, National Academy of Sciences of Ukraine, Institute of Mathematics, Kiev, *An adaptive discretization level choice for some nonlinear ill-posed problems regularized by projection*, April 16.

M. PICASSO, Ecole Polytechnique Fédérale de Lausanne, Département de Mathématiques, Switzerland, *Numerical simulation of three-dimensional free surface flows*, October 3.

V. POPOV, Technische Universität Berlin, Institut für Mechanik, *Numerical simulation of localized plastic flow and cracking in coated materials*, November 19.

K. PROMISLOW, Simon Fraser University, Department of Mathematics and Statistics, Burnaby, Canada, *Multi-species, multi-phase transport in polymer-electrolyte membranes*, October 4.

L. RECKE, Humboldt-Universität zu Berlin, Institut für Mathematik, *Anwendungen des Satzes über implizite Funktionen auf Variationsungleichungen*, April 17.

F. REDIG, Eindhoven University of Technology, Department of Mathematics and Computer Science, The Netherlands, *Loss and recovery of the Gibbs property in local stochastic evolutions*, January 30.

M. REISS, Humboldt-Universität zu Berlin, Institut für Mathematik, *Nonparametric inference for stochastic delay differential equations*, May 8.

V. REITMANN, Max-Planck-Institut für Physik komplexer Systeme, Dresden, *Attractor crises and dynamic buckling of elastic plates*, November 5.

A. REUSKEN, Rheinisch-Westfälische Technische Hochschule Aachen, Lehrstuhl für Numerische Mathematik, *Convergence analysis of multigrid methods for singularly perturbed elliptic problems*, October 4.

TH. RIECKMANN, Fachhochschule Köln, Fakultät für Anlagen, Energie- und Maschinensysteme, *Aktuelle verfahrenstechnische Probleme zur Kopplung von Transportphänomenen mit komplexen chemischen Reaktionen*, November 11.

G.J. RIX, Georgia Institute of Technology, School of Civil & Environmental Engineering, Atlanta, USA, *Near-surface site characterization using surface waves*, May 27.

J. ROBINSON, University of Warwick, Mathematics Institute, Coventry, UK, *A pitchfork bifurcation in a reaction-diffusion equation*, July 3.

A. ROGGAN, Celon AG medical instruments, Teltow, *Computergestütztes Planungssystem für Laser- und Hochfrequenzstromanwendungen in der Medizin*, February 25.

H.-G. ROSS, Technische Universität Dresden, Institut für Numerische Mathematik, *The discontinuous Galerkin method for singularly perturbed problems using layer adapted meshes*, October 3.

M.B. RUBIN, Technion Israel Institute of Technology, Faculty of Mechanical Engineering, Haifa, *Elimination of shear locking in thin elastic beams using the theory of a Cosserat point*, May 3.

W. RÜHAAK, Institut für Geowissenschaftliche Gemeinschaftsaufgaben, Sektion Geothermik und Grundwasserhydraulik, Hannover, *Modellierung des Grundwasserregimes in einem sedimentären Becken mit Hilfe von Bohrlochtemperaturen*, December 16.

S. SARDY, Ecole Polytechnique Fédérale de Lausanne, Département de Mathématiques, Switzerland, *ℓ_1-Markov random field-based estimators*, November 27.

B. SARTORIUS, Fraunhofer-Institut für Nachrichtentechnik, Heinrich-Hertz-Institut, Berlin, *Tutorial on 3R regeneration*, January 10.

W.H.A. SCHILDERS, Technical University of Eindhoven and Philips, The Netherlands, *Reduced order modelling with applications to electromagnetics and circuit simulation*, April 11.

——, *Preconditioning for indefinite linear systems*, November 14.

L. SCHIMANSKY-GEIER, Humboldt-Universität zu Berlin, Institut für Physik, *Theory of stochastic processes (Tutorial)*, July 4.

B. SCHMALFUSS, Fachhochschule Merseburg, Fachbereich Informatik und Angewandte Naturwissenschaften, *Invariant manifolds for random dynamical systems*, April 16.

