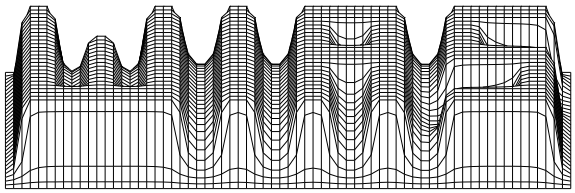
Weierstraß-Institut
für Angewandte Analysis und Stochastik
(WIAS)

im Forschungsverbund Berlin e. V.

Annual Research Report 2001



Berlin 2002

ISSN 1437-7489

Edited by Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)
Mohrenstraße 39
D – 10117 Berlin
Germany

Fax: + 49 30 2044975
E-Mail: preprint@wias-berlin.de
World Wide Web: http://www.wias-berlin.de/

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1 Vorwort / Foreword

Das Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS) legt hiermit Kollegen, Förderern und Kooperationspartnern des Instituts seinen Jahresforschungsbericht 2001 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 2001 to its colleagues, supporters, and cooperation partners. In its first part, the report informs about the progress made and the results obtained in 2001, 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 2001 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 2001 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, verstärkt Drittmittel aus der Wirtschaft einzuwerben; 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 2001, compared to last year's funds, and, much to our satisfaction, the institute succeeded in raising 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, im Bereich der Berufungen: Im Berichtsjahr 2001 ergingen drei Rufe an Mitarbeiter des Instituts auf C4-

The high rank of WIAS' research work in the scientific community becomes especially clear in the field of calls: in 2001, three calls to C4 (full) professorships were received by WIAS collaborators, including one abroad.

Professuren, davon eine im Ausland; seit der Gründung des Instituts im Jahre 1992 sind damit nunmehr schon 21 Rufe an Mitarbeiter des Instituts auf Professuren ergangen (davon elf auf C4-Professuren und sechs auf Professuren im Ausland), eine Bilanz, die sich bei einer Zahl von derzeit 54 etatisierten Wissenschaftlern wirklich sehen lassen kann.

Altogether, since the institute's foundation in 1992, 21 calls have been received by collaborators of WIAS (including eleven to C4 professorships and six 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 dabei der Zusammenarbeit mit den Berliner Hochschulen. Besonders erfreulich war die Tatsache, dass die gemeinsame Berufung des Leiters der Forschungsgruppe *Stochastische Algorithmen und Nichtparametrische Statistik*, Prof. Spokoiny, auf eine C4-S-Professur für *Angewandte Statistik* an der Humboldt-Universität zu Berlin erfolgreich abgeschlossen werden konnte. Ferner wurde nach der Humboldt- und der Freien Universität nunmehr auch mit der Technischen Universität Berlin ein Kooperationsvertrag abgeschlossen, der unter anderem die gemeinsame Berufung des Leiters der Forschungsgruppe *Nichtlineare Optimierung und Inverse Probleme* auf eine C4-S-Professur für *Numerische nichtlineare Optimierung* vorsieht. Inzwischen ist die Ausschreibung für diese Stelle erfolgt und das gemeinsame Berufungsverfahren angelaufen, so dass zu hoffen ist, dass am Ende des Jahres 2002 insgesamt vier gemeinsame Berufungen auf C4-S-Professuren mit den Berliner Universitäten realisiert sein werden.

The cooperation with the mathematical institutions in Berlin and its environs, having already been intensive, has been further strengthened. Our main attention was directed to the cooperation with the Berlin universities. We are especially pleased that the joint appointment of the head of the research group *Stochastic Algorithms and Nonparametric Statistics*, Prof. Spokoiny, to a C4 special professorship for *Applied Statistics* at Humboldt University of Berlin could successfully be concluded. After contracts with the Humboldt University and the Free University of Berlin, in the year under review, a cooperation contract was signed with the Technical University of Berlin, planning among other things the joint appointment of the head of the research group *Nonlinear Optimization and Inverse Problems* to a C4 special professorship for *Numerical Nonlinear Optimization*. In the meantime, the position has been advertized and the joint appointment procedure has been started, and we hope that at the end of the year 2002 altogether four joint appointments to C4 special professorships with the Berlin universities will be concluded.

Neben diesen Aktivitäten wurde die Zusammenarbeit mit den Hochschulen durch die vielfältigen von Mitarbeitern des WIAS abgehaltenen Lehrveranstaltungen, durch die Beteiligung an Sonderforschungsbereichen, Schwerpunktprogrammen und Graduiertenkollegs der DFG, durch die gemeinschaftliche Bearbeitung von Forschungsprojekten sowie durch die Betreuung von Examensarbeiten mit Leben erfüllt.

Beside these activities, the cooperation with the universities meant manifold teaching activities by WIAS collaborators, the participation in DFG Collaborative Research Centres, Priority Programs, and Graduate Colleges, cooperation in research projects as well as the supervision of graduation papers.

Unverändert bleibt es das übergeordnete Ziel

Our primary aim remains unchanged: to join

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.

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 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.

In organisatorischer Hinsicht war die Arbeit des Instituts durch die Einführung der *Kosten- und Leistungsrechnung* zum 01.01.2001 gekennzeichnet. Als Resultat dieser Bemühungen sind damit am WIAS die wichtigsten Elemente eines internen Controlling-Systems implementiert.

In the administrative respect, the institute's work was marked by the introduction of the *Cost and Activity Accounting*, which started on January 1, 2001. As a result of these efforts, WIAS has thus implemented the most important elements of an internal controlling system.

Die Herausforderungen im Jahre 2002 werden für das WIAS erheblich sein. Das Institut sollte aufgrund seiner wissenschaftlichen Leistungsfähigkeit in der Lage sein, die zukünftigen Probleme bewältigen zu können; das WIAS hat allen Grund, optimistisch in die Zukunft zu blicken.

The challenges in 2002 will be considerable for WIAS. But on the basis of its scientific productivity the institute should be able to master future problems. WIAS has every reason to look optimistically into the future.

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 2002 / in January 2002

J. Sprekels
Direktor / Director

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 Wissenschaftsgemeinschaft Gottfried Wilhelm Leibniz e. V. (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.

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

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

As a member of Wissenschaftsgemeinschaft Gottfried Wilhelm Leibniz e.V. (Gottfried Wilhelm Leibniz Science Association/WGL), *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.

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.

- Micro-, nano-, and optoelectronics,
- Optimization and control in process engineering,
- 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)
- Simulation von mikroelektronischen Schaltkreisen und von Mikrowellenschaltungen (in FG 3)
- Modellierung von Halbleiterlasern (in FG 1, FG 2 und FG 3)
- Diffraktive Optik (Simulation und Optimierung optischer Gitter; in FG 4)

- Microelectronic devices (technology and device simulation of semiconductor devices, in FG 1 and FG 3)
- Simulation of microelectronic circuits and of microwave circuits (in FG 3)
- Modeling of semiconductor lasers (in FG 1, FG 2, and FG 3)
- Diffractive optics (simulation and optimization of optical gratings, in FG 4)

3.1.2 Optimierung und Steuerung in der Verfahrenstechnik / Optimization and control in process engineering

- Simulation und Steuerung chemischer Anlagen (in FG 2, FG 3 und FG 4)
- Robotik (Optimierung und inverse Modellierung von Mehrkörpersystemen; in FG 4)
- Probleme des Optimal Shape Design (in FG 1)

- Simulation and control of chemical plants (in FG 2, FG 3, and FG 4)
- Robotics (optimization and inverse modeling of multi-body systems, in FG 4)
- 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)
- Phasenfeldmodelle (Simulation von Formgedächtnislegierungen, flüssig-fest-Übergängen und Phasenseparation; in FG 1, FG 3 und FG 7)
- Stochastische Modellierung von Phasenübergängen und Spingläsern (in FG 5)

- Heat treatment and welding processes for steels (modeling and simulation, in FG 1)
- Phase-field models (simulation of shape-memory alloys, liquid-solid transitions and phase separation, in FG 1, FG 3, and FG 7)
- Stochastic modeling of phase transitions and spin glasses (in FG 5)

[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.

– Verfahren der Züchtung von SiC- und GaAs-Einkristallen (in FG 1 und FG 7)

– 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)

– Stochastic particle systems and kinetic equations (modeling and simulation of coagulation processes and gas flows, in FG 5, FG 6, and FG 7)

– Modellierung von Aktien-, Zins- und Wechselkursen (in FG 6)

– Modeling of stock prices, interest rates, and exchange rates (in FG 6)

– Bewertung von Derivaten, Portfolio-Management und Risikobewertung (in FG 6)

– Evaluation of derivatives, portfolio management, and evaluation of risk (in FG 6)

– Nichtparametrische statistische Methoden (Bildverarbeitung, Finanzmärkte, Ökonometrie; in FG 6)

– Nonparametric statistical methods (image processing, financial markets, econometrics, in FG 6)

– Datenanalyse (Cluster- und Diskriminanzanalyse, Credit-Scoring; 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)

– Navier-Stokes equations (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)

– 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)

– Thermomechanik poröser Körper und granularer Stoffe (Schall- und Stoßwellen, Streuung und Beugung; in 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

– Numerical solution of partial differential equations (finite-volume and finite-element methods, preconditioners, grid generation, error estimators, and adapt-

und Adaptivität; in allen Forschungsgruppen, insbesondere in FG 3)

- Numerik von Algebro-Differentialgleichungen (in FG 3)
- Numerik von Integralgleichungen (Randelementmethoden, Waveletalgorithmen; in FG 4)
- Verfahren der nichtlinearen Optimierung (in FG 4)
- 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. 236; in FG 1, FG 2, FG 3, FG 4 und FG 6)

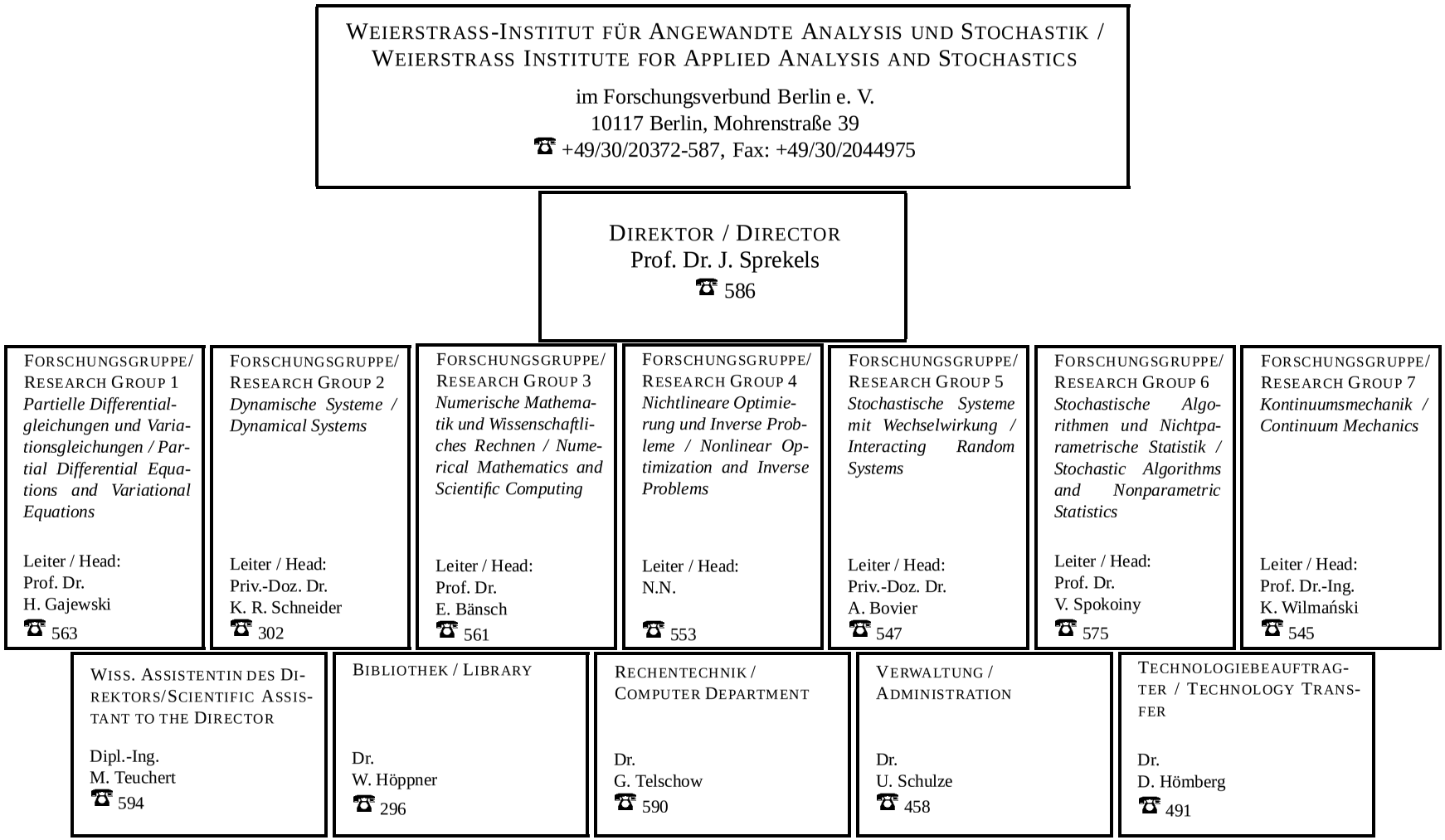
ivity, in all research groups, especially in FG 3)

- Numerics of differential–algebraic equations (in FG 3)
- Numerics of integral equations (boundary-element methods, wavelet algorithms, in FG 4)
- Nonlinear optimization techniques (in FG 4)
- 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 236; 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 2001 nach fachspezifischen Gesichtspunkten in sieben Forschungsgruppen gegliedert; hinzu kamen die wissenschaftlich-technischen Dienste. Im Folgenden sind die Aufgaben dieser Abteilungen angegeben. Dabei ist zu bemerken, dass zur Lösung konkreter Anwendungsprobleme in der Regel *längerfristig kooperierende interdisziplinäre Projektgruppen* zusammen mit Anwendern gebildet werden, in die Institutsmitarbeiter aus verschiedenen Fachrichtungen ihre jeweilige mathematische Expertise einbringen. Diese Arbeitsweise nutzt die spezifischen Möglichkeiten eines außeruniversitären Instituts und trägt mit zur *horizontalen Vernetzung* innerhalb des Instituts bei. Die Verbesserung dieser Vernetzung innerhalb des Instituts im Sinne eines möglichst effektiven Einsatzes der personellen Ressourcen ist eine ständige Aufgabe des Instituts.

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. In addition, there are *interdisciplinary project groups* including prospective users where collaborators from different fields contribute their respective mathematical expertise to the solution of application problems. Usually, these project groups persist over a longer period of time. Thus, the specific possibilities given to a nonuniversity institute are taken advantage of, and the *horizontal linking-up* within the institute is strengthened. It is a permanent task of the institute to improve the horizontal linking-up within WIAS in order to employ its personnel resources as effectively as possible.


WEIERSTRASS-INSTITUT FÜR ANGEWANDTE ANALYSIS UND STOCHASTIK / WEIERSTRASS INSTITUTE FOR APPLIED ANALYSIS AND STOCHASTICS
im Forschungsverbund Berlin e. V.
10117 Berlin, Mohrenstraße 39
☎ +49/30/20372-587, Fax: +49/30/2044975
DIREKTOR / DIRECTOR
Prof. Dr. J. Sprekels
☎ 586
FORSCHUNGSGRUPPE/ RESEARCH GROUP 1
Partielle Differentialgleichungen und Variationsgleichungen / Partial Differential Equations and Variational Equations
Leiter / Head:
Prof. Dr.
H. Gajewski
☎ 563
FORSCHUNGSGRUPPE/ RESEARCH GROUP 2
Dynamische Systeme / Dynamical Systems
Leiter / Head:
Priv.-Doz. Dr.
K. R. Schneider
☎ 302
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Numerische Mathematik und Wissenschaftliches Rechnen / Numerical Mathematics and Scientific Computing
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Prof. Dr.
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Nichtlineare Optimierung und Inverse Probleme / Nonlinear Optimization and Inverse Problems
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N.N.
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Stochastische Systeme mit Wechselwirkung / Interacting Random Systems
Leiter / Head:
Priv.-Doz. Dr.
A. Bovier
☎ 547
FORSCHUNGSGRUPPE/ RESEARCH GROUP 6
Stochastische Algorithmen und Nichtparametrische Statistik / Stochastic Algorithms and Nonparametric Statistics
Leiter / Head:
Prof. Dr.
V. Spokoiny
☎ 575
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Leiter / Head:
Prof. Dr.-Ing.
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D. Hömberg
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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 2001 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 2001, 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 Dynamische Systeme / Research Group Dynamical Systems

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

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.

ordinary and partial differential equations as well as of large systems of differential–algebraic equations. The main task of the research group was the development, the theoretical substantiation and the implementation of numerical methods to solve such systems. The studies concentrated upon the topics

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

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

Die 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,
- Optimale Steuerung in der chemischen 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,
- Optimal control in chemical 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 nonstandard 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 An-

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 sci-

wendungsproblemen aus Naturwissenschaften und Technik auftreten. Die Arbeitsschwerpunkte lagen dabei in den Bereichen

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

ences 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 und führt die auf klassische und moderne Technologien gestützte Literaturinformation durch. Dies geschieht in enger Zusammenarbeit mit der im Bereich der Rechentechnik angesiedelten *Fachinformation*. Gehalten werden Zeitschriften, Serien, Monographien, Preprints, Reports und CD-ROM.
Die Gruppe *Rechentechnik* ist zuständig für die Versorgung des Instituts mit den Kapazitäten im Bereich der EDV, die zur Erfüllung der wissenschaftlichen Aufgabenstellung des Instituts benötigt werden. Ihr obliegt neben der Hardware- und Software-Wartung das gesamte Systemmanagement und ferner die Betreuung des hausinternen Rechnernetzes.
Die *Verwaltung* erledigt die für die Arbeitsfähigkeit des Instituts notwendigen verwaltungstechnischen und organisatorischen Aufgaben. Das WIAS ist mit derzeit sieben weiteren naturwissenschaftlichen Forschungsinstituten im Forschungsverbund Berlin e. V. (FVB) rechtlich zusammengeschlossen. Administrative Aufgaben werden im FVB zwecks einer effizienten einheitlichen Verwaltungsleistung arbeitsteilig von der *Gemeinsamen Verwaltung des FVB* und den *Institutsverwaltungen* erbracht. Zentrale administrative Leistungen und Servicefunktionen sind der Gemeinsamen Verwaltung zugeordnet, während institutsspezifi-

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, and providing literature information based on classical and modern technologies in close cooperation with the *Science Information* which is part of the Computer Department. The library offers journals, series, monographs, preprints, reports, and CD-ROMs.

The *Computer Department* is responsible for supplying the institute with electronical data processing facilities that are necessary for the accomplishment of the institute's scientific mission. 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.

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 administrative tasks. Central administrative work and service is assigned to the Common Administration whereas institute-related administrational pro-

sche Verwaltungsvorgänge und „Interface-Funktionen“ im Verhältnis zur wissenschaftlichen Arbeit direkt im Institut wahrgenommen werden. Die Zusammenarbeit zwischen Gemeinsamer Verwaltung, Geschäftsführung, Institutsleitung und Institutsverwaltung wird durch die *Geschäftsordnung des FVB* geregelt. Dem *Geschäftsführer* des FVB obliegt danach die Führung der Verwaltungsgeschäfte. Er ist der Beauftragte des Institutshaushaltes im Sinne der haushaltsrechtlichen Bestimmungen und übt die Fachaufsicht in den administrativen Angelegenheiten unter Berücksichtigung der personalrechtlichen und sachlichen Entscheidungsbefugnisse des Institutsdirektors aus.

ceedings and “interface functions” with respect to the scientific work are to be realized directly in the institute. The cooperation between the Common Administration, the FVB management, the institute’s management, and the institute’s administration in regularized in the *Rules of Procedure of FVB*. The *Manager* of FVB accordingly attends to the administrative business. He is in charge of the institute’s budget in accordance with the budgetary law and supervises the administrative business taking into account the factual competence of the institute’s director as well as his competence in the field of the institute’s personnel.

4 Research Results and Applied Projects

4.1 Research Group Partial Differential Equations and Variational Equations

4.1.1 Overview

Die Forschungsgruppe hat ihre im WIAS-Forschungsprogramm konzipierten Arbeiten zur mathematischen Modellierung und Analyse von mikro- und optoelektronischen Bauelementen sowie von Phasenumwandlungen fortgesetzt. Das Spektrum der analytischen Arbeiten reicht 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. Schwerpunkte lagen dabei auf den Gebieten:

- Ladungstransportvorgänge in Halbleitern, unter Einbeziehung thermoelektrischer, optischer und quantenmechanischer Effekte,
- Reaktions-Diffusionsgleichungen zur Beschreibung des Transports von Fremdatomen in Festkörpern,
- Phasenfeldmodelle zur Beschreibung diffusiver Phasenübergänge,
- Modellierung von Shape-Memory-Phänomenen.

Im Berichtsjahr konnte Dr. Annegret Glitzky mit der Schrift „Elektro-Reaktions-Diffusionssysteme mit nichtglatten Daten“ ihr Habilitationsverfahren an der Humboldt-Universität zu Berlin abschließen.
Ein wesentlicher Teil der Forschungsarbeiten der Gruppe wurde durch Drittmittel finanziert. Dazu gehören die im Rahmen des BMBF-Programms „Neue Mathematische Methoden in Industrie und Dienstleistungen“ geförderten Projekte:

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 installation of solution algorithms at cooperation partners.

Our main topics are:

- Charge carrier transport processes in semiconductors including thermoelectric, optical, and quantum mechanical effects,
- Reaction-diffusion equations for dopant transport in solids,
- Phase-field models for diffusive phase transitions,
- Modeling of shape-memory phenomena.

In the year under review Dr. Annegret Glitzky received the degree Dr. habil. from the Humboldt-University of Berlin with the paper “Elektro-Reaktions-Diffusionssysteme mit nichtglatten Daten” (Electro-reaction-diffusion systems with nonsmooth data).

An essential part of the research work of the group has been funded from external sources: The projects

- 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

have been supported by the BMBF Program "New Mathematical Methods in Industry and Services".

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.

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 a Schrödinger-Poisson system 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.

Von der Industrie finanziert wurden die Projekte:

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

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

Studies on infrared RW lasers

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

Cooperation with: F. Fidorra, Ch. Radüge (MergeOptics GmbH, Berlin), J. Kreissl (Heinrich-Hertz-Institut für Nachrichtentechnik (HHI) Berlin GmbH)

Supported by: MergeOptics GmbH

Investigations on InP-based 1.55 μm-emitting Ridge Waveguide semiconductor lasers with strained Multi Quantum Well active region by MergeOptics GmbH have been performed for improving their performance. The simulations have been based on the device simulator `WIAS-TeSCA`, which allows for a selfconsistent treatment of the optical, electrical, and thermal behavior of semiconductor devices (see Fig. 1).

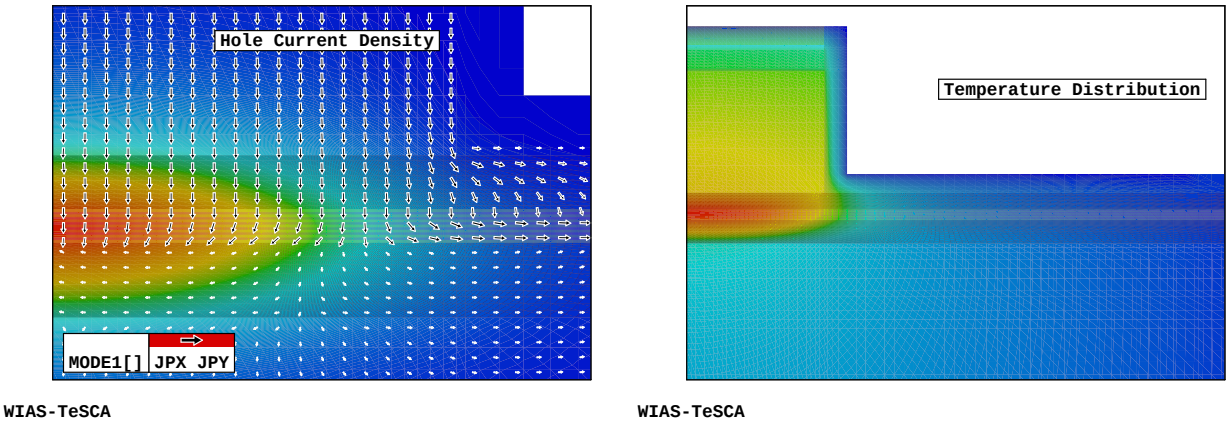

Fig. 1: Simulated hole injection current density and power distribution (left) and temperature distribution (right) in a part of the transverse cross-section of a RW-MQW laser

Among others, simulation results have been compared with measurements, which have been performed at HHI Berlin ([2]). Simulated device characteristics showed a good agreement with experimental findings, cf. the power-current characteristics in Fig. 2. Besides the behavior in the non-thermal regime (below 100 mA in Fig. 2) also the impact of the internal heating (Fig. 1, right) at higher injection currents is displayed properly by the simulations.
Based on this fact, further simulations have been used to predict properties with relevance for applications of possible future devices with changed geometry.

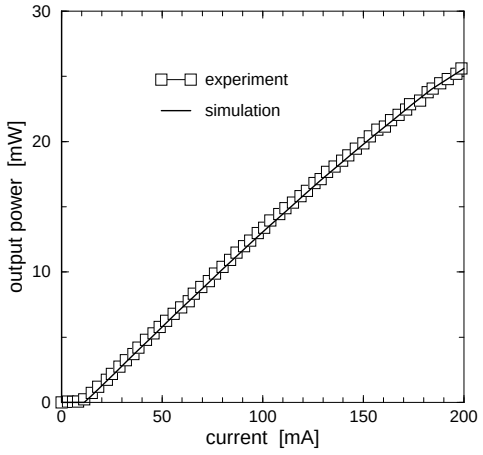

Fig. 2: Power-current characteristics, measured for a set of devices (boxes) and simulated with `WIAS-TeSCA` (solid line)

Using the optical field distribution at the facet of the laser, which has been obtained as one of the outputs of `WIAS-TeSCA`, also the farfield distribution has been calculated in a postprocessing procedure ([1]). Again, such farfield distributions have been compared with experimental data which have been obtained from measurements at HHI. Some typical farfield intensity patterns are displayed within Fig. 3.

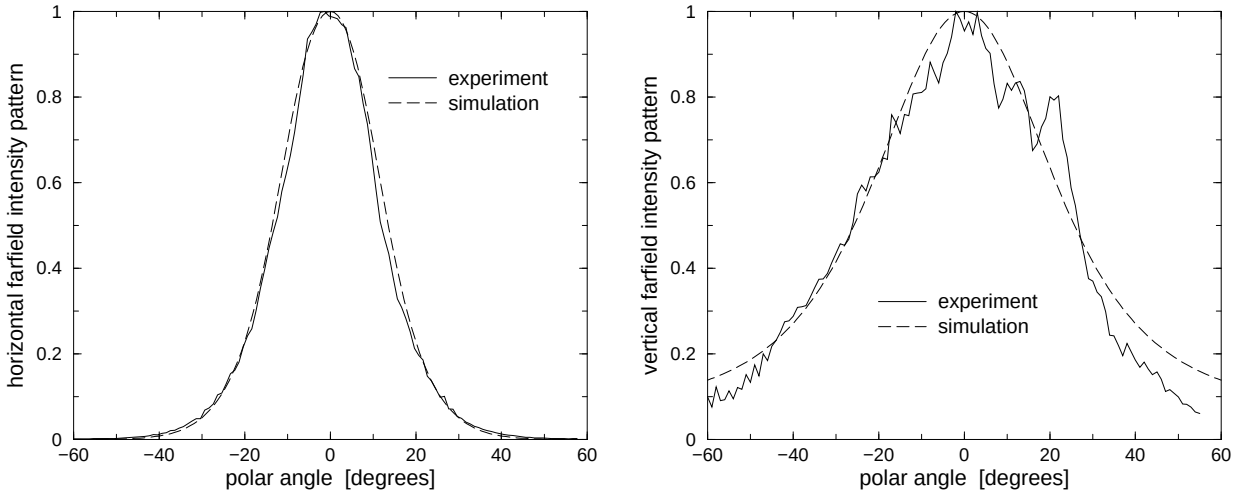

Fig. 3: Farfield intensity pattern, left: horizontal direction (parallel to the quantum wells), right: vertical direction (perpendicular to the quantum wells). Solid lines: experiment, dashed lines: simulation.

Basic farfield characteristics, as FWHM[1]-parameters and basic diffraction effects could be reproduced by the simulations in good agreement with the measurements, see Fig. 3. However, some details, especially of the vertical farfield intensity pattern (Fig. 3, right) are very difficult to be resolved by the model implemented so far. For the investigation of such effects future work would be required.

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[1]Full Width of Half Maximum.

Open quantum systems driven by a macroscopic current

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

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

The general goal of this research is the modeling of semiconductor multi quantum well lasers on the basis of a mixed model: One part is governed by van Roosbroeck's system while a neighborhood of the active zone is described by quantum mechanics. To that end we aim at an embedding of a quantum mechanically described structure into a macroscopic flow. The problem is that usually in quantum mechanics selfadjoint Schrödinger operators (including selfadjoint boundary conditions) are regarded, but selfadjoint Schrödinger operators necessarily lead to vanishing currents within the substructure. This consequence, however, is unacceptable from a physical point of view. Having in mind a current continuity condition for both the quantum and macroscopic current, in [6]/[7] the following setup for the description of an open quantum system driven by an adjacent macroscopic flow was proposed:
Let the open quantum system be situated in a bounded spatial domain Ω of $\mathbb{R}^d$, $d \leq 3$. There we regard the Schrödinger equation

$$-\frac{\hbar^2}{2}\nabla\cdot\left(m^{-1}\nabla\psi\right)+V\psi = f \qquad \text{in } \Omega \tag{1}$$

with a mass tensor m, a complex-valued potential V, and the boundary condition

$$\hbar\,\nu\cdot m^{-1}\nabla\psi = i\,\psi\,\nu\cdot\mathfrak{v} \qquad \text{on } \partial\Omega, \tag{2}$$

where ν denotes the outer unit normal on $\partial\Omega$. This system is partly driven by an adjacent macroscopic flow acting on the boundary $\partial\Omega$ of Ω. The macroscopic flow is assumed to be of the form $J = -U\,\mathfrak{v}$, where U is the density of the macroscopic transport quantity and $\mathfrak{v}$ is the corresponding velocity density. In particular, we have in mind a gradient flow $J = -DU\nabla\Phi$ with $U = F(\Phi)$ which is governed by a reaction-diffusion equation

$$\frac{\partial U}{\partial t}+\nabla\cdot J = R(U,J) \tag{3}$$

in a neighborhood of Ω. With non-smooth coefficients and mixed boundary conditions such an equation allows only for little regularity of the flow it governs ([1]). That is why we make only weak assumptions on the regularity of the flow acting on the boundary of Ω. The crucial point is that the boundary condition (2) cannot be implemented by using the usual boundary integral within the weak formulation, but has to be defined by a more subtle form approach, due to the deficient regularity of the adjacent macroscopic flow. Additionally, non-vanishing imaginary parts of the Schrödinger potentials, reflecting absorptive and dispersive properties of the substrate, have to be included in this context. Naturally, in a first step, the spectral properties of the—essentially non-selfadjoint—Schrödinger operators are of interest. The abstract framework for the rigorous definition and spectral analysis of the Schrödinger-type operator (1), (2) is the form perturbation method with a symmetric principal part and a non-symmetric part which is form-subordinated to it. In [4] under minimal (and realistic ([1])) assumptions on the macroscopic flow, the following assertions about the thus defined Schrödinger operator have been proven:

1. Its resolvent belongs to the same summability class as the resolvent of the free Hamiltonian (with Neumann boundary conditions).

2. It generates an analytic semigroup on L^2.

3. It has no real eigenvalues and is, consequently, completely non-selfadjoint.

4. In the two- and three-dimensional case there is an Abel basis of root vectors in L^2; in the one-dimensional case one obtains a Riesz basis of root vectors.

5. If the non-selfadjoint Schrödinger operator is dissipative, then the imaginary part of the potential must be positive, and the boundary form is given by a positive measure times the imaginary unit.

In the situation of a closed quantum system the Schrödinger-Poisson system ([2], [3], [6], [7]) turned out to give an adequate description of the occurring physical quantities such as carrier densities and electrostatic potential. This was the reason for our attempt to re-establish a Schrödinger-Poisson system in the situation of an open quantum system. At first, physical notions as carrier and current densities have to be re-defined in the case of open quantum systems. The key for doing so is the observation that the open quantum system always may be embedded by dilation theory into a closed one at least if the corresponding Hamiltonian is dissipative (or anti-dissipative) ([4]). In the spatially one-dimensional case the enlarged Hilbert space and the corresponding selfadjoint operator admit an explicit description ([5]), this is why we first investigated this situation. In [5] the required dilation of the non-selfadjoint Schrödinger operator is performed, the characteristic function is determined and a (generalized) eigenfunction expansion is carried out. On the basis of this, the fundamental notions of steady state, carrier density, and current density can be defined, and the concept of a dissipative Schrödinger-Poisson system can be established. The electron/hole densities u^+, u^- are determined by

$$\int_\omega u^{+/-}\,dx = tr(\rho^{\pm}\chi_\omega), \tag{4}$$

where ω is any Borel subset of the interval Ω, and ρ^+, ρ^- are density matrices, related to the Schrödinger-type operators (1)–(2) for holes and electrons, respectively, which act on the Hilbert space $L^2(\Omega)$. The dependence of the carrier density on the Schrödinger potential has been investigated concerning estimates and continuity properties. Having these things at hand, we intend to prove the existence of a solution for the dissipative Schrödinger-Poisson system.

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On a nonlocal phase separation model

Collaborators: H. Gajewski, K. Zacharias

We consider a binary alloy with components A and B occupying a spatial domain Ω. We denote by u and $1-u$ the (scaled) local concentrations of A and B, respectively. Let $(0,T)$ denote a time interval, ν the outer unit normal on the boundary $\Gamma=\partial\Omega$, and $Q=(0,T)\times\Omega$, $\Gamma_T=(0,T)\times\Gamma$.
To describe phase separation in binary systems, one usually uses the Cahn-Hilliard equation. This equation is derived ([1]) from a free energy functional of the form

$$F_{CH}(u)=\int_\Omega\Big\{f(u)+\kappa u(1-u)+\frac{\lambda}{2}\Big|\nabla u\Big|^2\Big\}dx. \tag{1}$$

Here f is a convex function with the property that $f(u)+\kappa u(1-u)$ (for sufficiently large κ) forms a so-called double well potential. Minimizing F_{CH} under the constraint of mass conservation, one identifies the Lagrange multiplier v via the associated Euler-Lagrange equation

$$v=f'(u)+\kappa(1-2u)-\lambda\Delta u \tag{2}$$

as chemical potential. Now one postulates that $-\nabla v$ is the driving force for the mass flux $\mathbf{j}$, i.e.

$$\mathbf{j}=-\mu\nabla v$$

with a suitable mobility μ. Considering the mass balance, one ends up with the Cahn-Hilliard equation

$$\frac{\partial u}{\partial t}-\nabla\cdot[\mu\ \nabla(f'(u)+\kappa(1-2u)-\lambda\Delta u)]=0\text{ in }Q,\quad \nu\cdot(\mu\nabla v)=0\text{ on }\Gamma_T, \tag{3}$$

where the Neumann boundary condition guarantees mass conservation

$$\int_\Omega u(t,x)dx=\int_\Omega u(0,x)dx.$$

Inspecting Cahn-Hilliard's arguments ([1]) establishing (1) as the free energy of the binary system, it seems to be reasonable and even more adequate ([7]) to choose an alternative nonlocal expression like

$$F(u)=\int_\Omega\Big\{f(u)+u\int_\Omega\mathcal{K}(|x-y|)(1-u(y))\,dy\Big\}dx, \tag{4}$$

where the kernel $\mathcal{K}$ of the integral term describes nonlocal interaction. By a simple calculation, we find from (4) the corresponding chemical potential v as the gradient of F in the form

$$v=f'(u)+w,\quad w(x)=\int_\Omega\mathcal{K}(|x-y|)(1-2u(y))\,dy. \tag{5}$$

Replacing (2) by (5), one gets instead of (3) the problem

$$\frac{\partial u}{\partial t}-\nabla\cdot(\mu\nabla(f'(u)+w))=0\text{ in }Q,\quad \nu\cdot(\mu\nabla v)=0\text{ on }\Gamma_T. \tag{6}$$

In the standard case $f(u) = u\log u + (1-u)\log(1-u)$, we have $f'(u) = \log\left(\frac{u}{1-u}\right)$, and hence by (5)

$$u = \mathcal{F}(w-v), \quad \mathcal{F}(s) := 1/(1+e^s).$$

The image of the Fermi function $\mathcal{F}$ is the interval $[0,1]$, so that the nonlocal model automatically satisfies the physical requirement $0 \le u(x) \le 1$. This property cannot be guaranteed for solutions of the original Cahn-Hilliard equation, since for fourth-order equations no maximum principle is available. Moreover, by physical reasons it is desirable to admit mobilities μ depending on u and $|\nabla v|$. A natural choice is $\mu = a(|\nabla v|)/f''(u)$ ([2], [7]) with a function a such that $s \mapsto a(s)s$ is monotone. Then problem (6) can be rewritten as

$$\frac{\partial u}{\partial t} - \nabla \cdot \left[a\left(\nabla u + \frac{\nabla w}{f''(u)} \right) \right] = 0 \text{ in } Q, \quad \nu \cdot \left[a\left(\nabla u + \frac{\nabla w}{f''(u)} \right) \right] = 0 \text{ on } \Gamma_T. \tag{7}$$

It seems worth mentioning that diffusion equations with a nonlocal drift term of this form also model transport processes in semiconductor ([4]) and chemotaxis ([5]) theory.
In this project we proved existence and uniqueness of a global solution u to (7). Moreover, we studied the asymptotic behavior as time going to infinity and characterized the asymptotic state by a variational principle ([6]). An extension to non-isothermal situations was also given ([3]).

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Generalized electro-reaction-diffusion systems in heterostructures

Collaborators: A. Glitzky, R. Hünlich

Cooperation with: K. Gröger (Humboldt-Universität zu Berlin)

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)

Models describing the transport of dopants in semiconducting materials via pair diffusion mechanisms are considered at very different modeling levels. Generally, such models contain continuity equations, a Poisson equation, and often nonlocal relations which express invariance properties such as global charge conservation. There exists a hierarchy of such models which is based on physically motivated assumptions concerning the time scales of different kinetic subprocesses (see [1, Chap. 5]). Starting from a basic model where all relevant species (electrons, holes, dopants, defects, and dopant-defect pairs) are balanced by continuity equations, one can finally reach a reduced model where only the total amount of each dopant is balanced. Most of such model equations at the different reduction levels can be written in a unified way as a generalized electro-reaction-diffusion system which we have studied last year. Many other problems in the field of electro-diffusion fit into this general setting, too.
We consider m species X_i where only the first l ones are assumed to underly drift-diffusion processes. Let z_0 denote the electrostatic potential, let $z = (z_0, \dots, z_k)$, where the components z_j, $j = 1, \dots, k$, are some additional quantities representing the electrochemical potential of species eliminated by the foregoing model reduction. The functions $p_i(\cdot, z)$ are suitably chosen reference densities of the special structure

$$p_i(x,z) = p_{0i}(x)\, \mathrm{e}^{P_i(z)}, \quad i = 1, \dots, m.$$

The problem is formulated in terms of the vector u of particle densities u_i, of the vector b of chemical activities $b_i = u_i / p_{0i}$, and of the vector z. The investigated model equations consist of m continuity equations

$$\begin{aligned}
\frac{\partial u_i}{\partial t} + \nabla \cdot j_i + \sum_{(\alpha,\beta)} (\alpha_i - \beta_i) R^{\Omega}_{\alpha\beta} &= 0 \quad \text{on } (0,\infty) \times \Omega, \\
\nu \cdot j_i - \sum_{(\alpha,\beta)} (\alpha_i - \beta_i) R^{\Gamma}_{\alpha\beta} &= 0 \quad \text{on } (0,\infty) \times \partial\Omega, \quad i = 1, \dots, l, \\
\frac{\partial u_i}{\partial t} + \sum_{(\alpha,\beta)} (\alpha_i - \beta_i) R^{\Omega}_{\alpha\beta} &= 0 \quad \text{on } (0,\infty) \times \Omega, \quad i = l+1, \dots, m, \\
u_i(0) &= U_i \quad \text{on } \Omega, \quad i = 1, \dots, m,
\end{aligned} \tag{1}$$

which are coupled with a nonlinear Poisson equation

$$\begin{aligned}
-\nabla \cdot (\varepsilon \nabla z_0) + \frac{\partial H}{\partial z_0}(\cdot, u, z) &= f_0 \quad \text{on } (0,\infty) \times \Omega, \\
z_0 &= 0 \quad \text{on } (0,\infty) \times \Gamma_D, \\
\nu \cdot (\varepsilon \nabla z_0) + \tau z_0 &= 0 \quad \text{on } (0,\infty) \times \Gamma_N,
\end{aligned} \tag{2}$$

and other nonlocal conservation laws

$$\int_\Omega \frac{\partial H}{\partial z_j}(\cdot,u,z)\,\mathrm{d}x = f_j \quad \text{on } (0,\infty), \quad j=1,\dots k. \tag{3}$$

Here ε is the dielectric permittivity, f_0 is a fixed charge density, and f_j represent prescribed values of invariants. The function H is given by

$$H(x,u,z) = h(x,z) - \sum_{i=1}^m P_i(z)\,u_i,$$

with some function h which is determined by the reduction scheme. The particle fluxes for the mobile species X_i, $i=1,\dots,l$, have the form

$$j_i = -D_i(\cdot,b,z)p_{0i}\big[\nabla b_i + Q_i(z)\,b_i\nabla z_0\big],\ i=1,\dots,l\,,$$

where $Q_i(z) = \frac{\partial P_i}{\partial z_0}(z)$ denote the charge numbers depending on the state z in our setting. The continuity equations contain volume source terms resulting from a lot of reversible reactions

$$\alpha_1 X_1 + \dots + \alpha_m X_m \rightleftharpoons \beta_1 X_1 + \dots + \beta_m X_m,$$

where $\alpha,\beta \in \mathbb{Z}_+^m$ are the vectors of stoichiometric coefficients. According to the mass action law, the corresponding reaction rates $R^\Omega_{\alpha\beta}$ are written as

$$R^\Omega_{\alpha\beta}(x,b,z) = k^\Omega_{\alpha\beta}(x,b,z)\Big[\prod_{i=1}^m a_i^{\alpha_i} - \prod_{i=1}^m a_i^{\beta_i}\Big],\ x\in\Omega,\ b\in\mathbb{R}^m_+,\ z\in\mathbb{R}^{k+1},\ a_i = b_i\mathrm{e}^{P_i(z)}.$$

For all immobile species X_i, $i=l+1,\dots,m$, there should be a special reaction of the form

$$R^\Omega_{\alpha\beta} = k^\Omega_{\alpha\beta}\big[\prod_{j=1}^l a_j^{\alpha_j} - a_i^2\big]. \tag{4}$$

Additionally, we take into account boundary reactions between the mobile species with reaction rates $R^\Gamma_{\alpha\beta}$. The kinetic coefficients D_i, $k^\Omega_{\alpha\beta}$, and $k^\Gamma_{\alpha\beta}$ are allowed to depend on the space variable and on the state (b,z). Moreover, unlike our former investigations of electro-reaction-diffusion systems, also immobile species, initial densities U_i vanishing on sets of positive measure and nonsmooth data (heterostructures) are treated.

In [4] we proved an existence result for (1)–(3) at a special level in the hierarchy of pair diffusion models. But there we considered only homogeneous structures with smooth boundaries, and all species were assumed to be mobile. In [2] we derived global estimates for solutions of that model but now involving heterostructures and immobile dopants. The existence theory for these model equations is contained in [3].

In the weak formulation of (1)–(3), both the Poisson equation (2) and the nonlocal conservation laws (3) are formulated as a generalized Poisson equation $\mathcal{E}(z,u)=0$. For every fixed u, the operator $\mathcal{E}(\cdot,u)$ is a strongly monotone potential operator. By means of the potential of this operator and of the usual chemical ansatz, the free energy functional

$$F(u) = \int_\Omega \Big\{\frac{\varepsilon}{2}|\nabla z_0|^2 - H(\cdot,u,z) + \sum_{j=0}^k \frac{\partial H}{\partial z_j}(\cdot,u,z)\,z_j\Big\}\,\mathrm{d}x + \int_{\Gamma_N}\frac{\tau}{2}z_0^2\,\mathrm{d}\Gamma$$
$$+ \int_\Omega \sum_{i=1}^m p_{0i}\Big\{\frac{u_i}{p_{0i}}\big(\ln\frac{u_i}{p_{0i}} - 1\big) + 1\Big\}\,\mathrm{d}x, \quad u\in L^2_+(\Omega,\mathbb{R}^m)$$

is derived, where z is the unique solution of $\mathcal{E}(z,u)=0$. The functional F turns out to be a Ljapunov functional. Under the assumption of no false equilibria in the sense of Prigogine, there is a thermodynamic equilibrium which is uniquely defined by the structure of the stoichiometric subspace and by the initial state. Exploiting the existence of reactions of the form (4), an estimate of the free energy by the dissipation rate

$$\begin{aligned}\mathcal{D}(u) &= \int_\Omega \sum_{i=1}^{l} 4D_i(\cdot,b,z)p_i(\cdot,z)|\nabla\sqrt{a_i}|^2\,\mathrm{d}x \\ &\quad + \int_\Omega \sum_{(\alpha,\beta)} 4k^\Omega_{\alpha\beta}(\cdot,b,z)\Big|\prod_{i=1}^{m}\sqrt{a_i}^{\alpha_i} - \prod_{i=1}^{m}\sqrt{a_i}^{\beta_i}\Big|^2\,\mathrm{d}x \\ &\quad + \int_\Gamma \sum_{(\alpha,\beta)} 4k^\Gamma_{\alpha\beta}(\cdot,b_1,\dots,b_l,z)\Big|\prod_{i=1}^{l}\sqrt{a_i}^{\alpha_i} - \prod_{i=1}^{l}\sqrt{a_i}^{\beta_i}|^2\,\mathrm{d}\Gamma,\end{aligned}$$

where $\mathcal{E}(z,u)=0$, $b_i=u_i/p_{0i}$, $a_i=b_i\,\mathrm{e}^{P_i(z)}$, guarantees the exponential decay of the free energy along trajectories. This leads to essential tools for the proof of global upper bounds of solutions. Starting with two preliminary estimates, a Moser iteration scheme supplies the global bounds for the particle densities of the mobile species. Then a corresponding assertion for the immobile species can be obtained straightforward. Using these global estimates, the exponential decay of densities u_i, chemical activities b_i, and potentials z_0 and z_j to their equilibrium values can be verified.