A. SCHMIDT, Universität Bremen, Zentrum für Technomathematik, *Adaptive multi mesh finite element methods for coupled systems of PDEs*, October 2.

H. SCHMIDT, Freie Universität Berlin, Forschungsbereich Numerische Mathematik/Scientific Computing, *Numerik zur Berechnung turbulenter vorgemischter Verbrennung unter Berücksichtigung instationärer Frontstrukturen*, February 14.

R. SCHNEIDER, Technische Universität Chemnitz, Fakultät für Mathematik, *Recent results on wavelet approximation of operator equations*, September 17.

S. SCHRAMOWSKI, M. STURM, Macron GmbH, Berlin, *Stochastisches Dithering im Inkjetdruck*, February 18.

M. SEAÏD, Technische Universität Darmstadt, Fachbereich Mathematik, *Efficient preconditioning of linear systems arising from the discretization of radiative transfer equation*, October 2.

E. SHCHEPAKINA, Samara State University, Department of Differential Equations and Control Theory, Russia, *Modeling of critical phenomena in applied problems*, October 31.

M. SHEARER, North Carolina State University, Department of Mathematics, Raleigh, USA, *The dynamics of thin liquid films and the motion of contact lines*, October 10.

A. SHILNIKOV, Georgia State University, Department of Mathematics and Statistics, Atlanta, USA, *Curious effects in slow-fast flows and maps*, May 14.

L. SHILNIKOV, Institute for Applied Mathematics and Cybernetics, Nizhny Novgorod, Russia, *Bifurcations of attractors*, December 10.

E. SHKARUPA, Russian Academy of Sciences, Institute for Applied Mathematics and Mathematical Geophysics, Novosibirsk, *Error estimation and optimization of the functional Monte Carlo algorithms for globally estimating the solution of an equation*, November 13.

H. SI, Hangzhou, Zheijiang, China, *Algorithms used in TetGen*, March 21.

J. SIEBER, University of Bristol, Department of Engineering Mathematics, UK, *Bifurcation analysis*, November 28.

D. SILVESTER, University of Manchester, Institute of Science and Technology, UK, *Black-box multigrid preconditioning for elliptic PDEs*, October 3.

I.V. SKRYPNIK, National Academy of Sciences of Ukraine, Institute of Applied Mathematics and Mechanics, Donetsk, *On degree theory for (S_+) perturbations of maximal monotone operators and applications*, July 10.

M. SLODICKA, Ghent University, Faculty of Engineering, Belgium, *Comprehensive models for wells*, November 7.

O. STENKIN, Imperial College, London, UK, *Conservative and nonconservative dynamics in reversible maps with homoclinic tangencies*, May 7.

B. STINNER, Universität Regensburg, Naturwissenschaftliche Fakultät I — Mathematik, *Zur Phasenfeld-Modellierung von Erstarrungsprozessen mehrkomponentiger Legierungen*, September 18.

G. SUCHANECK, Technische Universität Dresden, Institut für Festkörperelektronik, *Experimentelle Untersuchungen der Domänenstruktur, der Phasenübergänge und der Selbstpolarisation von PZT-Dünnschichten*, July 1.

J. SWART, Universität Erlangen-Nürnberg, Mathematisches Institut, *Trimmed trees and embedded particle systems*, May 8.

T. SZÁNTAI, Technical University of Budapest, Department of Differential Equations, Hungary, *PERT network analysis*, October 29.

J. TAMINE, Université Aix Marseille III, France, *Smoothed influence function: Another view at robust nonparametric regression*, July 3.

C. TAMMER, Universität Halle, Institut für Optimierung und Stochastik, *Minimalpunkttheoreme in Produkträumen und Anwendungen*, June 4.

L. TOBISKA, Otto-von-Guericke-Universität Magdeburg, Institut für Analysis und Numerik, *Finite element methods for coupled problems in ferrohydrodynamics*, October 3.

F. TRÖLTZSCH, Technische Universität Berlin, Institut für Mathematik, *Error estimates for the optimal control of elliptic equations*, October 2.

ST. TUREK, Universität Dortmund, Institut für Angewandte Mathematik und Numerik, *Recent developments for incompressible flow simulations regarding nonconforming FEM discretization and multigrid solution techniques*, October 5.

S. UBAL, Universidad Nacional del Litoral, INTEC, Santa Fe, Argentina, *Numerical analysis of two-dimensional Faraday waves*, November 14.

H. UHLIG, Humboldt-Universität zu Berlin, Institut für Statistik und Ökonometrie, *What moves real GNP?*, April 24.

P. VALLOIS, Université Nancy I, Institut Élie Cartan, France, *A solution to Skorokhods embedding for linear Brownian motion*, February 6.

P. VASSILEVSKI, Lawrence Livermore National Laboratory, Center for Applied Scientific Computing, USA, *Spectral agglomerate AMGe for unstructured finite element elliptic problems*, October 4.

S. VESSELLA, Università degli Studi di Firenze, Dipartimento di Matematica per le Decisioni, Italy, *Three cylinder inequalities and stability estimates in inverse boundary problems of parabolic type*, July 16.

A. VLADIMIROV, St. Petersburg State University, Russia, *Synchronization of semiconductor laser arrays by delayed global coupling*, December 12.

A. VLADIMIRSKY, Cornell University, Department of Mathematics, Ithaca, USA, *Ordered upwind methods for optimal control and dynamical systems*, October 5.

R. VODÁK, Palacky University, Faculty of Science, Olomouc, Czech Republic, *The existence and asymptotic behaviour of solutions to Navier-Stokes equations for compressible isothermal fluids with nonlinear stress tensor*, September 18.

A. VOGLIANO, Technische Universität Berlin, Institut für Mechanik, *Experiment und FE-Analyse Hand in Hand: Erzeugung phasengemittelter Last-Verformungs-Kurven durch Nanoindentation und Simulation des Nanoindenter-Eindruck-Vorgangs durch das FE-Programm ABAQUS*, November 19.

P. VOGT, University of Bath, Department of Mathematical Sciences, UK, *Solution of a non-linear boundary value problem using catalytic branching*, December 16.

A. VOIGT, Center of Advanced European Studies and Research, Bonn, *Multiscale simulations of industrial crystal growth*, July 18.

ST. VOLKWEIN, Karl-Franzens Universität Graz, Institut für Mathematik, Austria, *Affin-invariante Konvergenzanalysis für inexakte SQP-Verfahren*, February 21.

M. WABRO, Johannes Kepler Universität Linz, Institut für rechenbetonte Mathematik, Austria, *Coupled algebraic multigrid methods for the Oseen problem*, October 3.

N. WALKINGTON, Carnegie Mellon University, Mathematical Sciences Department, Pittsburgh, USA, *Macroscopic models of fluids with microstructure*, October 3.

D. WAN, Universität Dortmund, Institut für Angewandte Mathematik, *Numerical simulation of viscous flows with moving interfaces by the VOF method*, January 31.

——, *The fictitious boundary method for simulating flows with complex moving boundaries*, October 3.

A. WATHEN, Oxford University Computing Laboratory, Department of Numerical Analysis, UK, *Preconditioning and fast solvers for the incompressible Navier-Stokes equations*, October 3.

H.-J. WÜNSCHE, Humboldt-Universität zu Berlin, Institut für Physik, *Dynamics of multisection DFB lasers: Theory — control — application*, July 18.

Y. XIA, University of Cambridge, Department of Zoology, USA, *An adaptive estimation of dimension reduction space*, April 17.

J. XIONG, University of Tennessee, Department of Mathematics, Knoxville, USA, *A stochastic log-Laplace equation*, June 10.

J. XU, Pennsylvania State University, Department of Mathematics, USA, *Asymptotically exact a posteriori error estimates for unstructured grids*, October 2.

M. YAMAMOTO, University of Tokyo, Department of Mathematical Sciences, Japan, *Global uniqueness in the inverse conductivity problem*, May 14.