For the existence proof we carry out two steps of regularization and consider problems (P_N) and (P_M). The first step (P_N) contains regularizations in the volume and boundary reaction terms of the continuity equations only. By means of energy estimates and Moser iteration we derive a priori estimates which are independent of the regularization level N. A further regularization in the drift terms of (P_N) leads to a problem (P_M). The existence of solutions of (P_M) follows by two fixed-point iterations (Banach's fixed-point theorem for the equations of the immobile species, Schauder's fixed-point theorem for the equations of the mobile species). Moreover, we verify estimates for the solutions of (P_M) which are independent of the regularization level M which finally leads to the existence result.

The presented results concerning the generalized electro-reaction-diffusion system (1)–(3) and their proofs can be found in [1, Chap. 8].

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Optimal control of surface heat treatments

Collaborators: D. Hömberg, W. Weiss

Cooperation with: LASERVORM Volumen- und Oberflächenbearbeitung (Mittweida), probeam HÖRMANN GmbH (Neukirchen), J. Sokołowski (Université de Nancy I, France), H.-J. Spies (TU Bergakademie Freiberg), S. Volkwein (Karl-Franzens-Universität Graz, Austria)

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.

A. Laser and electron beam hardening.
Last year's work in our industrial project on simulation and control of laser and electron beam hardening was concerned with aspects of modeling, software engineering, and optimal control.

- Modeling

  Here, the main focus was on a model for the electron radiation flux in electron beam hardening. Compared to the laser hardening technology, the electron beam technology is much more flexible and can easily generate a wealth of different radiation profiles. Figure 1 shows two typical situations. The radiation flux profile on the left is applied for tasks where the workpiece is moved in one direction. The profile on the right-hand side corresponds to a ring-shaped exposure without workpiece movement.

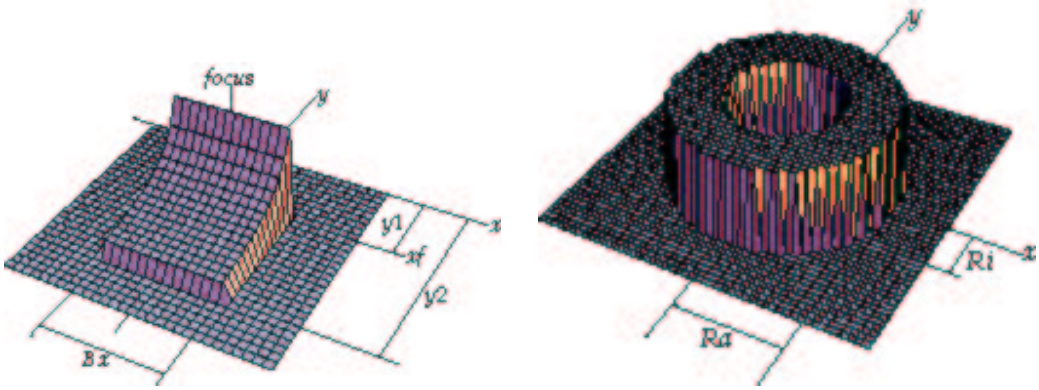

Fig. 1: Typical radiation flux profiles in electron beam hardening

- Software engineering

  Based on *pdelib*, a new software for electron and laser beam surface hardening, called *WIAS-SHarP*, has been developed. It contains additional routines to describe the phase transition kinetics during a heat treatment cycle (cf. [2]). 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 (cf. Fig. 2).

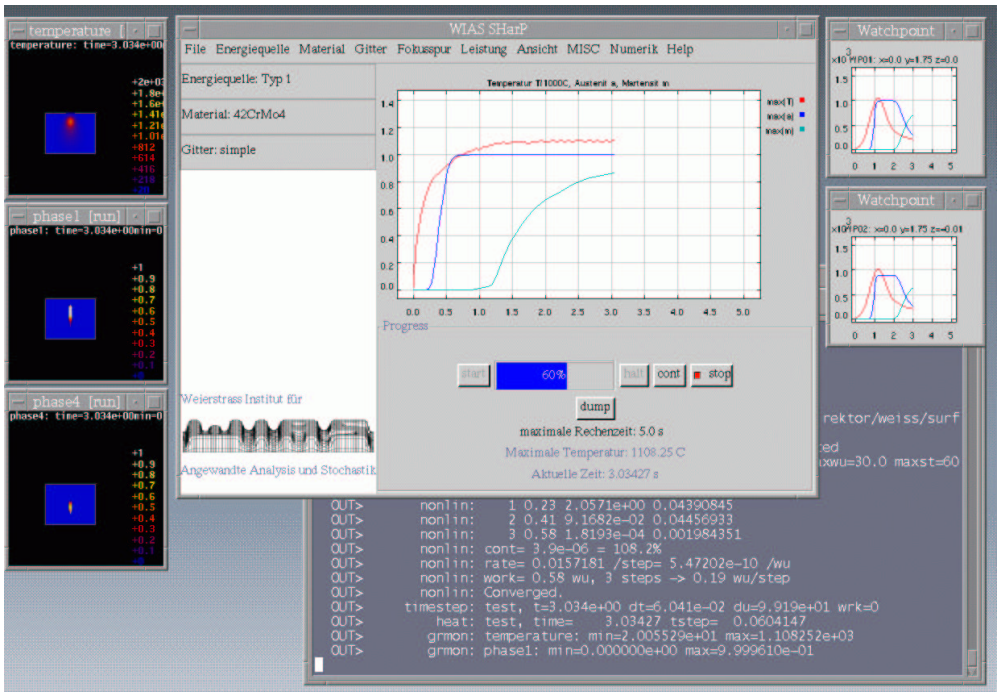

Fig. 2: Graphical user interface of the new software *WIAS-SHarP* (screenshot)

- Optimal control

  The goal of surface hardening is to achieve a desired distribution of martensite in the boundary layers of a workpiece, avoiding a melting of the surface. This goal can easily be formulated in terms of an optimal control problem. As usual, the complete control problem with PDE constraints is too big to be treated numerically. Therefore, in [3] we have used a POD ansatz for model reduction. The results (so far only in 2-d) are quite satisfactory.

  However, it turns out that the special structure of our control problem with a moving heat source, which is more or less a smeared-out point source, admits the derivation of a heuristic control strategy (cf. Fig. 3).

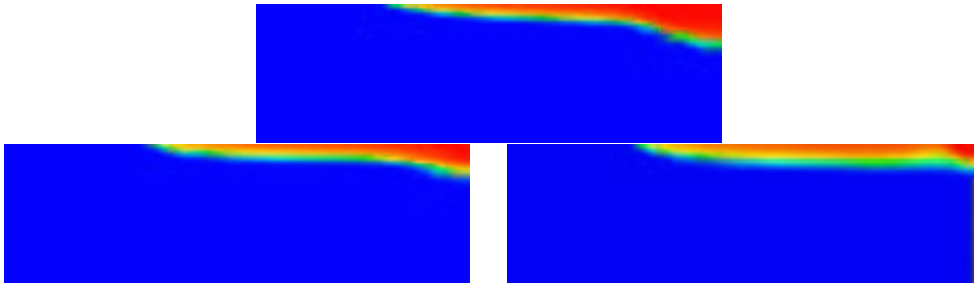

Fig. 3: Control of laser surface hardening to achieve a constant hardening depth: uncontrolled (top); with constant surface temperature (bottom left); with constant hardening profile in a fixed distance from the surface (bottom right).

B. Induction hardening.
In [1] a rather complete mathematical treatment of induction hardening has been given. The resulting system of model equations consists of an elliptic equation for the scalar potential, a

degenerate parabolic system for the magnetic vector potential, a quasistatic momentum balance coupled with a nonlinear stress-strain relation, and a nonlinear energy balance equation. Owing to the quadratic Joule heat term and a quadratic mechanical dissipation term in the energy balance, we obtain a parabolic equation with L^1 data. We prove existence of a weak solution to the complete system using a truncation argument.
Unfortunately, in most cases the geometry of the region to be hardened does not allow to have a simple annular inductor shape. But even when the principal topology of the inductor is already fixed, the coupling distance between inductor and workpiece and the spacing of the coil turns have to be adjusted carefully in order to obtain the desired heating or hardening pattern.
This problem is also addressed in [1]. A major issue in this connection is to find a decent mathematical formulation of the design problem. We show that induction coils can conveniently be described as tubes, constructed from space curves. To investigate the shape sensitivity with respect to perturbations of the coil, we employ the speed method for an admissible velocity field. We prove the existence of strong material derivatives for the state variables. An application of the structure theorem then allows us to conclude that the shape gradient only depends on normal variations of the velocity field. This normal velocity component, however, can be computed from a perturbation of the curve. Therefore, we are able to give a necessary optimality condition in terms of perturbations of the curve.
Probably, this new procedure of characterizing the optimal configuration of tubes will admit further applications, for instance in optimal design problems related to the flow of liquids through pipelines.

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Hysteresis operators in phase-field equations

Collaborators: O. Klein, J. Sprekels

Cooperation with: N. Kenmochi (Chiba University, Japan), P. Krejčí (Academy of Sciences of the Czech Republic, Prague), U. Stefanelli (Università di Pavia, Italy), C. Verdi (Università di Milano, Italy), S. Zheng (Fudan University, Shanghai, China)

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 diffusive effects as well as hysteretic phenomena.
(a) The hysteretic phenomena are modeled by hysteresis operators. A typical example is the *multi-dimensional stop operator $\mathcal{S}_Z$ with the characteristic set Z*, which is defined for a convex, closed subset Z of $\mathbb{R}^m$. For a final time $T > 0$, this operator maps a pair (u, x^0) consisting of an input function $u : [0,T] \to X$ and some $x^0 \in Z$ to the solution $x : [0,T] \to X$ to the variational inequality

$$\begin{cases} u(t) = x(t) + \xi(t), \quad x(t) \in Z, \quad \forall t \in [0,T], \\ \langle \xi_t(t), x(t) - y \rangle \geq 0, \quad \forall y \in Z, \quad \text{for a.e.} \quad t \in (0,T), \\ x(0) = x^0, \end{cases} \tag{1}$$

where $\langle \cdot, \cdot \rangle$ denotes the inner product on $\mathbb{R}^m$. The stop operator is used to define the corresponding *multi-dimensional Prandtl-Ishlinskii operators*

$$\mathcal{H}[u](t) = \int_0^\infty \phi(r) \mathcal{S}_{rZ}[u, x_r^0](t) \, \mathrm{d}r, \tag{2}$$

where $\phi \geq 0$ is a real-valued function and, for $r \geq 0$, $x_r^0 \in rZ := \{rz \in \mathbb{R}^m : z \in Z\}$ is an initial value for the stop operator S_{rZ} with the characteristic set rZ. In [9], these hysteresis operators are investigated, and for a phase-field system involving multi-dimensional Prandtl-Ishlinskii operators the existence of a unique solution is proved. This is an extension of results in the previous work ([8]), since it is no longer required that the domain Z must be polyhedral. More general classes of multi-dimensional Prandtl-Ishlinskii operators have been studied in [11].
The mathematical modeling of nonlinear thermo-visco-plastic developments leads to the following system

$$\rho u_{tt} - \mu u_{xxt} = \sigma_x + f(x,t), \tag{3}$$

$$\sigma = \mathcal{H}_1[u_x, w] + \theta \mathcal{H}_2[u_x, w], \tag{4}$$

$$(C_V \theta + \mathcal{F}_1[u_x, w])_t - \kappa \theta_{xx} = \mu u_{xt}^2 + \sigma u_{xt} + g(x,t,\theta), \tag{5}$$

$$\nu w_t + \mathcal{H}_3[u_x, w] + \theta \mathcal{H}_4[u_x, w] = 0, \tag{6}$$

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 [12], this system has been derived, the thermodynamic consistency of the model has been proved, and the existence of a unique strong solution to an initial-boundary value problem for this system has been shown. A large time asymptotic result for this system is presented in [5]. For almost the same problem with a

more general boundary condition, similar existence and asymptotic results have been derived. An approach used in [5] to derive uniform estimates for the solutions to partial differential equations involving hysteresis operators has been further investigated in [6]. Moreover, in [6], generalizations of the scalar Prandtl-Ishlinskii operators are introduced and investigated with respect to their thermodynamic consistency.
The system (3)–(6) can be simplified by adding u_{xxxx} on the left-hand side of (3). The corresponding system has been considered in [13].

(b) Phase-field systems of Penrose-Fife type are models for diffusive phase-transition phenomena, see [14]. For a non-conserved scalar order parameter χ, one gets the system

$$(C_V\theta + \lambda(\chi))_t - \kappa_0\Delta(\alpha(\theta)) = g, \tag{7}$$

$$\eta\chi_t - \varepsilon\Delta\chi + s'(\chi) = -\frac{\lambda'(\chi)}{\theta}. \tag{8}$$

In this system C_V, κ_0, and ε are given positive constants, and λ, α, s, g are given functions.
In [7], an a posteriori error estimate has been derived for a time-discrete scheme for the system (7)–(8), with η being a positive constant, and $\alpha(\theta) = -1/\theta$.
The system (7)–(8) with η depending on $\nabla\chi$ can be used to model the anisotropic solidification of liquids. The existence of a solution to this system has been shown in [4].
Following [1, 2], the system (7)–(8) is modified by replacing $-\Delta\chi$ in (8) by an integral operator and allowing η to be a function of θ. For an integrodifferential (non-local) system derived in this way, results concerning global existence, uniqueness, and large-time asymptotic behavior have been derived in [15].
In another modification of the phase-field system, the energy balance (7) is coupled with two order parameter equations:

$$w_t - \gamma\Delta w - \kappa_0\alpha(\theta)\lambda'(\chi) = 0, \tag{9}$$

$$\eta\chi_t - \varepsilon\Delta\chi + \partial I_Z(\chi) + \sigma(\chi) \ni w_t, \tag{10}$$

where w is a scalar-valued order parameter, χ is an order parameter with values in $\mathbb{R}^m$, and ∂I_Z is the subdifferential of the indicator function I_Z of a bounded, closed, convex set $Z \subset \mathbb{R}^m$. Formally, this system can be considered as a diffusive approximation of the corresponding multi-dimensional stop operator $\mathcal{S}_Z$. Results concerning existence, uniqueness, and continuous dependence on data have been presented in [3].
In [10], it has been proved for another phase-field system that the solutions are approximations for the evaluation of the stop operator.

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Optimization of curved mechanical structures

Collaborators: J. Sprekels, D. Tiba

The aim is to develop new approaches to the analysis and the optimization of curved mechanical structures like curved rods and shells. This is a continuation of the investigations on arches [1] and beams and plates [4]. Much attention is paid to the relaxation of the smoothness assumptions on the geometry of the mechanical structures.

(a) Control variational methods.
In the case of arches and plates, a new variational approach based on optimal control theory allows minimal regularity assumptions: plates with discontinuous thickness and absolutely continuous arches. In the latter case, if the tangent vector is non-zero a.e., then the classical reparametrization gives Lipschitzian representation of the arches with unit tangent vectors. It should be noted that the classical variational formulation of the Kirchhoff–Love model for arches requires three times bounded derivability of the parametrization. Moreover, the new method allows to prove the continuity and the Gâteaux/Fréchet differentiability of the mapping coefficient $\mapsto$ solution, in very weak norms. These results can be found in the papers [1], [5].

(b) Optimization of curved rods.
We are using a model that has been developed and studied, both from a theoretical and a numerical point of view, in [2]. It consists of a system of nine ordinary differential equations with null boundary conditions (the rod is clamped). Besides the deformation of the line of centroids, the cross-section may change its shape as well. The class of admissible geometries for the optimum problem is obtained by first generating the unit tangent vectors

$$\bar{t} = (\sin\varphi\cos\psi, \sin\varphi\sin\psi, \cos\varphi),$$

and by obtaining the parametrization via integration

$$\bar{\theta}(s) = \int_0^s \bar{t}(\tau)\,d\tau, \quad s \in [0,L].$$

The given cross-section is not necessarily constant. The mappings φ, ψ are in $C^1(0,L)$. The local frame can be obtained directly,

$$\begin{aligned} \bar{n} &= (\cos\varphi\cos\psi, \cos\varphi\sin\psi, -\sin\varphi), \\ \bar{b} &= (-\sin\varphi, \cos\psi, 0). \end{aligned}$$

In this way, the obtained three-dimensional curves have automatically a prescribed length L, which is an essential requirement in the study of the corresponding optimal design problems. Moreover, avoiding the usage of the Frenet frame allows to consider $C^2(0,L)^3$-parametrizations, which is an improvement over the existing literature, where C^3 assumptions are required.
The examined problem consists of the minimization of a general cost functional depending on the unknown geometry $\bar{\theta} \in C^2(0,L)^3$ and the deformation $\bar{y} \in H_0^1(0,L)^9$

$$\text{Min}\Big\{ j(\bar{\theta},\bar{y}) \Big\}, \qquad \textbf{(P)}$$

under the constraint $\bar{\theta} \in \mathcal{K} \subset C^2(0,L)^3$, a closed bounded subset. Important examples are quadratic cost functionals j and conditions that may be included in the definition of $\mathcal{K}$:

$$0 \leq \varphi \leq \frac{\pi}{2} - \varepsilon \quad \text{a.e. in } [0,L]$$

($\bar{\theta}$ has no multiple points),

$$\int_0^L t_1(\tau)\, d\tau = \int_0^L t_2(\tau)\, d\tau = 0$$

(periodicity conditions for θ_1, θ_2), etc.
Continuity and Gâteaux differentiability with respect to φ, ψ of the deformation $\bar{y}$ are proved in $C^1(0,L)^2 \times H_0^1(0,L)^9$, equipped with the strong topologies. This allows to establish the existence of optimal shapes $\bar{\theta}^*$ for problem **(P)** and the writing of the first order optimality conditions. Numerical tests will be performed as well, [7].

(c) Optimization of shells.
We consider the Naghdi-type shell model introduced in [6]. It is assumed that the middle surface of the shell is the graph of a function $p \in C^2(\bar{\omega})$, $\omega \subset \mathbb{R}^2$ open, bounded, (multiply) connected, and the thickness is constant.
The shape optimization problem is expressed as above, by the minimization of a general cost functional depending on the geometry $p \in C^2(\bar{\omega})$ and on the deformation $\bar{y} \in H^1(\omega)^2$. Constraints of the type $p \in \mathcal{K} \subset C^2(\bar{\omega})$, closed bounded subset, may be as well imposed.
To study the continuity and the differentiability properties of the mapping $p \mapsto \bar{y}$ is very difficult, since Korn-type inequalities with constants independent of the unknown geometry p are necessary. We have proved such inequalities by using an extension method. In this way, we have established the existence of at least one optimal geometry, when $\mathcal{K} \subset C^2(\bar{\omega})$ is compact, and the first order optimality conditions [8]. It should be noted that the uniform Korn inequality is valid for a small enough thickness of the shell, and the uniform constants depend in a bad way on the thickness. Consequently, instabilities are to be expected in the numerical tests and special approaches are necessary.

(d) Error estimates in the discretization of control problems.
In the work [3], the above question is discussed in connection with optimal control problems governed by (elliptic) variational inequalities. In the case of convex control problems, it is known that they are equivalent with the first order system of optimality conditions. Therefore, the error estimates results valid for the finite element discretization of PDEs can be extended to optimal control problems. However, in nonconvex problems as described in the points (a), (b), (c) or in problems with constraints on the state, very little is known and high difficulties arise. The work [3] is a contribution in this respect and continues the research from [9].

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4.2 Research Group Dynamical Systems

4.2.1 Overview

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

Forschungsschwerpunkte sind

- Modellierung, Analyse und Simulation der Dynamik von Mehrsektions-Halbleiterlasern mit dispersiver Rückkopplung,
- komplexe Dynamik und Attraktoren,
- Stabilitätswechsel in Mehrskalensystemen.

Zu den Höhepunkten der Arbeit unserer Forschungsgruppe im Berichtszeitraum gehören das Erscheinen des zweiten Bandes der Monographie „Methods of Qualitative Theory in Nonlinear Dynamics“, die in Zusammenarbeit mit dem Humboldt-Preisträger Prof. L. Shilnikov entstand, die erfolgreiche Verteidigung der hervorragenden Doktorarbeit „Longitudinal dynamics of semiconductor lasers“ von Jan Sieber und die Durchführung des internationalen Workshops „Dynamics of Semiconductor Lasers“ am WIAS.

Die Erfolge unserer kleinen Forschungsgruppe basieren 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 is 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

- Modelling, analysis, and simulation of the dynamics of multi-section semiconductor lasers with dispersive feedback,
- Complex dynamics and attractors,
- Exchange of stabilities in multi-scale systems.

As highlights of the work of our research group during the report period we want to specify the appearance of the second (main) volume of the monograph “Methods of Qualitative Theory in Nonlinear Dynamics” as a joint work with the Humboldt laureate Prof. Leonid P. Shilnikov, the successful defence of the outstanding PhD thesis “Longitudinal dynamics of semiconductor lasers” by Jan Sieber and the international workshop “Dynamics of Semiconductor Lasers” organized by our group at WIAS.

The successes of our small research group are 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, D. Turaev, M. Wolfrum

Cooperation with: B. Sartorius, D. Hoffmann, H.-P. Nolting, O. Brox, S. Bauer (Heinrich-Hertz-Institut für Nachrichtentechnik, Berlin), H.-J. Wünsche (Institut für Physik, Humboldt-Universität zu Berlin), L. Recke (Institut für Mathematik, Humboldt-Universität zu Berlin), H. Wenzel (Ferdinand-Braun-Institut für Höchstfrequenztechnik, Berlin), 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")

Optoelectronic devices play a central role in modern telecommunication systems: at the interface between electronical generation and optical transmission of data signals, and more and more also for all optical data processing which opens a perspective to much higher than the conventional processing in the electrical domain. Typically, the semiconductor laser devices which are used in telecommunication systems do not operate in a stationary state but show a complicated dynamical behavior on the timescale of nanoseconds. Dynamical components e.g. for pulse generation, clock recovery, signal regeneration, or fast switching are of particular interest [6, 7, 15].
For the mathematical investigation of such complicated spatio-temporal dynamical behavior, the application and further development of methods from dynamical system theory as well as of special numerical algorithms is necessary. In this way, we can numerically simulate these effects and obtain a theoretical understanding which allows to optimize existing devices or to find new design concepts.
This research project is concerned with a broad range of questions, including modelling, numerical simulation, and optimization as well as the theoretical investigation of the models and their dynamical properties. The software *LDSL-tool* provides a comprehensive toolkit to simulate and analyze monolithically integrated edge emitting multi-section lasers. It is used in the framework of an industrial cooperation project to optimize the performance and robustness of an electrically modulated pulsating laser (see §3).
Our analytical and numerical investigations are based on models of the structure

$$\begin{aligned} \frac{\partial}{\partial t}E &= H(n)E, \\ \frac{\partial}{\partial t}n &= f(n) - \langle E^*, g(n)E\rangle. \end{aligned} \tag{1}$$

The quantity E represents the complex valued electro-magnetic field and is typically resolved in one spatial dimension. $H(n)$ is a hyperbolic differential operator specifying wave propagation, internal refraction, and dispersion. The quantity n is typically a real scalar or finite-dimensional vector. It describes the section-wise spatially averaged carrier density. The software *LDSL-tool*

is able to treat also extensions and reductions of model (1). This way, we can optionally include or exclude physical effects like, e.g., gain dispersion, hole burning, or gain saturation.
A central theme of the report period was the investigation of the *mode degeneracy* (see §1, [3, 4]). It turned out that this singularity is caused by delayed optical feedback. Hence, the feedback configuration of Fig. 1 is already able to exhibit many different dynamical regimes of practical interest: excitability (see §2), DQS self-pulsations, mode beating self-pulsations, chaotic behavior (see §1). Using analytical methods of bifurcation theory and numerical path-following techniques, we were able to obtain a complete description of the complicated dynamics (see Fig. 2). Moreover, this analysis served as a guide to find the phenomenon of excitability in numerical simulations of model (1) and also, for the first time, in corresponding laser experiments (see §2, [8, 10]).

1 Bifurcations induced by delayed optical feedback (J. Sieber, M. Wolfrum, M. Radziunas, D. Turaev). Already in [3, 4] it has been suggested that a mode degeneracy of the linear operator $H(n)$ (see (1)) is the organizing center for many nonlinear phenomena in semiconductor lasers. It turns out that the presence of delayed optical feedback implies the existence of a mode degeneracy. The theoretical understanding of the mode approximations (see WIAS Annual Report 2000[1]) permits a complete unfolding of this singularity using two physically relevant parameters, the feedback strength η and the feedback phase φ.

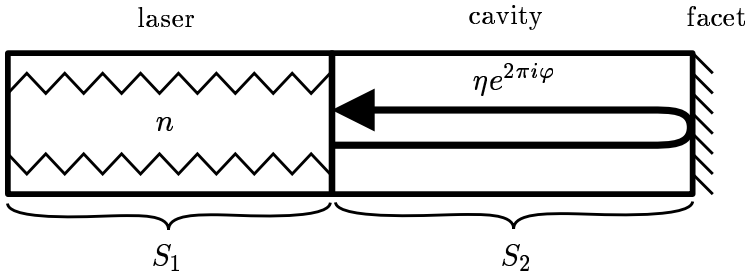

Fig. 1: Configuration of the two-section laser investigated in [10]. The variable n is a scalar and describes the spatially averaged carrier density in section S_1.

In [10], we perform a numerical bifurcation analysis for a multi-section laser device implementing a classical delayed optical feedback experiment (see Fig. 1). This laser consists of an active DFB section S_1 acting as a laser and a passive Fabry-Perot section S_2 providing accurately tunable delayed optical feedback.
The bifurcation diagram in Fig. 2 shows how the dynamics of this laser depends on the parameters η and φ, which can be controlled in the experiments by changing the temperature and the current input of section S_2.

[1] http://www.wias-berlin.de/publications/annual_reports/00/node29.html

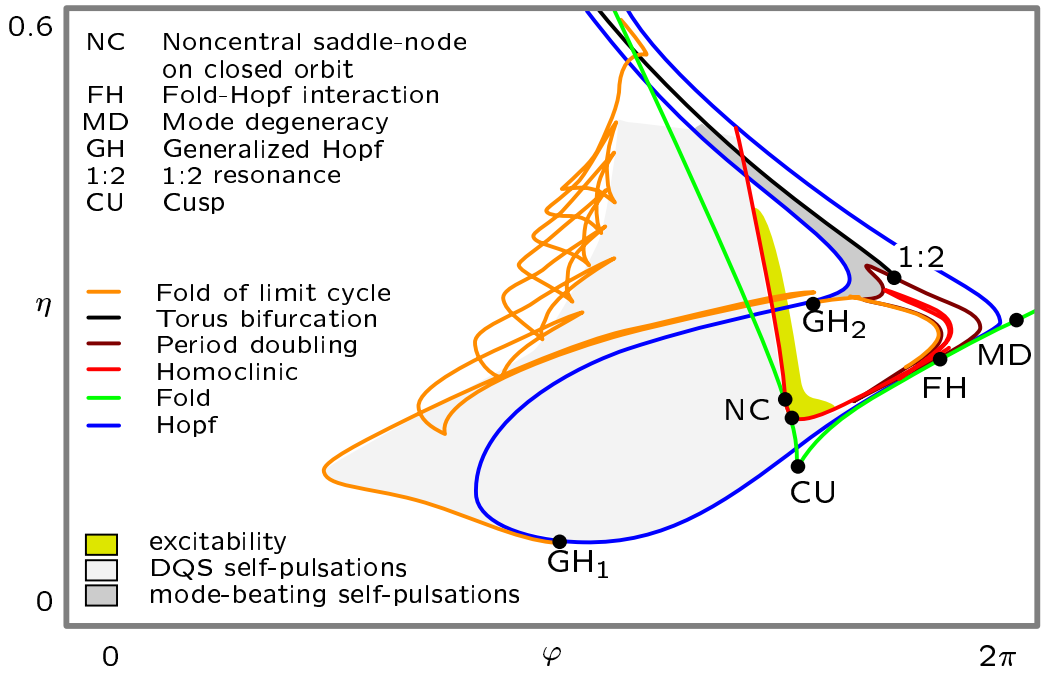

Fig. 2: Bifurcation diagram for a multi-section laser configuration as depicted in Fig. 1 varying the parameters η and φ. Colored lines represent bifurcations of codimension 1, black points represent bifurcations of codimension 2.

Fig. 2 has been obtained using the two-mode approximation including the two eigenvalues of $H(n)$ which have a critical mode degeneracy at *MD* (double eigenvalue of $H(n)$ on the imaginary axis). It reveals the sources of many nonlinear phenomena observed in experiments and simulations and locates them in the parameter plane. The following is of particular interest for applications:

- The region of *DQS self-pulsations* (light grey colored in Fig. 2, frequency less than 10 GHz, non-harmonic, fairly large amplitude, see WIAS Annual Report 1999[2]) is bordered by curves representing Hopf bifurcations, folds of limit cycles, and homoclinic bifurcations. Approaching the curve of homoclinic bifurcations, the frequency tends to zero.

- The region of mixed mode or *mode-beating* self-pulsations (dark-grey colored in Fig. 2, frequency larger than 10 GHz, nearly harmonic, small amplitude in n) is a narrow channel between a Hopf and a torus bifurcation. Its lower border is formed by curves describing a period doubling bifurcation and a fold of limit cycles. This mode-beating mechanism is of another nature than the mechanism reported in WIAS Annual Report 2000[3]. This type of mode-beating could be of great practical use in case it is possible to enlarge the corresponding parameter region.

- Close to the homoclinic bifurcation, there is a region where the system is *excitable* (yellow colored in Fig. 2, see also §2). The appearance of a saddle-node on a closed orbit between the two NC points is a classical excitability scenario.

[2] http://www.wias-berlin.de/publications/annual_reports/99/node31.html
[3] http://www.wias-berlin.de/publications/annual_reports/00/node29.html

- Some of the homoclinic orbits tend to a saddle-focus which satisfies the conditions of Shilnikov's theorems implying *complicated dynamics*. Moreover, the 1:2 resonance and the fold-Hopf interaction are also well-known sources of complicated behavior.

Fig. 2 shows that a simple multi-section laser device implementing a classical delayed optical feedback experiment is able to exhibit many different dynamical regimes of practical interest: excitability (see §2), DQS self-pulsations, mode beating self-pulsations, chaos, etc. Future investigations should focus on the question how modifications of the laser design (Fig. 1) or inclusion of other physical effects influence the bifurcation diagram presented in Fig. 2.

2 Excitability (J. Sieber, K.R. Schneider, M. Radziunas). It was demonstrated theoretically and experimentally in [7, 8] how an injected sufficiently strong short optical pulse is able to excite a two-section DFB laser (see Fig. 1) operating at a stationary lasing state. The response of the system is almost independent of the strength of injection, if the power of the injected pulse is below or above some threshold (see Fig. 3).

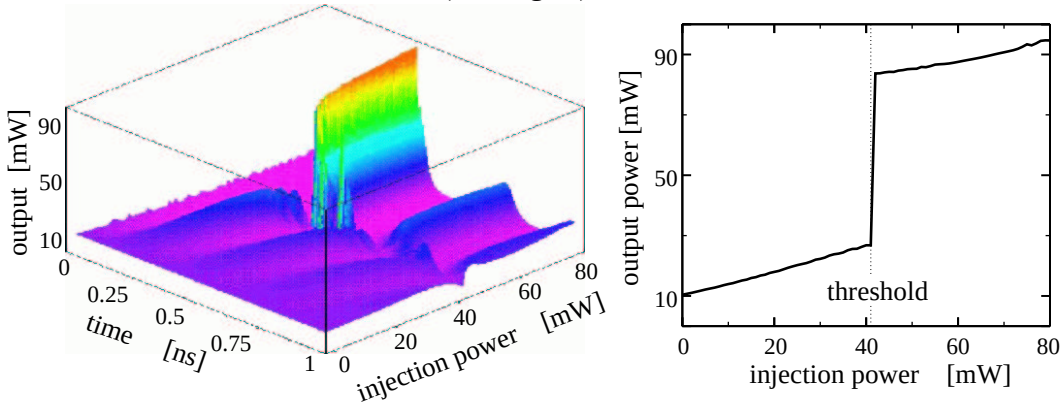

Fig. 3: Left: response of the system due to injection of an optical signal. Right: nonlinear response function measuring the maximum of the responding signal.

The theoretical study of this problem is based on the traveling wave (TW) model (1) and its two-mode approximation system. It has allowed to adjust suitable experimental conditions and to find excitability in real DFB lasers (see [8]).
The simulations of the TW model have shown that the parameter region where an excitable stable stationary state exists is neighboring a parameter region with self-pulsating solutions. By using the two-mode approximation system we were able to identify homoclinic bifurcations which separate the parameter region of stable self-pulsations from the region where excitability has been observed (see the red line in Fig. 2).
Now the mechanism of excitability can be easily explained by Fig. 4, presenting suitable projections of two stable and of saddle-type stationary states (solid and empty big points), unstable limit cycle (green curve), already broken homoclinic loop (blue trajectories tending to and outgoing from the saddle), and the trajectory of the responding signal (red curve). In these figures, yellow and blue shaded areas indicate carrier densities supporting the growth of the first and of the second mode, respectively.

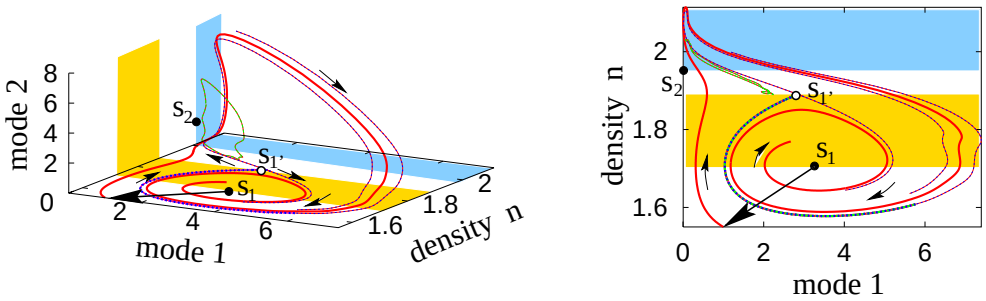

Fig. 4: Three- and two-dimensional projections of the phase space of the excitable system

At the beginning, the system is operating at the stable stationary state s_1. Then, a perturbation caused by an injected pulse is acting along the thick arrow. If the perturbation is small, the field-density state remains close to the stationary state s_1, and after some decaying oscillations the trajectory returns to this state.
In the case when the perturbation is strong enough, the field-density state point can be kicked to the left side of the thick blue curve which indicates a part of the stable manifold of the saddle and defines the threshold perturbation. The response trajectory makes a large excursion in the phase space bypassing the saddle stationary state $s_{1'}$ and entering the blue shaded region where the second mode becomes dominant. After returning to the plane where the first mode dominates (yellow shaded part and below in the right part of Fig. 4), the trajectory is attracted by the state s_1.

3 Synchronization of a three-section DFB laser to current modulation (M. Radziunas). Synchronization of high-frequency (up to hundreds of GHz) self-pulsations observed in multi-section semiconductor lasers with an external modulated signal is highly desired for practical applications in all optical data transmission systems (see [6, 7, 14, 15]). We want to investigate the quality of self-pulsations and to study the question of their synchronization with a modulated electrical signal. This work is a part 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 order to demonstrate locking in the model, the modulation frequency f_{ext} should be sufficiently close to the frequency f_0 of self-pulsations in the free running laser. Then, if the modulation amplitude is big enough, one can expect to have the required locking (see blue shaded area in the left diagram of Fig. 5).

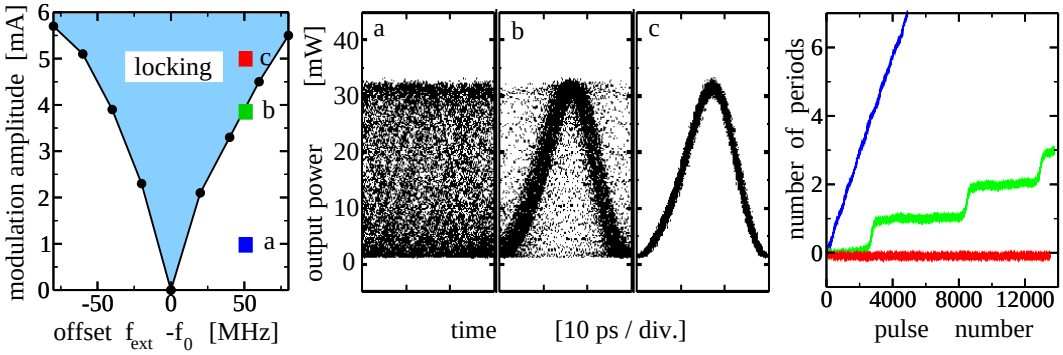

Fig. 5: Left: range of modulation frequency and amplitude which is sufficient to achieve locking. Middle: eye diagrams of unlocked (a), almost locked (b) and locked (c) self-pulsations. Right: drift of the pulse maxima in the eye diagrams.

To demonstrate locking we apply a sampling technique and draw eye diagrams used frequently in engineering (see the three middle diagrams of Fig. 5). The considered three cases show the behavior of the TW model (1) with included optical field noise terms when the current modulation of the DFB section was applied. The frequencies and amplitudes of this modulation are indicated by coloured small squares in the left diagram of Fig. 5. An open eye in the third of the middle diagrams indicates locking of the self-pulsations to the frequency of modulation. Finally, the right part of Fig. 5 shows the drift of pulse maxima in the eye diagram. The drift along the horizontal line (red trace in the right part of Fig. 5) indicates an almost constant position of each pulse in the eye diagram, and, therefore, guarantees an open-eye diagram. On the contrary, if the pulse maximum is drifting over more than one period (blue and green traces in the right part of Fig. 5), then the eye in the corresponding diagram will be closed.
This way, the pictures show how the developed software allows to analyze the quality of the self-pulsations and to determine the locking regions.

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Estimates of the dimension for attractors of evolutionary PDEs and homoclinic bifurcations

Collaborator: D. Turaev

Cooperation with: S. Zelik (Moscow State University, Faculty of Mathematics and Mechanics, Russia)

One of the great achievements of the theory of evolutionary PDEs is the theory of attractors of semiflows in infinite-dimensional spaces. Here, the main idea due to works of Ladyzhenskaja, Yorke, Vishik, Temam, Hale, and others is that although the phase space is infinite dimensional, all the orbits may be attracted by an invariant set A (the attractor) of a finite dimension, so that the dynamics can possibly be understood by methods of the qualitative theory of ordinary differential equations. The crucial question here is to get realistic estimates on the dimension of the attractor. The best known upper estimates are obtained by the Douady-Oesterle-Iljashenko method which yields the estimate

$$\dim_H A < k, \tag{1}$$

provided the semiflow contracts k-dimensional volumes.

The only working method which has been used, until now, to obtain estimates from below employs the idea that $\dim A$ is greater than the dimension of the unstable manifold of any equilibrium state in A. However, there exist classes of equations for which the gap between the lower estimates obtained by this method and the upper estimate given by (1) is very large. The question whether estimate (1) is optimal is a longstanding problem in the theory.

The goal of our research was to resolve this problem. Our idea is that the upper estimate (1) must be sharp whenever the dynamics of the system is recurrent. Different to this situation is the case of gradient-like systems where the dynamics on the attractor is, in a sense, trivial and where the dimension of the unstable manifolds of the equilibria gives a correct estimate for the dimension of the attractor, no matter what the volume-contraction properties of the system are. Our approach is based on the ideas from [1] where the notion of effective dimension d_{eff} of homoclinic bifurcations was introduced and where it was argued that the maximal dimension of invariant sets which can be born at a homoclinic bifurcation must be equal to d_{eff} no matter how small a dimension of the unstable manifolds of the involved saddle equilibria is. This principle is known to hold true for many different examples of homoclinic bifurcations.

This idea yields a radically new and very powerful method of obtaining realistic lower estimates of the dimension of attractors of systems which are not gradient-like: If the dynamics is recurrent, then it is plausible that some homoclinic bifurcations can be detected. Therefore, the corresponding value of d_{eff} estimates $dim A$ from below. We note that the definition of the effective dimension from [1] is strongly based on the volume contraction arguments, so that the lower estimates obtained by our method must be close to the upper estimate (1) indeed.

An important example of systems, where a tremendous gap exists between the upper estimate (1) and the usual lower estimates, is provided by a class of damped nonlinear hyperbolic equations

$$u_{tt} + \gamma u_t + Au + \Phi(u) + F(u, u_t) = 0, \tag{2}$$

where u is an element of an abstract Hilbert space H, the operator A is positive definite, self-adjoint, and has a compact inverse, Φ is a gradient-type nonlinearity, F is a bounded nonlinearity in an appropriate norm, γ is a small parameter (damping). We assume that the nonlinear damping terms in $F(u, u_t)$ are smaller than γu_t, i.e. $\|F'_v(u, v)\| \ll \gamma$ in an appropriate

norm. One can see that the best possible estimate from above to the dimension of the attractor which can be obtained here by volume-contraction arguments is

$$\dim_H A < \frac{c}{\gamma}, \tag{3}$$

where c is some constant. On the other hand, the dimension of the unstable manifold of saddle equilibria which may exist here is bounded from above by a constant independent of γ. Hence, when the damping constant γ is small, the old methods give a very large gap between lower and upper estimates. Therefore, we choose this example to test our method.

In [2] we show that if system (2) is not gradient-like, then the following homoclinic bifurcation can typically be encountered: The system has an equilibrium state O of saddle type with one-dimensional unstable manifold W^u which contains two trajectories (separatrices) which leave O in opposite directions, one of these separatrices returns to O as $t \to +\infty$, forming a homoclinic loop; moreover, it returns to O along the most stable direction. The spectrum of characteristic exponents of O has the following structure: One exponent, λ_0, is real and positive and bounded away from zero at small γ, one exponent, λ_1, is real and negative and bounded away from zero, and the rest of characteristic exponents are typically complex and have real parts of order γ.

According to [1], the effective dimension of this homoclinic bifurcation is of order γ^{-1}. In [2] we prove the following result.

Theorem. A $d_{eff}/2$-dimensional invariant torus densely filled with quasiperiodic trajectories can be born by an arbitrarily small smooth perturbation of the homoclinic loop under consideration.

Of course, such an invariant torus must lie in the attractor of the system so that the dimension of the attractor cannot be less than the dimension of this torus. Hence, we obtain the lower estimate comparable with the upper estimate (3), i.e. (3) cannot be improved. This proves, maybe contrarily to an intuitive believe, that unless the nonlinearity has a gradient-like structure, the dimension of the attractor of a weakly damped hyperbolic equation is extremely large and is given by (3). We stress again that such a kind of result is absolutely beyond the reach of the methods which existed before.

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Long-time dynamics in adaptive gain control systems

Collaborator: K.R. Schneider

Cooperation with: G.A. Leonov (St. Petersburg University, Russia), A. Ilchmann (Technische Universität Ilmenau)

We assume that the plant to be controlled can be described by a finite dimensional single input single output linear time invariant system that can be stabilized by a high gain output feedback. Such systems can be represented in the form

$$\begin{aligned} \frac{dx}{dt} &= Ax+by, \\ \frac{dy}{dt} &= -c^T x - dy + u, \end{aligned} \tag{1}$$

where u is the input, y the output, $(x,y) \in R^n \times R$ is the state of the system. We apply the adaptive feedback law

$$\begin{aligned} u &= -zy+e, \\ \frac{dz}{dt} &= -\sigma z + y^2, \quad z(0) > 0, \end{aligned} \tag{2}$$

where e is the control offset error.
Control systems of such type have been investigated, e.g., by I. Mareels et al. [5] and A. Ilchmann [4]. An essential aim of [5] was to show by a bifurcation analysis and by numerical investigations that already in the case $n = 1$ the long-time dynamics of (1), (2) can be very rich, including chaotic behavior. Therefore, from the point of control theory it is desirable to find conditions for (1), (2) to be globally stable or to minimize the region G containing the global attractor.
The goal of the project was to study the long-time dynamics of (1), (2). To this end we constructed an appropriate Lyapunov function. An essential part of this function is some quadratic form defined by means of a symmetric positive definite matrix H. For the existence and also for the construction of H we used frequency domain methods, in particular, we applied some version of the Yakubovich-Kalman frequency domain theorem (see, e.g., [3]).
This way we were able to estimate the global attractor and to derive conditions that (1), (2) were globally asymptotical stable which improve corresponding results in [5].
Using a theorem of Douady-Oesterle ([1]) we were able to estimate the Hausdorff dimension of the global attractor and to derive conditions for the global stability in the case of a vanishing control offset error.
Furthermore, we could establish an upper bound for the Hausdorff dimension of the global attractor.
The results have been presented in [2], a corresponding publication appeared in Lecture Notes in Control and Information Sciences ([6]).

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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 interessante 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.

Unsere thematischen Schwerpunkte waren:

- Numerische Verfahren und Softwarekomponenten für die Lösung von Systemen partieller Differentialgleichungen (WIAS-Schwerpunktthemen: *Strömungs- und Transportprobleme in Kontinuen, Mikro-, Nano- und Optoelektronik, Phasenübergänge*),
- Simulation von Höchstfrequenzschaltungen (WIAS-Schwerpunktthema: *Mikro-, Nano- und Optoelektronik*),
- Dynamische Simulation chemischer Prozesse (WIAS-Schwerpunktthema: *Optimierung und Steuerung in der Verfahrenstechnik*).