——, *Stability in determination of point sources by the marriage theorem*, September 27.

S. YANCHUK, National Academy of Sciences of Ukraine, Kiev, *Synchronization of semiconductor lasers*, April 25.

M. ZAKS, Humboldt-Universität zu Berlin, Institut für Physik, *Delayed bifurcations and slow-fast dynamics in weakly desynchronized chaotic oscillators*, June 4.

H. ZESSIN, Universität Bielefeld, Fakultät für Mathematik, *On the conceptual foundations of random simplicial complexes with interaction (simplicial quantum gravity)*, January 16.

P. ZUNINO, Ecole Polytechnique Fédérale de Lausanne, Département de Mathématiques, Switzerland, *Mathematical and numerical modelling of solute dynamics in blood flow and arterial walls*, October 3.

6.11 Membership in Organizing Committees of non-WIAS Meetings

E. BÄNSCH, member of the Local Organizing Committee and of the Scintific Committee, co-organizer, *9th Workshop on Numerical Methods for Free Boundary Problems (Interphase 2001)*, College Park, Maryland, USA, January 9–12.

——, member of the Scientific Program Committee, *Conference on Scientific Computing (ALGORITMY 2002)*, Podbanské, Slovakia, September 8–13.

A. BOVIER, member of the Organizing Committee, *Stochastic Models from Statistical Physics III*, EURANDOM, Eindhoven, The Netherlands, October 7–11.

K. FLEISCHMANN, member of the Organizing Committee, *Workshop on Spatially Distributed and Hierarchically Structured Stochastic Systems*, Université de Montréal, Centre de Recherches Mathématiques, Canada, April 4–10.

H. GAJEWSKI, organizer of the minisymposium "Modelling and Analysis in Semiconductor Technology" (together with A. Jüngel, Universität Konstanz), *GAMM Annual Conference 2002*, Universität Augsburg, Institut für Mathematik, March 25–28.

——, member of the Program Committee, *International Conference on Numerical Simulation of Semiconductor Optoelectronic Devices*, Zurich, Switzerland, September 25–27.

G. HEBERMEHL, member of the Scientific Advisory Committee, *Scientific Computing in Electrical Engineering (SCEE-2002)*, University of Technology, Eindhoven, The Netherlands, June 23–28.

R. HENRION, co-organizer, *DECHEMA continuation course "Optimierung verfahrenstechnischer Prozesse"*, Technische Universität Berlin, September 23–25.

S. JASCHKE, member of the Organizing Committee, *Computational Finance Research Conference*, Berlin, August 24–25.

K.K. SABELFELD, co-organizer and member of the Program Committee, *The International Conference on Computational Mathematics*, Novosibirsk, Russia, June 24–28.

K.R. SCHNEIDER, chairman, *GAMM Annual Conference*, Universität Augsburg, Institut für Mathematik, March 25–28.

——, member of the Organizing Committee, *International Conference on Differential and Functional Differential Equations, Satellite Conference of the International Congress of Mathematicians (ICM) 2002 in Beijing*, Moscow, Russia, August 11–17.

——, chairman, *Annual Conference of DMV*, Universität Halle, September 16–20.

——, member of the Editorial Board, *Vth International Congress on Mathematical Modeling*, Dubna, Russia, September 30 – October 6.

V. SPOKOINY, member of the Local Organizing Committee, *15th Conference on Computational Statistics (Compstat 2002)*, Berlin, August 24–28.

J. SPREKELS, member of the Scientific Committee, *Workshop "Frost Resistance of Concrete: From Nano-Structure and Pore Solution to Macroscopic Behaviour and Testing"*, Essen, April 18–19.

——, member of the Scientific Committee and of the Organizing Committee, *Workshop "Free Boundary Problems: Theory and Applications"*, Trento, Italy, June 5–8.

——, member of the International Program Committee, *International Conference "Analysis and Optimization of Differential Systems"*, Constanta, Romania, September 10–14.

——, co-organizer, *Workshop "Interfaces and Singularly Perturbed Interface Evolutions"*, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, November 29–30.

D. TIBA, member of the Organizing Committee, *International Conference "Analysis and Optimization of Differential Systems"*, Constanta, Romania, September 10–14.

6.12 Software

For detailed information about our software products please see also http://www.wias-berlin.de/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: F. Grund, phone: +49 30/20372-583)
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 to 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 2k 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 power plant environment for example.
Detailed information: http://www.wias-berlin.de/publications/annual_reports/2002/nummath-1.

ClusCorr98® (contact: H.-J. Mucha, phone: +49 30/20372-573)
The statistical software ClusCorr98® is an interactive statistical computing environment based on both Visual Basic for Application (VBA) and the Excel spreadsheet environment. It performs exploratory data analysis mainly by using adaptive methods of cluster analysis, classification and multivariate visualization. Typically it aims at the extraction of knowledge from huge samples of numerical and alphanumerical data. Some of the available methods are: model-based cluster analysis, hierarchical clustering, K-means clustering, core-based clustering. Multivariate visualization of both the data and the results makes it easier to formulate hypotheses about the data at hand. ClusCorr98® runs under Microsoft Windows taking advantage of

the Excel environment, but it is not restricted to Excel because the programming language VBA is based on object models of various Microsoft Office components.
Please find further information under
http://www.wias-berlin.de/publications/annual_reports/2002/ClusCorr98.

COG (contact: I. Schmelzer, phone: +49 30/20372-463)
`COG` is a software package for grid generation and geometry description. It allows to generate Delaunay grids with local and anisotropic refinement for arbitrary geometries.
The volume-oriented geometry description allows to describe geometries with implicit functions, pixmaps, voxmaps, grids in a dimension-independent way. They may be combined as unions or intersections and transformed using nonlinear coordinate transformations.
Please find further information under
http://www.wias-berlin.de/publications/annual_reports/2002/cog.

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 the grating geometry, 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.
Please find further information under
http://www.wias-berlin.de/publications/annual_reports/2002/optik.

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/publications/annual_reports/2002/~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.
Please find further information under
http://www.wias-berlin.de/publications/annual_reports/2002/LDSL-tool.

NUMATH (contact: G. Hebermehl, phone: +49 30/20372-562)
`NUMATH` is a well-documented library of FORTRAN subroutines for solving problems in linear algebra; approximation, interpolation and differentiation of functions; computation of integrals; nonlinear equations; optimization; ordinary differential equations; integral equations; special functions; and partial differential equations.
The hierarchical structure of `NUMATH` consists of three levels: problem solvers, primary routines, and basic modules and routines for matrix manipulation.
The routines of `NUMATH` can be tested using the modules of the `NUMATH` test library.
Please find further information under
http://www.wias-berlin.de/publications/annual_reports/2002/~NUMATH.

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.
Please find further information under
http://www.wias-berlin.de/publications/annual_reports/2002/~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. 43) supported by the BMBF.
Please find further information under
http://www.wias-berlin.de/publications/annual_reports/2002/WIAS-HiTNIHS.

WIAS-SHarP (contact: D. Hömberg, phone: +49 30/20372-491)
Based on pdelib a new software for electron and laser beam surface hardening, called WIAS-SHarP, has been developed. Based on a data bank with material parameters for 20 important steels, it contains 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/publications/annual_reports/2002/laeserhaerten.html.

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 (PowerPC).
For more information please look up:
http://www.wias-berlin.de/publications/annual_reports/2002/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. For more information please look up: http://www.wias-berlin.de/publications/annual_reports/2002/WIAS-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)

  D3: "Global singular perturbations" (FG 2)

[1] research group

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)

“Modeling and optimization of phase transitions in steel” (FG 1)

– Collaborative Research Centre (SFB) 373, Humboldt-Universität zu Berlin, “Quantifikation und Simulation ökonomischer Prozesse” (Quantification and simulation of economic processes)

  “Kurvenschätzung und Resampling” (Curve estimation and resampling methods, FG 6)