Im November 2001 wurde von der Forschungsgruppe ein initialer Workshop zum Thema „Direct Methanol Fuel Cells“ veranstaltet (siehe S. 215), der einen repräsentativen Überblick über die Modellierung, Simulation und experimentelle Forschung in Deutschland in diesem Bereich gab.

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.

Our main research topics were:

- Numerical procedures and software modules for the solution of systems of partial differential equations (focal points at WIAS: *Flow and propagation phenomena in continua, Micro-, nano- and optoelectronics, Phase transitions*),
- Simulation of high-frequency circuits (focal point at WIAS: *Micro-, nano- and optoelectronics*),
- Dynamic simulation of chemical processes (focal point at WIAS: *Optimization and control in process engineering*).

In November 2001, the group held a workshop on “Direct Methanol Fuel Cells” (see page 215), which gave a representative overview of the modeling, simulation, and experimental research that has been performed in this field in Germany. This was the first in a planned series of workshops to be presented by the group.

Die Forschungsgruppe hat an den nachfolgend genannten forschungsgruppenübergreifenden Projekten mitgearbeitet:

- Enveloppenfunktionsapproximation für elektronische Zustände in Halbleiter-Nanostrukturen (siehe S. 156) zusammen mit den FGn 1 und 4 (WIAS-Schwerpunktthema: *Mikro-, Nano- und Optoelektronik*) und
- Modellierung und Simulation blau-emittierender Halbleiter-Nanostrukturen (siehe S. 157) zusammen mit der FG 1 (WIAS-Schwerpunktthema: *Mikro-, Nano- und Optoelektronik*).

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

- Envelope function approximation for electronic states in semiconductor nanostructures (see page 156) in cooperation with research groups 1 and 4 (focal point at WIAS: *Micro-, nano- and optoelectronics*) and
- Modeling and simulation of blue-emitting semiconductor nanostructures (see page 157) in cooperation with research group 1 (focal point at WIAS: *Micro-, nano- and optoelectronics*).

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. 163),
  - Optimale Steuerung der Oberflächenhärtung von Stahl (siehe S. 31),
  - Spannungsanalyse einer dünnen Wafer-Platte aus einkristallinem Gallium-Arsenid (siehe S. 153).
- 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 163),
  - Optimal control of surface heat treatments (see page 31),
  - Stress analysis of a thin wafer plate of single crystal gallium arsenide (see page 153).
- Development of special modules and features for *pdelib*, general advice for questions on numerical issues,
- Visualization.

4.3.2 Projects

Uniaxial, extensional flows in liquid bridges

Collaborator: E. Bänsch

Cooperation with: C. Berg (Universität Bremen, ZARM)

Owing to their constant deformation rates linear flow fields are commonly used for rheological tests, e.g., to measure the fluid viscosity or the deformation behavior of the whole sample or components in it.
Experimentally, these flow fields may be realized as extensional flows in a stretched bridge of viscous liquid under microgravity conditions, where the bridge is held exclusively between two circular concentric support membranes. To derive an almost linear flow field, the stretching velocity has to increase exponentially in time. Furthermore, in order to achieve a deformation rate as constant as possible, both in space and time, in our case the radius of the membranes is decreased accordingly to maintain a (nearly) cylindrical shape during stretching.
A mathematical description of the system leads to a free boundary problem for the Navier-Stokes equations: Let $\Omega = \Omega(t)$ denote the—a priori unknown—domain occupied by the fluid. Find a vector-valued velocity field $\mathbf{v} = \mathbf{v}(t,\mathbf{x})$ and a pressure field $p = p(t,\mathbf{x})$ such that

$$\rho(\partial_t \mathbf{v} + \mathbf{v}\cdot\nabla\mathbf{v}) - \nabla\cdot\sigma = 0 \quad \text{in } \Omega, \tag{1a}$$

$$\nabla\cdot\mathbf{v} = 0 \quad \text{in } \Omega. \tag{1b}$$

Here, $\sigma = \sigma(p,\mathbf{v},\mu)$ denotes the stress tensor

$$\sigma = -p\mathbf{I} + \mu\,\mathbf{D} = -p\mathbf{I} + \mu(\nabla\mathbf{v} + \nabla\mathbf{v}^T)$$

with ρ the density and μ the viscosity of the fluid.
On the free surface Γ_f we have a balance of forces:

$$\sigma\mathbf{n} = \gamma(\frac{1}{R_1} + \frac{1}{R_2})\mathbf{n}, \tag{1c}$$

with γ the coefficient of surface tension, R_1, R_2 the principle curvatures of Γ_f, and $\mathbf{n}$ the normal vector to Γ_f. Finally, the kinematic condition

$$\mathbf{v}\cdot\mathbf{n} = V_f, \tag{1d}$$

with V_f the normal velocity of the free surface Γ_f, holds.
Since all data are axisymmetric and the flow is laminar we may assume a two-dimensional axisymmetric configuration.
For the numerical simulation of the problem we use a finite element method with the following key ingredients: a variational formulation of the curvature of the free boundary, yielding an accurate, dimension-independent and simple-to-implement approximation for the curvature; a stable time discretization, semi-implicit w.r.t. the treatment of the curvature terms, which on the one hand avoids a CFL-like restriction of the time step as in common “explicit” treatments of the curvature terms and on the other hand decouples the computation of the geometry from that of the flow field. This approach has proven to be both efficient and robust (see [2]).

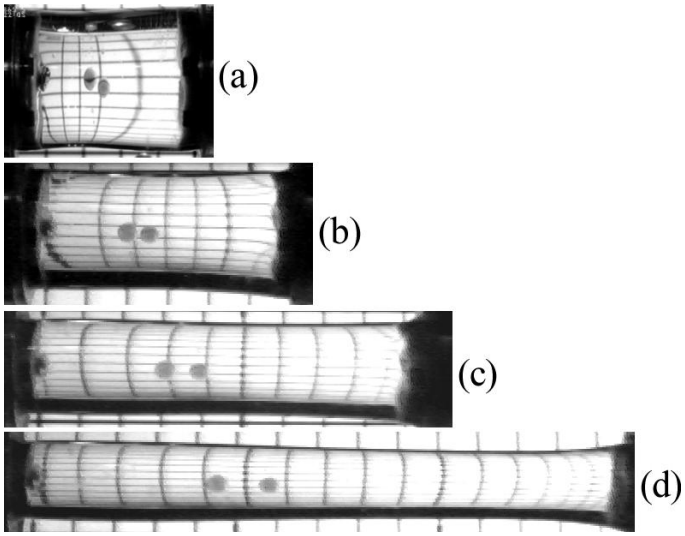

Fig. 1: Experiment, stretched bridge of castor oil at different time instants

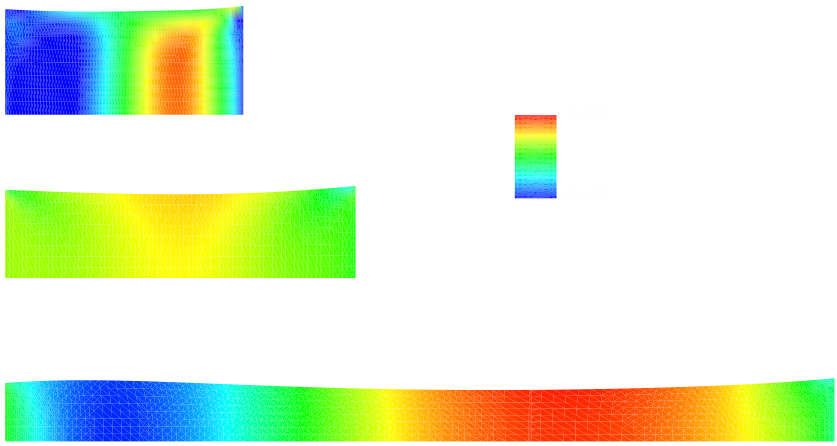

Fig. 2: Simulation, strain rate distribution of stretched bridge at different time instants

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Numerical aspects of unsteady incompressible non-Newtonian flows

Collaborator: N. Scurtu

In nature, there are many fluids that do not satisfy the Newtonian constitutive law. This is also the case for many fluids created for industrial purposes. Fluids like multi-grade oils, liquid detergents, shampoos, dyes, adhesives, biological fluids like blood, paints, greases, printing inks, industrial suspensions, polymer solutions, and polymer melts, fall within the category of non-Newtonian fluids. First, the Oldroyd-A and -B fluid models are considered but the intention is to study the behavior of the generalized Oldroyd-B model, introduced by Yeleswarapu in [8], which is an up-to-date model for blood. The projected investigations could be transferred to the case of a blood-centrifuge (with bio-medical practice at the dialysis).
The numerical simulation of many industrial problems has been carried out using viscoelastic models of the Oldroyd kind. As unknowns there are the tensorial stress-field τ, the vectorial velocity-field u, and the scalar pressure-field p. The dimensionless constitutive, momentum and continuity equations for the Oldroyd model yield the following system:

$$\begin{cases} We\left[\dfrac{\partial \tau}{\partial t}+(\mathbf{u}.\nabla)\tau+\beta_a(\tau,\nabla\mathbf{u})\right]+\tau-2\alpha D(\mathbf{u}) &= 0 \\ Re\left[\dfrac{\partial \mathbf{u}}{\partial t}+(\mathbf{u}.\nabla)\mathbf{u}\right]-div\tau-(1-\alpha)\Delta\mathbf{u}+\nabla p &= \mathbf{f} \\ div u &= 0 \\ + \text{ initial and boundary conditions} \end{cases}$$

where $\beta_a(\tau,\nabla\mathbf{u})=\dfrac{1-a}{2}(\tau\nabla\mathbf{u}+\nabla\mathbf{u}^T\tau)-\dfrac{1+a}{2}(\nabla\mathbf{u}\tau+\tau\nabla\mathbf{u}^T)$ and $a\in[-1,1]$ ($a=-1$ corresponding to the Oldroyd-A and $a=1$ to the Oldroyd-B model).
Three parameters characterize the flow: the Reynolds number $Re\geq 0$, the fraction of viscoelastic viscosity $\alpha\in(0,1]$, and the Weissenberg number $We\geq 0$. This system includes the Navier-Stokes system as a particular case ($We=0$), so it is favorable to develop a numerical method which can generalize an existing one used for the Navier-Stokes system.
There are two aspects which should be addressed for this system: the finite-element spatial discretization and the time discretization.
The solution of the Oldroyd problem by the finite-element method presents a difficulty due to the hyperbolic character of the constitutive equation, which is to be considered as a system in τ with $\mathbf{u}$ fixed (the mathematical nature of the global system is a difficult problem; loss of evolution and change of type can occur for $\alpha=1$). For some years the numerical solution of the Oldroyd system with convenient boundary conditions on $\mathbf{u}$ and τ was limited to the small Weissenberg number, because the hyperbolic character of the constitutive equation was not taken into account. This hyperbolic nature implies that some upwinding is needed. The choice of upwinding techniques depends on the choice of the finite-element space used to approximate τ. Since no continuity requirement is needed on τ at interfaces between elements, as shown in [2], this will be done by using the discontinuous Galerkin method, which allows the computation of τ on an element by element basis.

For fixed τ, the last two equations comprise a Stokes system in the variables **u** and p. To solve the Stokes system, a mixed finite-element method was used: the stable Taylor-Hood element was implemented on unstructured simplicial grids in 2-d and 3-d, i.e. piecewise-quadratic basis functions for the velocity and piecewise-linear for the pressure.
Major numerical problems for the unsteady Oldroyd system arise due to:

- the incompressibility condition;
- the strong nonlinearity in the momentum equation;
- the transport of the stress;
- the strong coupling of the unknowns;
- stability versus accuracy of the numerical scheme.

The decoupled computation of stress, velocity, and pressure is performed with an algorithm involving a time approximation based on the fractional-θ scheme ([3]) and on the splitting method introduced by Saramito ([6]). As an operator splitting method, the θ-scheme was used by Bänsch for the Navier-Stokes equations ([1]). The method consists of splitting each time interval $[t_n, t_{n+1}]$ of length Δt into 3 subintervals $[t_n, t_n + \theta\Delta t]$, $[t_n + \theta\Delta t, t_n + (1-\theta)\Delta t]$, and $[t_n + (1-\theta)\Delta t, t_{n+1}]$, and integrating the equations on each of these subintervals.
For the Navier-Stokes equations this scheme is 2nd order accurate, non-dissipative, and A-stable. Stability and convergence analysis of the fractional step θ-scheme for the unsteady Navier-Stokes equations are proven in [4] and [5]. Due to the complexity of the splitting method for the Oldroyd system, only the stability in the linearized case could be proven.
The splitting technique leads to three subproblems, a linear Stokes-like one, a nonlinear Burger-like one, and a stress-tensor transport problem. The first two subproblems have been solved by the finite-element methods described below and the last is in progress.
The method has been implemented in ALBERT, an adaptive finite-element toolbox ([7]).

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Convective mechanisms in full-zone liquid bridges

Collaborator: D. Davis

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

This project is chiefly concerned with the numerical investigation of nonlinear, convective mechanisms in liquid bridges of full-zone extent, with an aim to better understand the nature of time-dependent instability for low-Prandtl number (Pr) flows. This is especially pertinent in the field of semiconductor single-crystal growth via the floating-zone method, where such instabilities are known to be a major cause of striations in crystals ([1], [2]). Of particular importance are the rôles played by buoyancy in the melt region (Ω) and thermocapillarity (Marangoni convection) on the liquid/gas interface (Γ_{LG}) (see fig1).

The fluid motion and heat transport in Ω are modeled by the Navier-Stokes equations with Boussinesq approximation, the incompressibility condition, and the energy equation. The temperature is prescribed on all boundaries (in particular, having an axisymmetric, sinusoidal form on Γ_{LG}), while the no-slip condition is assumed to hold on the solid/liquid parts (Γ_{SL}). Also on Γ_{LG}, a tangential stress condition is applied to account for the Marangoni influence there; the liquid-gas interface is moreover assumed to be non-moving and cylindrical.

A variational form of the equations was chosen which could naturally incorporate the stress boundary condition ([3]); this can be characterized by the treatment of the steady Stokes part of the momentum equation, i.e. its conversion to a "strain" form:

$$\int_\Omega \{-\Delta\mathbf{u}+\nabla p\}\cdot\mathbf{v}d\Omega = \frac{1}{2}\int_\Omega D(\mathbf{u}):D(\mathbf{v})d\Omega - \int_\Omega p\nabla\cdot\mathbf{v}d\Omega - \int_{\Gamma_{LG}} \mathbf{n}\cdot\sigma\mathbf{v}ds,$$

where $\mathbf{u}$, p denote velocity and pressure in turn, σ is the fluid stress tensor, $\mathbf{n}$ is the unit outer normal to Γ_{LG}, and $D(\mathbf{u}) := \nabla\mathbf{u}+(\nabla\mathbf{u})^{\mathrm{T}}$ is the strain tensor, while $\mathbf{v}$ is an appropriately defined test function.

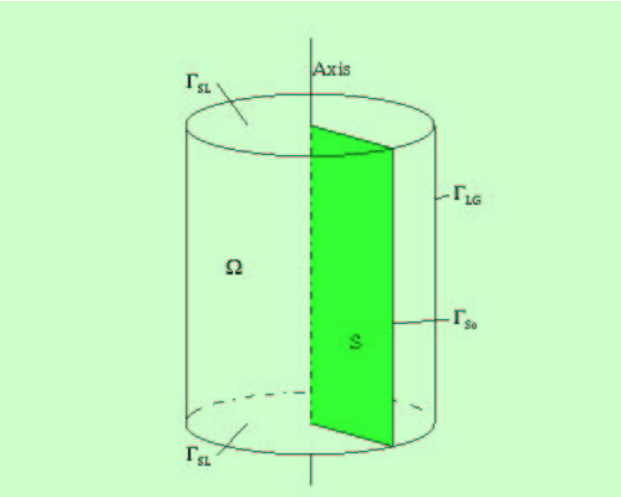

Fig. 1: Sketch of a cylindrical liquid-bridge domain

The flow is assumed to be steady and two-dimensional (2-d) axisymmetric, which is valid provided the maximum temperature deviation in the melt is sufficiently small. In particular then,

owing to rotational symmetry, the volume integrals that appear in the variational formulation can be reduced to plane integrals, since

$$\int_{\Omega} f d\Omega = 2\pi \int_{S} r f dr dz$$

holds for any continuous function $f(r,z)$ defined in the melt region Ω; here S is a vertical half-plane/cylinder intersection region of arbitrary azimuthal angle (as shown in fig1).

To better understand the possible influences of the underlying convective mechanisms on the flow and thermal development, and therefore be better placed to interpret any subsequent instability features that may emerge, a first study has been made for sub-critical parameter values. Here the relevant parameters are the Rayleigh number (Ra) and the Marangoni number (Ma), with the values Ra/Pr, Ma/Pr indicating the typical sizes of the buoyancy and thermocapillary forces. Their influence *relative to one another* can be observed in fig2, for example, where the Prandtl number is 0.01.

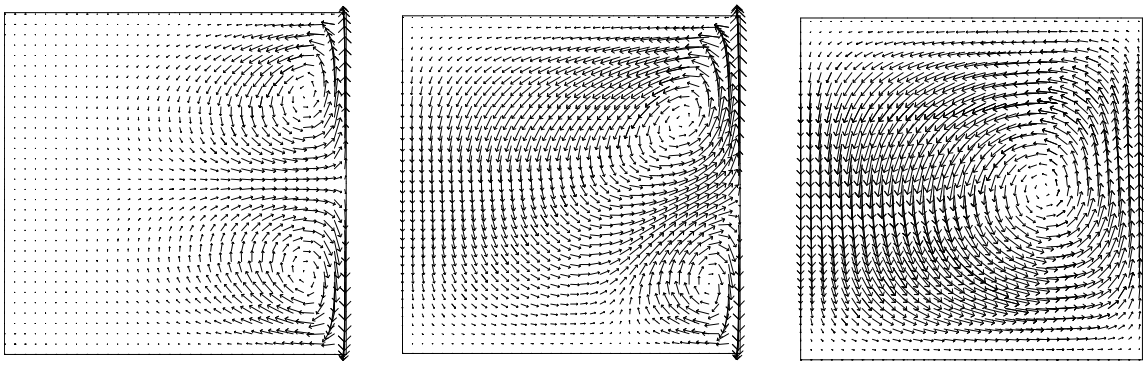

Fig. 2: Computed velocity field in a domain of unit aspect ratio for (a) pure thermocapillarity ($Ra/Pr = 0,\ Ma/Pr = 100$); (b) mixed buoyancy-thermocapillarity ($Ra/Pr = 100,\ Ma/Pr = 10$); (c) pure buoyancy ($Ra/Pr = 100,\ Ma/Pr = 0$)

Direct numerical simulations (numerical methodology described below) were performed for low-Prandtl number flows in domains of various aspect ratios, including slender and wide cases, and, allied with nonlinear theory, several nonlinear phenomena could be identified and interpreted ([4]). In particular, for slender domains, this includes a strong convective effect in a box-shaped Euler zone around the mid-horizontal plane of the melt zone, where bell-shaped local velocity profiles, associated with an increased relative Marangoni effect, are seen to emerge. Also high shears are evident in zones (again of Euler type) near the solid boundaries, where the flow turns. fig3 illustrates this effect.

For the spatial discretization of the governing system of equations, a standard Bubnov-Galerkin finite-element method is applied on 2-d simplicial meshes using globally-continuous, piecewise-quadratic basis functions for the discrete velocity and temperature spaces, and globally-continuous, piecewise-linear basis functions for the discrete pressure space, i.e. the $P_2 - P_1$ (Taylor-Hood triangular) element. The corresponding meshes are generated via new-node bisection from an initial coarse macro-triangulation of the discrete domain S_h.

To discretize in time, a fractional-θ scheme ([5]) is applied to the hydrodynamic part together with a first-order, semi-implicit, backward-Euler scheme for the energy equation. The principal advantage of the former is the full decoupling of the nonlinearity and incompressibility, which then yields two distinct types of sub-problem: a self-adjoint, quasi-linear, Stokes system for

velocity and pressure, and an asymmetric, nonlinear system for velocity only; the first of these is solved by applying a preconditioned conjugated-gradient method ([5]) to the associated Schur-complement equation for pressure, while the second is solved using the GMRES scheme ([6]).

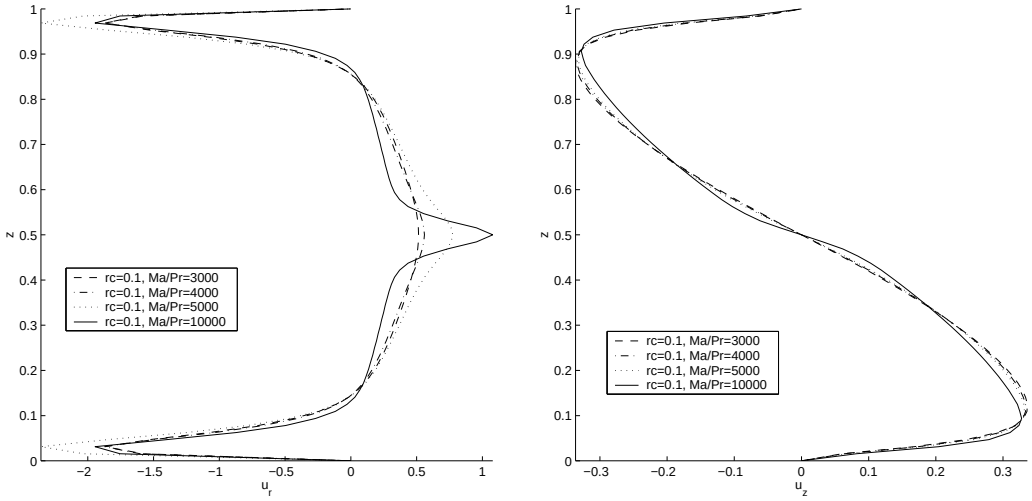

Fig. 3: Pure thermocapillary motion in a slender domain (aspect ratio of 0.1) for four cases, depicting axial variations along the mid-vertical line (of the plane S) of (a) the scaled radial velocity component, u_r (b) the scaled axial velocity component, u_z

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Numerical simulation of electro-chemical processes in a thin layer cell

Collaborators: E. Bänsch, J. Fuhrmann, M. Uhle

Cooperation with: H. Baltruschat, Th. Löffler (Rheinische Friedrich-Wilhelms-Universität Bonn, Institut für Physikalische und Theoretische Chemie)

We consider a new coupled thin layer cell (TLC) described in [1] suitable for analysing electro-chemical processes at metal electrolyte phase boundaries with differential electro-chemical mass spectrometry. A coupled thin layer cell (see Fig. 1) is characterized by separation of the area of electrodes (3) and an additional area which enables the electrolyte to flow through a membrane (6) to a mass spectrometer. They are connected by capillary vessels (11).

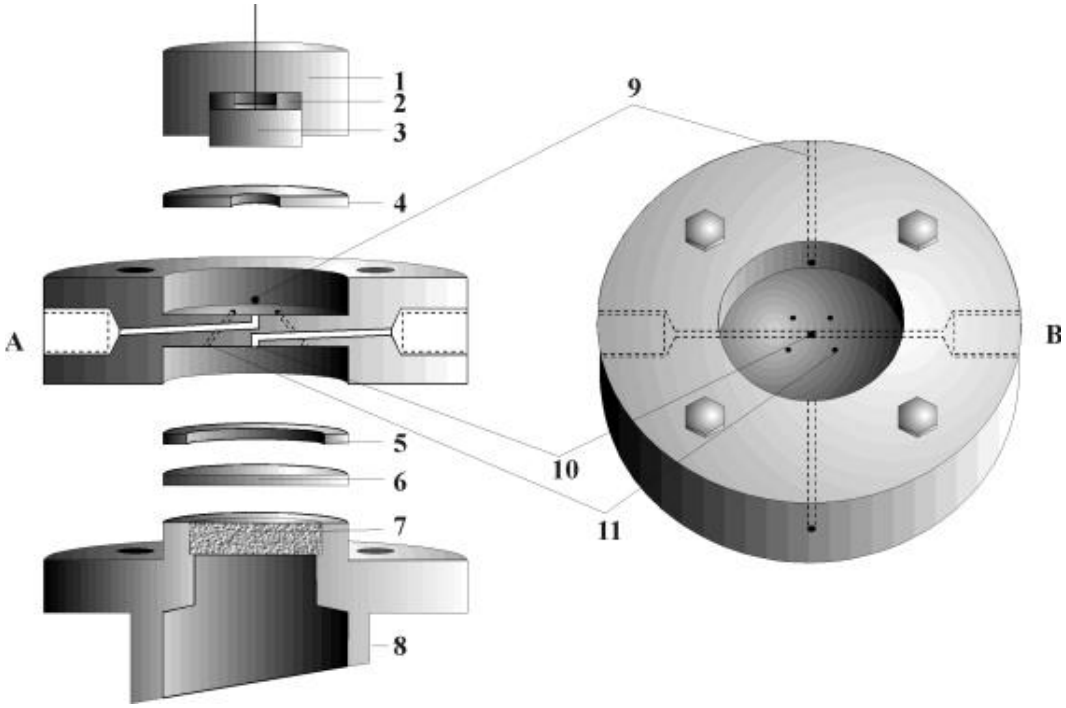

Fig. 1: Cross-section through a thin layer cell ([1])

We are planning to analyze the following experiment, which is important for basic research of fuel cells: a water-soluble substance (methane) streams from input (A) to an electrode (3), which has a large surface area to cell volume ratio, i.e. the layer (4) is very thin. At the surface of the electrode a chemical reaction occurs. The chemical products of the reaction stream through the capillaries (11) to the membrane (6) and through the steel frit (7) to the mass spectrometer, while other chemical products flow to output (B).

We are interested in the reaction rate on the electrode. The amount of source and target substance is measured by the mass spectrometer. By detecting the amount of molecules of the target substance, one can determine the rate of reaction at the electrode.

The geometry of thin layer cells, the drift of electrolyte, process and material parameters play crucial roles in the chemical reaction process, and in determining the kind of reaction products.

As a first means of modeling the chemical process, the TLC is assumed to be cylindrical. The model of the cross-section of the TCL is shown in Fig. 2 indicating the simulation area Ω as a bounded domain.

In this particular model, we consider the capillary vessels as radial passages to the membrane area. We further assume that there are no external forces acting on the TLC. Also, the drift components of the electrolyte in the azimuthal direction are neglected.

Essentially, two basic physical processes need to be formulated: the drift of the electrolyte, and the diffusion and the concentration of the reaction products.

The hydrodynamics of the process is modeled by the incompressible Navier-Stokes equations:

$$\begin{aligned} \rho\ [\ \partial_t \vec{u}\ +\ (\ \vec{u}\cdot\nabla)\ \vec{u}]\ -\ \eta\ \vec{\Delta}\vec{u}\ +\ \nabla p\ &=\ 0 \\ \nabla\cdot u\ &=\ 0 \end{aligned} \tag{1}$$

on Ω x (0,T), where ρ is the density of fluid, p is the pressure, η is the so-called dynamical viscosity, and u describes the velocity field of the electrolyte. We consider the Navier-Stokes equations in cylindrical coordinates. Based on the above assumption for the drift components, we disregard azimuthal variations and rotation inside the electrolyte:

$$u_\phi = \partial_\phi u_r = \partial_\phi u_\phi = \partial_\phi u_z = \partial_\phi p = 0.$$

The flow in the TLC through Γ_1 (see Fig. 2) is modeled by a quadratic profile

$$u_z|_{\Gamma_1} = U[1-(\frac{r}{r_o})^2], \quad u_\phi|_{\Gamma_1} = 0, \quad u_r|_{\Gamma_1} = 0,$$

where U is the so-called characteristic velocity and r_o the radius of the electrolyte input on Γ_1. The Reynolds number calculated by process and material parameters ranges from 0.1 to 100. Initial numerical results have been obtained for the velocity field of the electrolyte (see Fig. 3).

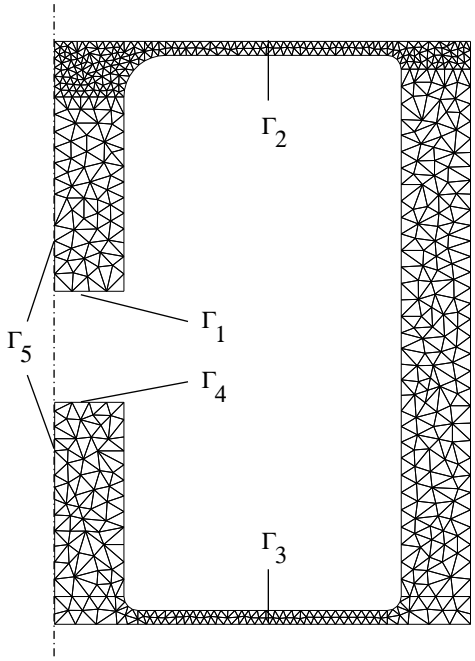

Fig. 2: Cylinder-symmetric discretization

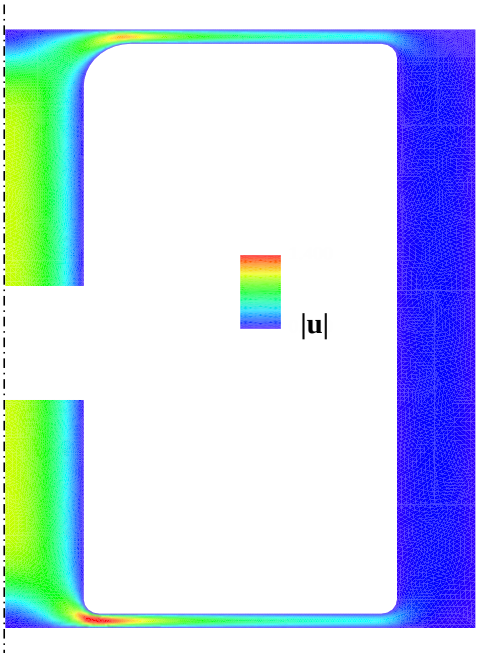

Fig. 3: Velocity field of the electrolyte

The rate of concentration is calculated by the following equation with given velocity $\vec{u}$:

$$\partial_t c\ +\ \vec{u}\ \nabla c\ -\ \nabla\cdot D\ \nabla c\ =\ 0, \tag{2}$$

on Ω x (0,T), where c is the rate of concentration and D is the diffusion coefficient.
Boundary conditions which fulfil equation (2) need to be addressed: first, the electrolyte is taken to be homogeneous at input (Γ_1), i.e. $c|_{\Gamma_1} = 1$; secondly, we assume the source substance is fully converted at the electrode (Γ_2), i.e. $c|_{\Gamma_2} = 0$; thirdly, only the reaction products can diffuse through the membrane ($c|_{\Gamma_3} = 0$); finally, homogeneous Neumann conditions are defined at all other boundaries ($\partial_\nu c = 0$).

The computations are carried out in cylindrical coordinates using algorithm [3]. As yet, attemps at numerical simulation have led to problems, mainly caused by different local spatial discretization schemes; whereas the finite-volume scheme [3] for equation (2) assumes a divergence-free velocity field, the finite-element method developed in [2] for equation (1) can only guarantee this property to hold approximately.
The solution of this problem, calculations of reaction rates near the electrode surface, and a detailed modeling of the electro-chemical process will be addressed in current and future work.

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

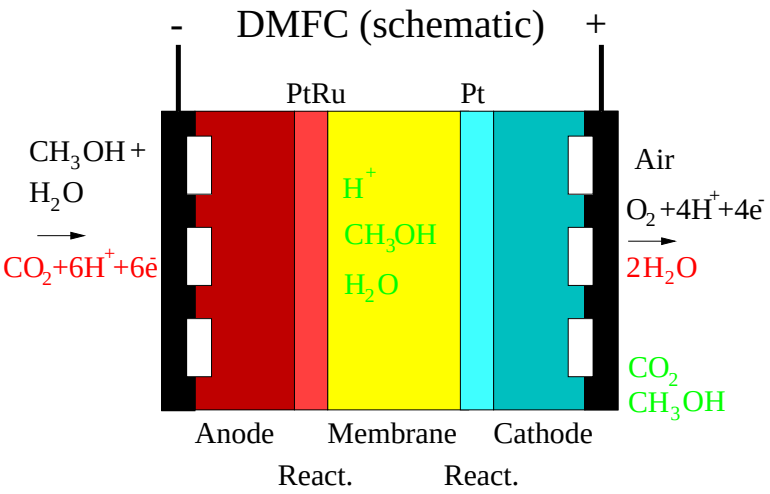
Collaborators: J. Fuhrmann, K. Gärtner

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

Supported by: IWV-3 Jülich

During the second year of the project we have focused on:
- support and adaptation for use at Forschungszentrum Jülich GmbH, IWV-3,
- the extension of the CH_3OH kinetics to Pt/Ru catalysts,
- a model taking into account mixed wettability by negative capillary pressures,
- some code extensions for fuel cells using H_2 rich gas mixtures,
- the energy balance equation and temperature dependence of the parameters,
- the fit of experimental data.

Short general description of a DMFC:



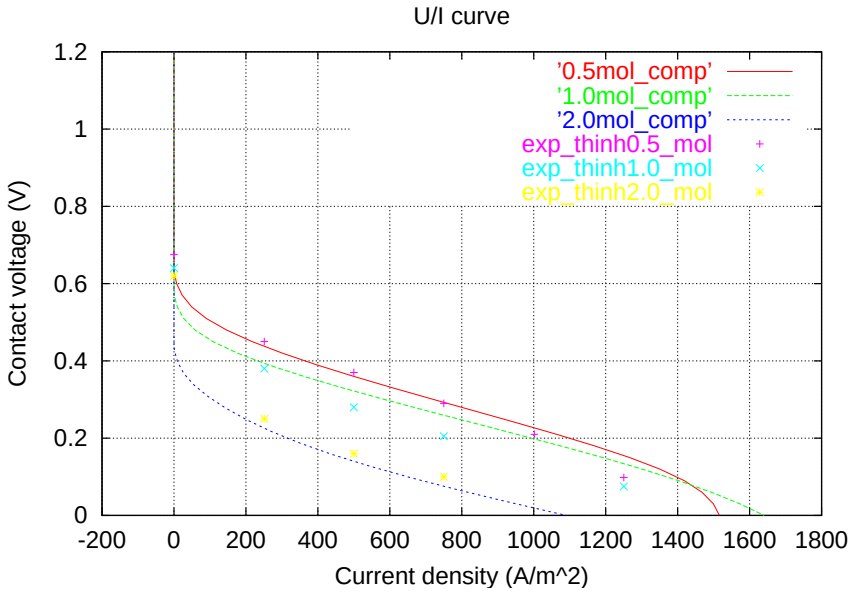
Methanol (0.5 ... 2.0 mol) dissolved in fluid water enters through channels of the diffusion layer (anode, left). At the *PtRu* catalyst grains CO_2, H^+, e^- are produced. The membrane transports H^+, the skeleton transports e^- to contacts and at the *Pt* catalyst grains the H^+, e^-, and O_2 react to water. This water must be removed and competes with the O_2 diffusing from the cathodic (right) channel to the reaction zone.

The following table summarizes the different variables present at the different locations (gases: red, true fluids: blue, solved tracers: green, electrochemical potentials: yellow, temperature: black, the immobile variables describe the fraction of the occupied catalytic sites by the species produced in different electrochemical reaction steps):

Layer	Mobile Species	Immob.	Composition
An. diff.	H_2O; CO_2, CH_3OH; H_2O, CO_2, CH_3OH; e^-; T	0	graphite, teflon
An. react.	H_2O; CO_2, CH_3OH; H_2O, CO_2, CH_3OH; e^-, H^+; T	8 or 10	graphite, teflon, nafion, Pt, PtRu
Membrane	H_2O; CO_2, CH_3OH; H^+; T	0	nafion
Cath. rea.	H_2O; CO_2, CH_3OH; H_2O, N_2, O_2; e^-, H^+; T	8+4	graphite, teflon, nafion, Pt
Cath. diff.	H_2O; CO_2, CH_3OH; H_2O, N_2, O_2; e^-; T	0	graphite, teflon

Due to methanol transport through the membrane, a parasitic reaction of methanol takes place at the cathodic reaction layer. Depending on the width of the reaction zone (and the concentration profile of CH_3OH and O_2), the reaction may be mainly chemical or electro-chemical. This

parasitic reaction is responsible for the non-monotonic dependence of the performance of the cell on the methanol concentration: measurements and computations show a decreasing performance from 0.5 to 2.0 mol/l methanol concentration:



An ideal transport assumption (no methanol permeation) would yield increasing performance with concentration.
Further experimental data are needed especially to improve the water transport models.
To improve the overview and interaction of the different (DMFC-related) research communities in Germany and to present information on simulation possibilities, a workshop focusing on all processes around the membrane was organized at WIAS (November 23/24; 30 participants, 14 talks, 3h round table discussion, see also: http://www.wias-berlin.de/dmfc/workshop/workshop-prog.html). Some further details on the model equations can be found in a talk given by J. Divisek at the Annual Congress of DECHEMA ([1]).

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Dynamics of thermal convection in sedimental basins

Collaborators: J. Fuhrmann, K. Gärtner

Cooperation with: GeoForschungsZentrum Potsdam

As a continuation of previous work, a careful investigation of two-dimensional solutions of the thermal convection system

$$\begin{aligned} \text{Mass balance:} \quad & \partial_t(\varphi\tilde{\rho}_f) - \nabla\cdot(\tilde{\rho}_f\mathbf{v}) = 0 \\ \text{Darcy law:} \quad & \mathbf{v} = \frac{k}{\mu}(\nabla p - \rho_f\mathbf{g}) \\ \text{Energy balance:} \quad & \partial_t(((1-\varphi)\rho_s c_s + \varphi\tilde{\rho}_f c_f)T) - \nabla\cdot\mathbf{q} = \mathbf{0} \\ \text{Fourier law:} \quad & \mathbf{q} = (\varphi\lambda_\mathbf{f} + (\mathbf{1}-\varphi)\lambda_\mathbf{s})\nabla\mathbf{T} - \mathbf{T}\tilde{\rho}_\mathbf{f}\mathbf{c}_\mathbf{f}\mathbf{v} \end{aligned} \tag{1}$$

in sedimental basin geometries has been undertaken. With high probability, the fluctuations of the solutions obtained can be associated with quasi-periodical and chaotical behavior of the underlying physical system. In order to obtain relevant statements in this direction, nonlinear time series analysis has been used to investigate the time series of the Nusselt number which reflects the heat transfer through the system. Visual inspection as well as time-series-based estimates of Lyapunov exponents strongly suggest that the hypothesis of chaos is true.
This corresponds well with analytical investigations undertaken during this project.

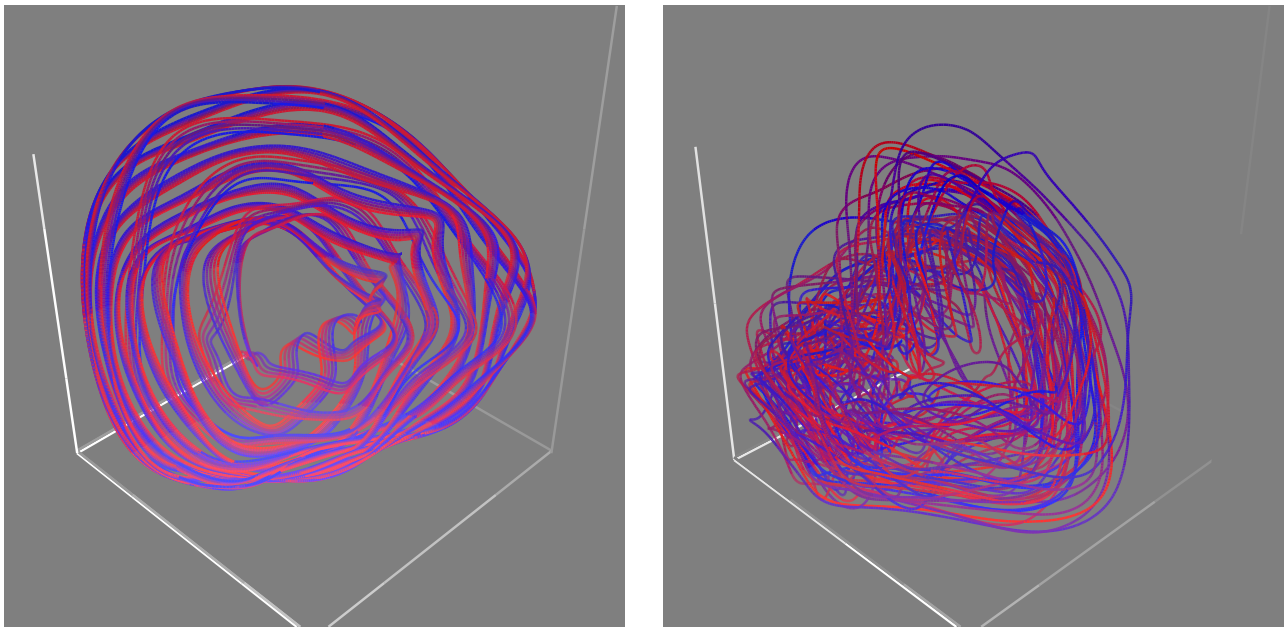

Fig. 1: Quasi-periodic and chaotic behavior of flow field (time delay embedding of Nusselt number time series)

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

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

The aim of this project is the maintenance and further development of *pdelib*, a toolbox of software components for the numerical solution of partial differential equations. Recent tasks within this project can be grouped into three main parts:

Maintenance. The code has now been successfully ported to all actual Unix systems (Linux/Intel, Compaq Tru64 Unix, IBM AIX, HP UX, Sun Solaris, SGI Irix). This took considerable effort mainly for the installation system. A CVS release policy has been formulated. New revisions of integrated software have been added. Noteably, version 4.0 of the extension language Lua with more convenient scripting possibilities is available for the *pdelib* users.

New Features. Newly added features have been influenced mainly by application projects. The main effort here went into the multiphysics capabilities of the *pdelib/sysconlaw* code for the solution of systems of viscous nonlinear conservation laws. For a system of partial differential equations it is possible to allow a particular variable to exist only in a subdomain. This takes into account the situation in fuel cells where one has to be able to couple different physical processes in the diffusion layer, the reaction zones, and the membrane.
A similar aim is followed in the development of the 3-d version of `WIAS-TeSCA` . Here, a flexible material management scheme is tested, which will enable the user to describe complex heterogeneous physical models.
For Lua input scripts, a library of all SI Units has been developed. Thus, in applications, scaling of physical units can be managed in a safe way.

Projects. Within the research group, a considerable effort went into the simulation of Direct Methanol Fuel Cells and the simulation of thermal convection in sedimental layers. Collaboration with the Research Group *Partial Differential Equations and Variational Equations* (see page 19) has been established. Here, the support of existing projects concerning the three-dimensional simulation of semiconductor devices, the numerical handling of $k \cdot p$ Schrödinger operators, the simulation of resistance welding and crystal growth have been continued. Recent new projects are the simulation bending of gallium arsenide plates, and the GUI-based laser treatment simulator.

Future Directions. Discussions and draft code studies have been started in order to develop the successor of *pdelib*, *pdelib2*. Aims of this effort are:

- increased efficiency, parallelization in order to be able to treat large three-dimensional problems,
- flexible management of degrees of freedom at nodes, edges, faces of a discretization, higher-order finite elements,
- adaptivity and geometry evolution based on Delaunay meshing/refinement techniques,
- easy-to-understand API for the implementation of new problems,
- improved user interface.

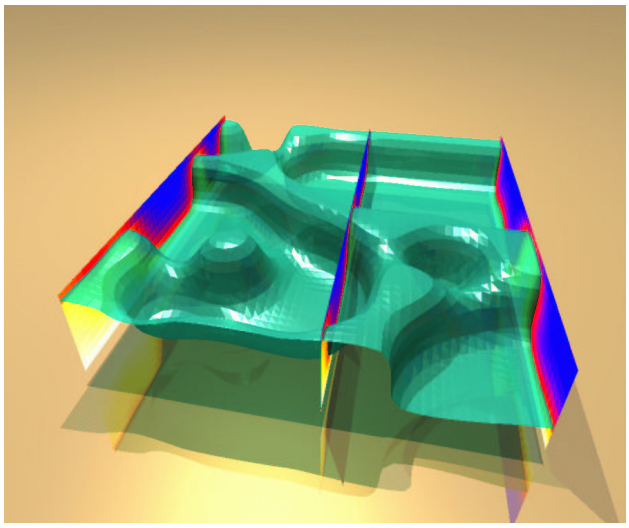

Fig. 1: Thermal convection in a three-dimensional porous layer. Ray-traced scene generated with gltools and povray.

Simulation of microwave and optoelectronic devices

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

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

Supported by: DFG: "Finite-Integrations-Methode mit Tetraedergitter zur elektromagnetischen Simulation von Mikrowellenschaltungen" (Electromagnetic simulation of microwave circuits using finite integration techniques with tetrahedral meshes), FBH

The design of microwave and optoelectronic devices requires efficient CAD tools in order to avoid costly and time-consuming redesign cycles. The fields of application are mobile communications, radio links, automobile radar systems, optical communications, and material processing. The commercial applications of microwave circuits cover the frequency range between 1 GHz and about 100 GHz, special applications in radioastronomy use even higher frequencies up to 1 THz. For optoelectronic devices, frequencies about several hundred THz are common.

The structures under investigation can be described as an interconnection of infinitely-long transmission lines, which have to be longitudinally homogeneous. Ports are defined on the transmission lines. The junction, the so-called discontinuity, may have an arbitrary structure. The whole structure may be surrounded by an enclosure.

For numerical treatment, the computational domain has to be truncated by electric or magnetic walls or by so-called Absorbing Boundary Conditions (ABC) simulating radiation effects. Among the ABCs, the Perfectly Matched Layer (PML) technique represents the most powerful formulation.

The scattering matrix describes the structure in terms of wave modes at the ports, which can be computed from the electromagnetic field. A three-dimensional boundary value problem can be formulated using the integral form of Maxwell's equations in the frequency domain in order to compute the electromagnetic field and subsequently the scattering matrix:

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

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

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

The boundary value problem 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.

In the period under report, studies were made in the following areas:
(A) Eigenmode problem ([1]): We are interested only in a few modes having the smallest attenuation. These are the modes with the smallest magnitudes of the imaginary part, but possibly with a large real part of associated propagation constants. First the method to find all eigen modes within a certain region of the complex plane was developed for microwave structures ([3], [4]). The modes 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 number of the corresponding propagation constants increases using PML. Due to the short wavelength, the dimension and the number of eigenvalue problems grows strongly for applications in optoelectronics (self-aligned stripe (SAS) laser) ([7]) in comparison to microwave circuits. All propagation constants which are located in the long strip of the complex plane covered by a sequence of Cassini curves (see Fig. 1) must be found. New strategies to handle these problems in a feasible time were developed. To reduce the execution times, in a first step, the problem is solved using a coarse grid in order to find approximately the locations of the propagation constants of interest. The accurate modes are calculated in a second step for an essentially reduced region, using a fine grid. Examining the eigenfunctions, in an additional step, nonphysical PML modes are eliminated.

(B) Boundary value problem ([2]): Using a finite volume approach with staggered nonequidistant rectangular grids, Maxwell's equations are transformed into a set of Maxwellian grid equations. The corresponding high-dimensional systems of linear-algebraic equations are solved using Krylov subspace methods with preconditioning techniques ([6]). Depending on the PML, the number of iterations increases strongly in some cases. To get feasible execution times, techniques how to choose the PML and the PML cell sizes have been developed.

(C) Tetrahedral grids ([9]): For the above-mentioned methods, the geometry to be analyzed is subdivided into elementary rectangular cells using three-dimensional nonequidistant rectangular cells. Due to the high spatial resolution, CPU time and storage requirements are very high. Supported by DFG and FBH, a finite volume method using unstructured meshes (tetrahedrons) was developed for the boundary value problem, with the aim to reduce the number of elementary cells by improved possibilities of local grid refinement and to improve the treatment of curved boundaries. Using a Delaunay triangulation (grid generator COG (see page 76) and *lbg*) and corresponding Voronoi cells, Maxwell's equations are transformed into a set of Maxwellian grid equations. The circumcenter of a generated tetrahedron can be located outside the tetrahedron. This is taken into account when generating the matrix. Substituting the components of the magnetic flux density, the number of unknowns is reduced by a factor of two.

The new research results have been published in [4] – [9].

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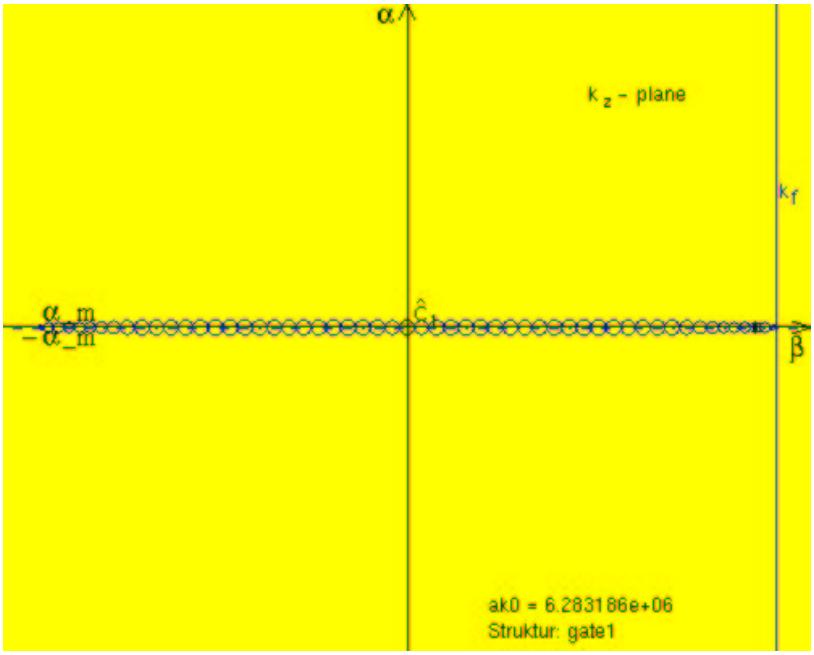

Fig. 1: Cassini curves cover the region of propagation constants with the smallest attenuation.

Large-scale dynamic process simulation

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

Cooperation with: S. Kurz (Robert Bosch GmbH, Stuttgart), A. Rogowski (EMS Inventa-Fischer, Berlin), D. Zeitz (Alstom (Switzerland) AG, Baden)

Supported by: Robert Bosch GmbH, Stuttgart

Over the last three decades, dynamic process simulation has become an indispensable tool for process design, analysis, and operation in chemical industry. Due particularly to an improved accuracy of mathematical process models and an increasing degree of integration in process modeling, the sizes of the problems which have to be solved numerically have grown considerably within this time. As a result, the plantwide dynamic process simulation has become a challenging field of application for parallel numerical methods.
For a dynamic process simulation of complex, highly interconnected plants, initial value problems for large-scale systems of coupled differential and algebraic equations (DAEs) have to be solved. Generally, the differential equations arise from balances of energy, mass, and momentum, while the algebraic relations result from constitutive relations for phenomenological quantities or different constraints. These DAE systems are highly nonlinear and can involve several tens of thousands of equations or even more. Usually their solution components process at different time scales. The process models depend on numerous parameters and are often characterized by discontinuities.

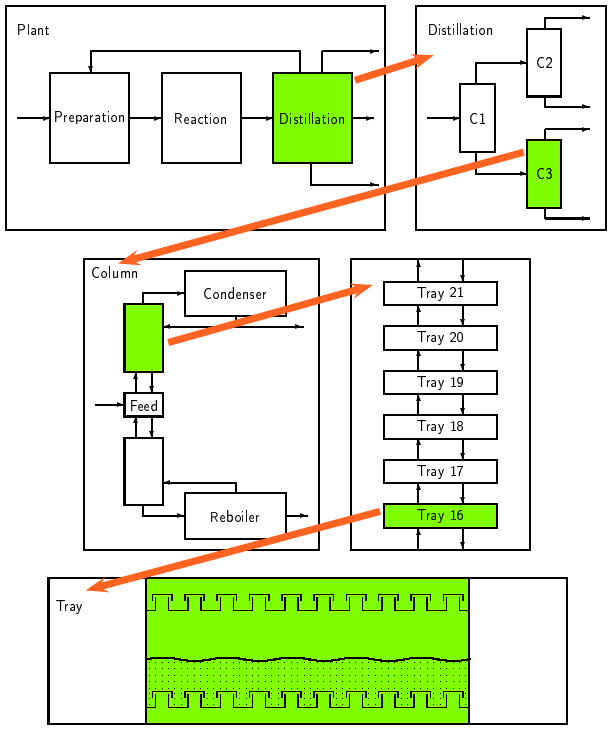

Fig. 1: Hierarchical modular structure of a sample plant

Our simulation concept is based on divide-and-conquer techniques and exploits the hierarchical, modular structure of chemical plants for large-scale dynamic process simulation on parallel computers. For that, a plant is considered as a network of connected process units like reactors, pumps, heat exchangers, or trays of distillation columns (see Fig. 1). In an equation-based flowsheet technique, a parameter-dependent mathematical model, describing the unit operations, is assigned to each unit type, and the units are connected, e.g., by mass and energy streams. With it, the corresponding system of DAEs is structured into subsystems according to the units and can be appropriately partitioned into blocks, which can be treated almost concurrently. The approach has been implemented in the Block Oriented Process simulator *BOP* that uses its own compiler to generate a hierarchically structured data interface from a process description with our modeling language.
In the period under report, we have mainly worked on improving the homogeneous simulation approach within *BOP*, in which the entire plant is modeled by a hierarchically structured,

block-partitioned system of DAEs

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

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

where the vectors $Y_j(t)$ and $U_j(t)$ denote the unknown and coupling variables of the blocks, respectively, and $u(t)$ the parameter functions. Within this approach, we use efficiently parallelizable block-structured Newton-type methods ([1]) to get a widely applicable parallel approach, covering "exact" methods as well as relaxation techniques. This approach has been improved concerning block partitioning, an adaptive relaxation decoupling, as well as the treatment of analytical derivatives for procedures, and a continuation method has been included into the simulator. With it, the parallel performance of *BOP* has been further improved ([2]).
The numerical solution within *BOP* requires a repeated solution of linear systems with the same pattern structure of sparse, unsymmetric coefficient matrices, and with multiple right-hand sides. Usually the linear solver requires between 50 and 80 percent of the total amount of computing time in large-scale applications. Our direct solver *GSPAR* is used to solve the linear system $Ax = b$. It uses advanced direct methods based on the Gaussian elimination method

$$\begin{aligned} PAQ &= LU, \\ Ly = Pb, \qquad & UQ^{-1}x = y. \end{aligned}$$

The row permutation matrix P is used to provide numerical stability, and the column permutation matrix Q is chosen to control sparsity. In a new approach, at each step of the elimination, the algorithm is searching for columns with a minimal number of nonzero elements, and a partial pivoting technique is used to maintain numerical stability.

Table 1: CPU times (in seconds) for factorization: *GSPAR2* compared with *UMFPACK V3*

			GSPAR2		*UMFPACK V3*	
			First	Second	Symb.+Num.	Redo
Matrix	N	NNZ	Factorization	Factorization	Factorization	Factorization
bayer01	57 735	277 774	1.583	0.328	1.600	0.917
lhr34c	35 152	764 014	11.713	2.735	3.133	1.833
circuit_4	80 209	307 604	2.736	0.098	950.012	930.063
shermanACb	18 510	145 149	6.846	2.011	25.499	23.949

Our new linear solver *GSPAR2* has proven to be successful in simulating several real-life problems. For linear systems with matrices arising from different technical problems, it has been compared with the solver *UMFPACK V3* (T.A. Davis, University of Florida, USA) concerning computing time. The results ([5]) are given in Table 1. Here N denotes the order and NNZ the number of nonzeros of the matrices. The first two matrices are from chemical process simulation, while the last two are from circuit simulation. The computations have been performed on a Compaq AlphaServer GS80 6/731 with 9 GB memory and alpha EV6.7 (21264A) processors, which operate at 731 MHz.
The generation of the data interface for the simulator *BOP* consists of three phases that can be controlled separately. To improve the usage of the compiler, a graphical user interface (GUI)

has been implemented in JAVA. The GUI (see Fig. 2) enables the selection of examples, the editing of the model and process description, the selection of different compiler phases, the setting of compiler parameters, and the evaluation of the resulting data interface. The compiler itself has been improved regarding the analysis and treatment of modeling errors.

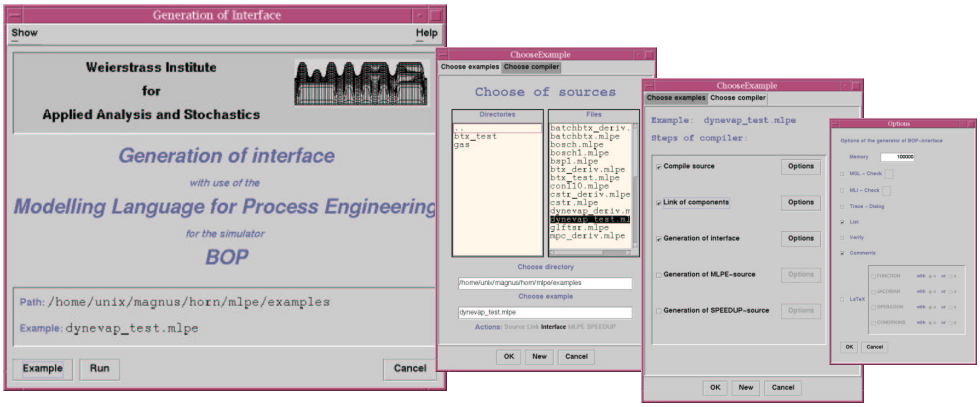

Fig. 2: GUI of the modeling language compiler for the simulator *BOP*

In the period under report, a continuing interest of industrial partners in our simulation concept has been maintained. The work concerning the realization of a continuation method within *BOP* for solving a special industrial problem has been successfully finished and was fully financed by the cooperation partner. Due to the request of another industrial partner, a PC version of *BOP* running under WindowsNT is in preparation. Finally we have started work to adapt a SPICE-like description language in the area of electric circuit simulation to our process description language, so that in the future, the simulator *BOP* will be applicable to circuit simulation problems as well.
First results concerning an inhomogeneous simulation approach have been reported in [3], [4].

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Grid generation

Collaborator: I. Schmelzer

The development of the grid generation and geometry description package COG has been continued.
The main focus was on the development of a graphical user interface to simplify the use of COG. A first version of the user interface has been implemented. This version allows many features of the package COG to be used. On the other hand, further improvement is necessary.

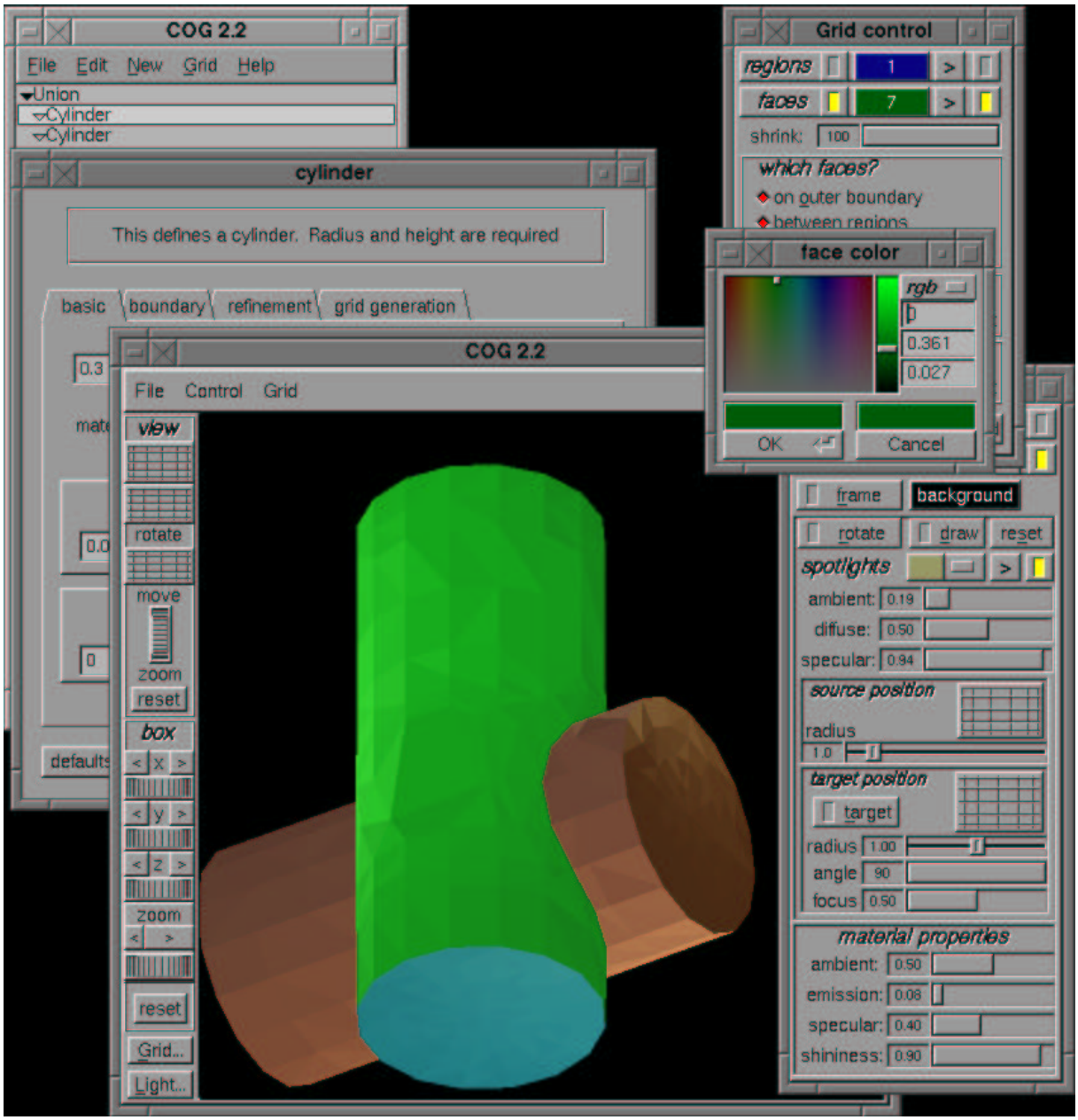

Fig. 1: COG User Interface

Another major issue has been the improvement of the stability of the algorithm. The Steiner

point insertion algorithm has been completely redesigned. This has allowed to improve the stability of the COG algorithm in transitional domains between different local coordinate charts, which has been a major problem of COG in the past.

For geological applications with very thin skew layers, a two-dimensional algorithm which allows the creation of sparse, slightly non-Delaunay grids has been generalized to the three-dimensional case and implemented:

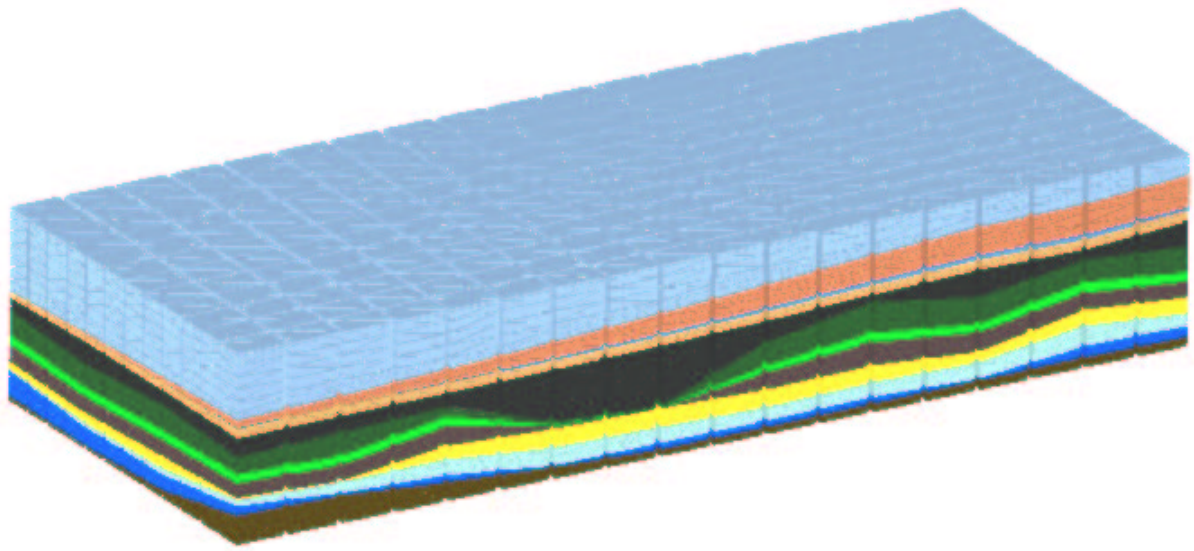

Fig. 2: 3-d grid for a geological profile with thin layers

Last but not least, parts of a future PhD thesis about grid generation have been completed.

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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 successfully been continued. For the Research Groups 1 and 7, videos were produced in MPEG and VHS formats.

It was also necessary to transform some of these videos to a format compatible for PCs (such as AVI and Quicktime).

Some complex graphical presentations of mathematical objects (non-simple curves such as Cassini's curve (see page 70) and other complex designs (Fig. 1)) were created directly using the programming language C and the OpenGL-API (application programming interface).

Our hardware equipment was supplemented by a digital video recorder (miniDV format), which allows high-quality videos to be archived. The recorder can also be used as playback equipment when connected to a normal television set. It can further be used for lecture presentations.

It was shown that our anticipatory policy of purchasing equipment pays dividends. The visual workstation Silicon Graphics Octane2 (tm) with the high-performance graphics subsystem VPro V12 was a basic necessity for establishing cooperation with an industrial partner (see page 86).

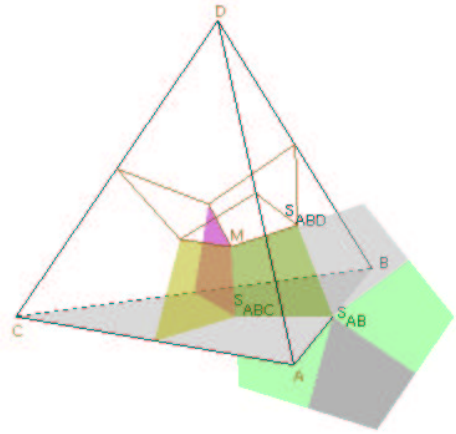

Fig. 1: Tetrahedron with Voronoi cells directly created by a code in the programming language C with the OpenGL-API

4.4 Research Group Nonlinear Optimization and Inverse Problems

4.4.1 Overview

Die Arbeit der Forschungsgruppe konzentriert sich auf die analytische und numerische Behandlung von nichtlinearen Optimierungsproblemen und inversen Problemen in aktuellen Anwendungsfeldern der Natur- und Ingenieurwissenschaften. Im Berichtszeitraum wurde die Bearbeitung der folgenden zentralen Projekte der Gruppe erfolgreich weitergeführt:

- Direkte und inverse Probleme der diffraktiven Optik (gefördert durch das BMBF-Mathematikprogramm „Neue Mathematische Verfahren in Industrie und Dienstleistungen“ und die DFG im Rahmen der Zusammenarbeit mit Japan),
- Optimierungsprobleme mit zufälligen und nichtglatten Daten (gefördert durch das DFG-Schwerpunktprogramm „Echtzeitoptimierung großer Systeme“),
- Bahnplanung für Industrieroboter und Menschmodelle (Industriekooperation mit einem schwäbischen Softwarehaus für Produktionsplanung),
- Parameterschätzung bei Mehrphasenströmungen (gefördert durch die DFG).

Im September 2001 organisierte die Forschungsgruppe einen Workshop zum Thema „Inverse Problems in Applications“, der insbesondere aktuellen Problemen der inversen Modellierung und ihrer Numerik gewidmet war.
Im Folgenden werden die im Berichtszeitraum erzielten wissenschaftlichen Ergebnisse näher dargestellt.

The work of the research group concentrates on the analytical and numerical treatment of nonlinear optimization and inverse problems occurring in real world applications in natural sciences and engineering. In 2001 the following main projects were successfully continued:

- Direct and inverse problems in diffractive optics (supported by the BMBF mathematics program “New Mathematical Methods in Industry and Services” and by the DFG in the framework of the cooperation with Japan),
- Optimization problems with random and nonsmooth data (supported by the DFG Priority Program “Real-time Optimization of Large Systems”),
- Path planning for robots and human models (industrial cooperation with a South German software company for production planning),
- Parameter estimation in multiphase flow (supported by the DFG).

In September 2001 the research group organized a workshop on Inverse Problems in Applications, which was particularly devoted to the challenges that practical applications pose to inverse modeling and computation.
In the following, the research activities and the results obtained will be described in more detail.

4.4.2 Projects

Direct and inverse problems in diffractive optics

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), J. Cheng (Fudan University, Shanghai, China), M. Yamamoto (University of Tokyo, Japan)

Supported by: BMBF: "Modellierung und Optimierung mikrooptischer Oberflächenstrukturen" (Modeling and optimization of microoptic surface structures – 03ELM3B5), DFG: "Scientific cooperation with Japan: Inverse problems in electromagnetics"

1 Accurate FEM simulation of diffraction by polygonal gratings (J. Elschner, A. Rathsfeld, G. Schmidt).
As is well known, the diffraction of electromagnetic plane waves by optical gratings (i.e. devices which are independent in one direction, say, in the direction of the x_3 coordinate, and the cross section of which in the $x_1 - x_2$ plane is periodic in another direction, say, in that of the x_1 coordinate) can be reduced to various boundary value problems for the Helmholtz equation. From their solution all interesting features, including the reflected/transmitted energy, the reflection/transmission efficiencies (percentage of the light reflected/transmitted in a finite number of predetermined directions), and of course the near field behavior can be derived.

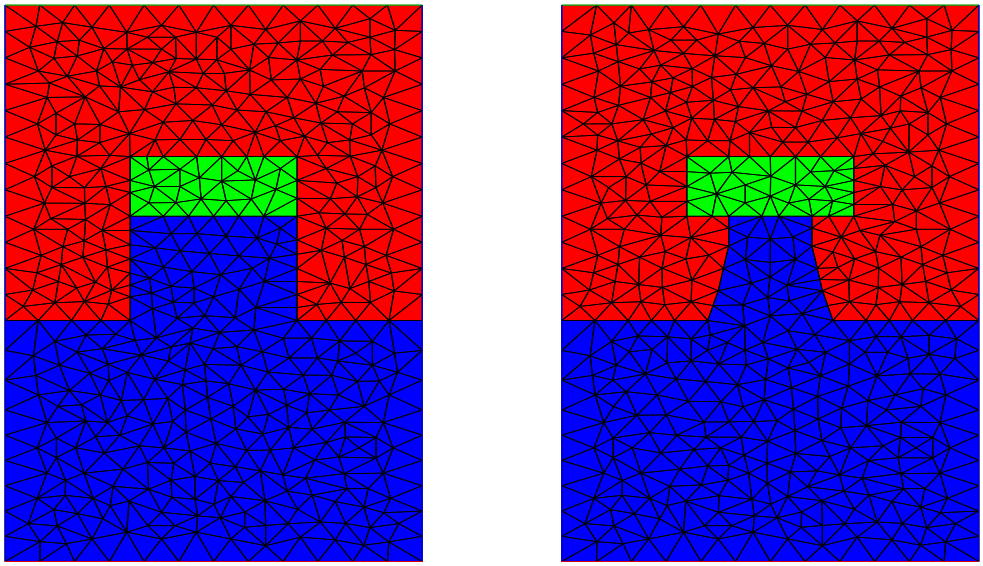

Fig. 1: One period of coated binary grating, exact and overetched

We developed a new code DPOGTR (direct problem, optical grating, triangular grid) for the FEM solution of the diffraction problems by gratings of polygonal shape and by gratings bounded by smoothly parameterized curves (for the theoretical background, cf. [8, 5]). The field components for the TE (transverse electric) and TM (transverse magnetic) polarization are determined as continuous piecewise linear functions defined over triangular meshes. For instance, the grating in Fig. 1 with a period of 1.7 μm, consisting of cover material air (red), a

coated layer of photoresist (green), and substrate material (blue), leads to the efficiencies shown in Fig. 2 if TM polarized red light (wave length 633 nm) is illuminating the grating under various incident angles. This new code DPOGTR is based on subroutines of the previously developed package DiPoG treating the case of lamellar gratings (all edges parallel to the coordinate axis) with rectangular meshes and bilinear trial function. Furthermore, in cooperation with colleagues of the Research Group *Numerical Mathematics and Scientific Computing* we adapted the corresponding PDELIB subroutines for the assembling of the stiffness matrix and the solution of the linear system of equations. The most time- and storage-consuming part of the computation is the solution of the FEM system which is ill-conditioned for large wave numbers. We implemented an iterative solver based on preconditioned CGS and on a simple algebraic domain decomposition.

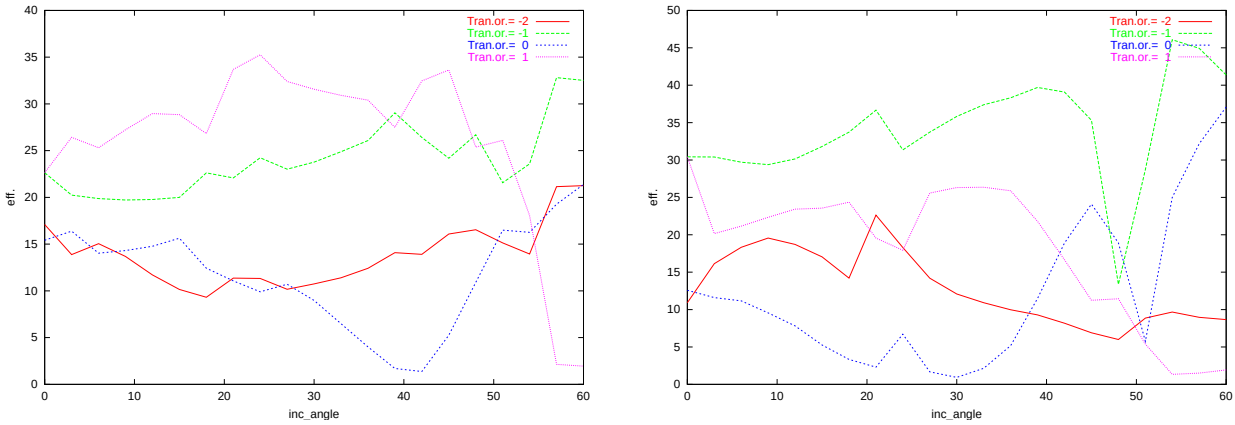

Fig. 2: Resulting transmission efficiencies of orders 1, 0, -1, -2

The main difficulty in the FEM approach is to deal with large wave numbers requiring small step sizes and, therewith, the solution of huge systems of equations. However, the technological progress allows to produce smaller devices, and the FEM solution of the resulting boundary value problems with moderate wave numbers becomes more and more attractive. Nevertheless, there is still a need to solve problems with larger wave numbers, e.g., problems for coated echelle gratings with “larger” periods. Therefore, the old package DiPoG contains a generalized FEM with reduced so-called pollution error. Unfortunately, the basic idea of this method relies on uniform partitions. We started to consider an alternative generalized FEM on triangular grids. This uses a new basis of trial functions which are locally the approximate solution to the Helmholtz equation. The first results are promising. However, the parameters still need to be adjusted and the code must be optimized. In other words, the work on the generalized FEM will be continued.

Finally, for our cooperation partner in Oberkochen, we rendered an expert opinion on several aspects of the integral equation method applied to diffraction gratings.

2 Reconstruction of grating profiles (G. Bruckner, J. Elschner, G. Schmidt).
The problem of recovering a periodic structure from illuminating the structure by incident plane waves is of great practical importance in modern diffractive optics, e.g., in quality control and optimal design of diffractive elements (see [1]). The efficient numerical solution of inverse problems of this type is challenging due to the fact that they are both nonlinear and severely ill-posed in general. So far we considered scattering of time-harmonic plane electromagnetic waves in the TE (transverse electric) mode by a two-dimensional perfectly conducting periodic structure, which is modelled by the Dirichlet problem for the Helmholtz equation. The results will be extended to the inverse TE and TM transmission problems for diffraction gratings in the near future.
Let the profile of the diffraction grating be given by the graph $\{(x_1, f(x_1)) : x_1 \in \mathbb{R}\}$ of a 2π-periodic Lipschitz function, and suppose that a plane wave given by $\exp(i\alpha x_1 - i\beta x_2)$ is incident from the top. Here the wave number k is a positive constant, $\alpha = k\sin\theta$, $\beta = k\cos\theta$, and $\theta \in (-\pi/2, \pi/2)$ is the incident angle. In the inverse or *profile reconstruction problem*, one tries to determine the profile function f from measurements of the scattered field, e.g., from the Rayleigh coefficients of the propagating modes (possibly for several wave numbers and/or incident angles).
The conditional (global) stability of this problem for smooth profile curves and small wave numbers was proved in [3]. The method is based on a Carleman estimate for the Laplace operator and originates from the inverse problem of determining an unknown part of the boundary modelled by the Laplace equation. The consequences for Tikhonov regularized reconstruction procedures are studied in [4], where a logarithmic convergence rate is obtained. Local stability estimates of Lipschitz type for nonsmooth grating profiles were derived in [6], using a new approach based on the material derivative method.
In [4], [7], we studied the performance and convergence of an effective inverse method, which is based on an approach by Kirsch and Kress (for acoustic obstacle scattering; see [2]) and avoids the solution of the direct scattering problem. In this method, the inverse problem is decomposed into the severely ill-posed linear problem of reconstructing the scattered wave from its far-field pattern, and into the well-posed nonlinear problem of determining the unknown profile curve as the location of the zeros of the total field. The convergence analysis covers the practically important case of nonsmooth grating profiles and is based on new perturbation and stability results for the direct problem, see [7].
The discretization of the resulting optimization problem then leads to a nonlinear least-squares problem which is solved iteratively by the Levenberg-Marquardt algorithm. In the case of Fourier gratings our method proved to be rather efficient if the grating grooves are not too deep. First numerical results are also obtained for piecewise linear profile curves.

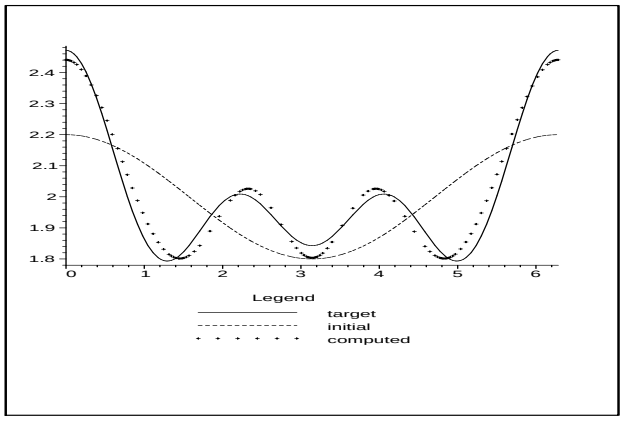

Fig. 3: Profile reconstruction for a Fourier grating with seven modes

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Optimization problems with random and nonsmooth data

Collaborators: R. Henrion, A. Möller

Cooperation with: W. Römisch (Humboldt-Universität (HU) zu Berlin), G. Wozny (Technische Universität (TU) Berlin), M. Steinbach (Konrad-Zuse-Zentrum für Informationstechnik (ZIB) Berlin), T. Szántai (Technical University of Budapest, Hungary), J. Outrata (Institute of Information Theory and Automation (UTIA) Prague, Czech Republic), A. Jourani (Université de Bourgogne, Dijon, France)

Supported by: DFG: Priority Program "Echtzeitoptimierung großer Systeme" (Real-time optimization of large systems)

The emphasis of this research project is on the solution of applied optimization problems containing random parameters. The analysis of these problems leads to algorithmic challenges and raises new questions about structure and stability.
The first application deals with a robust control of a continuous distillation process under random feed conditions. A sketch is given in Fig. 1. This subject has been analyzed in cooperation with G. Wozny (TU Berlin) and co-workers in the framework of a DFG project entitled *Real-Time Optimization of Distillation Columns under Probabilistic Constraints* (http://www-iam.mathematik.hu-berlin.de/dfg2/). The peculiarity here is the need to cope with random parameters given by feed characteristics like inflow rate, composition, and temperature, which are observed only after a decision on the control (feed extraction, heating profile) has been made. The basic approach is a model formulated by means of probabilistic constraints. In previous work, just the inflow rate was assumed to be random. Inside this setting, the focus shifted from rates assumed as a Gaussian process towards rates with an arbitrary deterministic profile affected by random initial time. Numerical results are presented in [1] and [2], whereas structural properties of the arising problems are analyzed in [3] and [4]. Additionally incorporating random composition, however, leads to more complicated structures and requires more sophisticated algorithmic techniques. A first step in this direction has been made by developing (jointly with T. Szántai and J. Bukszár) a method for calculating functional values and gradients of polyhedral chance constraints. The algorithm compares favourably with competing approaches in moderate dimension, but its efficiency has to be improved at dimensions relevant in the application.
A third field of research concerns the investigation of Lipschitz properties of multifunctions arising in general (nonsmooth) optimization problems. Here, an intensive cooperation with J. Outrata (Prague) and A. Jourani (Dijon) shall be continued. The focus of analysis is on subdifferential conditions for the so-called calmness property of constraint mappings which has direct consequences for many important issues of nonlinear optimization like multiplier rules, constraint qualifications, local error bounds, sensitivity or weak sharp minima. First results dealing with Lipschitz data in finite dimensions ([5]) have been extended in [6] to convex data in Banach spaces. The most recent work ([7]) is devoted to more general constraint structures, to applications in complementarity problems, and to the characterization of the stability of solutions. A major challenge to be attacked in the future is the case of Lipschitz data in Banach spaces.

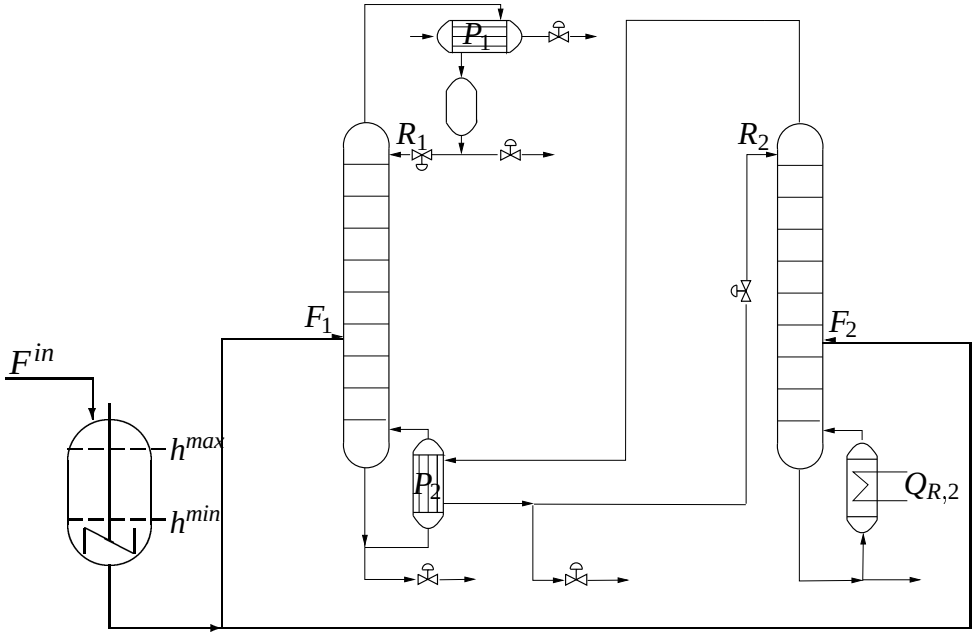

Fig. 1: Flow chart of the distillation unit under parallel operation

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Path planning for robots and human models

Collaborators: I. Bremer, V. Schulz

Cooperation with: a South German software company for production planning

Work from last year[1] has been continued.

Aims:

- Theoretical insights about the
  - attainability of (welding) points,
  - choice of robot type,
  - placement of robots, workpieces, grippers, etc.
  - cycle times,
- offline computation of robot controls,
- visualization of the whole process (movements of robot and man),
- direct coupling of robot control to the simulation software,
- generation of programs for the robot control,
- processing of the original robot programs.

In the field of path planning for robots, the work is built up on previous joint efforts with the industrial partner and is focused on practice-related extensions for synchronization and modification. Among other things, the preservation of speed limits for the TCP (tool center point) for linear paths has been realized.
The path planning for human models has been implemented in a first attempt analogously to the one of the robot models. We are proceeding on the assumption of a simplified axes model. The overparametrization of the final position and final hand orientation is resolved by independently determining the positions of the trunk and the shoulder.

Inverse kinematics

The position and the orientation of a point in space are given by six coordinates, three for the position vector (v) and three for the local orientation.
The orientation is described by a rotation matrix (R) to be produced by rotations executed one after the other on three independent axes.
A transformation of an oriented point consists of a translation and a rotation. A point can be identified by the transformation of the point of origin ($v_0 = (0,0,0), R_0 = \mathrm{Id}$).
Thus, the transformations form a (noncommutative) group as far as the execution one after the other is concerned.
Point coordinates and orientation can be given absolutely, i.e. in connection with a world coordinate system, or relatively, i.e. in respect of a local coordinate system.
The transformation in local coordinates corresponds to the multiplication on the left-hand side, the transformation of the global coordinates to the transformation on the right-hand side.

[1] http://www.wias-berlin.de/publications/annual_reports/2000/node47.html

Transformation on the left-hand side
(local coordinate system)

$$\begin{aligned} T_r(v,R): \qquad (v_n,R_n) &= T_r(v,R)(v_a,R_a), \text{ with} \\ v_n &= v_a + R_a * v \\ R_n &= R_a * R \end{aligned}$$

Transformation on the right-hand side

(global coordinate system)

$$\begin{aligned} T_l(v,R): \qquad (v_n,R_n) &= T_l(v,R)(v_a,R_a), \text{ with} \\ v_n &= v + R * v_a \\ R_n &= R * R_a \end{aligned}$$

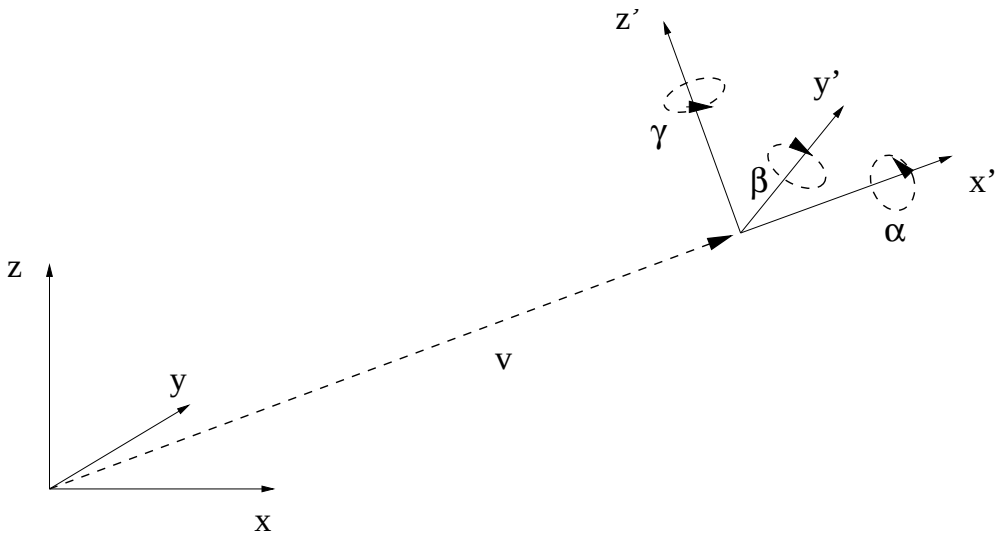


Fig. 1: Simulated ramps in comparison with measured ones

The direct kinematics
consist of the calculation of the position and orientation of a point in space by multiplying individual parameter-dependent transformations. In the case of robot kinematics, these parameters are the lengths and the angles of the axes. The lengths of the axes are (in general) fixed. Some angles are determined by the position of the motor in the joints. Thus they are free. In addition, the temporal changes of the parameters being given, the path is calculated in its final point, as a function of time.

The inverse problem
consists of the calculation of the transformation parameters (positions of the axes) from given point coordinates and orientations and the calculation of the angular speed for given paths.

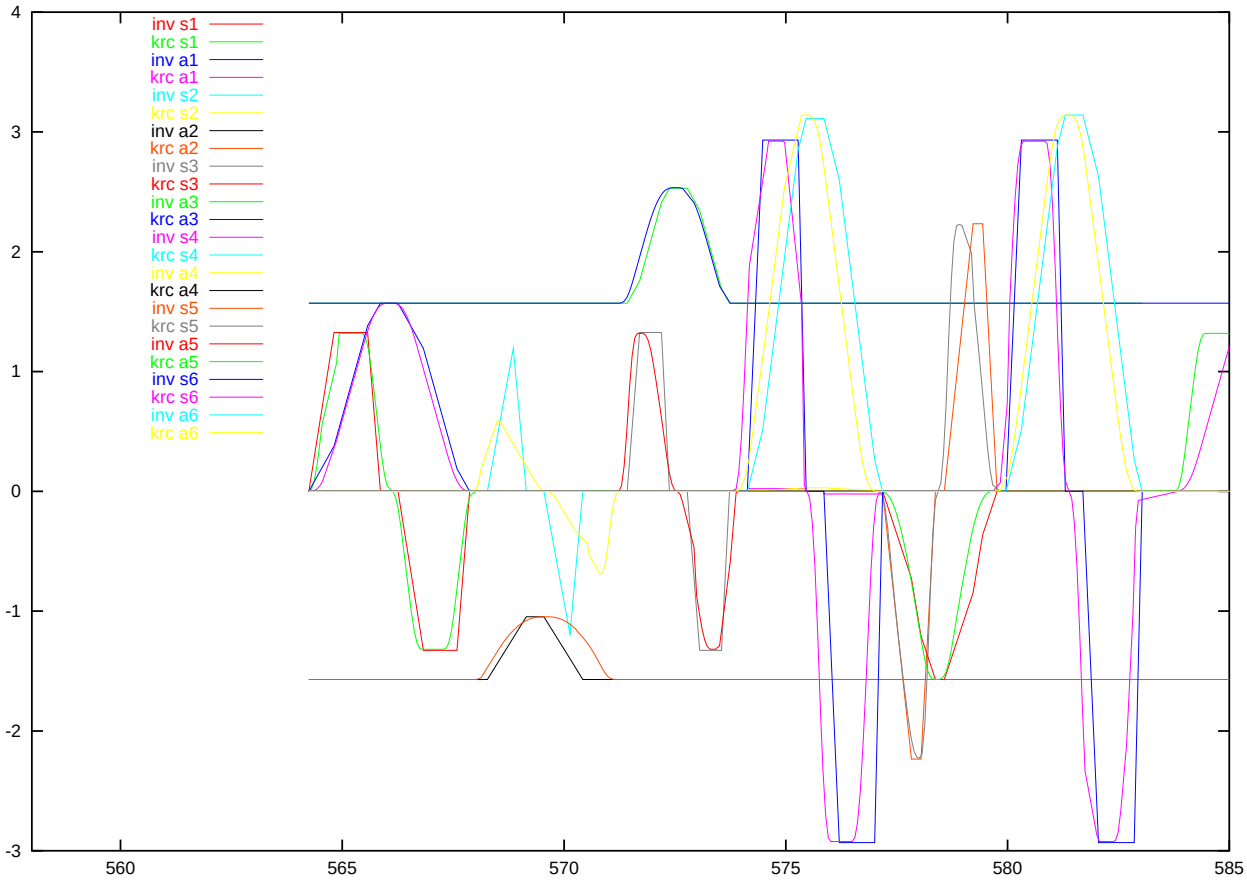
Ramp model

The real robot controls realize the axial movements in so-called ramps, i.e. the velocity profile is, in its idealized form, piecewise linear.

$$\omega(t) := \begin{cases} b_a t, & t \leq t_1 \\ b_a t_1, & t_1 < t \leq t_2 \\ b_a t_1 - b_e(t - t_2), & t_2 < t \end{cases}$$

For a simple movement, consisting of a phase of acceleration to a constant velocity and a phase of deceleration, this results in the form of a trapezoid for the velocity graph.
For each axis, the lengths of the phases of acceleration and of the interval with constant angular speed are computed for given angle differences and time slices.
Since all axes are supposed to conclude their movement synchronously, we first compute, for each axis, the minimal time to reach the new position. Then we determine the time slice for the whole movement as the maximum of these times.
The axis requiring the longest time for its movement is called the leading axis. This one works with maximum velocity and determines the time slice for all other axes.
The calculation of the ramp profiles for given time slices entails piecewise quadratic equations.
A path leading through several points is constructed from individual ramp profiles.
In a PTP (point to point) run with zero velocity in the point to be reached, the ramps are clearly defined and directly to be determined.
In a “sliding over” run, the point is passed by without stopping. This is realized by subsidiary points in which the velocity has not to be zero.
Thus we get an optimization problem with free velocities in the individual points of the path.