  “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 nanostructure, 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)

– **Normalverfahren (Individual Grants)**

  “Hysterese-Operatoren in Phasenfeld-Gleichungen” (Hysteresis operators in phase-field equations, FG 1)

  “Zur Analysis von thermodynamischen Modellen des Stoff-, Ladungs- und Energietransports in heterogenen Halbleitern” (Analysis and thermodynamic models for the transport of mass, charge, and energy in heterogeneous semiconductors, 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, Humboldt-Universität zu Berlin
  “Angewandte Mikroökonomik” (Applied microeconomics, FG 6)

– 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 (FG 2)

– Scientific cooperation with Japan: “Inverse problems in electromagnetics” (FG 4)

– Scientist exchange with the Czech Republic (FG 1)

– Scientist exchange with Russia (FG 1, 6)

Alexander von Humboldt-Stiftung (Alexander von Humboldt Foundation)

– 1 Humboldt Laureate (FG 2) and 3 scholarship holders (FG 5, 6, 7), see page 248

Deutscher Akademischer Austauschdienst (German Academic Exchange Service), Bonn

– 1 short-term fellowship (FG 2)

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:** “Stochastic modelling of aerosol particle transport and reacting pollutants in the atmosphere” (FG 6)
- **(EU) INTAS:** “Random walk models for the footprint problem in the turbulent atmosphere” (FG 5, 6)
- **NATO Linkage Grant:** “Stochastic modelling of aerosol particle transport and reacting pollutants in the atmosphere” (FG 6)
- **ESF** (European Science Foundation) Programme “Phase transitions and fluctuation phenomena for random dynamics in spatially extended systems” (FG 5)

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)

Mission-oriented research

- Alstom Power(Switzerland) Ltd., Baden: “Prozesssimulation für Gasturbinen” (Gas turbine process simulation, FG 3)
- Bankgesellschaft Berlin AG: “Monte Carlo Simulation” (FG 6)
- Bundesanstalt für Materialforschung und -prüfung, Berlin: “Statistisch-methodische Verfahrensentwicklung zur Zertifizierung von Referenzmaterialien” (Statistical methods for certification of reference materials, FG 6)
- Ferdinand-Braun-Institut für Höchstfrequenztechnik, Berlin: “Simulation von Mikrowellenschaltungen unter Berücksichtigung von Perfectly-Matched-Layer-Randbedingungen” (Simulation of microwave circuits including Perfectly Matched Layer boundary conditions, FG 3)
- Ferdinand-Braun-Institut für Höchstfrequenztechnik, Berlin: “Finite-Integrations-Methode mit Tetraedergitter zur elektromagnetischen Simulation von Mikrowellenschaltungen” (Electromagnetic simulation of microwave circuits using finite integration technique with tetrahedral grids, FG 3)
- Forschungszentrum Jülich: “Numerische Simulation von Methanol-Brennstoffzellen (DMFC)” (Numerical simulation of Direct Methanol Fuel Cells (DMFC), FG 3)
- Freiberger Compound Materials GmbH: “Spannungs- und Dehnungsanalyse an GaAs-Waferplatten” (Stress and strain analysis of GaAs wafer plates, FG 7)
- Macron GmbH, Berlin: consulting and cooperation (FG 6)

- MergeOptics GmbH, Berlin: “Simulation und Optimierung von MQW-Lasern” (Simulation and optimization of MQW lasers, FG 1)
- Science & Tec, Lisieux, France: “Techniques d’apprentissage, méthodes d’exploration aléatoire” (FG 5)
- Rücker Ges.m.b.H, Graz, Austria: “Bahnplanung für Industrieroboter und Menschmodelle” (Path planning for robots and human models, FG 4)

Advanced training courses

- Technische Universität Berlin: “Einführung in Methoden der stochastischen Optimierung” (Introduction to methods of stochastic optimization), in: DECHEMA continuation course “Optimierung verfahrenstechnischer Prozesse” (Optimization in process engineering, FG 4)

Index