The approximate solution
of the optimization problem for paths through several points is obtained by a direct method, starting out from maximal transit velocities and taking only the accessibility of the next point into consideration. In this process, it is possible that an already calculated ramp has to be corrected in case that the transit velocities have been too high to reach the arrival point exactly.
The figure shows a relatively good agreement of the ramp model with the real robot control.



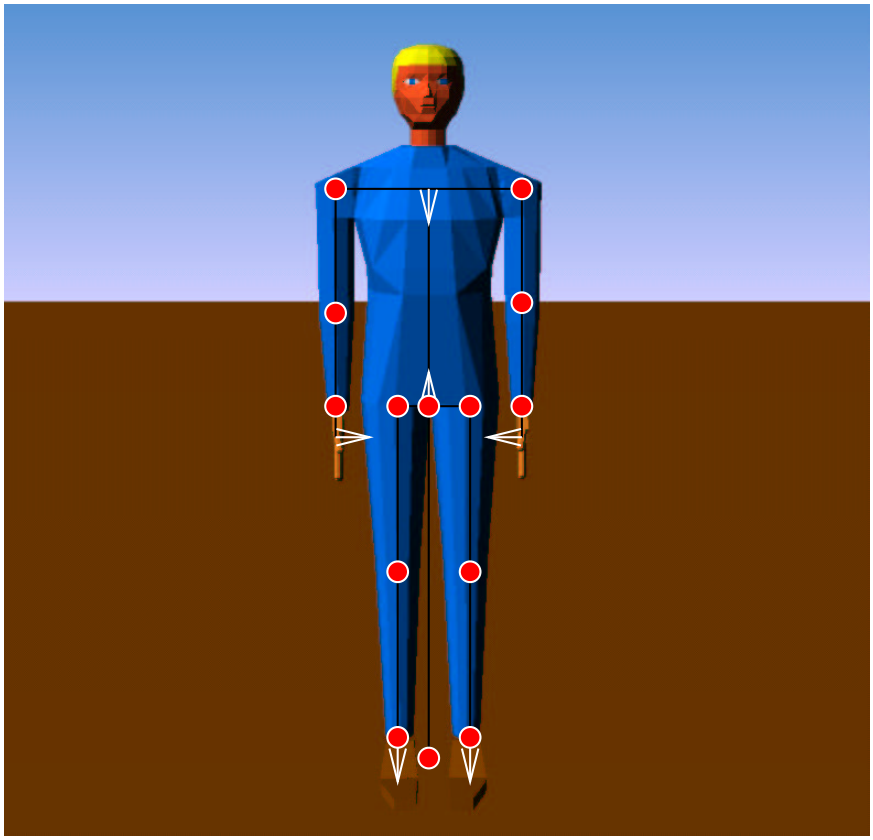


Fig. 2: Axes in the human model

Human model

Kinematics for the „worker“

- Position of the local coordinate system to the world coordinate system fixes the pelvis area.
- The upper part of the body is fixed with reference to the pelvis (i.e. in the local coordinate system),
- the arms relatively to the shoulders (determined by the upper part of the body), and
- the legs relatively to the hip (determined by the pelvis).

Inverse problem

given: position of hands and feet in world coordinates.

searched: angles for all joints

Reduced inverse problem

given: position of pelvis, hands, and feet

searched: angle for the rotation of the upper part of the body and of the joints of arms and legs

Path calculation for motion sequences

Example: walking straight ahead

- Decomposition of the motion sequence into three sub-sequences: “foot up”, “foot forward”, “foot down”,
- positioning of the trunk in the intermediate points,
- positioning of the legs, one foot fixed,
- positioning of the hands for balancing movements of the arms,
- independent path calculation for the individual kinematics,
- on-line correction of the fixed foot on the surface of the path (by use of SQP methods).

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Parameter estimation in multiphase flow

Collaborator: V. Schulz

Cooperation with: S.B. Hazra, G. Wittum (Universität Heidelberg)

Supported by: DFG: “Inverse Modellierung von Strömungs- und Transportvorgängen im heterogenen Untergrund auf der Basis von Mehrgitterverfahren” (Inverse modeling of flow and transport in a heterogeneous subsurface with multigrid methods)

Multiphase flow is of high importance, e.g., for waste removal in the subsurface. The basic mathematical models are described by certain nonlinear partial differential equations which involve also empirical relationships. For example, the capillary pressure saturation relationship is described by a Brooks-Corey formulation with two constitutive parameters: the entry pressure p_d and another parameter λ. These parameters are a priori unknown and cannot be measured or derived from other relationships. For realistic computational simulations of planned in situ remediation processes, these parameters have to be determined via parameter estimation from other magnitudes which can be directly measured.
In our problem, they are to be determined from pointwise measurements of the capillary pressure or saturation of water at several time instances. We employ an output-least-squares approach resulting in a nonlinear optimization problem with PDE constraints. This yields in particular two difficulties: the high dimension of the discretized optimization problem and its nonlinearity. Since it is well-known that single shooting strategies result in numerical instabilities, we have developed a multiple shooting approach, where we have to take into account that we are dealing with an instationary PDE rather than with an ordinary differential equation involved in the classical multiple shooting formulation. Therefore we have developed a variant employing the weak formulation of the continuity conditions. In order to cope with the high dimensionality of the problem, reduced Gauss-Newton methods are used, where derivatives are computed according to the principle of internal numerical differentiation.
We have started out in the year 2000 with academic formulations of parameter estimation problems for the isothermal case. The multiple shooting approach has been implemented within the PDE software toolbox *ug*. Now we have enlarged the problem class so that we are able to treat non-isothermal three-phase three-component models, which leads to even more pronounced nonlinearities. On the other hand, we now also incorporated real measurement data. Fig. 1 presents one such result where the parameters λ and a (scaled absolute permeability) are determined using the measurements of saturation from a one-dimensional column experiment carried out at the VEGAS, University of Stuttgart. The figure shows the comparison of computed saturation, using the parameters determined by our method, with the experimental ones. The latter developments are described in detail in [2].

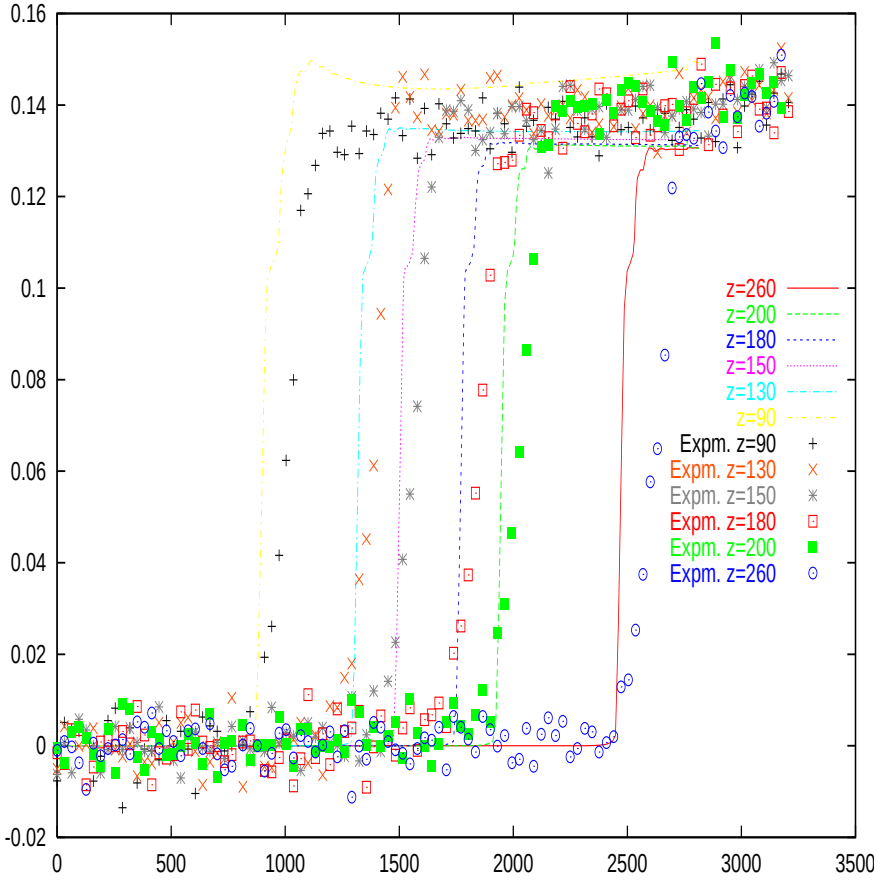

Fig. 1: Comparison of saturation of water phase with experimental values

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Optimization and filtering design

Collaborators: J. Tseng, V. Schulz

Cooperation with: K.L. Teo (Hong Kong Polytechnic University, China), A. Cantoni (University of Western Australia, Perth), Z. Zang (Australian Telecommunications Research Institute, Perth), R.H.W. Hoppe, S.I. Petrova (Universität Augsburg)

This project is concerned with the application of optimization techniques to signal processing where the design of a filter can often be cast as a constrained optimization problem. The envelope-constrained (EC) filtering problem is a specific constrained optimization problem. In this problem, we are concerned with the design of a linear time-invariant filter with impulse response $u(t)$ to process a given input signal $s(t)$ which is corrupted by an additive random noise. The objective is to design a filter such that its squared L^2 norm is minimized, whereas its noiseless output response with respect to a specified input signal stays within a prescribed pulse-shape envelope defined by the lower and upper boundaries. Traditionally, problems of this type were often handled by minimizing the weighted least-mean-square (LMS) difference between the output of the filter and a desired pulse shape. By using output envelope constraints, the EC filtering approach, however, is more relevant than the LMS approach in a variety of signal processing fields such as robust antenna and filter design, radar and sonar detection, and seismology. The continuous-time envelope-constrained filtering problem is then posed as a QP problem with linear inequality constraints:

$$\begin{aligned} \min \quad & \|u\|_2^2 \\ \text{subject to} \quad & \varepsilon^-(t) \le \psi(t) \le \varepsilon^+(t), \forall t \in [0,\infty), \end{aligned}$$

where $\psi(t) = \int_0^\infty u(\tau)s(t-\tau)d\tau$. Although QP problems have been studied extensively, and a number of efficient optimization algorithms are now available, these algorithms are not suitable for on-line or adaptive applications when the continuous-time domain is substituted by a discrete-time representation. The reason is that their computation requirements at each iteration for the search direction and the corresponding step-size are rather demanding. The goal of this project is to develop an adaptive algorithm based on the gradient flow and space transformation method for solving the filtering problem in a stochastic environment ([1], [2], [3]). Furthermore, we have begun to generalize the methods developed for the solution of linear quadratic programs in this special case to efficient iterative solution techniques for high-dimensional QP subproblems within SQP methods for nonlinear discretized optimization problems.

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4.5 Research Group Interacting Random Systems

4.5.1 Overview

Im Berichtsjahr konzentrierte sich die Forschung weiterhin auf die Thematik der stochastischen dynamischen Systeme. Es wurde eine Vielzahl bemerkenswerter Resultate erzielt. Diese betreffen vor allem die stochastische Dynamik ungeordneter Spin-Systeme, wobei die Analyse des Phänomens des „Alterns“ im Mittelpunkt stand, zeitabhängige stochastische dynamische Systeme, wo Phänomene wie „stochastische Resonanz“ und „Hysterese“ untersucht wurden, sowie interagierende Verzweigungsprozesse und stochastische Teilchensysteme für die numerische Lösung von Koagulationsprozessen und die Dynamik verdünnter Gase. Die Mitarbeit von S. Rœlly seit dem Herbst erlaubt es uns nunmehr, wechselwirkende Diffusionsprozesse auch von der Seite der Gibbs-Maße her zu betrachten.

The research in the past year has further focused on stochastic dynamical systems, where a number of remarkable results could be obtained. These concern in particular the stochastic dynamics of disordered spin systems, where the analysis of “aging” phenomena has been a key objective, time dependent stochastic dynamical systems, where phenomena such as “stochastic resonance” and “hysteresis” were investigated, interacting branching diffusions, and stochastic particle systems for the numerical solutions of the coagulation processes and rarefied gas dynamics.
In the fall, S. Rœlly joined our group which allows us now to develop a Gibbsian viewpoint on interacting diffusion processes.

A. Eibeck hat im Jahr 2001 seine Dissertation an der Humboldt-Universität zu Berlin eingereicht. Ebenfalls im Jahr 2001 habilitierte Chr. Külske an der Technischen Universität Berlin.

In 2001, A. Eibeck has submitted his Ph.D. thesis to the Humboldt University of Berlin, while Chr. Külske completed his Habilitation at the Technical University of Berlin.

Herauszustellen ist im Berichtsjahr die Beteiligung von Mitgliedern der Forschungsgruppe an der Organisation internationaler Tagungen und Workshops. Dies betrifft die Mitorganisation der Tagung „Stochastics in the Sciences“ am Mathematischen Forschungsinstitut Oberwolfach sowie zweier Miniworkshops: „Aging and Glassy Systems“ und „Stochastic Models for Coagulation Processes“, ebenfalls am Mathematischen Forschungsinstitut Oberwolfach. Des Weiteren wurde der Workshop „Stochastic Methods from Statistical Physics“ in Blaubeuren mitorganisiert, der im Rahmen des DFG-Schwerpunktprogramms „Interagierende Stochastische Systeme von hoher Komplexität“ stattfand.

Members of the group have been particularly active in the organization of international meetings and workshops. At the Mathematical Research Institute of Oberwolfach we participated in the organization of a Meeting “Stochastics in the Sciences”, as well as of two miniworkshops on “Aging and Glassy Systems” and “Stochastic Models for Coagulation Processes”. Moreover, we participated in the organization of a Workshop “Stochastic Methods from Statistical Physics” in Blaubeuren in the framework of the DFG Priority Program “Interacting Stochastic Systems of High Complexity”.

Über die wissenschaftlichen Ergebnisse des letzten Jahres wird im Folgenden detailliert berichtet.

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

4.5.2 Projects

Low temperature phases in models with long range interactions

Collaborators: A. Bovier, C. Külske

Cooperation with: M. Zahradník (Charles University, Prague, Czech Republic)

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

Models of statistical mechanics with weak long range interactions have been introduced by V. Kac half a century ago to obtain a rigorous version of the van der Waals mean field theory. Today we see these models anew as interesting candidates to reach a better understanding of disordered spin systems and in particular the relation between mean field theory and lattice models in the context of disordered systems. In this project we are undertaking a long-term effort to investigate such models and to develop appropriate mathematical tools for their analysis.

In the past year one of the main goals of this project could be achieved. In [1] we have developed a contour model representation for a large class of spin systems with interactions of Kac type that allows to analyze these systems in a domain of parameters that is uniform in the range of the interaction. The difficulties in achieving this arise from the fact that to gain uniform control on the energy of the so-called "contours", the definition of these objects must be quite non-local. As a consequence, the so-called "restricted ensembles", i.e. the regions in space that are free of contours, must satisfy non-local constraints. The crucial step, namely the cluster-expansion of the restricted ensembles is therefore quite non-standard, and a careful adjustment between the requirements for the convergence of this expansion and the necessity to obtain uniform estimates on the energies of contours necessitates a delicate balancing. The final formulation of the contour model with non-local interactions between contours that is provided in [1] allows then to use the Pirogov-Sinai theory to give a complete description of the phase diagram of the model ([3]).

In a separate development, an important step was taken to prepare the analysis of the random field Kac-Ising model. One of the challenges here is to control the low-temperature phase asymptotically up to the critical temperature of the mean field model, as was done in the ferromagnetic case in [2]. To do so requires a block transformation of the spin variables. While in the ferromagnetic case, one can work with suitable bounds on the resulting distribution of the block variables, in the random case one needs complete control of the effective action of the blocked model. This is achieved in [4] for suitably chosen block sizes as functions of the range of the interaction. The effective Hamiltonian of the blocked model is then represented as the desired "mean-field" type term plus a well-controlled "small" correction that arises from a high-temperature expansion. A conceptually interesting side-result is that the measure on the blocked variables is indeed a Gibbsian measure.

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Stochastic dynamics

Collaborators: A. Bovier, B. Gentz

Cooperation with: G. Ben Arous (Ecole Polytechnique Fédérale, Lausanne, Switzerland), N. Berglund (Eidgenössische Technische Hochschule Zürich, Switzerland), V. Gayrard (Centre de Physique Théorique, Marseille, France and Ecole Polytechnique Fédérale, Lausanne, Switzerland), M. Klein, F. Manzo (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. E.g., 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 an entirely 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, we have been building on the methods and results of [2] in various directions.
In [4] we have shown that the results of [2] naturally apply in the context of reversible Markov chains with exponentially small transition probabilities and that, in this setting, all key quantities can be computed up to multiplicative errors that tend to one in terms of properties of the energy function. As a particularly interesting example we considered the stochastic Ising model in finite volume when the temperature is a small parameter. In this context we could compute the mean nucleation time, e.g., in the presence of a positive external field, from a metastable state of negative magnetization to the stable $+$-state including the precise prefactor. Following the general theory of [2], this quantity was also shown to be the inverse of the spectral gap of the generator.
A far more challenging program was the extension of the methods of [2] to disordered spin systems with an unbounded number of "metastable states". In this situation, on the time-scale where transitions between the involved metastable states occur, one may observe the appearance of an effective non-Markovian dynamics. These phenomena have received considerable attention in the physics literature under the name of "aging", in particular in materials such as *glasses* and *spin glasses*, or *glassy polymers*. The current state of the art in the physical literature involves the ad-hoc introduction of a simple effective dynamics on the set of metastable states that can then be analyzed exactly (so-called "trap models"). The literature on these models as well as the observed phenomenology is abundant. However, the rigorous derivation of these effective models is missing, and the very first results were obtained last year in the context of the random energy model (REM), one of the simplest spin glass models ([5, 6, 7]). The REM is considered

in the physics literature as one of the basic paradigms for the study of the phenomenon of *aging*. However, all work has previously been based on an ad-hoc simplification of the model that consists in effectively replacing the dynamics on the underlying spin-space by an effective Markov chain defined in terms of transitions between the "meta-stable" states only. The same procedure is used in much more general situations to get an idea of the long-time dynamics of highly disordered systems. In the references cited above, a mathematically *rigorous* derivation of the results based on the trap model ansatz could be given for the first time in the context of the REM. Let us mention that the results on the equilibrium properties of the REM obtained in [3] (see also [1]) have been instrumental for this work. Extensions of this analysis towards the more complex Generalized Random Energy Model are now under way.

A second direction of research that has made substantial progress last year is the investigation of slow explicit time dependence in the parameters of random dynamical systems. These are of major importance in applications where stochastic resonance or hysteresis are observed, such as ring lasers, electronic circuits, neurons, and climate models, for instance for the Atlantic thermohaline circulation.
We used the methods developed in [8] to study the overdamped motion of a Brownian particle in a periodically modulated Ginzburg–Landau potential in a regime of moderately low frequency of the modulation: In [9], we obtained a precise mathematical understanding of the behavior of sample paths in the case when the amplitude of the modulation is too small to allow for transitions between wells in the absence of noise. There is a threshold value for the noise intensity as a function of amplitude and frequency of the modulation. Below threshold, typical sample paths remain in the same potential well for many periods while above threshold, typical paths switch wells twice per period. The probability of atypical paths decays exponentially, with an exponent scaling with the small parameters of the problem. Inter-well transitions are concentrated in small windows around the instant of minimal barrier height and the width of these windows depends only on the noise intensity.
In [10], the area of random hysteresis cycles in the same model is investigated. There are three qualitatively different regimes. Below a critical noise intensity, the area enclosed by a sample path over one period is concentrated near the deterministic area, which is microscopic for small amplitudes and macroscopic for larger amplitudes. Above the critical noise intensity, noise causes transitions regardless of the amplitude, and the typical hysteresis area depends, to leading order, on the noise intensity only. We estimated the probability of deviations from the typical area in all three regimes.
In addition, we also discussed the effect of colored noise instead of Gaussian white noise and applications to simple climate models, see [11] and [12], respectively.

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Mutually catalytic branching processes

Collaborators: K. Fleischmann, A. Sturm

Cooperation with: S. Athreya (Indian Statistical Institute, New Delhi), D.A. Dawson (Carleton University Ottawa, Canada), A.M. Etheridge (University of Oxford, UK), A. Klenke (Universität Erlangen), P. Mörters (University of Bath, UK), C. Mueller (University of Rochester, USA), L. Mytnik (Technion, Haifa, Israel), E.A. Perkins (University of British Columbia, Vancouver, Canada), A. Stevens (Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig), J. Swart (Universität Erlangen), V.A. Vatutin (Steklov Mathematical Institute, Moscow, Russia), A. Wakolbinger (Johann Wolfgang Goethe-Universität Frankfurt), J. Xiong (University of Tennessee, Knoxville, USA)

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

Mutually catalytic branching processes describe the evolution of two materials, which randomly move, split, and possibly disappear in space. The system is interactive in that the branching rate of each material is proportional to the local density of the other one. This interaction destroys the usual basic independence assumption in branching theory. In particular, the connection to reaction-diffusion equations is lost. The model was created by Dawson, Perkins, and Mytnik in [1], [2] in the one-dimensional Euclidean space $\mathbb{R}$ and in the lattice space $\mathbb{Z}^d$. After some time of controversial discussions, the non-degenerate *existence of a two-dimensional continuum model* of mutually catalytic branching processes was verified in the last year, and is now comprehensively presented in the trilogy [3], [4], [5]. Here, the second part complements the first one by extending it to infinite measure states. In the third part, *uniqueness* in the martingale problem is resolved. One of the remarkable properties of this model is that at almost all times the states are absolutely continuous with disjoint densities. At the same time, these densities are unbounded at the interface of both types. This explains how interaction works in the model despite the segregation of densities. The long-term behavior of this process is well-understood: Only one of the types may survive in the long run.

In the case of the simpler catalytic branching processes, with only a one-sided influence of a catalyst on a reactant, further aspects have been studied. In [6] open problems from [7] are answered. It is shown that for the continuous super-Brownian reactant in $\mathbb{R}$ with *stable point catalysts* under a mass-time-space scaling, asymptotic clusters appear that are macroscopically isolated as in the constant medium case. They continuously change in a non-Markovian way and are distributed in the domain of attraction of a stable law of index smaller than two. These results contrast the constant medium case. For the proof of this functional limit theorem, a Brownian snake approach in this catalytic setting is established, which is meanwhile slightly generalized in [8].

For the super-Brownian reactant in $\mathbb{R}$ with *super-Brownian catalyst*, a universal mass-time-space scaling limit is derived ([9]): If both substances are started in uniform states, the limit reactant exists and is uniform, for all scaling indices. This is done in a setting of convergence of finite-dimensional distributions, and for certain scaling indices also in terms of a functional limit theorem.

Related models, where the branching rate of the material is affected by a *continuous correlated random environment*, have also been studied. Ground work on such models has been done

in [10]. In [11], existence and uniqueness have been established for a model with a similar branching mechanism which, as in the mutually catalytic branching process case, allows for the absolute continuity of states in higher dimensions, in this case on $\mathbb{R}^d$. This is of particular interest since the densities solve stochastic partial differential equations and thus extend the connections of such solutions to super-Brownian motions.

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Phase transitions and statistical mechanics

Collaborator: S. Rœlly

Cooperation with: P. Dai Pra (Università degli Studi di Padova, Italy), P.-Y. Louis (Université Lille 1, France)

Probabilistic Cellular Automata (PCAs) are discrete time Markov chains with parallel updating and local updating rules ([1]). PCAs are natural stochastic algorithms for parallel computing and as such have become widely used numerical tools in a large number of fields.
A key question in the theory of PCAs concerns the classification of their invariant measures according to their nature as stationary, reversible, or Gibbsian measures. This question was addressed in [2] for general PCAs, and the results were illustrated in the context of a class of reversible PCAs that were introduced by Lebowitz, Maes, and Speer ([4]). In fact, it has been known for a long time ([3]) that if a PCA is reversible with respect to a Gibbs measure corresponding to a potential Φ, then all its reversible measures are Gibbsian with respect to the same potential. In [2], a similar statement is now proven for the set of stationary measures:
For a general PCA, if one shift invariant stationary measure is Gibbsian for a potential Φ, then all shift invariant stationary measures are Gibbsian w.r.t. the same potential Φ. This induces that for a class of local, shift invariant, non-degenerated, reversible PCAs the reversible measures coincide with the Gibbsian stationary ones.
Applying this general statements to a particular class of reversible PCAs, it is shown in [2], using contour arguments that, for sufficiently small values of the temperature parameter, *phase transition* occurs, that is there are several Gibbs measures w.r.t. Φ. Furthermore, unlike what happens with sequential updating, a Gibbs measure which is not stationary for the associated PCA is exhibited.

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Infinite systems of interactive diffusions and their equilibrium states

Collaborator: S. Rœlly

Cooperation with: P. Dai Pra (Università degli Studi di Padova, Italy), D. Dereudre (École Polytechnique, Palaiseau, France), M. Thieullen (Université Paris VI, France), H. Zessin (Universität Bielefeld)

The concept of reciprocal processes can be traced back to E. Schrödinger. They form a class of stochastic processes that generalize the notion of Markov processes and are defined via a temporal Markovian field property. They play an important role in the context of Quantum Diffusions, Nelson's stochastic mechanics, and several variational problems such as entropy maximization on path space.
In a collaboration with M. Thieullen ([1]) we characterize real-valued reciprocal processes associated to a Brownian diffusion as a solution of an integration-by-parts formula. In this characterization appears a function, called reciprocal characteristics, that turns out to play the same role as the Hamiltonian in statistical mechanics. This approach is systematically applied in the context of periodic Ornstein-Uhlenbeck processes. The same approach was also carried through in the multi-dimensional setting. The next major goal of this project is an extension to infinite-dimensional situations, where the reciprocal process is the solution of a stochastic partial differential equation.
In collaboration with P. Dai Pra and H. Zessin, we have developed a characterization of the stationary law of interacting diffusion processes indexed by the lattice $\mathbb{Z}^d$ as Gibbsian measures. Let $X = \{X_i(t), i \in \mathbb{Z}^d, t \in \mathbb{R}\}$ be the weak solution of the Stochastic Differential Equation

$$(*) \qquad dX_i(t) = \Big(-\frac{1}{2}\varphi'(X_i(t)) + \mathbf{b}_{i,t}(X) \Big) dt + dB_i(t) \ , i \in \mathbb{Z}^d, t \in \mathbb{R},$$

where $\mathbf{b}_{i,t}$ is a measurable bounded local functional on the path space, a priori non Markovian. Then the law Q of X can be interpreted as Gibbs distribution on $\Omega = \mathcal{C}(\mathbb{R},\mathbb{R})^{\mathbb{Z}^d}$, with a priori measure P the product of Wiener measures drifted by $-\frac{1}{2}\varphi'$ and a certain interaction potential Φ. The main result in [2] shows the following equivalence

- Q is a stationary solution of the SDE (*).
- Q is a space-time shift invariant Gibbs state.
- Q minimizes the free energy $\mathcal{H}^{\mathbf{b}}(Q') = \mathcal{H}(Q') - E_{Q'}(\Phi)$, where $\mathcal{H}(Q')$ denotes the specific entropy of Q' with respect to P.

The technique is based on Girsanov transformation, stochastic analysis, and the classical variational principle of Statistical Mechanics.
In [3], the above results are completed by an existence result for the solution of (*). The authors use a space-time cluster expansions method, well adapted when the coupling parameter $\mathbf{b}$ is sufficiently small.

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Stochastic particle systems as numerical tools for problems in aerosol dynamics

Collaborators: W. Wagner, A. Eibeck

Cooperation with: H. Babovsky (Technische Universität Ilmenau), M. Kraft (University of Cambridge, UK), A. Lushnikov (Karpov Institute of Physical Chemistry, Moscow, Russia), J. Norris (University of Cambridge, UK), K. Sabelfeld (FG 6)

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

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. A basic element of the existing convergence proofs is the uniqueness of the solution to the limiting equation. However, this uniqueness has been established only up to the gelation point

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

which is finite for sufficiently fast increasing coagulation kernels. Thus the problem of convergence after that point is open for general kernels, and numerical observations concerning the behavior of the stochastic processes are of special interest.
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 [2]. Its convergence behavior, when the number of particles tends to infinity, was investigated under appropriate assumptions on the coagulation kernel. The derivation is based on some transformation of equation (1) (first used in [1]), and on the approximation of the modified solution. The new algorithm based on the mass flow process

has several important features compared to the standard model. First it leads to a considerable variance reduction, when functionals of the solution are calculated. Secondly it shows better approximation properties (faster convergence), especially in the case of gelling kernels. Thus, the mass flow process provides a very efficient tool for studying the gelation effect numerically. Some conjectures based on detailed numerical observations have been stated in [3], [5]. In particular, a new approach to the approximation of the gelation point (2), for a particular class of kernels, has been presented in [5].

An interesting aspect of the mass flow model is the emergence of infinite clusters in finite time for gelling kernels. It has been conjectured in [2] that the (random) explosion times τ_∞^n of the stochastic system converge (as $n \to \infty$) to the gelation time t_{gel}. This would connect the gelation effect (a property of the limiting equation) with the explosion phenomenon of a stochastic process, thus representing the physical interpretation of gelation. In this respect we refer to recently announced results ([4]) concerning the explosion behavior of some appropriately scaled tagged particle in the direct simulation process.

The topic of studying coagulation processes by stochastic models has attracted much interest in recent years. Some of the latest results in this field have been reported at a workshop in Oberwolfach last summer (cf. [6]). In particular, a better theoretical understanding of the gelation phenomenon, as well as the study of the spatially inhomogeneous case, are a challenge for future research.

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Efficient control of stochastic particle methods for rarefied gas flows

Collaborators: W. Wagner, A. Eibeck, I. Matheis

Cooperation with: K. Aoki (Kyoto University, Japan), S. Ermakov (St. Petersburg University, Russia), A. Garcia (San Jose State University, USA), C. Lécot (Université de Savoie, Chambéry, France), S. Rjasanow (Universität des Saarlandes, Saarbrücken), S. Ukai (Yokohama National University, Japan)

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

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

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 S^2 denotes the unit sphere in the Euclidean space $\mathbb{R}^3$, 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 $(n \sim 10^6 - 10^7)$ system of particles

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

approximating the behavior of the real gas. Here $x_i(t) \in D \subset \mathbb{R}^3$ and $v_i(t) \in \mathbb{R}^3$ denote the position and the velocity of the i-th particle at time t.
Stochastic particle methods for kinetic equations like (1) provide results which are subject to random fluctuations. Thus, the construction of algorithms with reduced fluctuations is an important problem (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 has been developed, which is based on an alternative interaction mechanism. In [3] an extension of this so-called stochastic weighted particle method for the numerical treatment of the Boltzmann equation is presented. A new procedure for modeling the inflow boundary condition is introduced, which contains

an appropriate control mechanism for the particle flow. Its performance is tested in a two-dimensional example with strong density gradients. A gain factor of several orders of magnitude in computing time is achieved in specific situations.
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 [1] a theoretical foundation for this algorithm was established by deriving the limiting kinetic equation.
This equation generalizes the classical Boltzmann equation (1). A further investigation of its relationship to the Enskog equation was the subject of [2]. 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 turn out to be the same as for the Enskog equation. These results confirm previous derivations, based on the virial, of the corresponding equation of state.

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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 Stochastik und Finanzmathematik im Rahmen der Institutsforschungsprojekte *Statistische Datenanalyse, Angewandte Finanzmathematik* und *Numerische Methoden*.

Die theoretische Basis des Forschungsprogramms bilden moderne nichtparametrische statistische Verfahren für komplexe Zusammenhänge, stochastische Partikel-Methoden und stochastische Differentialgleichungen. Der Schwerpunkt in der Finanzmathematik liegt auf der Entwicklung von Verfahren zu Risikomessung und -management sowie der Modellierung von Risikofaktoren. Auf diesen Gebieten, die sowohl bei der Lösung von Problemen in Technologie und Umweltforschung als auch bei der Risikomessung und Bewertung von Finanzderivaten Anwendung finden, hat sich die Forschungsgruppe in den vergangenen Jahren mit wichtigen mathematischen Beiträgen und mit der Entwicklung anerkannter statistischer Software eine führende Stellung erworben.

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

- Nichtparametrische statistische Methoden der Bildverarbeitung, Finanzmärkte, Ökonometrie, Cluster- und Diskriminanzanalyse,
- Angewandte Finanzmathematik, speziell Risikomessung und -steuerung, Bewertung und Simulation von Zinsmodellierung, Kalibration und Bewertung exotischer Derivate,
- Stochastische Modelle in numerischer Mathematik und Monte-Carlo-Verfahren, Anwendungen bei turbulenten Strömungen, Nukleations- und Koagulationsprozessen und stochastischen Algorithmen für hochdimensionale Randwertprobleme.

The research group works on problems from Applied Stochastics and Financial Mathematics within the institute's research projects *Statistical Data Analysis, Applied Financial Mathematics,* and *Numerical Methods*.

Modern nonparametric statistical approaches for the analysis and modeling of complex systems and numerical methods to investigate stochastic models form the theoretical foundation of the research program. Within Financial Mathematics the work focuses on the development of methods for risk evaluation, for risk management and on the modeling of risk factors. With important mathematical contributions and the development of statistical software, over the last years, the research group has reached a leading position in these fields. This includes solutions for problems in technology and environmental research as well as risk evaluation and option pricing in finance.

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,
- 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

Inference for complex statistical models

Collaborators: S. Jaschke, P. Mathé, G.N. Milstein, H.-J. Mucha, J. Polzehl, J. Schoenmakers, V. Spokoiny

Cooperation with: K. Hahn (GSF-IBB, München), F. Godtliebsen (University of Tromsø, Norway), F. Baumgart (Leibniz-Institut für Neurobiologie, Magdeburg), P. Qiu (University of Minnesota, USA), A. Juditski (INRIA, Grenoble, France), M. Hristache (Université de Rennes, France), W. Härdle (SFB 373, Humboldt-Universität zu Berlin), L. Dümbgen (Medizinische Universität Lübeck), J. Horowitz (University of Iowa, USA), S. Sperlich (University Carlos III, Madrid, Spain), D. Mercurio (Humboldt-Universität zu Berlin), B. Grund (University of Minnesota, USA), O. Bunke, B. Droge, H. Herwartz (SFB 373, Humboldt-Universität zu Berlin), A.W. Heemink (Technische Universiteit Delft, The Netherlands), E. Heimerl (Universität Salzburg, Austria), O. Lepski, J. Golubev (Université de Marseille, France), A. Samarov (Massachusetts Institute of Technology, Cambridge, USA), S.V. Pereverzev (Academy of Sciences of Ukraine, Kiev), R. von Sachs (Université Louvain-la-Neuve, Belgium), S. Zwanzig (Uppsala University, Sweden)

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

Many interesting applications of statistics in economics, finance, and life sciences are based on large databases and complex, high-dimensional models. In these cases, the first goals of statistical analysis are exploratory data analysis, qualitative description of properties of the data, and dimension reduction for further analysis.
Statistical inference includes various methods in statistical modeling, goodness-of-fit tests, and tests of significance for properties identified in the exploratory data analysis.

1. Adaptive techniques for image processing (J. Polzehl, V. Spokoiny).
Large amounts of two- or three-dimensional images are generated in many fields including medicine, environmental control, meteorology, geology, and engineering. Often decisions have to be based on certain features in the image. To do this the quality of noisy images has to be improved and the features have to be identified. Examples are satellite images, tomographic images, magnetic resonance images (MRI), and ultrasonic images.
Within the project we have developed two new adaptive smoothing techniques, pointwise adaptation and adaptive weights smoothing. The first method, described in [32], allows to estimate grey-scale images that are composed of large homogeneous regions with smooth edges and observed with noise on a gridded design. The procedure searches, in each point, for the largest vicinity of the point for which a hypothesis of homogeneity is not rejected. Theoretical properties of the procedure are studied for the case of piecewise constant images. We present a nonasymptotic bound for the accuracy of estimation at a specific grid point as a function of the number of pixel, of the distance from the point of estimation to the closest boundary, and of smoothness properties and orientation of this boundary. It is shown that the proposed method provides a near optimal rate of estimation near edges and inside homogeneous regions.

The second method, Adaptive Weights Smoothing (AWS) (see [33]), is based on the idea of structural adaptation. The method employs the structural assumption of a specified local model within an iterative procedure. The resulting method has many desirable properties like preservation of edges and contrast, and (in some sense) optimal reduction of noise. The method considerably improves on classical smoothing procedures as soon as the local model provides a reasonable approximation to the image.
Fig. 1 illustrates the reconstruction of a local constant image from a noisy version.

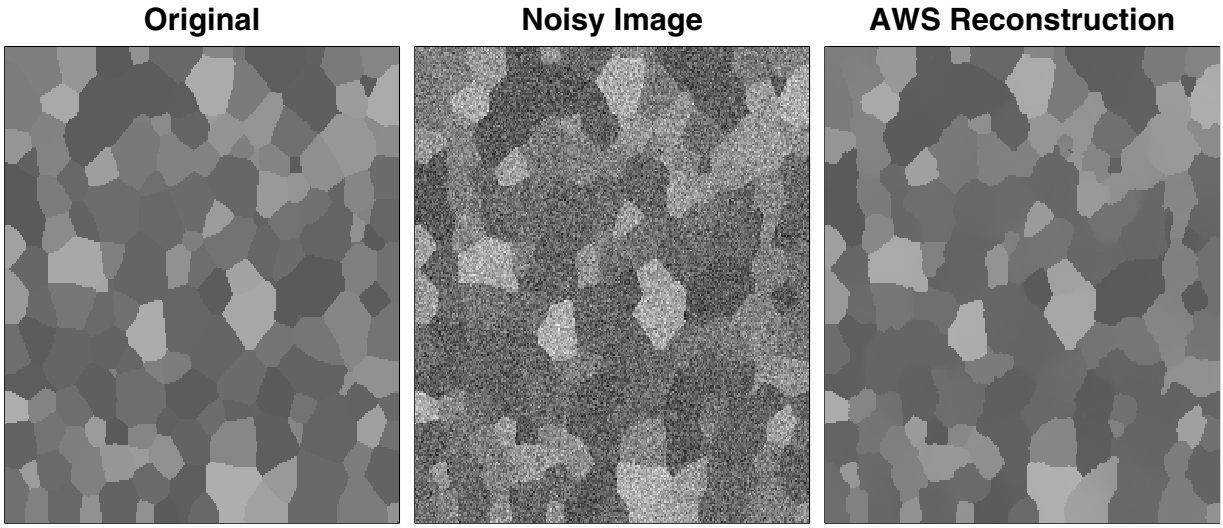

Fig. 1: Original (left), image with additive noise (central) and AWS reconstruction from the noisy image (right)

The idea underlying AWS can be applied to many other types of data. We shortly present an application to classification in dynamic MRI, see [34]. The data, illustrated in Fig. 2, consist of 30 MR images showing, in each voxel, the effect of a contrast agent over time.

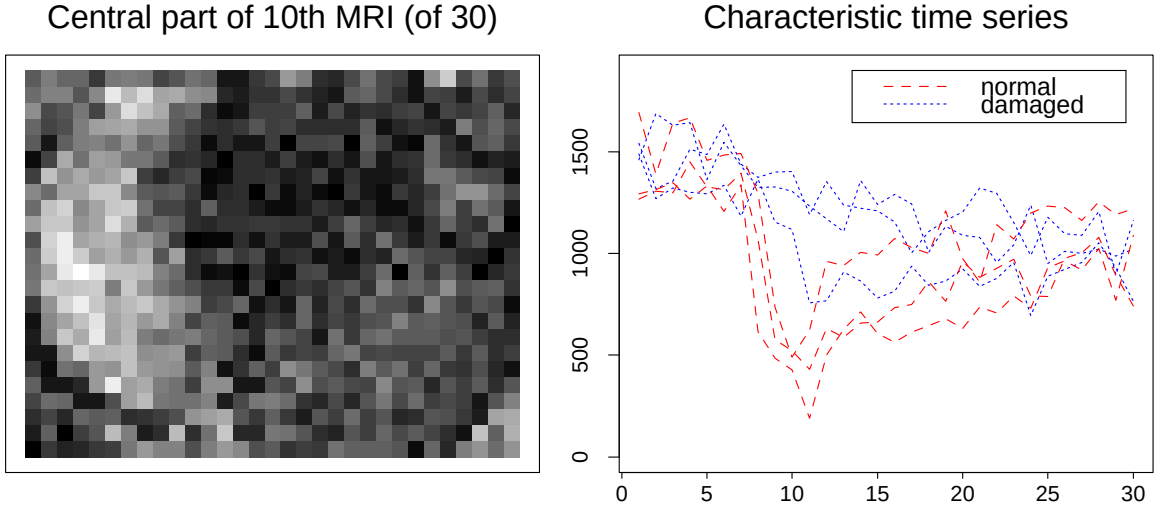

Fig. 2: Dynamic MRI: 10^{th} MR Image (left) and typical time series of gray values (right)

The different behavior in pathologic areas provides the necessary contrast for tissue classification. In this context a vectorized version of AWS can be used to improve tissue classification by adaptive spatial smoothing. Fig. 3 shows the results without (raw data) and with (AWS) spatial adaptive smoothing for two classification criteria.

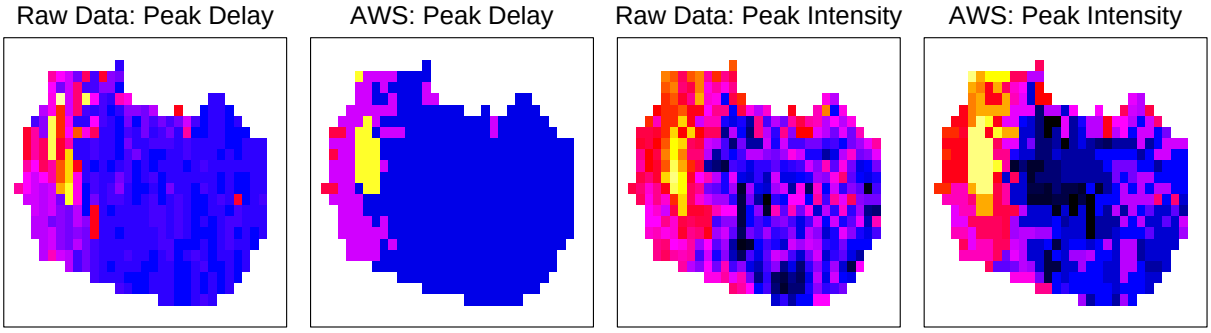

Fig. 3: Tissue classification from dMRI data

Currently several generalizations of the structural approach are under development. This especially includes local polynomial adaptive smoothing, varying coefficient models and likelihood-based methods, e.g., for binary response models.
Research in this field is supported by the DFG Priority Program 1114.

2. Effective dimension reduction (J. Polzehl, V. Spokoiny).
In many statistical problems one is 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). Such models generalize classic linear models and they can be viewed as a reasonable compromise between too restrictive linear and too vague pure nonparametric modeling. For the corresponding analysis, the targets are typically index vectors which allow to reduce the dimensionality of the data without essential loss of information. The existing methods of index estimation can be classified as direct and indirect. The indirect methods 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 [17]. 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 [36], [35] and [4].
Another direct method of index estimation for a single-index model is proposed in [14]. This method can be regarded as a recursive improvement of the average derivative estimator. The results show that after a logarithmic number of iterations, the corresponding estimator becomes root-n consistent. The procedure is fully adaptive with respect to the design and to unknown smoothness properties of the link function, and results are valid under very mild model assumptions.
For the multi-index situation, [15] proposed a new method of dimension reduction which extends the procedure from [14] and is based on the idea of structural adaptation. The method applies for a very broad class of regression models under mild assumptions on the underlying regression function and the regression design. The procedure is fully adaptive and does not require any prior information. The results claim that the proposed procedure delivers the optimal rate $n^{-1/2}$ of estimating the index space provided that the effective dimensionality of the model is not larger than 3. The simulation results demonstrate an excellent performance of the procedure for all considered situations. An important feature of the method is that it is very

stable with respect to high dimensionality and for a non-regular design.
Fig. 4 illustrates the results of a simulation study using a bi-index model $Y_i = f(X_i^T\beta_1, X_i^T\beta_2) + \varepsilon$ with Gaussian errors ε. The box-plots display the values of a numerical criterion characterizing the quality of the estimated index space for a covariance-based SIR, the "best" one-step estimate and after the first, second, fourth, eighth, and final iteration for $d = 10$, $m = 2$, and different sample size n. The results displayed are obtained from $N = 250$ simulations.

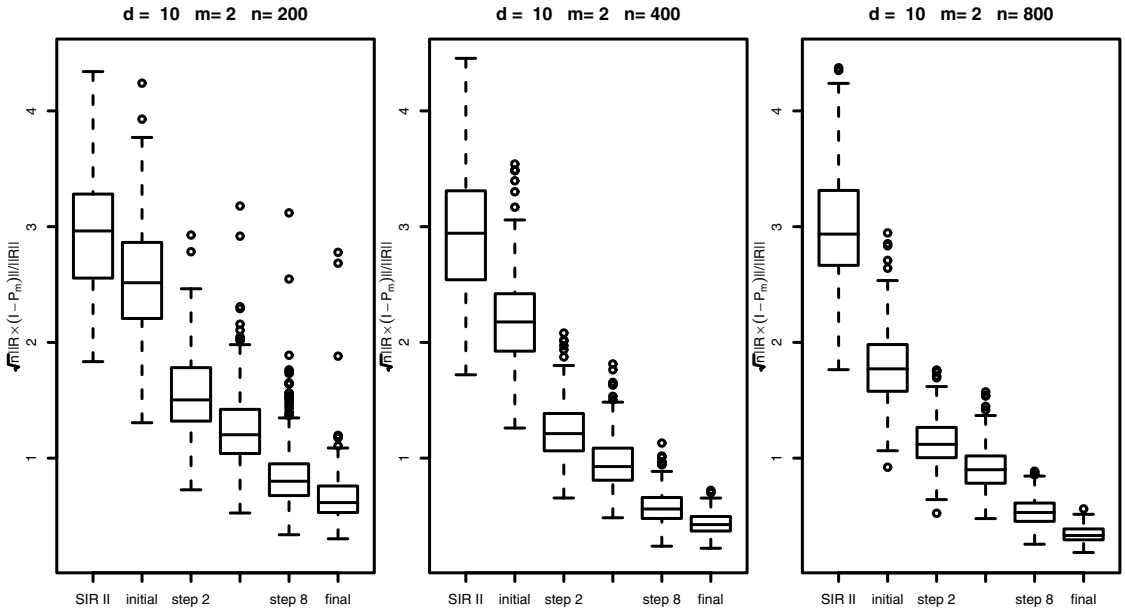

Fig. 4: Simulation results for a bi-index model for $m = 2$, $d = 10$, and $n = 200, 400, 800$. Estimates obtained by SIR II, the initial estimate, 2nd, 4th, 8th, and final iteration.

3. Statistical inference for time-inhomogeneous finance time series (J. Polzehl, V. Spokoiny). Log-Returns R_t of the price or currency process in the speculative market are typically modeled using the *Conditional Heteroscedasticity* assumption:

$$R_t = \sigma_t \varepsilon_t,$$

where ε_t is a noise process (e.g., white noise) and σ_t is a *volatility* process. One typical goal of statistical analysis is a few-step-ahead forecasting of the volatility which can be used for portfolio management or Value-at-Risk evaluation. The volatility process is usually modeled using a parametric assumption like ARCH, generalized ARCH (GARCH), stochastic volatility, etc. ([5]). All such models are time homogeneous and therefore fail to capture structural changes of the underlying processes. We developed alternative methods which are based on the assumption of local time homogeneity. More precisely, we assume that the underlying process is time homogeneous within some unknown time interval and the idea of the method is to describe this interval, in a data-driven way. Afterwards one can estimate the current volatility value or one-step volatility forecast simply by averaging over the interval of homogeneity, see [8], [25].
The paper [7] offers an extension of the proposed method to multiple volatility modeling for high-dimensional financial data. The approach involves data transformation, dimension reduction, and adaptive nonparametric smoothing as building blocks.
Fig. 5 demonstrates the results of an adaptive weights smoothing procedure for time series using the structural assumption of a local ARCH(20) model for the logarithmic returns of

the US $ / DM exchange rates in the period 1988–2000. The bottom plot illustrates the segmentation into homogeneous time intervals obtained by the procedure.

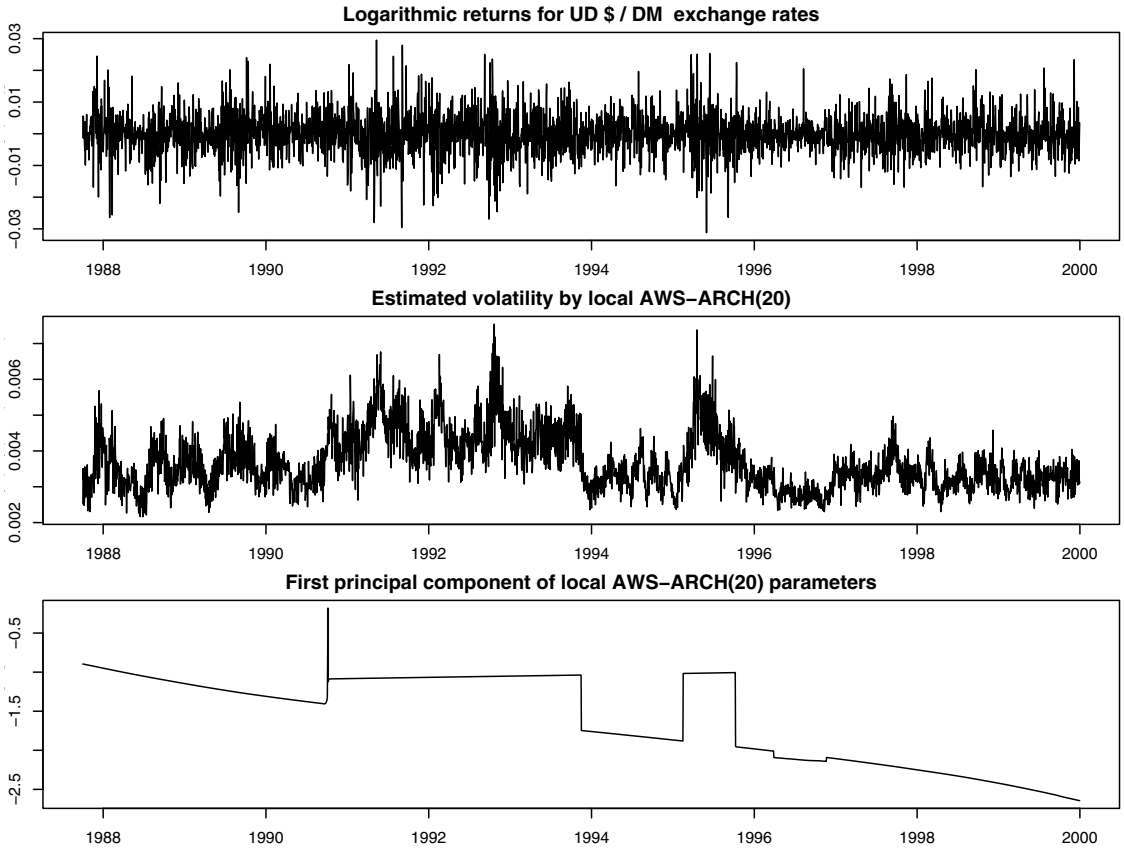

Fig. 5: Logarithmic returns of US $ / DM exchange rates in the period 1988–2000 (top), estimated volatility within a local ARCH(20) model (center), and first principal component of local parameter estimates

4. Robust nonparametric hypothesis testing (J. Polzehl, V. Spokoiny).
Linear quantile regression models are often used in applications. See [2], [18], [20], among others. In contrast to mean regression models, quantile regression models do not require the individual errors to have moments, are robust to outlying values of the observations, and permit exploration of the entire conditional distribution of the dependent variable. However, there has been little research on testing the hypothesis of linearity. To our knowledge, only [38] and [1] have developed tests of parametric quantile regression models against nonparametric alternatives. In contrast, there is a broad range of literature on testing mean regression models against nonparametric alternatives, see [12] and the references therein.
Paper [13] proposed a new test of the hypothesis that a conditional median function is linear against a nonparametric alternative. The test adapts to the unknown smoothness of the alternative model, does not require knowledge of the distribution of the possibly heterogeneous noise components of the model, and is uniformly consistent against alternative models whose distance from the class of linear functions converges to zero at the fastest possible rate. This rate is slower than $n^{-1/2}$. In addition, the new test is consistent (though not uniformly) against local alternative models whose distance from the class of linear models decreases at a rate that is only slightly slower than $n^{-1/2}$. The results of Monte Carlo simulations and an empirical application have illustrated the usefulness of the new test.
In the semiparametric additive hazard regression model of McKeague and Sasieni ([24]) the

hazard contributions of some covariates are allowed to change over time while contributions of other covariates are assumed to be constant. In [6] bootstrap-based test procedures for parametric hypotheses in nonparametric additive survival models are developed, which can be used to identify covariates with constant hazard contributions.

5. Cluster analysis, multivariate graphics, data mining (H.-J. Mucha).
Clustering, in data mining, aims at finding interesting structures or clusters directly from the data without using any background knowledge. The notion of cluster analysis encompasses a great family of methods. Synonyms in use are numerical taxonomy (because of its biological roots), automatic classification, and unsupervised learning. There are model-based as well as heuristic clustering techniques. At most one will set up new hypotheses about the data. At least they aim at a practical useful division of a set of objects into subsets (groups, clusters). This task of subdivision can be attained at the lowest level simply by reordering or sorting techniques. In any case, high-dimensional data visualization (multivariate graphics, projection techniques) and matrix reordering techniques are very useful for visualizing structures and clusters within data ([28]). This indeed is a highly recommended way for a better understanding of both the multivariate high-dimensional data and the results of clustering.

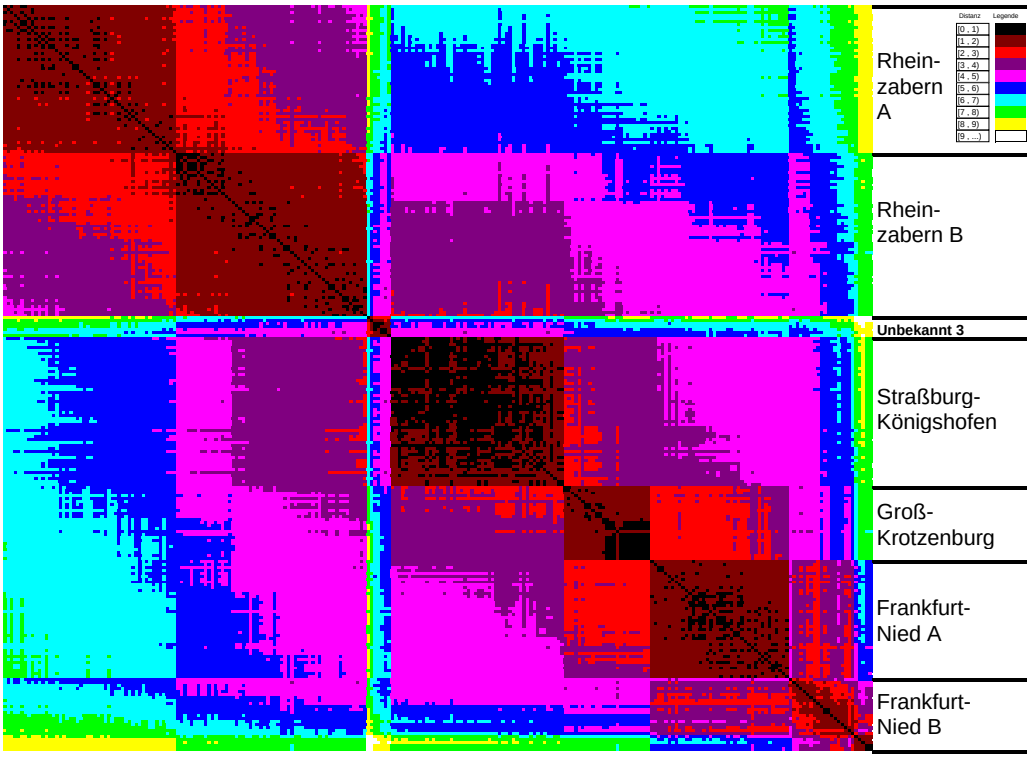

Fig. 6: Fingerprint of a distance matrix (data: Roman bricks)

Our statistical software `ClusCorr98`® performs exploratory data analysis mainly by using adaptive methods of cluster analysis, classification, and multivariate graphics. Having data mining applications in mind, some new cluster analysis tools are under development. For example, new model-based clustering techniques using cores are based on weighted observations in order to handle huge data sets effectively ([3]). Intelligent clustering based on dual scaling can handle mixed data. `ClusCorr98`® is written in Visual Basic for Applications (VBA) ([29]). It runs under Microsoft Windows taking advantage of the Excel environment including its database facilities.

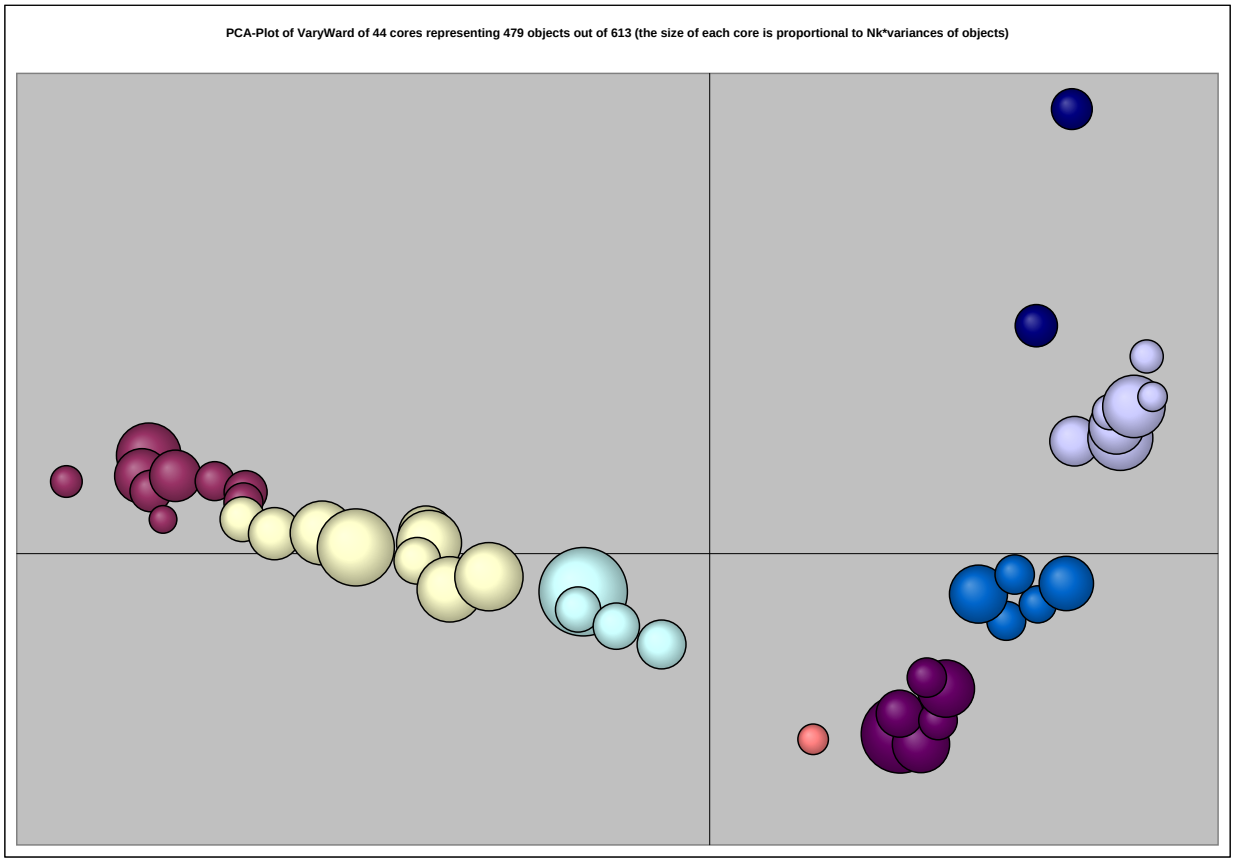

Fig. 7: Principal components plot of eight clusters of cores obtained by modified Ward's method (data: Roman bricks)

6. Numerical analysis of statistical ill-posed problems (P. Mathé).
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. Unless special methods, such as Tikhonov regularization, are used, it is often impossible to get sensible results.
In collaboration with S.V. Pereverzev this area of problems is studied for statistical 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 is 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 ([30]). 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. For these reasons *variable Hilbert scales* were introduced by Hegland ([9]). 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. Roughly speaking, in a Hilbert scale with generator L, the norm $\|x\|_s := \|L^{-s}x\|$ is replaced by $\|x\|_\varphi := \|\varphi(L^{-1})x\|$, where φ is some non-negative function (on the spectrum) of L.
The analysis of ill-posed problems in variable Hilbert scales was further developed in [10] and [37]. In this project the following problems were analyzed.

- How does a given regularization react to smoothness? What has to be assumed about the source condition in order to automatically make use of the given regularization?

  For certain source conditions (power functions or logarithms), first answers were known, see [19], [11], and [31]. In [23] the role of certain geometric properties of the source condition, in particular their concavity, was analyzed.

- A further aspect concerns discretization. Most previous studies were based on spectral theoretical analysis. This restricts consideration to discretizations *along the spectrum*, which is not realistic. In [21] the authors have indicated how methods from approximation theory allow a more general analysis. This could now be generalized to the context of variable Hilbert scales in [22].

This research constitutes the basis for further investigations of numerical problems in variable Hilbert scales. It shall be continued, supported by the DFG.

7. Statistic and Monte Carlo methods for estimating transition densities for stochastic differential equations (SDEs) (G. Milstein, J. Schoenmakers, V. Spokoiny).
In many applications, for instance in financial and environmental modeling, it is useful to have an efficient algorithm to determine the transition density of a, for example, financial or environmental process given by a stochastic differential equation,

$$dX = a(s,X)ds + \sigma(s,X)dW(s),\ t_0 \le s \le T,$$

where X and a are d-dimensional vectors, W is an m-dimensional standard Wiener process, σ is a $d \times m$-matrix, $m \ge d$.
In a cooperation project with "Applied mathematical finance" and "Numerical methods for stochastic models" we constructed a Monte Carlo estimator for the unknown transition density $p(t,x,T,y)$ for fixed t,x,T,y, which improves upon classical kernel or projection estimators based on approximate realizations of $X_{t,x}(T)$ directly. For example, the kernel (Parzen-Rosenblatt) density estimator with a kernel K and a bandwidth δ is given by

$$\hat{p}(t,x,T,y) = \frac{1}{N\delta^d} \sum_{n=1}^{N} K\left(\frac{X_n - y}{\delta}\right),$$

where X_n, $n = 1,...,N$, are independent approximate realizations of $X_{t,x}(T)$. It is well-known that even an optimal choice of the bandwidth δ leads to an error of order $N^{-2/(4+d)}$. For $d > 2$, this would require a huge sample size N for providing a reasonable accuracy of estimation. In the statistical literature this problem is referred to as "curse of dimensionality". Classical Monte Carlo methods allow for an effective estimation of functionals $I(f) = \int p(t,x,T,y) f(y)dy = Ef(X_{t,x}(T))$ by forward diffusion. We derive general reverse diffusion equations for Monte Carlo estimation of functionals $I^*(g) = \int g(x)p(t,x,T,y)dx$. The obtained probabilistic representations and the numerical integration of stochastic differential equations (SDEs) together with ideas of mathematical statistics are used for a density estimation by forward-reverse diffusion (see

[27]). It is shown that density estimation based on forward-reverse representations allows for essentially better results in comparison with usual kernel or projection estimation based on forward representations only (root-N accuracy instead of $N^{-2/(4+d)}$). The following table gives comparative results of a forward-reverse estimator (FRE) with a forward estimator (FE) for an Ornstein-Uhlenbeck-type process ($d = 1$).

N	FRE	$2\sigma_{FRE}$	$\sigma^2_{FRE}N$	(sec.)	FE	$2\sigma_{FE}$	$\sigma^2_{FE}N^{4/5}$	(sec.)
10^4	0.522	0.031	2.40	2	0.524	0.036	0.51	2
10^5	0.519	0.010	2.50	20	0.515	0.016	0.64	18
10^6	0.5194	0.0031	2.45	203	0.5164	0.0064	0.65	183
10^7	0.5193	0.0010	2.50	2085	0.5171	0.0026	0.68	1854

Table 1: true $p = 0.518831$

The developed methods have recently been presented in the Netherlands (Universities of Delft and Amsterdam). These presentations have led to a new scientific cooperation with the group "Large Scale Systems" of the Delft University.
Further, in [16] we proposed asymptotically efficient procedures for estimating the linearized drift of SDEs. Some extremal problems related to nonparametric maximum likelihood estimation of a signal in white noise are investigated in [26].

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Applied mathematical finance

Collaborators: S. Jaschke, G.N. Milstein, O. Reiß, J. Schoenmakers, V. Spokoiny, J.-H. Zacharias-Langhans

Cooperation with: A. Bachi (University of Twente, The Netherlands), B. Coffey (Merrill Lynch, New York, USA), J.P. Dogget (Risk Waters Group, London, UK), H. Föllmer, W. Härdle, U. Küchler, R. Stehle (Humboldt-Universität zu Berlin), H. Haaf (Münchener Rückversicherung AG, München), A.W. Heemink, H. van der Weide (Technische Universiteit, Delft, The Netherlands), P. Kloeden (Johann Wolfgang Goethe-Universität, Frankfurt am Main), J. Kremer, C. März, T. Sauder, T. Valette (Bankgesellschaft Berlin AG, Berlin), O. Kurbanmuradov (Turkmenian Academy of Sciences, Ashkhabad), M. Schweizer (Technische Universität Berlin/Universität München), G. Stahl (Bundesaufsichtsamt für das Kreditwesen), U. Wystup (Commerzbank AG, Frankfurt am Main)

Supported by: Bankgesellschaft Berlin AG, SWON Netherlands (Dutch Research Association), BMBF: "Effiziente Methoden zur Bestimmung von Risikomaßen" (Efficient methods for valuation of risk measures – 03SCM6B5)

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. These problems of risk measurement and risk modeling are the subject of the BMBF project "Efficient methods for valuation of risk measures", which started in January 2001 in cooperation with and with support of the Bankgesellschaft Berlin AG.
Methods for the valuation of transition densities of diffusions, or more generally, stochastic differential equations are useful in financial modeling. In joint work with the projects "Inference for complex statistical models" and "Numerical methods for stochastic models" we discovered a general root–N consistent Monte Carlo estimator for a diffusion density ([16]).
Within the SWON Netherlands project new progress has been made with respect to the unified modeling of stocks and interest rates. This was presented at RISK Europe 2001 (Paris) ([20]).

1. Risk management for financial institutions (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.

In cooperation with Bankgesellschaft Berlin AG we work on a project concerning the problem of efficient valuation of complex financial instruments, for example American options and convertible bonds. For standard American options our objective was to increase the speed and accuracy of various algorithms, for example by Richardson extrapolation. Further we focused on the problem of how to incorporate credit risk in the valuation of highly complex instruments like, e.g., ASCOTs (Asset Swapped Convertible Option Transactions). The close cooperation with traders in the bank proved to be very fruitful in testing and comparing several models that combine credit and market risk.

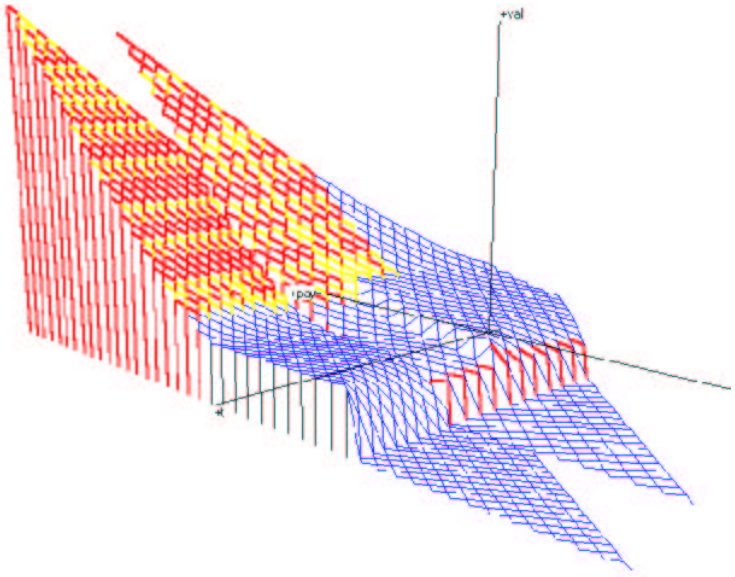

Fig. 1: A graphical analysis of a convertible bond. The different colors indicate different exercise strategies of call and put options.

In preparation of the lecture “Risk Management for Financial Institutions”, given by Stefan Jaschke in the winter terms 2000/01 and 2001/02, 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.

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 ([10]). An overview of the approximation methods in the context of delta-gamma-normal models was given by [13].

The relation between coherent risk measures, valuation bounds, and certain classes of portfolio optimization problems was established in [12]. One of the key results is that coherent risk measures are essentially equivalent to generalized arbitrage bounds, also called “good deal bounds” by Cerny and Hodges. The results are economically general in the sense that they work for any cash stream spaces, be it in dynamic trading settings, one-step models, or deterministic cash streams. They are also mathematically general as they work in (possibly infinite-dimensional) linear spaces. The valuation theory seems to fill a gap between arbitrage valuation on the one hand and utility maximization (or equilibrium theory) on the other hand. Coherent valuation bounds strike a balance in that the bounds can be sharp enough to be useful in the practice of pricing and still be generic, i.e. somewhat independent of personal preferences,

in the way many coherent risk measures are somewhat generic. Coherent risk measures are so important because of the deficiencies of the currently used quantile-VaR, which is not coherent. These deficiencies of quantile-VaR as a risk measure are discussed and contrasted with the properties of coherent risk measures in [11], which was submitted to the Basel Committee in the consultation period of the "Basel II" proposal. Generalizations of coherent risk measures are currently being studied by S. Jaschke and P. Mathé.
In the context of the BMBF project "Efficient methods for valuation of risk measures" we concentrated on the problem of estimating the Value-at-Risk for large portfolios by full Monte Carlo valuation. In this respect we closely work together with the project "Numerical methods for stochastic models". In order to obtain fairly accurate results by this method in acceptable time, variance reduction techniques like importance sampling or stratified sampling have to be used ([7]). To apply these techniques one typically needs some a priori estimation of the value to be determined. The industrial standard delta-gamma-normal approximation poses, while being standard, computational problems which demand careful analysis. We developed well-adapted algorithms for the generalized eigenvalue problem and for the Fourier inversion arising in this context.

2. Interest rate modeling, calibration, and pricing of non-standard derivatives (G.N. Milstein, O. Reiß, J. Schoenmakers).
Previously we established a conceptual approach of deriving parsimonious correlation structures suitable for the implementation in the LIBOR/EurIBOR market model given by

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

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 $\mathbb{P}_n$. By imposing additional constraints on a known ratio correlation structure, motivated by economically sensible assumptions concerning forward LIBOR/EurIBOR correlations, we yield a semi-parametric framework of non-degenerate correlation structures from which we derive systematically low parametric structures with, in principle, any desired number of parameters [14, 22, 23]. See (1) for an example correlation structure with three parameters $\eta_1, \eta_2, \rho_\infty$, where m is the number of LIBORs involved.

$$\begin{aligned} \rho_{ij} \;=\; & \exp\left[-\frac{|j-i|}{m-1}\left(-\ln\rho_\infty + \eta_1 \frac{i^2+j^2+ij-3mi-3mj+3i+3j+2m^2-m-4}{(m-2)(m-3)}\right.\right. \\ & \left.\left. -\eta_2 \frac{i^2+j^2+ij-mi-mj-3i-3j+3m+2}{(m-2)(m-3)}\right)\right], \\ & i,j = 1,\ldots,m, \quad 3\eta_1 \ge \eta_2 \ge 0,\ 0 \le \eta_1+\eta_2 \le -\ln\rho_\infty. \end{aligned} \tag{1}$$

As a result, such correlation structure combined with a suitable parametrization of the norm of the deterministic LIBOR/EurIBOR volatility provides a parsimonious multi-factor model with a realistic correlation structure. This allows for stable simultaneous calibration to caps and swaptions via approximative swaption formulas. In the global markets the payment dates of swaps and caps are differently settled. In this respect we improved existing approximation

methods for swaptions by taking this issue into account. Further we proposed the incorporation of a stabilizing penalty factor in the RMS object function which prevents the calibration routine from running into degenerate parameter regions. By this penalty function calibration remains stable even if the market data set under consideration contains some internal misalignments. Within the thus constructed framework we carried out various calibration tests which has led to new insights concerning the relationship between the cap and swap markets. Our results will be presented at Risk Europe 2002.
Within an economical context we study the concept of assets and interest rates in a unified model which is completely specified by the assets alone. This allows endogenous derivations of dynamic relations between assets and interest rates from global structural assumptions (homogeneity and some spherical symmetry) on the market. For instance, if c is the drift and b_0 the volatility of the short rate, $\bar{\mu}$ the drift and $\bar{\sigma}$ the volatility of the stock index, and $\rho_{I,r}$ the correlation between short rate and index, we obtained:

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

We analyzed such relations further and studied connections among the numeraire portfolio (which is in fact the inverse of the pricing kernel), observable indices, interest rate dynamics, and risk premia. This research was presented at Risk Europe 2001 ([20]).
Within the framework of a risk management system it is necessary not only to validate financial instruments but also to compute their derivations, the so-called Greeks. Due to symmetry relations in a financial market or homogeneity relations of a financial product we obtained relations between the Greeks of a derivative. These results can be used to avoid usually instable numerical differentiations ([21]).
In [15] we developed a Monte Carlo approach for computing option sensitivities. There we find these quantities by Monte Carlo simulation of a corresponding system of stochastic differential equations using weak solution schemes. It turns out that with one and the same control function a variance reduction can be achieved simultaneously for the claim value as well as for the deltas. Recently, we started to investigate Monte Carlo methods for the determination of exercise boundaries of certain American options. The idea is to extend an exercise boundary known up to a certain maturity time by a Monte Carlo procedure. In this procedure we utilize a more sophisticated algorithm for the simulation of stochastic differential equations in the neighborhood of a boundary ([17]).

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Numerical analysis of complex stochastic models

Collaborators: P. Mathé, G.N. Milstein, K.K. Sabelfeld

Cooperation with: S. Orszag (Yale University, USA), T. Vesala (Helsinki University, Finland), P.K. Yeung (Georgian Institute of Technology, USA), O. Kurbanmuradov (Phys. Tech. Institute, Turkmenian Academy of Sciences, Ashkhabad), I.A. Shalimova (Institute of Computational Mathematics and Mathematical Geophysics, Russian Academy of Sciences, Novosibirsk), O. Smidts (Université Libre de Bruxelles, Belgium), G. Wei (Hong Kong Baptist University), M. Tretyakov (University of Wales, Swansea, UK)

Supported by: INTAS Project INTAS-99-1501, Nato Linkage Grant N 971664

Complex physical phenomena are conventionally governed by deterministic differential and integral equations, but the advanced measurements and modern technology require nowadays a development of stochastic research methods. The basis of these methods are stochastic models, so the main effort is often related to the creation of an adequate stochastic model which mimics, in a probabilistic sense, the desired physical phenomena. Next, these models should be efficiently modelled by computer. Mathematical analysis of the model and the implementation algorithm is an important part of research. A new type of stochastic model is developed for solving transport problems in saturated porous media which is the first stochastic Lagrangian model of Langevin type for porous media. We develop also stochastic algorithms for solving some examples of Cauchy and boundary value problems for nonlinear parabolic PDEs. The study is accomplished with an analysis of algorithms for high-dimensional integration.

1. Stochastic simulation models for transport in porous media (K.K. Sabelfeld).
It is well-known that stochastic models are well-developed for solving transport problems in turbulent flows like the transport in the atmospheric boundary layer (see, e.g., [24], [23]). This technique was extended to a wide class of flows, in particular, to rivers ([2]), to flows in porous media (see [4]). 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 simulation), 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, we suggest 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. It is worth to mention that the same scheme has been carried out in the atmospheric transport problem (see our recent work [8], [7], [26], [25] and [9]). The basis for the Langevin-type approach comes from the Kolmogorov similarity theory of fully developed turbulence ([22]) 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 study if in the porous media, this kind of linear law can be observed. This problem is studied by the DSM. Detailed derivation of the Langevin-type

model is given. Numerical simulations and comparisons with the random displacement model confirm that the new Lagrangian approach is highly efficient.

In many general flow conditions, the phenomenological Darcy law forms the basis of the theory of flow through porous media. It is a consequence of the linearity of the equations of slow viscous flow which are obtained from the Navier-Stokes equations by neglecting the inertial terms. For time-independent flow conditions and saturated porous media, it is written as

$$\mathbf{q}(\mathbf{r}) = \theta(\mathbf{r})\,\mathbf{u}(\mathbf{r}) = -K(\mathbf{r})\nabla\phi(\mathbf{r}),$$

where $\mathbf{q}$, θ, $\mathbf{u}$, K, and ϕ are all macroscopic variables depending on space vector $\mathbf{r}$, θ is the effective (or kinematic) porosity. This porosity takes into account the volumes of voids effectively concerned with ground-water flow (that is, for instance, without the dead-end pores and the adherence volume of the fluid to the grains). It is upper bounded by total porosity which is the volume occupied by the pores divided by the volume of the bulk medium, $\mathbf{q}$ is called Darcy's velocity and represents the ground-water flow rate, that is, the volume of water crossing a unit area of porous medium per unit time; $\mathbf{q}$ is a measurable quantity whereas $\mathbf{u}$ is the pore velocity, that is, the flow rate per unit area of fluid (which is equivalent to consider that only fluid is present). ϕ is the hydraulic potential (or pressure head). It is defined by $\phi = p/\rho g + z$ where p is the fluid pressure, ρ the volumetric mass of the fluid, g the gravitational constant, and z the height. In ϕ, the kinematic term is always neglected due to small ground-water velocities in common applications. Finally, K, the proportionality coefficient between Darcy's velocity and the gradient of the hydraulic potential, is called hydraulic conductivity. This parameter (and also permeability) is recognized as a key parameter for ground-water flow. Several experimental techniques (of which mainly: pumping tests, sedimentary analysis, but also seismic, geoelectrical or tracer methods) are used to intensively measure this parameter in the laboratory or in the field scale. These measurements have put in evidence the (highly) heterogeneous behavior of K in space and have suggested the use of stochastic models.

In the stochastic models, the hydrogeological parameters (like K and θ) are represented by Random Space Functions (RSF). A RSF h is regarded as a random variable with an infinite number of components. Thus, with the random function $h(\mathbf{r})$ depending on the spatial coordinate $\mathbf{r}$, h_i is defined as the value of h at a point $r = r_i$ and the joint probability distribution function (Pdf) $F(h_1, h_2, \ldots, h_N)$, with $N \to \infty$, contains the probability information about h. We can also regard $h(\mathbf{r})$ as an ordinary function of the space coordinates in each realization and the ensemble underlying F, the Pdf, is that of the values of h at the set of points $\mathbf{r}_i$ ($i = 1, 2, \ldots, N$). Law ([10]) was the first to apply RSF in porous media and to propose, on the basis of core analysis data from a carbonate oil field reservoir, a **log-normal** probability density function (Pdf) for K. Since this proposition, there is now a large body of direct evidence to support the statement that the Pdf for hydraulic conductivity is log-normal ([1]), ([4]). Hydraulic log-conductivity $Y = \ln K$ is therefore commonly used and assumed to be distributed according to a Gaussian distribution $N(m_Y, \sigma_Y)$, where $m_Y = < Y >$, and σ_Y is the standard deviation.

Solving the Darcy equation with the random (log-normal) hydraulic conductivity, we have found the statistical characteristics required for the construction of the stochastic Lagrangian model in the form of a Langevin equation. The main difficulty was the unique derivation of this equation.

The results of the numerical simulation on the basis of the developed stochastic Lagrangian model are highly efficient, but what is especially important, is that the new model is free of many limiting assumptions used in the conventional models. In addition, the method calculates not only the mean concentration but also the flux of the concentrations.

2. A probabilistic approach to the solution of boundary value problems. Numerics for problems of stochastic dynamics (G.N. Milstein).

A probabilistic approach to constructing new numerical methods for solving Cauchy and boundary value problems for nonlinear parabolic PDEs is based on making use of the well-known probabilistic representations of solutions to linear PDEs and ideas of the weak sense numerical integration of SDEs. It takes into account a coefficients dependence on the space variables and a relationship between diffusion and advection in an intrinsic manner and allows to obtain a number of new effective numerical algorithms. The approach is applied to the numerical solution of the Dirichlet problem for nonlinear parabolic equations in [21].

In [15], some random walks for the general Dirichlet problem for linear elliptic and parabolic PDEs are proposed. They are based on the weak Euler approximation and on linear interpolation. Due to this, it is possible to suggest a number of efficient Monte Carlo algorithms.

Stochastic systems, phase flows of which have integral invariants, are considered in [16], [18], and [19]. In particular, the Hamiltonian systems perturbed by additive noise belong to systems with integral invariants. For such systems, numerical methods preserving a number of important features of the original phase flows are constructed. They demonstrate superiority in comparison with nonsymplectic methods in numerical experiments (see Fig. 1).

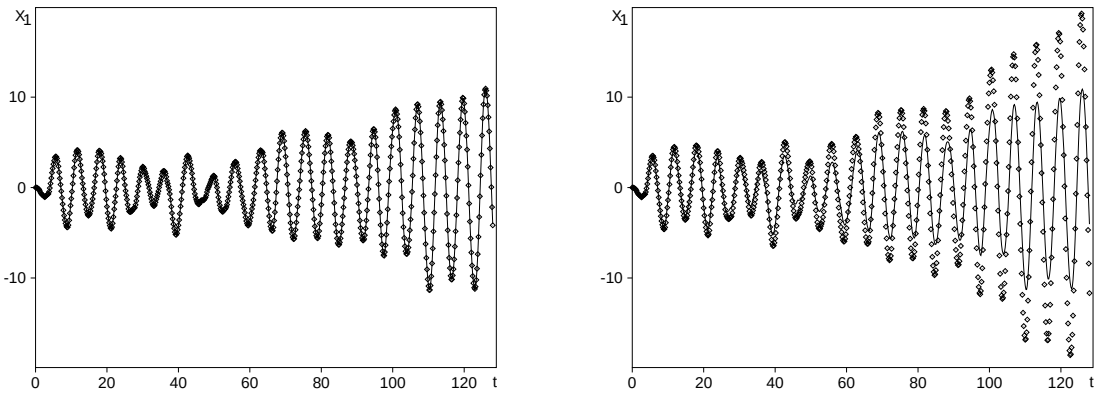

Fig. 1: A sample trajectory of a solution to an oscillator with noise obtained by the exact formulae (solid line), a symplectic method (points on the left figure), and the Euler method (points on the right figure). The symplectic and Euler methods are of the same order.

Some theoretical and numerical investigations of stochastic systems connected with such phenomena as stochastic resonance and noise-induced unidirectional transport are reported in [20].

Stability properties of stochastic systems are studied in [5] and [17].

3. Monte Carlo and Quasi-Monte Carlo methods for integration (P. Mathé).

Many physically relevant quantities are means or require to compute certain means intermediately. Therefore, we investigate numerical methods for the efficient computation of integrals. Precisely, for a fixed probability π on some space X, we aim at approximating $\int_X f(x)\,\pi(dx)$ by means of a sample mean of random variables arising from an ergodic Markov chain with transition kernel K, having π as its invariant distribution. Thus, if ν is an initial distribution,

then we use, for a given f on X, the sample mean

$$\vartheta_N(f) := \frac{1}{N}\sum_{j=1}^{N} f(X_j),$$

where $X_1,\ldots,X_N$ are the consecutive steps of our Markov chain. Typically, the error is measured in mean square sense, i.e.

$$e(f,\vartheta_N,\nu,K) := \left(\mathbf{E}\left|\frac{1}{N}\sum_{j=1}^{N} f(X_j) - \int_X f(x)\,\pi(dx)\right|^2\right)^{1/2}$$

denotes the individual error of the sample mean at function f. Previous analysis, see [11], was restricted to uniformly ergodic Markov chains. It is, however, known that on general state space, most Markov chains will not be uniformly ergodic, see [6]. Therefore, as in [14], we extended our study to V-uniformly ergodic Markov chains. Another goal was to establish the interaction between ergodicity properties of the kernel K, respective classes F of functions to be integrated, and initial distributions ν.
Let $V \geq 1$ be a real valued function on X. By $L_\infty(V)$ we denote the Banach space of all functions f on X, for which $\|f\|_V := \text{ess-sup}\,|f(x)/V(x)| < \infty$. The Harris-Markov chain K is called *V-uniformly ergodic*, if, for the transition operator P, we have

$$\|\,\mathrm{P}^n - \mathrm{E}\colon L_\infty(V) \to L_\infty(V)\| \to 0.$$

We established a series of consequences of this definition, using tools from interpolation theory. The intrinsic rôle of the weight function V became transparent.
Convergence results for the sample mean towards the integral are presented in terms of the following (quadratic) functional

$$\Phi(f) := \langle \pi, [(\mathrm{I}-\mathrm{P})^{-1}(\mathrm{I}+\mathrm{P})(\mathrm{I}-\mathrm{E})f][(\mathrm{I}-\mathrm{E})f]\rangle.$$

A typical result can be stated as follows. For all initial distributions ν with $\int V(x)\,\nu(dx) < \infty$ and bounded sets F in the weighted Hilbert space $L_2(V)$ we have

$$\lim_{N\to\infty} \sup_{f\in F} \left|Ne^2(f,\vartheta_N,\nu,K) - \Phi(f)\right| = 0.$$

The convergence results are then extended to classes of functions which are no longer square integrable.
A further aspect was the study of QMC methods for functions over unbounded domains, in particular integrals $\mathrm{Int}_\rho(f) := \int f(\mathbf{x})\rho(\mathbf{x})\,d\mathbf{x}$ over $\mathbb{R}^d$ with probability weight function ρ. These can be evaluated with the aid of QMC algorithms using a proper decomposition of the domain $\mathbb{R}^d$ and arrangement of the low discrepancy points over a series of hierarchical hypercubes. Precisely, we proposed

$$S_{m,\mathbf{n}}(f,\rho) := \sum_{j=0}^{m} \frac{q_j}{n_j}\sum_{i=1}^{n_j} f(\mathbf{y}_{ij})\rho(\mathbf{y}_{ij})\chi_{I_j}(\mathbf{y}_{ij}),$$

where $m+1$ is any number of cubes and $\mathbf{n} := (n_0,\ldots,n_m)$, where each n_j is the number of points used within cube Q_j, $j = 0,\ldots,m$, and the χ_{I_j} are the indicator functions of $I_j := Q_{j+1} \setminus Q_j$.

Furthermore,

$$\begin{aligned} q_j &= \text{Volume}(Q_j) = 2^{(j+1)d}, \\ \mathbf{y}_{ij} &= -2^j\mathbf{1} + 2^{(j+1)} * \mathbf{x}_{ij},\ 0 \le j \le m,\ 1 \le i \le n_j, \\ P_j &= \left\{\mathbf{x}_{ij} : 1 \le i \le n_j\right\} \subset [0,1]^d,\ 0 \le j \le m. \end{aligned}$$

The total amount of function evaluations is $N = \sum_{j=0}^{m} n_j$. The P_j s are some low-discrepancy point sets, consisting of n_j points, respectively.
By arranging the number of hypercubes as well as the number of low-discrepancy points properly, the proposed method can be seen to be optimal for power/exponential decaying weights. This was joint work with G. Wei, Hong Kong Baptist University, see [13]. Emphasis was on results which allow application to mathematical finance. Therefore we could assume smooth weights, but less smoothness for the integrands, in order to cover the evaluation of financial products.

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4.7 Research Group Continuum Mechanics

4.7.1 Overview

Die Forschungsgruppe hatte im Berichtszeitraum zwei Hauptforschungsrichtungen:

- Dynamik und Thermodynamik von porösen und granularen Materialien,
- Mikro-Makro-Übergänge.

Seit mehreren Jahren wird in der Forschungsgruppe ein makroskopisches thermodynamisches Mehrkomponentenmodell für poröse und granulare Materialien entwickelt. Die grundlegende Struktur dieses Modells ist für gesättigte Materialien sowohl für nichtlineare wie auch lineare Prozesse vollständig erarbeitet. Einige wichtige Fragen zur Beziehung zu anderen Modellen wie auch zu Stabilitätseigenschaften und zur Ausbreitung verschiedener dynamischer Störungen sind jedoch noch nicht vollständig beantwortet. Sie wurden in den letzten drei Jahren erforscht.
Es wurde gezeigt, dass sich das linearisierte Modell wesentlich von dem am häufigsten benutzten Modell von Biot unterscheidet. Dieser Unterschied beruht im Wesentlichen auf der thermodynamischen Unzulässigkeit des Biot-Modells. Es wurde bewiesen, dass das Biot-Modell zwei wichtige kontinuumsthermodynamische Prinzipien verletzt, nämlich die materielle Objektivität und den zweiten Hauptsatz der Thermodynamik. Einige eigene Modellalternativen (z. B. beide Komponenten kompressibel und Porosität beschrieben durch eigene Bilanzgleichung; manche Komponenten inkompressibel oder Höhere-Gradienten-Modelle) wurden vorgeschlagen und ihre praktischen Anwendungsmöglichkeiten in der Geophysik diskutiert.
Es wurde bewiesen, dass eindimensionale stationäre Strömungen durch poröse und granulare Materialien zu Instabilitäten führen können. Einige von ihnen sind notwendig, um

During the time covered by this report the research group has worked on two main research fields:

- Dynamics and thermodynamics of porous and granular materials,
- Micro-macro transitions.

For many years a macroscopic thermodynamical multicomponent model for porous and granular materials has been constructed in the research group. The fundamental structure of this model is already fully developed for both nonlinear and linear processes in saturated materials. However, some important questions concerning relations to other available models as well as stability properties and the propagation of various dynamical disturbances have not yet been answered. During the last year, three of these questions have been investigated. It has been shown that the linearized model differs considerably from the most commonly used model of Biot. It has been demonstrated that this difference is primarily related to the lack of thermodynamical admissibility of Biot's model. It has been proved that Biot's model violates two important principles of continuum thermodynamics: material objectivity and the second law of thermodynamics. A few own alternative models (e.g., both components compressible and the porosity described by a balance equation; some of the components incompressible, higher gradient models) have been proposed and their practical applications in geophysics have been discussed.
It has been proved that 1-d steady state flows through porous and granular materials may lead to instabilities. Some of them are needed in order to describe threshold effects leading to the liquefaction. Some others are not desired. However they appear solely on the border of

„Threshold“-Effekte, die zu Fluidisierung führen, zu beschreiben. Andere sind unerwünscht. Sie treten allerdings auch nur für praktisch kaum beobachtete Werte für die Volumen- und Flächendurchlässigkeiten, die die Stabilitätsbereiche steuern, auf.

practically admissible values of bulk and surface permeabilities controlling the region of stability.

Im Rahmen der Dynamik poröser Medien wurden wesentliche Erweiterungen zur Oberflächenwellenanalyse ermittelt. Zusätzlich zur Hochfrequenzasymptotik, die schon in den vergangenen Jahren hergeleitet wurde, wird jetzt eine Langwellenapproximation (niedrige Frequenzen) für Oberflächenwellen entwickelt. Dies ist besonders in der Praxis von Interesse, weil in geophysikalischen Anwendungen niedrige Frequenzen in der Größenordnung von 1–10 Hz vorherrschen. Außerdem wurde die Erforschung von Oberflächenwellen in heterogenen Materialien begonnen.

Within the frame of dynamics of porous media essential extensions of the surface wave analysis have been investigated. In addition to high-frequency asymptotics which has been developed previously, surface modes of propagation in the long-wave approximation (low frequency) are investigated. This has a particular practical bearing because most of the practical geophysical applications are made for low frequencies of the order of 1–10 Hz. In addition, research on the field of surface waves in heterogeneous materials has been initiated.

Die Aktivitäten der Forschungsgruppe Kontinuumsmechanik im Bereich der Mikro-Makro-Übergänge gliedern sich in vier Unterprojekte.

The activities of the research group “Continuum Mechanics” in the field of micro-macro transitions are divided into four subprojects

- Phasenübergänge, teilweise gefördert im BMBF-Programm „Neue Mathematische Verfahren in Industrie und Dienstleistungen“ unter der Nummer 03DRM3B5

  Zurzeit ist dieses Projekt in fünf Teile aufgegliedert: 1. Für das Referenzmaterial *Zinn-Blei-Legierung* wurden experimentelle Tests durchgeführt, und diese wurden mit Simulationen des WIAS-Standard-Phasenfeldmodells verglichen, 2. Eine Konvergenzstudie wurde für die Neumann-Reihen durchgeführt, welche im mechanischen Teil des WIAS-Modells auftreten, 3. Existenz- und Eindeutigkeitsstudien einer vereinfachten Version des Standardmodells, 4. Aufstellung von nichtlokalen Modellen zur Beschreibung von Phasenseparationsprozessen in thermomechanischen Spannungsfeldern, 5. Keimbildung von flüssigen Arsentropfen in einkristallinem Gallium-Arsenid.

- Phase transitions, supported in parts within the BMBF program “New Mathematical Methods in Industry and Services” under the contract 03DRM3B5

  This project is currently divided into five subprojects: (1) Experimental tests and comparison of the reference material tin/lead alloy with simulations of the WIAS standard phase-field model, (2) A convergence study of Neumann series appearing in the mechanical part of the WIAS standard phase-field model, (3) Existence and uniqueness studies of a simplified version of the standard model, (4) Formulation of nonlocal models of phase separation processes under thermomechanical stress fields, (5) Nucleation of liquid Arsen droplets within single crystal gallium arsenide.

- Kinetische Lösungen der Boltzmann-Peierls-Gleichung und ihrer Momentensysteme, gefördert durch die DFG innerhalb des Schwerpunktprogrammes „ANumE — Analysis und Numerik von Erhaltungsgleichungen“ unter Nummer DR 401/2-2

  Eine spezielle Klasse hyperbolischer Systeme enthält Systeme, die auf einer darunterliegenden kinetischen Gleichung basieren. Mitglieder dieser Klasse haben die besondere Eigenschaft, dass Anfangs- und Randwertprobleme durch sehr mächtige und allgemeine mathematische Methoden gelöst werden können, welche sich auf Mikro-Makro-Übergänge und das *Maximum-Entropie-Prinzip* gründen. Im Berichtszeitraum haben wir die Boltzmann-Peierls-Gleichung sowie ihre zugehörigen hyperbolischen Systeme studiert. Das wichtigste Resultat ist ein kinetisches Schema, welches beide Typen von Gleichungen durch eine einheitliche Methode löst, so dass ein Vergleich der Lösungen der kinetischen Gleichungen und der hyperbolischen Systeme durchgeführt werden kann. Seit Juli 2001 wird dieses Projekt, welches vorher im DFG-Normalverfahren finanziert wurde, im Schwerpunktprogramm ANumE gefördert.

- Multiskalenmodellierung von thermoelastischen Körpern, gefördert durch die DFG innerhalb des Schwerpunktprogramms SPP 1095 „Analysis, Modellbildung und Simulation von Mehrskalenproblemen“, unter der Nummer SP 212/15-1. Dies ist ein Gemeinschaftsprojekt von Dreyer (FG 7) und Sprekels (FG 1).

  Zur Zeit werden rigorose Grenzübergänge etabliert, die von mikroskopischen Bewegungsgleichungen zu makroskopischen Feldgleichungen führen.

- Kinetic solutions of the Boltzmann-Peierls equation and its moment systems, supported by the DFG within the Priority Program “ANumE — Analysis and Numerics of Conservation Laws” under the contract DR 401/2-2

  A special class of hyperbolic systems contains systems that are based on an underlying kinetic equation. What is special for members of this class, is that initial and boundary value problems can be solved by very powerful and generic mathematical methods which rely on micro-macro transitions and the *Maximum Entropy Principle.* During the period of this report we have studied the Boltzmann-Peierls equation as well as its corresponding hyperbolic systems. The most important result is a kinetic scheme that solves both types of equations by a unified method, so that a comparison of the solutions of the kinetic equation and of the corresponding hyperbolic system becomes practicable. Since July 2001 this project, which was previously financed within the *DFG Individual Grant Program,* has been sponsored within the DFG Priority Program *ANumE*.

- Multi-scale modeling of thermoelastic bodies, supported by the DFG within the Priority Program SPP 1095 “Analysis, Modelling and Simulation of Multiscale Problems” under the contract SP 212/15-1, which is a joint project of Dreyer (Research Group 7) and Sprekels (Research Group 1)

  Currently, rigorous limits are established that lead from microscopic equations of motions to macroscopic field equations.

- Außerdem wurde ein rein industrielles Projekt im Berichtszeitraum beendet: Spannungsanalyse einer dünnen Waferplatte aus einkristallinem Gallium-Arsenid. Es wurde finanziert durch die Freiberger Compound Materials GmbH Freiberg (FCM).

  Die von uns vorgeschlagene von Kármán-Theorie zur Lösung dieses Problems erwies sich als äußerst angemessen. Die große Herausforderung resultierte aus folgenden extremen Skalenunterschieden: Ein Plattendurchmesser von 150 mm, eine Plattendicke von 0,5 mm sowie eine Fläche von 0,1 mm^2, auf welcher die Kraft eingeleitet wurde, stehen sich gegenüber.

- Furthermore, a purely industrial project was completed within the last period: Stress analysis of a thin wafer plate of single crystal gallium arsenide, financed by the Freiberger Compound Materials GmbH Freiberg (FCM)

  The proposed von Kármán theory turned out to be the appropriate model. The great challenge resulted from extreme differences of various scales: A plate diameter of 150 mm, a plate thickness of 0.5 mm, and a contact area of 0.1 mm^2, where the external load is introduced, have to be taken into account.

4.7.2 Projects

Wave propagation in porous and granular materials

Collaborator: K. Wilmanski

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

Aims and results of the project
The project is devoted to a theoretical analysis of weak discontinuity waves on the basis of the own model [1], [2], as well as practical geotechnical applications particularly in a nondestructive testing of soils. Three main topics are in the process of investigation:

1. Long wave approximations of surface waves on the vacuum/porous body and fluid/porous body interfaces,
2. Approximate solutions by the method of propagators of the bulk and surface waves in vertically heterogeneous semispace,
3. Estimations of porosity by means of measurements of speeds of bulk waves.

The first problem is the continuation of the research carried out in the group during the last two years. The analysis of surface waves has been performed primarily in the limit of high frequency which yields the speeds of propagation of impulses ([3]). Such an approximation has the disadvantage of not corresponding to the frequency ranges used in geotechnical applications (approx. 1 to 10 Hz in contrast to some kHZ used in our work). For this reason a new asymptotic approximation has been designed. It seems to give correct results (a preliminary report is due to appear ([4])) but some singularities for different modes of propagation still require an explanation. Let us mention that such singularities (phase speeds going to infinity for low critical frequencies of monochromatic surface waves) appear also in the analysis of classical Rayleigh waves in heterogeneous materials.
The second problem is related to the first one because it concerns surface wave solutions for heterogeneous materials. Under the assumption that material properties depend on the variable z measuring the distance from the surface of the semispace, the wave analysis leads to a differential eigenvalue problem of the following form

$$\frac{d\mathbf{f}}{dz} = A(z)\,\mathbf{f}, \quad \mathbf{f} \in \Re^4, \quad \mathbf{A} \in \Re^4 \times \Re^4, \tag{1}$$

where in the single component solid the vector $\mathbf{f}$ and the matrix $\mathbf{A}$ are defined as follows

$$\mathbf{f} := (U, W, f_3, f_4)^T, \quad f_3 := \mu\left(\frac{dU}{dz} - kW\right), \quad f_4 := (\lambda + 2\mu)\frac{dW}{dz} + k\lambda U,$$

$$\mathbf{A} := \begin{pmatrix} 0 & k & \mu^{-1} & 0 \\ -k\lambda\,(\lambda+2\mu)^{-1} & 0 & 0 & (\lambda+2\mu)^{-1} \\ k^2\zeta - \omega^2\rho & 0 & 0 & k\lambda\,(\lambda+2\mu)^{-1} \\ 0 & -\omega^2\rho & -k & 0 \end{pmatrix}, \quad \zeta := 4\mu\frac{\lambda+\mu}{\lambda+2\mu}. \tag{2}$$

In these relations λ, μ, ρ are z-dependent material parameters, k, ω are the wave number and frequency, respectively. U, W denote the amplitudes of disturbances.
In order to solve this problem, i.e. in order to find a relation between k and ω, a method of successive approximations has been developed. The method is based on the assumption that the deviation of the matrix $\mathbf{A}$ from its average $\mathbf{A}_0$ with respect to z is a small quantity

$$\frac{\|\mathbf{A}-\mathbf{A}_0\|}{\|\mathbf{A}_0\|} \ll 1. \tag{3}$$

The method has been tested on the classical problem of Rayleigh waves, and it shall be applied in the future to surface waves in two-component heterogeneous systems as well as in some flow stability problems in such systems.
The third problem is related to a nondestructive testing of soils. It is attempted to develop a systematic acoustic method of *in situ* measurements of such quantities as the porosity of soils. The first result of this form has been obtained in [5], [6]. It is based on very simple relations between macroscopic material parameters and the porosity. One obtains the following relation between porosity n and the speeds of propagation of the longitudinal P1-wave c_{P1}, the longitudinal P2-wave c_{P2}, and the shear S-wave c_S

$$n = \frac{\rho^{SR} - \sqrt{\rho^{SR2} - 4\rho^{FR}(\rho^{SR}-\rho^{FR})\frac{c_{P2}^2}{(c_{P1}^2-\varphi c_S^2)}}}{2(\rho^{SR}-\rho^{FR})}, \quad \varphi := \frac{2(1-\nu)}{1-2\nu}, \tag{4}$$

where ρ^{SR}, ρ^{FR} are real mass densities of components and ν denotes Poisson's ratio (approx. $0.155-0.20$). Comparison of these results with measurements on the site of Pisa tower ([5]) shows a very good agreement.

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Thermodynamical modeling of porous and granular materials – flaws of Biot's model

Collaborator: K. Wilmanski

Cooperation with: I. Edelman (Alexander von Humboldt fellow in WIAS, Russian Academy of Sciences, Moscow), T. Wilhelm (Universität Innsbruck, Austria), C. Lai (Studio Geotecnico Italiano, Milano), R. Lancellotta (Politecnico di Torino, Italy)

Aims and results of the project
Most of the linear multicomponent models used in contemporary applications in soil mechanics and geophysics are derived from Biot's model developed at the beginning of the fourties. This model describes mechanical processes in saturated poroelastic materials by means of a two-component linear continuum. It has two essential features:

1. In addition to classical partial accelerations in two-momentum balance equations it contains coupling terms. Momentum balance equations for the solid and fluid components have then the following form

$$\begin{aligned} \rho^S \frac{\partial \mathbf{v}^S}{\partial t} + \rho_{12} \frac{\partial \mathbf{v}^F}{\partial t} &= div \mathbf{T}^S - \hat{\mathbf{p}}, \\ \rho^F \frac{\partial \mathbf{v}^F}{\partial t} + \rho_{12} \frac{\partial \mathbf{v}^S}{\partial t} &= div \mathbf{T}^F + \hat{\mathbf{p}}, \end{aligned} \tag{1}$$

   where $\mathbf{T}^S, \mathbf{T}^F$ are partial stress tensors, $\mathbf{v}^S, \mathbf{v}^F$ denote velocities, ρ^S, ρ^F are partial mass densities, $\hat{\mathbf{p}}$ is the diffusive force of interaction, and ρ_{12} is a mass density describing the dynamical coupling of components. It is usually related to a so-called added mass effect, and some experimentalists claim that it is related to the tortuosity of porous and granular materials.

2. There exists a static interaction between the components which leads to the following constitutive relations for partial stresses

$$\begin{aligned} \mathbf{T}^S &= \lambda \left(\text{tr } \mathbf{e}^S \right) \mathbf{1} + 2\mu \mathbf{e}^S + Q\varsigma \mathbf{1}, \\ \mathbf{T}^F &= -\left(M\varsigma + Q \,\text{tr } \mathbf{e}^S \right) \mathbf{1}, \end{aligned} \tag{2}$$

   where $\mathbf{e}^S$ is the Almansi-Hamel tensor of small deformations, ς describes volume changes of the fluid component, λ, μ, M, Q are material constants. The constant Q is responsible for interactions introduced to the model by Biot (e.g., [1]).

In the series of papers we show that such a model contradicts basic principles of continuum thermodynamics.
It is a rather easy task to prove that the dynamical contribution with the interaction mass density ρ_{12} violates the principle of material objectivity ([2]). Namely, if we assume that constitutive relations must be invariant with respect to the time-dependent orthogonal transformation in the space of motion $\Re^3$

$$\mathbf{x}^* = \mathbf{O}(t)\mathbf{x} + \mathbf{d}(t), \quad \mathbf{O} \in Orth, \quad \mathbf{x}^*, \mathbf{x} \in \Re^3, \quad \mathbf{d} \in V^3, \tag{3}$$

then a dependence of the diffusive force $\hat{\mathbf{p}}$ on the relative acceleration $\frac{\partial \mathbf{v}^F}{\partial t} - \frac{\partial \mathbf{v}^S}{\partial t}$ must vanish identically. Consequently, ρ_{12} must be identically zero.
Even if we ignored the principle of material objectivity, contributions of this dynamical interactions would have to be very small. This is also shown in the work [2].
More sophisticated is the argument concerning the coupling constant Q of Biot's model. It is based on the evaluation of the second law of thermodynamics for isothermal processes. Direct substitution of linear constitutive relations in the entropy inequality does not give reliable results because such an evaluation is inconsistent with orders of magnitude of contributions to the inequality. Consequently, one has to rely on the evaluation for the nonlinear model and then one has to make a transition to the linear version with respect to both geometric and kinematical contributions. Such a procedure is not unique and it depends on the structure of a chosen nonlinear model. The following nonlinear models have been investigated ([3, 4]):

1. A fully nonlinear thermomechanical model of a two-component system with either a balance equation of porosity or a constitutive relation for porosity,

2. Three hybrid incompressible nonlinear models with either a balance equation of porosity or a constitutive relation for porosity,

3. A nonlinear model with an incompressible real fluid component, and without a balance equation for porosity.

We present a scheme of argument on the last example.
It is assumed that the mass density of the fluid component ρ^F is related to the real mass density $\rho^{FR} = const$ by the formula $\rho^F = n\rho^{FR}$. Then the partial mass balance equation becomes the equation for the porosity

$$\frac{\partial n}{\partial t} + \operatorname{div}\left(n\mathbf{v}^F\right) = 0. \tag{4}$$

Exploitation of the second law of thermodynamics yields the following constitutive relations for partial stresses

$$\begin{aligned} \mathbf{T}^S &= \lambda\left(tr\mathbf{e}^S\right)\mathbf{1} + 2\mu\mathbf{e}^S - n_0 N\varsigma\mathbf{1}, \\ \mathbf{T}^F &= -M\varsigma\mathbf{1}, \end{aligned} \tag{5}$$

where n_0 denotes a reference porosity, and the constant N appears also as a coefficient in the diffusive force

$$\hat{\mathbf{p}} = \pi\left(\mathbf{v}^F - \mathbf{v}^S\right) + N\operatorname{grad} n. \tag{6}$$

If we consider the model without a constitutive dependence on $\operatorname{grad} n$, the constant N is equal to zero and there is no coupling between partial stresses.
Certainly there is no way in which the above relations (5) can be transformed into Biot relations (2). The same conclusion has been proved for all other models. Consequently the classical Biot model seems to be violating two most important conditions of the continuum thermomechanics. In spite of these flaws practical results which follow from Biot's model seem to be acceptable. This has been checked for numerous problems of practical bearing. As mentioned above the nonobjective contributions are extremally small and cannot be observed in experiments conducted under normal conditions (e.g., on the turntable rotating with angular velocities much smaller than 1 MHz). The influence of Biot's coupling constant Q on the propagation conditions

of bulk and surface waves is solely quantitative and there is no change in the number and character of modes of propagation ([5]). The onset of some instabilities such as liquefaction of granular materials is also not influenced by this constant ([6]). The latter arguments seem to advocate the much simpler two-component model developed and investigated in WIAS (e.g., [4]).

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Stability and relaxation of flows in porous materials

Collaborators: B. Albers, K. Wilmanski

Cooperation with: T. Wilhelm (Universität Innsbruck, Austria)

Aims and results of the project
The main aim of the project is the linear stability analysis of various flow processes coupled with the deformation of the saturated skeleton made of a poroelastic material. During the last two years three problems have been investigated:

1. Loss of stability of the 1-d steady state flow through a granular material due to liquefaction ([1]),
2. Relaxation properties of a longitudinal disturbance of a 1-d steady state flow through a poroelastic material ([3]),
3. Stability properties of a 1-d steady state flow through a poroelastic material with respect to a transversal disturbance.

It has already been reported that it is necessary to introduce a contribution that be nonlinear with respect to the relative velocity of components to the source of momentum in order to describe a threshold to the fluidized state of a granular material. This result has been well-confirmed by experiments performed at the University of Innsbruck (Austria).
The problem of stability of a 1-d flow through a saturated poroelastic material has been divided into two parts.
In the first part the steady state solution has been disturbed by a dynamical disturbance in the longitudinal direction. Such a flow through the immobile skeleton is described by the following field equations ([2])

$$\frac{\partial \rho^F}{\partial t}+\frac{\partial \rho^F v^F}{\partial x}=\hat{\rho}^A, \quad \rho^F\left(\frac{\partial c}{\partial t}+v^F\frac{\partial c}{\partial x}\right)=(1-c)\,\hat{\rho}^A,$$

$$\hat{\rho}^A:=-\rho^A_{ad}\frac{d\xi}{dt}, \quad \frac{d\xi}{dt}=\frac{1}{\tau_{ad}}\left[\frac{cp^F}{p_0}(1-\xi)-\xi\right],$$

$$\rho^F\left(\frac{\partial v^F}{\partial t}+v^F\frac{\partial v^F}{\partial x}\right)=-\frac{\partial p^F}{\partial x}-\pi v^F, \quad p^F=\overset{0}{p}{}^F+\kappa\,\overset{1}{\rho}{}^F. \tag{1}$$

The first two equations are, of course, mass balance equations for the fluid component and for the adsorbate in the fluid. The concentration of the adsorbate is denoted by c. ξ is the microstructural variable called the number of occupied sites. $\kappa, \pi, p_0, \tau_{ad}, \rho^A_{ad}$ are constants. We consider two cases. The first one is the longitudinal disturbance without mass exchange (i.e. $\hat{\rho}^A \equiv 0$). In the second one the adsorption in the nonsteady disturbance is different from zero.
The base steady state flow in a pipe is described for both cases by the following relations:

1. Skeleton is deformed and does not move any more,

2. Longitudinal velocity and pressure in the fluid satisfy the following relations

$$\begin{aligned} \overset{0}{v}^F &= f\,\frac{n_E\,(p_l-p_r)}{\pi l} = const., \\ \overset{0}{p}^F &= n_E\,p_l - f\,n_E\,(p_l-p_r)\,\frac{x}{l} - \frac{n_E\,(p_l-p_r)}{2+\frac{\alpha\pi l}{\rho_0^F}}, \\ f &:= \frac{\frac{\alpha\pi l}{\rho_0^F}}{2+\frac{\alpha\pi l}{\rho_0^F}}, \end{aligned} \tag{2}$$

where we use the following notation. p_l, p_r denote the external pressure at the left and right ends of the pipe, respectively. n_E is the constant porosity of the skeleton. ρ_0^F denotes the initial mass density of the fluid component, l is the length of the pipe, and π, α are material constants. The first one describes the bulk permeability, and the second one the surface permeability of the material. The above solution satisfies the boundary conditions of the third type describing the flow through a permeable boundary. In the special case $\alpha \to \infty$, this boundary condition becomes: $p^F\big|_{x=0} = p_l, \quad p^F\big|_{x=l} = p_r$, which is commonly used in Darcy-like models of flows.

The longitudinal disturbance may or may not lead to the exchange of mass between the fluid as a carrier of an adsorbate and the skeleton.
The main result of this work is that the flow (2) is stable with respect to any such disturbance. However, the analysis leads as well to some results on the relaxation properties of longitudinal disturbances related to different values of permeability coefficients π and α. We demonstrate these results in the two figures below.

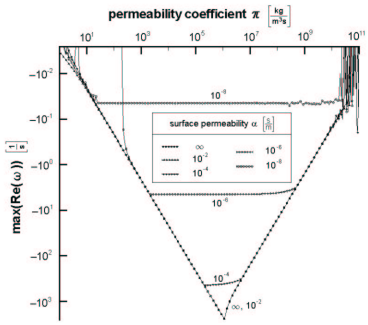

Fig. 1: Relaxation without adsorption

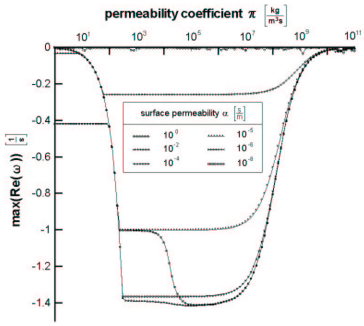

Fig. 2: Relaxation with adsorption

In Fig. 1 we show the inverse of the relaxation time of disturbance (in seconds) as a function of the bulk permeability π for the case of disturbance without mass exchange. It is seen that the relaxation is fastest for medium values of the permeability. The value appearing in the most common applications in soil mechanics is $\pi = 10^6 - 10^8 \quad \left[\frac{kg}{m^3 s}\right]$. Simultaneously there exists an essential influence of the surface permeability α. The relaxation time becomes longer for smaller values of this permeability. It should be mentioned that in the range of smaller values of the bulk permeability the dynamical disturbance yields not only damping but also vibrations. In Fig. 2 we show similar results under the presence of mass exchange. Qualitatively the changes in comparison to the previous case are not very big even though there appear additional plateaus. However, quantitatively the relaxation becomes much slower and it depends on the relaxation time of adsorption τ_{ad}.
The results for transversal disturbance of the same steady state flow are still preliminary. We consider the 2-d flow through a channel of the width $2b$. The boundary conditions in the direction of the channel are the same as before. The boundary conditions in the transversal direction are: $v_z^F\big|_{z=\pm b} = 0$, where v_z^F is the transversal component of the fluid velocity.
The flow becomes unstable in the range of high values of the bulk permeability π. The exchange of stability (Re $\omega = 0$, where ω is the complex frequency of the transversal disturbance) appears for the values of π which grow with the growing surface permeability α. This problem shall be further investigated in the next year.

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Phase transitions

Collaborators: W. Dreyer, F. Duderstadt

Cooperation with: S. Brodie, C.M. Brown (Heriot-Watt University Edinburgh, UK), P. Colli, G. Gilardi (Università di Pavia, Italy), S. Eichler (Freiberger Compound Materials GmbH (FCM)), T. Hauck (Motorola, München), W.H. Müller (Technische Universität Berlin), E. Radkevich (Lomonosov University, Moscow, Russia)

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 – 03DRM3B5)

Currently, the investigations on phase transitions were oriented towards the following tasks:
(1) In collaboration with W.H. Müller, S. Brodie, and C.M. Brown, AMF techniques have been used in order to study in-situ the motion of interfaces in various microstructures that were obtained from a melt by different cooling paths. In turn the morphological changes were compared with simulations. To this end, the grey colors of micrographs of tin/lead alloys are mapped onto concentrations so that the resulting mathematical microstructure serves as initial data for the phase-field model.
(2) For the evaluation of the mechanical part of the model, a Neumann series must be computed. This makes a convergence study necessary. It was shown that the convergence of the Neumann series depends sensitively on the different elastic tensors of tin and lead. To describe this quantitatively, various norms were compared in order to select the appropriate norm so that convergence of the Neumann series could be proved ([1]).
(3) For given initial and boundary data, the standard phase-field model that was used by Dreyer/Müller for numerical simulations of various phase separation processes in tin/lead alloys contains too many complexities. In particular, the quadratic dependence of the diffusion potential on the strain tensor renders the analysis difficult. Indeed, L^p estimates for ∇u are known to hold just for p close to 2 while global L^4 estimates were to be required. Therefore, in order that the problem turns out to be accessible from a mathematical point of view, some simplifications have been made concerning the matrices of mobilities, the stiffness matrix, and the matrix of surface tensions in their dependencies on the concentration and on the unisotropy. For the simplified model, existence and uniqueness results were established, [2].
(4) The aforementioned difficulties of a mathematical treatment of the standard phase-field models are among the motivations of Prof. Gajewski from WIAS, who proposed an alternative mathematical model for phase separation processes. The model is a nonlocal alternative to the classical Cahn/Hilliard model, where the fourth-order derivatives do not occur any more, but are modeled now by integrals with local kernels. For the simple Cahn/Hilliard model, Gajewski and Zacharias demonstrated that the nonlocal alternative allows for the powerful maximum principle, which fails to exist for the Cahn/Hilliard equation. The extension of Gajewski's ideas to phase separation processes under thermomechanical stress fields has now been established. There results the nonlocal version of the standard Dreyer/Müller model that describes phase separation processes by a coupling of a diffusion equation of Cahn/Hilliard type and the elliptic quasi-static mechanical system for the mechanical displacement. The central quantity of the

nonlocal model is the free energy functional, which is proposed according to

$$\begin{aligned}\Psi &= U_{ther}(T) + k_B \int_\Omega \left(c(t,X)\ln(c(t,X)) + (1-c(t,X))\ln(1-c(t,X))\right) d^3X * \\ &\frac{1}{d^6}\int_\Omega\int_\Omega d^3X d^3X' c(t,X)(1-c(t,X))\left(\varphi\left(\Delta^{XX'}\right) + \frac{1}{2}\Phi_{ij}(X,X')\Theta_i(t,X,X')\Theta_j(t,X,X')\right) + \\ &\frac{1}{d^6}\int_\Omega\int_\Omega d^3X d^3X' \frac{1}{2}\left(c(t,X)-c(t,X')\right)^2\left(\varphi\left(\Delta^{XX'}\right) + \frac{1}{2}\Phi_{ij}(X,X')\Theta_i(t,X,X')\Theta_j(t,X,X')\right) + \\ &\frac{1}{d^6}\int_\Omega\int_\Omega d^3X d^3X' \frac{1}{2}\left(c(t,X)+c(t,X')\right)^2\left(\tilde{\varphi}\left(\Delta^{XX'}\right) + \frac{1}{2}\tilde{\Phi}_{ij}(X,X')\Theta_i(t,X,X')\Theta_j(t,X,X')\right) + \\ &\frac{1}{d^6}\int_\Omega\int_\Omega d^3X d^3X' \left(\varphi_{AA}\left(\Delta^{XX'}\right) + \frac{1}{2}(\Phi_{AA})_{ij}(X,X')\Theta_i(t,X,X')\Theta_j(t,X,X')\right). \qquad (1)\end{aligned}$$

The first line gives the pure thermal part and the well-known entropic part. The further lines reflect the coupling between diffusion, which is indicated here by the concentration field $c(t,X)$, and the mechanical fields, which appear here in form of interaction potentials, $\varphi\left(\Delta^{XX'}\right), \tilde{\varphi}\left(\Delta^{XX'}\right), \varphi_{AA}\left(\Delta^{XX'}\right), \Phi_{ij}(X,X'), \tilde{\Phi}_{ij}(X,X'), (\Phi_{AA})_{ij}(X,X')$, and displacements, which are described by the functions $\Theta_i(t,X,X')$. The second line gives the already known local part of the interaction energy, while the third up to the last line represent the nonlocal contributions, which appear in the standard phase-field models as derivatives of second order.

This model and a further nonlocal model for the description of intermetallic phases, which need additionally nonconserved order parameters, form the basis of the WIAS proposal *Model of phase transitions with thermo-mechanical interactions* to the DFG Priority Program 1095 *Analysis, Modellbildung und Simulation von Mehrskalenproblemen* (Analysis, modeling and simulation of multiscale problems). Here the three WIAS groups Dreyer/Gajewski/Sprekels, in collaboration with Prof. W.H. Müller, Technische Universität Berlin, and T. Hauck, Motorola München, will investigate and compare mathematically, as well as numerically and experimentally, the properties of the standard phase-field model with higher derivatives with the nonlocal model represented by integro-differential systems, containing at most second-order derivatives. Furthermore a serious data basis for the two reference materials tin/lead (conserved order parameter) and silver/tin (nonconserved order parameters) will be established.

(5) The very first period of nucleation and the subsequent evolution of liquid arsenic droplets within single crystal gallium arsenide (GaAs) were modeled and studied in collaboration with the Freiberger Compound Materials GmbH (FCM). This study is sponsored by the BMBF. The outstanding and difficult problem arises from the following process:

In order that single crystal GaAs can be appointed as a semiconductor material there is an excess content $\Delta, 0 < \Delta < 0.0001$ of As above the ideal single crystal As concentration $c = 0.5$. The excess atoms occupy homogeneously in space interstitial sites, vacancy sites, and sites of the Ga sublattice. During necessary heat treatments under very high pressure, so that arsenic cannot evaporate, the excess As atoms start to diffuse and the process of liquid As-droplet formation sets in. Obviously, the initial and necessary homogeneity is lost. The objective of this project is (i) a simulation of the complete process, and (ii) the identification of the parameter which possibly can be adjusted, so that liquid droplets will not form.

The first year of this three-year project was devoted exclusively to the establishment of the mathematical model. After many discussions with the physicists in charge from FCM, it has turned out that the following items are important:

(i) There is an observed tendency that droplets appear in the vicinity of dislocations. The

diffusion process is thus modeled by the Dreyer/Müller standard phase-field model that describes diffusion under inhomogeneous stress fields, which are induced here, and introduced into the model, by a given random distribution of point dislocations.
(ii) The nucleation process itself is thermodynamically far from the instability region of the parent phase. Thus the critical energy barrier and the critical droplet size can be calculated according to the classical nucleation theory. This means that a reduction of the energy barrier, which might appear according to the more advanced Cahn/Hilliard nucleation theory, has not to be considered.
(iii) The evolution of the droplet formation from a locally given content of As atoms, according to (i), was first modeled and described in the last annual report, by a dynamic generalization of the stationary and well-accepted Becker/Döring theory. However, a preliminary numerical study of the explicit system of rate equations has revealed serious deficits. For example, this system predicts droplet formation for undercritical pressure! Thus a very detailed study of the pure nucleation problem became necessary. To this end we considered the nucleation of liquid droplets in vapor as a simple reference system.

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Kinetic solutions of the Boltzmann-Peierls equation and its moment systems

Collaborators: W. Dreyer, M. Herrmann

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

Supported by: DFG: 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 classical Fourier theory of heat fails to describe heat conduction at low temperatures, where the evolution of a phonon gas is governed by the Boltzmann-Peierls equation which is a kinetic equation for the phase density of phonons. For more details we refer to [4] and [5]. In [4] we have shown that the full Boltzmann-Peierls equation can be reduced to the simplified kinetic equation

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

In (1), φ is a reduced phase density depending on time t, space $\mathbf{x} = (x_1, x_2)$, and a normal vector $\mathbf{n} = (n_1, n_2) \in S^1$; and the positive constant c_D is the Debye speed. For simplicity we consider (1) in two space dimensions only. In addition to the reduced equation (1) we introduce a reduced definition of the (entropy density h / entropy flux Φ_i) pair according to

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

where μ is a given constant. We have proved that these definitions and the kinetic equation (1) imply the entropy inequality

$$\frac{\partial}{\partial t} h(\varphi)(t,\mathbf{x}) + \frac{\partial}{\partial x_i} \Phi_i(\varphi)(t,\mathbf{x}) \geq 0. \tag{3}$$

As well as the phase density, also the reduced phase density φ can be used to define moments. The following moments have an immediate physical interpretation

$$e(\varphi) = \hbar c_D \int_{S^1} \varphi(\mathbf{n})\, d\mathbf{n}, \qquad p_i(\varphi) = \hbar \int_{S^1} n_i \varphi(\mathbf{n})\, d\mathbf{n}, \tag{4}$$

$$Q_j(\varphi) = \hbar c_D^2 \int_{S^1} n_j \varphi(\mathbf{n})\, d\mathbf{n}, \qquad N_{ij}(\varphi) = \hbar c_D \int_{S^1} n_i n_j \varphi(\mathbf{n})\, d\mathbf{n}. \tag{5}$$

The fields e, p_i, Q_i, and N_{ij} denote the energy density, the momentum density, the heat flux, and the momentum flux, respectively. From a physical point of view, the moments of φ are more important than φ itself. On the right-hand side of (1) there are two collision operators Ψ_R and Ψ_N which are simplified models of two different kinds of interaction processes, which are called R-processes and N-processes. The N-processes describe phonon-phonon interactions and conserve the energy as well as the momentum, while the R-processes indicate interactions of

phonons with lattice impurities. The latter ones only conserve the energy. The Callaway ansatz for the collision operators reads

$$\Psi_\alpha \varphi = \frac{1}{\tau_\alpha}(\Theta_\alpha \varphi - \varphi), \quad \alpha \in \{R, N\}. \tag{6}$$

Here τ_R and τ_N are two relaxation times, and Θ_R and Θ_N describe the phase density in the limiting cases $\tau_R \to 0$ and $\tau_N \to 0$, respectively. In particular, $\Theta_R\varphi$ and $\Theta_N\varphi$ maximize the entropy according to

$$h(\Theta_R\varphi) = \max_{\varphi'}\Big\{h(\varphi) : e(\varphi') = e(\varphi)\Big\}, \tag{7}$$

$$h(\Theta_N\varphi) = \max_{\varphi'}\Big\{h(\varphi) : e(\varphi') = e(\varphi),\ p_i(\varphi') = p_i(\varphi)\Big\}. \tag{8}$$

The reduced Boltzmann-Peierls equation (1) induces an infinite number of balance equations. For any vector $\vec{m} = \vec{m}(\mathbf{n})$ of moment weights, there is a corresponding vector of densities $\vec{u}$, fluxes $\vec{F}_1$, $\vec{F}_2$, and productions P, according to

$$\vec{u}(\varphi) = \int_{S^1} \vec{m}(\mathbf{n})\varphi(\mathbf{n})\, d\mathbf{n}, \tag{9}$$

$$\vec{F}_i(\varphi) = c_D \int_{S^1} n_i \vec{m}(\mathbf{n})\varphi(\mathbf{n})\, d\mathbf{n}, \tag{10}$$

$$\vec{P}(\varphi) = \int_{S^1} \vec{m}(\mathbf{n})(\Psi_R\varphi + \Psi_N\varphi)(\mathbf{n})\, d\mathbf{n}. \tag{11}$$

With these definitions, the kinetic equation implies

$$\frac{\partial}{\partial t}\vec{u}(\varphi)(t,\mathbf{x}) + \frac{\partial}{\partial x_i}\vec{F}_i(\varphi)(t,\mathbf{x}) = \vec{P}(\varphi)(t,\mathbf{x}). \tag{12}$$

Physicists and engineers are not interested in the phase density itself, but in balance equations for moments as (12). It is a common strategy in Extended Thermodynamics (cf. [4, 1, 3, 5]) to consider in (12) the densities $\vec{u}(\varphi)$ as variables. However, since the fluxes and the productions are in general not functions of $\vec{u}(\varphi)$ there arises the so-called closure problem. An often used and powerful closure principle is the *Maximum Entropy Principle*. It has the advantages that

1. the resulting moment systems are hyperbolic, after a suitable transformation, they are even symmetric hyperbolic;

2. there exists a corresponding entropy inequality.

The *Maximum Entropy Principle* (MEP) can be formulated as follows. We start with a fixed vector of densities $\vec{u}$ with N components. In the first step, we determine the corresponding MEP projector Θ_M so that, for any given φ, there holds

$$h(\Theta_M\varphi) = \max_{\varphi'}\Big\{h(\varphi) : \vec{u}(\varphi') = \vec{u}(\varphi)\Big\}.$$

In the second step we use Θ_M in order to solve the closure problem of the system (12). When we replace formally the phase density φ by $\Theta_M\varphi$, we obtain the resulting MEP system

$$\frac{\partial}{\partial t}\vec{u}(\Theta_M\varphi)(t,\mathbf{x}) + \frac{\partial}{\partial x_i}\vec{F}_i(\Theta_M\varphi)(t,\mathbf{x}) = \vec{P}(\Theta_M\varphi)(t,\mathbf{x}), \tag{13}$$

which is indeed a closed system for the variables $\vec{u}$.
In the year 2001 we have studied the following problems:

1. **Derivation of the reduced equation and the corresponding reduced entropy inequality**
   We have proved that the reduced equation contains all important information on the solutions of the original Boltzmann-Peierls equation. Furthermore, we have derived the reduced entropy (2) from the original Bose entropy so that

   (a) there holds the entropy inequality (3),

   (b) the MEP applied to the original Boltzmann-Peierls equation and to the reduced equation (1) lead to identical moment systems.

2. **Existence of MEP-operators**
   The existence of MEP operators is a crucial problem. Junk has shown in [3] that in the most prominent application of the *Maximum Entropy Principle,* which is the Boltzmann equation for monatomic gases, MEP operators fail to exist within a reasonable domain of definition. In [1] we have proved that in the case of the Boltzmann-Peierls equation, the *Maximum Entropy Principle* will lead to well-defined MEP operators Θ_M, if it is applied to the reduced entropy.

3. **Kinetic approximations and kinetic schemes**
   Corresponding to the MEP system (13) there exists the following modified kinetic equation

   $$\frac{\partial\varphi}{\partial t} + c_D n_i \frac{\partial\varphi}{\partial x_i} = \Psi_R\varphi + \Psi_N\varphi + \frac{1}{\tau_M}(\Theta_M\varphi - \varphi),$$

   where Θ_M is the MEP operator corresponding to $\vec{u}$ (cf. [1]) and τ_M is an artificial relaxation time. The moment system (13) formally results in the limit $\tau_M \to \infty$. This approach illustrates the close connection between the kinetic equation and the MEP system.
   Furthermore there exists a class of consistent kinetic schemes containing schemes for the kinetic equation as well as for the moment systems. For the details we refer to [1].

4. **Numerical simulations**
   A numerical example shall illustrate that the MEP systems induce a sequence of approximations of the kinetic equation. To this end we study the evolution of an initial energy pulse as shown in Fig. 1.

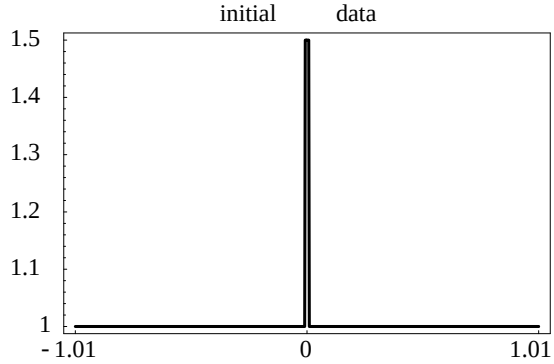
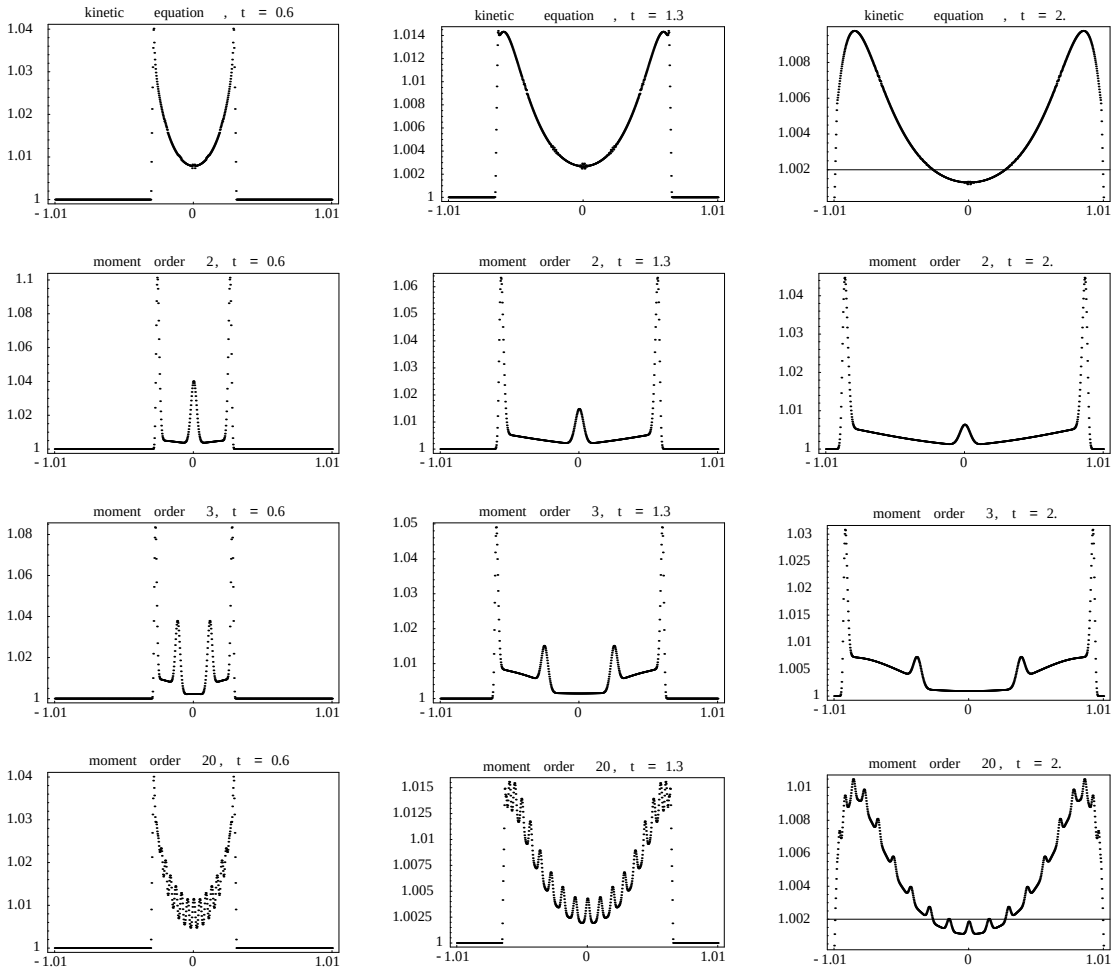


Fig. 1: Initial energy pulse

For simplicity we set $\tau_R = 0$, and we assume that all quantities do not depend on the x_2 direction. Furthermore we set $\tau_N = 0.7$, $c_D = 0.5$. The initial data ϕ_0 are determined by an equilibrium assumption, i.e. $\Theta_R \phi_0 = \phi_0$. The evolution of the energy pulse according to the kinetic equation is depicted in Fig. 2. The figures show the corresponding solutions of various MEP systems.



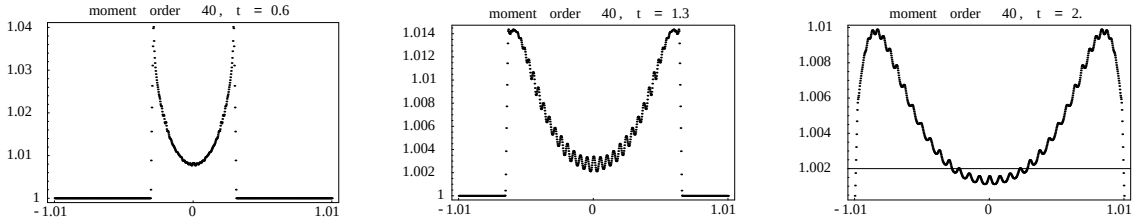


Fig. 2: Solution of a MEP system with 81 moments

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Stress analysis of a thin wafer plate of single crystal gallium arsenide

Collaborators: W. Dreyer, F. Duderstadt

Cooperation with: S. Eichler (Freiberger Compound Materials GmbH (FCM))

Supported by: Freiberger Compound Materials GmbH

In 2000 we have started a remittance study on the stress distribution in a thin wafer plate which is loaded by the steel sphere according to Fig. 1.

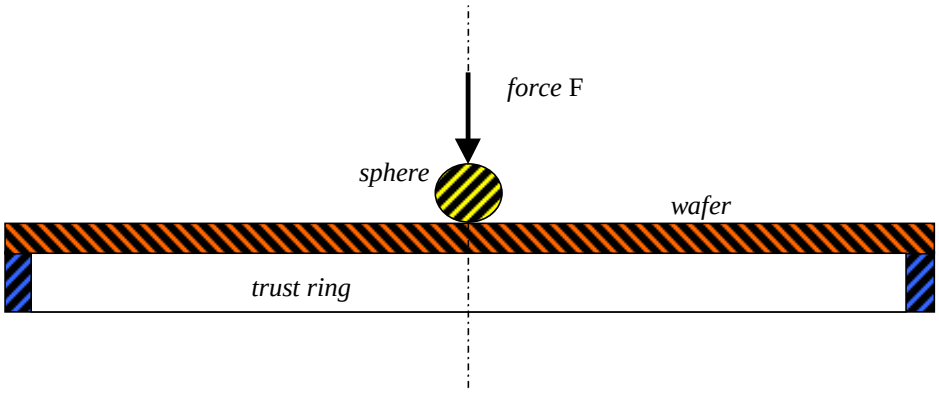

Fig. 1: Experimental device

The wafer plate's material is single crystal GaAs the [100] direction of which is parallel to the load axes. Preliminary studies have shown that the external load induces a deformation field that has small strain components, however, the rotational contribution to the deformation field is quite large, so that the appropriate field equations are the nonlinear von Kármán equations in Lagrangian coordinates. The complete elliptic von Kármán system is to be found in the WIAS Annual Report 2000, and we refer the reader to pp. 120–122. The von Kármán system results, by a limiting process, from the 3-d nonlinear elasticity system for the second Piola-Kirchhoff stress tensor

$$\frac{\partial}{\partial X_k}(\sigma_{ik} + \frac{\partial u_i}{\partial X_j}\sigma_{jk}) = 0, \quad \text{with} \tag{1}$$

$$\sigma_{ik} = (\lambda G_{nn} + \mu' G_{\underline{ii}})\delta_{ik} + 2\mu G_{ik} \quad \text{and} \quad G_{ik} = \frac{1}{2}(\frac{\partial u_i}{\partial X_k} + \frac{\partial u_k}{\partial X_i} + \frac{\partial u_n}{\partial X_i}\frac{\partial u_n}{\partial X_k}). \tag{2}$$

During the time of the current annual report we finished all necessary calculations, and we proceeded according to the following items:

1. The von Kármán system revisited
We have rederived the von Kármán system from a different point of view as it was considered in the year 2000. While we started at first from special kinematic assumptions in order to reduce the cubic anisotropic 3-d system of elasticity to the von Kármán system, the new derivation relies on some simple assumptions regarding the dependence of the displacement and stress components u_i and σ_{ij}, respectively, on the thickness h of the plate. In particular, we now conclude, relying on an asymptotic expansion for the displacement, that the main contributions

to the displacements are of the form

$$\begin{aligned} u_1 &= -\partial_X W(X,Y)\,Z + U(X,Y) + O(h^3), \\ u_2 &= -\partial_Y W(X,Y)\,Z + V(X,Y) + O(h^3), \\ u_3 &= W(X,Y) + O(h^2), \end{aligned} \tag{3}$$

while the second Piola-Kirchhoff stresses can be written as

$$\sigma_{\alpha\beta} = \sigma^P_{\alpha\beta} + O(h^3), \quad \sigma_{\alpha 3} = \sigma^P_{\alpha\beta} + O(h^4), \quad \sigma_{33} = \sigma^P_{33} + O(h^5). \tag{4}$$

2. The contact problem sphere/plate
The distribution of the load over the contact surface is given by

$$p(r,\varphi) = p_0 \sqrt{1 - (\frac{r}{R_k(\varphi)})^2}. \tag{5}$$

The anisotropic cubic symmetry is indicated by the function $R_k(\varphi)$, which gives the boundary of the contact area that induces the isotropic steel sphere on the upper surface of the anisotropic wafer plate.

3. The boundary conditions
It is crucial for the correct modeling of the actual technical problem that in particular the boundary conditions at the thrust ring are prescribed appropriately. A comparison of the maximal displacement according to the mathematical simulation with the experimental data has revealed that the material points of the plate that coincide initially with the inner circle of the thrust ring do not remain there, rather the plate may glide without friction. This fact leads to the phenomenon that the stress resultant tensor $n_{\alpha\beta}$ is continuous across the inner thrust line. Because the plate can additionally rotate freely here, the bending moment tensor $m_{\alpha\beta}$ is also continuous across the thrust line. From preliminary test calculations we know that there are only compressive forces along the thrust line, so that the 3-component of the displacement W vanishes here.
The outer boundary of the plate is free of stress:

$$n_{rr} = 0, \quad n_{r\varphi} = 0, \quad m_{rr} = 0, \quad \frac{\partial m_{rr}}{\partial X_r} + 2\frac{\partial m_{r\varphi}}{\partial X_\varphi} = 0. \tag{6}$$

4. The numerical simulation
The von Kármán system is numerically solved by a finite element method. The finite-element net consists of triangles that have 36 degrees of freedom. The 3- displacement W is given in each of the outer nodes of an element by a 6- parameter Hermitian ansatz which is C^1 continuous. Thus the value of the ansatz function and its two first derivatives can be described. The two other displacements U and V are given in each of the outer nodes of an element by a 3-parameter Hermitian ansatz which is C^0 continuous. Thus the value of the ansatz functions and their first derivatives can be described. Consequently, we obtain for each triangle an algebraic nonlinear coupled system for 36 unknowns with a symmetric Jacobian.

5. The Kirchhoff system
The accuracy of the used elements is tested by the Kirchhoff system, which results as the limiting case of the von Kármán system for very small bending. The elements used approximate

the analytic solution of the Kirchhoff system already up to five mantissae even for a very rough net.

6. The crucial test of accuracy

The FCM has compared the maximal displacement versus the external load according to the WIAS calculation of the von Kármán system with their own careful measurements. Figure 2 shows the perfect matching of the simulation with the experimental data. It is important to note that the WIAS result is in fact a prediction, and does not contain any fitting procedure. However, if the load is increased beyond 450 N, a difference between simulation and the experiment begins to grow. The range of applicability of the von Kármán system is reached, and further nonlinear contributions of the complete 3-d elasticity system must be incorporated.

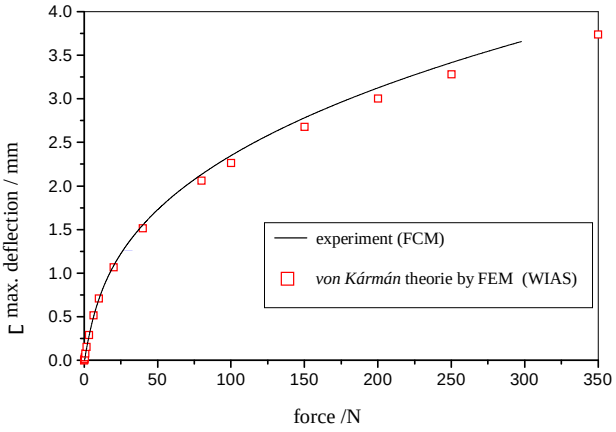

Fig. 2: Experiment versus prediction

7. The anisotropic behavior

The cubic symmetry of single crystal GaAs is reflected in Fig. 3, which shows the relevant stress components for three selected angles 0°, 22.5°, and 45°. We observe that the rr component of the stress deviates only weakly from the isotropic case. However, the shear component, i.e. $\sigma_{r\varphi}$, is nonzero, and depends considerably on the angle φ.

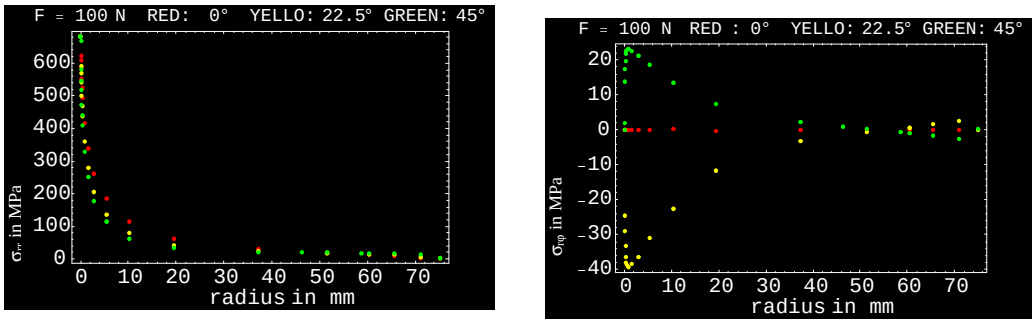

Fig. 3: Anisotropic behavior of stress components

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4.8 Projects interconnecting research groups

4.8.1 Projects

Envelope function approximation of electronic states in semiconductor nanostructures

Collaborators: U. Bandelow (FG 1), J. Fuhrmann (FG 3), H.-Chr. Kaiser (FG 1), Th. Koprucki (FG 3), G. Schmidt (FG 4)

Cooperation with: A. Arnold (Universität Münster), A. Jüngel (Universität Konstanz)

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

The role of semiconductor nanostructures will increase in the future due to the advent of quantum electronic devices which is assisted by the increasing sophistication of fabrication technology. To understand and to predict the physical properties of such devices, efficient and reliable computations of their electronic states is required.
The ab initio solution of the many-electron Schrödinger equations on the microscopic scale fails due to the immensity of the computational effort. To overcome this burden, it appears to be natural to utilize the presence of two scales inherent to the problem—the mesoscopic scale of the variation of the materials in the nanostructure and the microscopic scale of the atoms of each material.
The standard approach to this problem is the kp-method in combination with the *envelope function approximation*. Within the nanostructure, the wave function is represented in terms of *envelope functions*, which describe the slowly-varying mesoscopic part of the locally highly-oscillating microscopic wave functions. The envelope functions are eigenfunctions of matrix-valued $k \cdot p$ Schrödinger operators with *discontinuous* coefficients, whose spectral properties and applications have been investigated by us in previous projects. Usually kp-Schrödinger operators are constructed by a physically intuitive but heuristic transfer of the kp-theory for bulk materials to nanostructures. However, this approach to modeling has two main drawbacks: the ambiguity of boundary conditions across interfaces between two materials and the appearance of spurious modes for some materials.
A viable approach to a kp-theory for heterostructures was first given by Burt ([1]), who points out a way to derive equations for the envelope functions in terms of the microscopic potential. Following this approach, we obtain pseudodifferential equations for the envelope functions in real space or integral equations for Fourier-transformed envelope functions (cf. [2]). A certain limit of these equations leads to kp-Schrödinger operators of the same formal structure as the ones in the standard approach, but with microscopically derived boundary conditions. This leads to new tools for the computation of electronic states in nanostructures (cf. [2]).

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Modeling and simulation of blue-emitting semiconductor nanostructures

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

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

Although diode lasers have existed for more than 25 years, blue-emitting diodes have only recently been realizable. This closed the "gap" between devices emitting in the visible spectral range and gives rise to many applications with a big market potential. Such applications include active laser tv, increasing storage capacities on DVDs and very high-quality laser printers.
The technological breakthrough to the blue laser diodes came with the successful epitaxy of GaN-based nanostructures. Typically, these materials grow in crystallographic wurtzite configurations and display a large energy band gap, as well as other unusual features.

We have simulated such nanostructures using the eight-band kp-model for wurtzite semiconductors in WIAS-QW. This model is a generalization of [1] including strain, spin-orbit interaction, and crystal-field splitting. A primary result of such kp-calculations is the subband structure (dependence of the energy on the in-plane wave vector $k_{||} = (k_x, k_y)$), as depicted in Fig. 1.

As shown in Fig. 1, the subband structure exhibits some remarkable properties, which partially differ from those known from other laser materials:

- No warping (no angular dependence of the energy) is observed.
- The conduction subbands are nearly parabolic. This means low band mixing between conduction and valence bands, mainly due to the large band gap (see y-axes in Fig. 1).
- The valence subbands show a small curvature, indicating much higher hole masses than for other semiconductor laser materials. Also the in-plane heavy hole mass is high ($1.96 m_0$ for GaN).
- The valence subbands are nonparabolic, indicating the valence band mixing effects. Moreover, level crossings can be observed, see lower figure in Fig. 1.

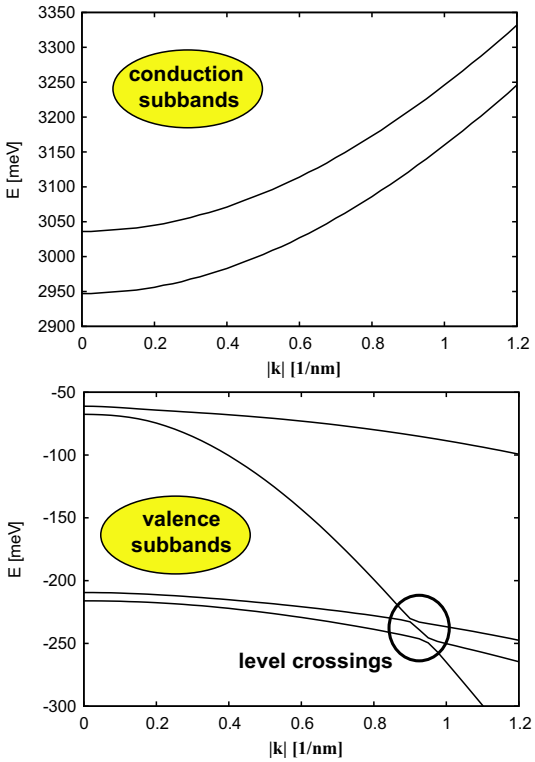

Fig. 1: Subband structure for a strained GaN/InGaN multi quantum well structure

Furthermore, eight-band kp-calculations allow for a realistic prediction of the matrix elements for the optical interband transitions ([3]), which are a prerequisite for the calculation of the optical response function for such nanostructures.

As a representation for the imaginary part of the optical response function, we have calculated the spectra of the optical material gain (TE-polarization has been assumed) for different sheet densities, as illustrated in Fig. 2. The gain increases monotonically with the carrier density, but much higher densities are required for the laser threshold, compared to other semiconductor materials. This is mainly due to the much higher effective masses in GaN-based materials, as discussed above, but in some part also due to the reduced interband mixing.

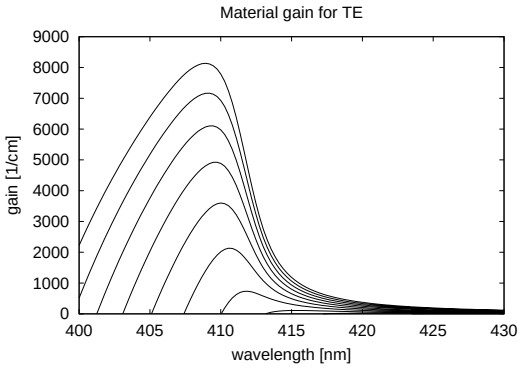

Fig. 2: Gain spectra of a GaN/InGaN MQW structure for different sheet densities $(1 \cdot 10^{12}/cm^2, \ldots, 10 \cdot 10^{12}/cm^2)$

Pure kp-calculations correspond to the exclusion of any Coulomb interaction between the carriers. Being charged fermions, their behavior can be drastically modified by such Coulomb effects. In particular, such impacts have been studied for GaN/InGaN quantum wells ([2]). For the calculation of some prominent Coulomb effects, we used a Kohn-Sham type model similar to [3], which has already been successfully applied to analyzing InP-based nanostructures. It includes the Hartree contribution via the Poisson equation and the bandgap shift via exchange-correlation potentials. As a result of such self-consistent calculations, the gain spectra experience a density-dependent red shift and a small enhancement, as observed by the difference between the curves in Fig. 3. In addition, the electrons become more strongly confined, whereas the holes stay untouched in the self-consistent case. This is in contrast to the situation of InP-based nanostructures ([3]) and can be explained by the large heavy hole mass.

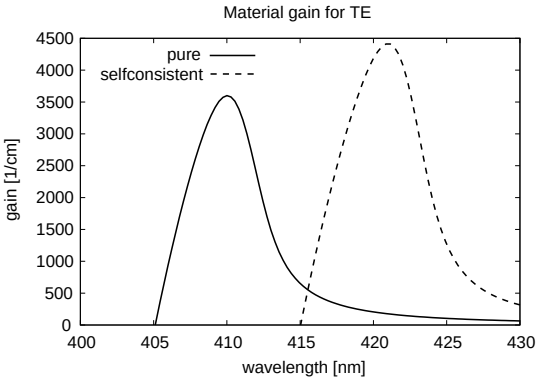

Fig. 3: Gain spectra for a sheet density of $6 \cdot 10^{12}/cm^2$. Solid: pure eight-band kp-calculation, dashed: as for left curve, but with self-consistent Hartree interaction and bandgap shift.

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Optoelectronical sensors

Collaborators: H. Gajewski (FG 1), R. Nürnberg (FG 1), G. Schmidt (FG 4)

Cooperation with: CiS Institut für Mikrosensorik gGmbH (Erfurt), Silicon Sensor International AG (Berlin), MPI-Halbleiterlabor (München)

Supported by: BMBF: "Optoelektronische Sensoren" (Optoelectronic sensors)

The project is concerned with the mathematical modeling and numerical simulation of optoelectronical semiconductor sensors for Microsystem Technology. Optical sensors and radiation detectors play a key role in robot engineering, materials science, X-ray microscopy, and many other areas of modern technology. In a variety of technical processes there is a need for sensors that are able to register external signals and process them for the control unit. Semiconductor structures are ideally suited for converting incoming information such as light, X-rays or particle radiation into an electrical signal. Their electrical properties change under the influence of radiation due to the generation of pairs of electrons and holes which are separated in the electrical field and are registered at the contacts as currents of electrons and holes, respectively. Semiconductor detectors have great advantages in terms of small dimensions, quantum efficiency, high signal amplification, and chip integrability.

A simultaneous mathematical modeling of light diffusion and absorption as well as charge generation and transport is needed for both the physical understanding and the optimization of optical semiconductor detectors. An adequate model are Maxwell equations for the optical processes and drift-diffusion and grid temperature equations for the electronical processes. These equations are coupled via optical, Avalanche, and thermal source terms.

The aim of the project is to extend and further develop the simulation program `WIAS-TeSCA` (Two- and three-dimensional Semi–Conductor Analysis package) with regard to new requirements in the development of these devices. This includes the analytical foundation, implementation, and testing of efficient solution algorithms for the coupled system of equations. The results will be evaluated with the help of real-life optical sensors, namely position sensors and Avalanche photodiodes, taken from the manufacturing line of our project partners.

In a first step the project was concerned with the integration of a module to calculate light diffusion in structured optical films. The interaction between light rays and charge transport is modeled with the generation rates in the corresponding partial differential equations. This optical charge generation is described with the ansatz

$$G_{opt}(x,y) = \frac{\lambda}{hc} \cdot \eta \cdot \alpha \cdot I(x,y)\,,$$

where λ represents the wave length of the incoming light, η is the quantum efficiency (number of generated electron-hole pairs per absorbed photon), α is the absorption constant, h is the Planck constant, c is the speed of light in a vacuum and I is the intensity of the electromagnetic field. On assuming a perpendicular rays direction, the light intensity can be approximated by $I(x,y) = \exp(-\alpha y) \cdot I(x,0)$, where y is the coordinate in the direction of the incoming light. In general, however, the light intensity also depends on the optical and geometric characteristics of the structure and on properties of the incoming light, such as spectral distribution, polarization, coherency, and contact angle. Since the wave length is comparable with the dimensions of relevant sensors, bending effects come into play. Hence geometrical optics approaches are no

longer sufficient, and the light intensity has to be obtained as a solution of the time-harmonic Maxwell equations.

Under the invariance assumptions valid here, depending on the light polarisation (TE or TM, resp.), these can be reduced to two-dimensional Helmholtz equations of the form

$$\Delta u + k_0^2 \varepsilon_{opt} u = 0 \quad , \quad k_0 = \frac{2\pi}{\lambda} I \,,$$

or

$$\nabla \cdot (\frac{1}{\varepsilon_{opt}} \nabla u) + k_0^2 u = 0, \qquad \text{respectively,}$$

where ε_{opt} denotes the complex-valued refractive index. The function u denotes the component of the electric (TE) or magnetic field (TM), respectively, which is perpendicular to the cross-section of the device. Additionally, the solution has to satisfy radiation conditions at infinity.

The optical equations have to be solved in an expanded two-dimensional domain. Due to the periodicity, the equations can be solved in a bounded periodic cell, capturing the details of the sensor structure, such as optical grids and micro lenses. The radiation conditions as well as the incoming light are modeled with the help of nonlocal boundary conditions.

To solve the Helmholtz equations we make use of the program DiPoG which was developed at WIAS to simulate and optimize periodic diffraction gratings. The program is based on the Finite-Element Method and the forward solver calculates the efficiency of gratings under conical incidence of plane electromagnetic waves. In order to integrate this module into the program `WIAS-TeSCA`, we implemented in particular an efficient method to model thick layers within the optical structure, different routines to postprocess the calculated field distributions and an effective exchange of the field and intensity distributions within the semiconductor structure.

We successfully performed test computations to simulate a position sensor for the project partner CiS Institut für Mikrosensorik gGmbH. In this case there are several optical layers on the CiS photodiode, two of which have a chrome strip and can be moved against each other. As the structure dimensions are within a few μm, the light diffusion in the optical grid is determined by diffraction effects. The computed entities are the characteristics of the photodiode, the photocurrent with fixed voltage depending on the lateral translations of the structured layers with respect to each other.

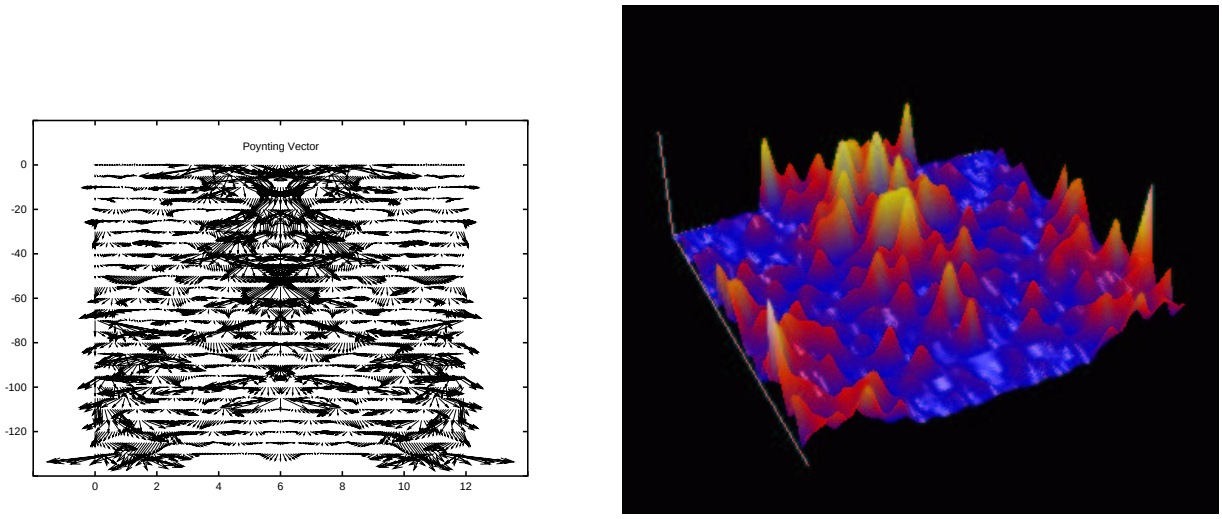

Fig. 1: Intensity distribution of the electromagnetic field and Poynting vector in the air film between the grid structures

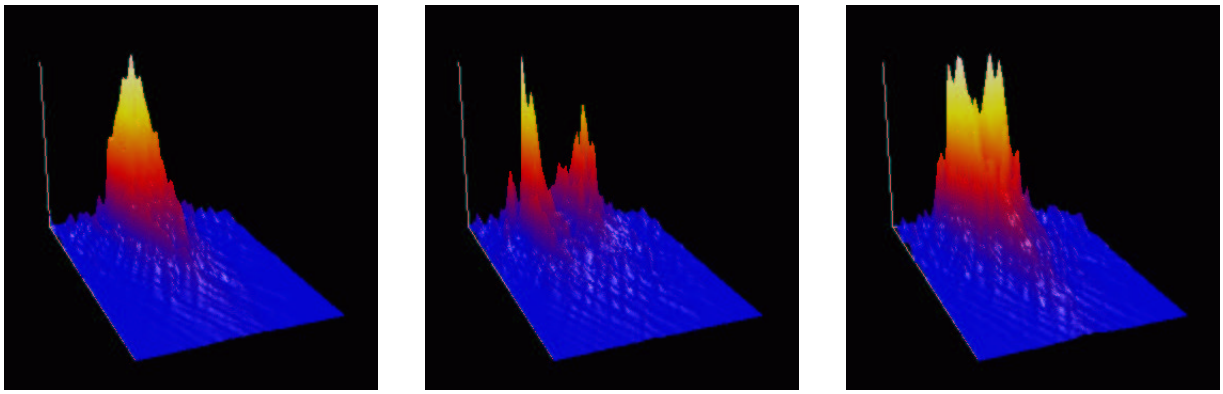

Fig. 2: Intensity distribution of the electromagnetic field within the photodiode for different relative positions of the strip structures

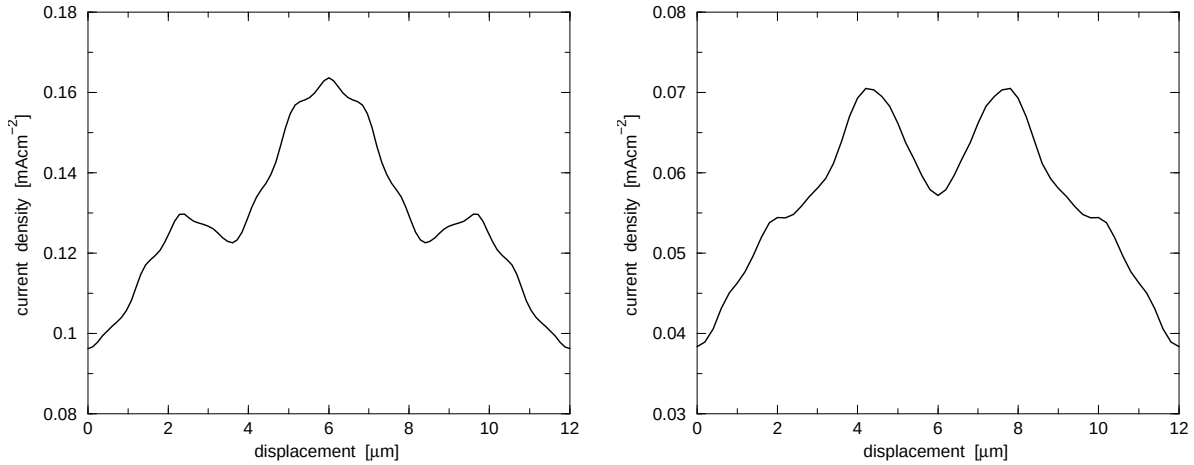

Fig. 3: Current-displacement characteristics of the position sensor for different strip and gap width

The simulations help to analyze the dependence of these characteristics on optical and geometric

parameters of the layer system, the properties of the incoming light, and the electrical features of the semiconductor structure.

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

Collaborators: O. Klein (FG 1), P. Philip (FG 1), J. Sprekels (FG 1), K. Wilmanski (FG 7)

Cooperation with: K. Böttcher, D. Schulz, D. Siche (Institut für Kristallzüchtung, Berlin)

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)

Owing to numerous technical applications in electronic and optoelectronic devices, such as lasers, semiconductors, and sensors, the industrial demand for high-quality SiC bulk single crystals remains large. It is still a challenging problem to grow sufficiently large SiC crystals with a low defect rate. Sublimation growth of SiC bulk single crystals via *physical vapor transport (PVT)*, also known as the *modified Lely method*, has been one of the most successful and most widely used growth techniques of recent years.
During PVT a graphite crucible (see Fig. 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 of some 3000 K. Inside the crucible, polycrystalline SiC source powder is evaporated, resulting in a gas mixture consisting of argon and molecules made up of silicon and carbon, Si, Si_2C, and SiC_2 being the predominant species. The SiC single crystal grows on an SiC single crystalline seed that is kept at a temperature below that of the SiC source. There is also a variant of PVT where tantalum is used as crucible material instead of graphite.

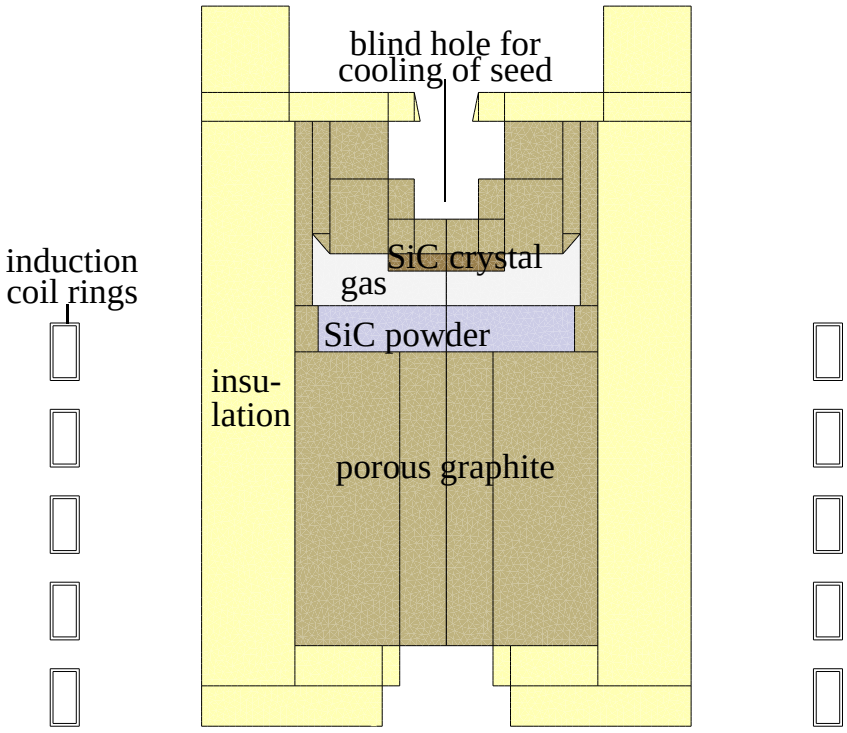

Fig. 1: Setup of growth apparatus according to [1]

Since reactor temperatures up to 3000 K make direct observations of the processes inside the growth chamber highly impractical, it is of paramount importance to have reliable theoretical models that allow the use of numerical simulation to improve the understanding of the growth procedure and to predict favorable growth conditions. Control parameters with respect to an optimization of the crystal growth are the design of the apparatus, the position of the induction coil, the heating power, and the inert gas pressure.

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 evaporating source powder.

The model of the gas mixture is based on continuous mixture theory and results in balance equations for mass, momentum, and energy, including reaction-diffusion equations. The energy balance in the gas mixture is coupled to the different energy balance equations in the various solid components of the growth apparatus via suitable interface conditions ([2]).

Due to the high temperatures, it is essential to include heat transfer by radiation between surfaces of cavities in the growth apparatus. In our model we account for the radiative heat transfer using the net radiation model. The semi-transparency of the single crystal is included via the band approximation model ([3, 4]).

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 the resulting current density and thus the heat sources to be calculated. Within the research of 2001 we refined our induction heating model to ensure the correct computation of the voltage distributions to the coil rings during axisymmetric and sinusoidal modeling ([5]).

Building on previous work, within the research year 2001 the model was used to create the prototypical numerical simulation software WIAS-*HiTNIHS* (see p. 238). In its current version the software constitutes an effective tool to simulate the evolution of the temperature inside the growth apparatus including heat sources caused by induction heating, heat transport by diffusion, radiation, and constant convection in good agreement with physical experiments. It can thus be used to test and optimize geometrical setups with respect to favorable growth conditions. See [6] for an account of parameter studies varying heating voltage and coil positions.

Figures 2 and 3 depict results of numerical simulations of the heating process for the configuration of Fig. 1.

On the left-hand side of Fig. 2 it can be seen that the evolution of the temperature in the center of the powder is quite different from T_{top} and T_{bottom}, i.e. from the temperatures that can be measured during the production process. The temperature $T_{\text{powdersurface}}$ is omitted in the left-hand figure, since in the depicted temperature scale it almost coincides with T_{seed}. The evolution of the difference between $T_{\text{powdersurface}}$ and T_{seed} is illustrated on the right-hand side of Fig. 2.

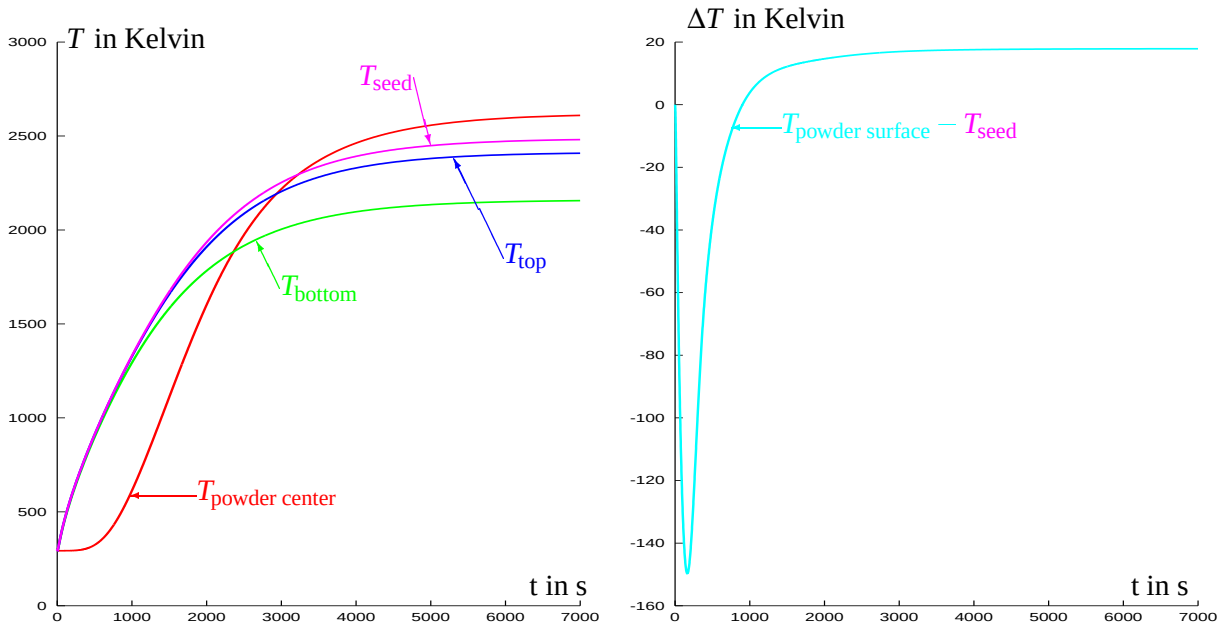

Fig. 2: Numerical results for the configuration of Fig. 1. Left-hand side: temperature evolution at the top and at the bottom (T_{top} and T_{bottom}), at the seed (T_{seed}), and in the center of the powder ($T_{\text{powdercenter}}$). Right-hand side: evolution of the temperature difference between powder surface and seed.

The computed temperature distribution and corresponding heat sources for the quasi-stationary state at the end of the heating process ($t = 30000$ s) are presented in Fig. 3. The temperature difference between neighboring isotherms in the left picture is 20 K. The minimal temperature T_{min} occurs at the outside of the insulation, whereas the maximal temperature T_{max} occurs inside the lower graphite body of the apparatus. In the right-hand picture the difference between isolevels is 0.1 kW/m^3, darker regions indicating larger heat sources. The depicted heat sources correspond to a total power $P_{\text{total}}^{[\text{apparatus}]} = 5.136$ kW. The maximal power density $\mu_{\text{max}}^{[\text{apparatus}]}$ occurs in the lower outside corner of the graphite.

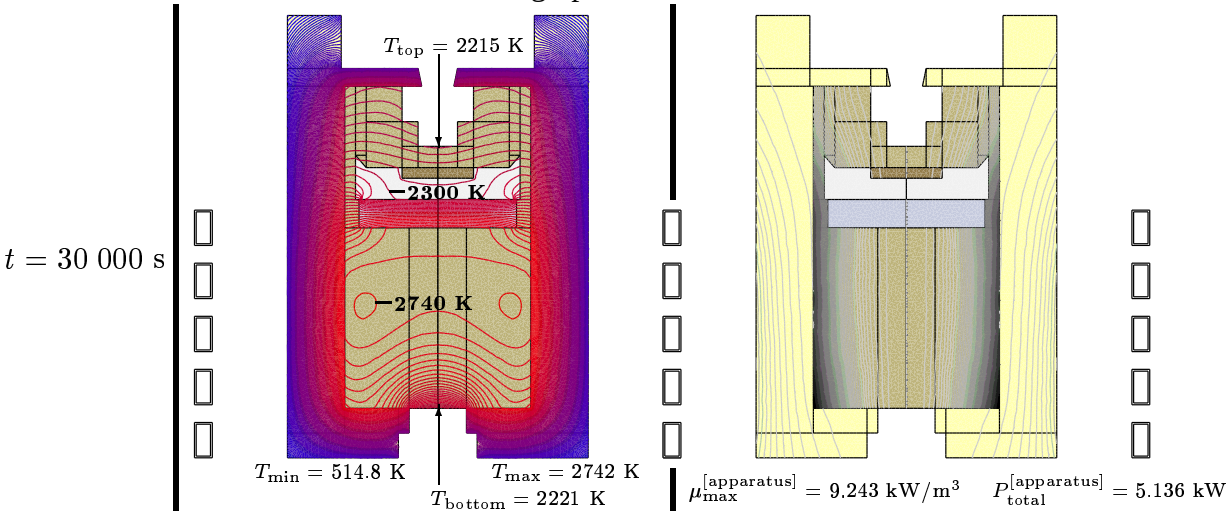

Fig. 3: Computed temperature distribution (left-hand side) and corresponding heat sources (right-hand side) at the end of the heating process for the configuration of Fig. 1

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Multiscale modeling of thermoelastic bodies

Collaborators: W. Dreyer (FG 7), M. Herrmann (FG 7), J. Sprekels (FG 1)

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

This is a joint project of Dreyer/Sprekels. In the last period two questions were posed and answered:

1. Is a continuum limit of a microscopic particle system automatically a macroscopic limit?
2. Is there a rigorous procedure so that the macroscopic limit of time means of microscopic observables can be written as means with macroscopic distribution functions?

Regarding the first question, we have shown that the answer is affirmative only for a special class of microscopic initial conditions, namely those that can be prepared macroscopically.
Regarding the second question, we have studied simple cases, where the microscopic observables only depend on time but not on the particle index. A well-known example is the oscillator motion of the atomic chain, which can be found in [1].
Let τ be the microscopic time. $f(r(\tau))$ denotes a microscopic observable that depends continuously on the microscopic variable $r(\tau)$ with $0 < r_- \le r(\tau) \le r_+$. The macroscopic time is defined by $t = \varepsilon\tau$, where ε is a small positive parameter, and the macroscopic limit can be established for $\varepsilon \to 0$. To this end we define

$$\overline{f}(\tau) \equiv \int_0^\infty \chi(\vartheta - \tau) f(r(\vartheta)) d\vartheta, \qquad \text{and} \qquad \overline{f}^\varepsilon(t) \equiv \overline{f}(\frac{t}{\varepsilon}), \qquad \overline{r}^\varepsilon(t) \equiv r(\frac{t}{\varepsilon}), \tag{1}$$

where $\chi(\tau)$ denotes a window function with a finite microscopic support. If $r(\tau)$ solves the Newtonian equation of the oscillator motion according to [1], then there holds

$$\lim_{\varepsilon\to 0} \overline{f}^\varepsilon(t) = \int_{r_-}^{r_+} f(r) w(r_-, r_+, r) dr, \tag{2}$$

where w is the distribution function of the oscillator motion, and r_-, r_+ are the statistical parameters, see [2] for details.
A second simple example serves to illustrate the suitable mathematics of the macroscopic limit. We consider the following Newtonian system that contains the small parameter ε :

$$\begin{aligned} \frac{d}{ds} Q(\tau) &= A\Big(Q(\tau)\Big) + \begin{pmatrix} 0 \\ f(\varepsilon\tau) \end{pmatrix}, \quad Q(0) = Q_0\,, \\ Q &= \begin{pmatrix} q \\ p \end{pmatrix}, \quad A(Q) = \begin{pmatrix} p \\ G(q) \end{pmatrix}. \end{aligned} \tag{3}$$

We interprete τ, q, p as microscopic time, position, and momentum, respectively, of a microscopic particle, and we assume that an external force f is given, which changes very slowly on the microscopic time scale. For simplicity, we consider the simplest case of a harmonic oscillator with $G = -q$.

The macroscopic time is defined by $t = \varepsilon\tau$, so that the force f varies only on the macroscopic scale, while the variable Q oscillates on the microscopic scale. Fig. 1 shows a typical example: There is a rapid oscillation for small ε from the macroscopic viewpoint.

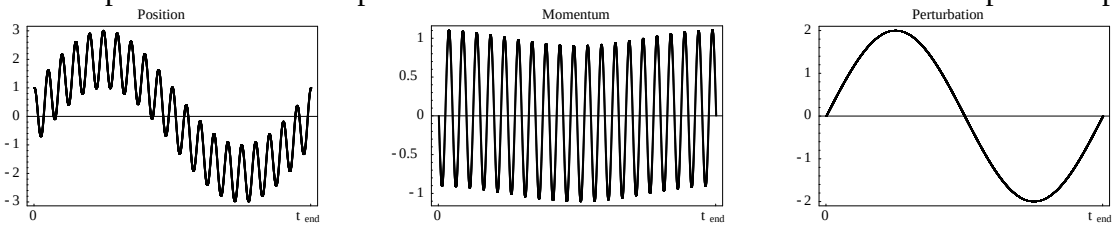

Fig. 1: Numerical example

For fixed ε and fixed macroscopic time t_{final} there exists, within the time interval $0 \le \tau \le \varepsilon^{-1} t_{final}$, a solution $Q_\varepsilon(\tau)$ of (3) that we rescale according to

$$\overline{Q}_\varepsilon(t) := Q_\varepsilon(\varepsilon^{-1}t), \quad 0 \le t \le t_{final}. \tag{4}$$

Next we consider various observables Ψ, which we define as continuous functions of Q and t. It is the objective to study the evolution of $\Psi(Q(t),t)$ on the macroscopic scale, i.e. we are interested in the function $\Psi_\varepsilon(\overline{Q}_\varepsilon(t),t)$ in the limit $\varepsilon \to 0$.
The most important observable is the energy e, which is given by

$$e(Q,t) = \frac{1}{2}p^2 + \frac{1}{2}q^2 - qf(t). \tag{5}$$

The rescaled energy is defined by $\overline{e}_\varepsilon(t) = e(\overline{Q}_\varepsilon(t),t)$ within $0 \le t \le t_{final}$. We expect that the microscopic and the macroscopic scale decouples in the limit $\varepsilon \to 0$ in a certain sense, and in fact this expectation can be described as follows:
The functions $\overline{Q}_\varepsilon$ and $\overline{e}_\varepsilon$ converge to Young measures μ and ν, respectively. Precisely we write $\mu = \mu(t,Q)$ and $\nu = \nu(t,e)$ although μ and ν are no functions but Young measures. The Young measures μ and ν are completely determined by the following properties

1. For almost every $0 \le t \le t_{final}$, the decomposition of μ at time t is a solution of the following time-dependent but stationary Liouville equation

$$\mathrm{div}_Q\left(\mu(t,Q)\cdot[A(Q) - \begin{pmatrix} 0 \\ f(t) \end{pmatrix}]\right) = 0. \tag{6}$$

2. Equation (6) implies that μ is completely determined by ν.

3. The Young measure ν is a solution to the following transport equation

$$\frac{\partial \nu}{\partial t}(t,e) - \dot{f}(t)f(t)\frac{\partial \nu}{\partial e}(t,e) = 0.$$

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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 wichtigste Funktion der Bibliothek besteht darin, das Institut mit der Literatur zu versorgen, die es zur Erledigung seiner Aufgaben braucht. Daneben ist die von der Bibliothek gesammelte Literatur auch den Gästen des Instituts zugänglich.
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. 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 main function of the library is to provide WIAS with the literature it requires to accomplish its work. The literature collected by the library is accessible to the guests of the institute, too.

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. 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.

Als Dienstleistung werden für die Mitarbeiter und Gäste des Instituts Bücher, Preprints usw. aus anderen Bibliotheken sowie einzelne Artikel aus am WIAS nicht gehaltenen Zeitschriften besorgt.
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. Die Mitgliedschaft in diesem Konsortium ist insbesondere eine Grundlage für den Zugriff auf elektronische Zeitschriften, wie er von mehreren Verlagen und Agenturen angeboten wird.

As a service for the WIAS collaborators and guests the library provides them with books, preprints etc. from other libraries, and single articles from journals not available in the WIAS library.
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. The membership in this consortium is especially a basis for the access to electronic journals as it is offered by several publishers and vendors.

Statistische Informationen über das Jahr 2001

Erwerbungen:
179 Bücher
288 gebundene Zeitschriftenbände
946 Preprints und Reports
52 Loseblattsammlungen

Aussonderungen:
313 Bücher

Entleihungen aus der WIAS-Bibliothek:
3151 Bücher

Aus anderen Bibliotheken beschaffte Literatur:
554 Bücher
628 Artikel

Statistical information about the year 2001

Acquisitions:
179 books
288 bound volumes of journals
946 preprints and reports
52 loose-leaf collections

Sorted out:
313 books

Lent from the WIAS library:
3151 books

Literature provided from other libraries:
554 books
628 articles

5.2 Fachinformation / Science Information

Die primäre Aufgabe der Fachinformation besteht darin, für die Forschungsgruppen des Instituts die erforderliche (Fach)-Informationsversorgung zu gewährleisten.
Dazu bietet die Fachinformation des WIAS unterschiedliche Recherchemöglichkeiten in bibliographischen Informations-Datenbanken und in Volltext-Datenbanken für alle Mitarbeiter des WIAS an:

- Im Vordergrund stehen die für die Mathematik wichtigsten Datenbanken „Zentralblatt MATH/Database“ und „MathSci“ (Mathematical Reviews).
- Zur Versorgung der anwenderprojektorientierten Forschung werden auch Zugangsmöglichkeiten zu natur- und ingenieurwissenschaftlichen Online-Datenbanken vorgehalten.
- 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.

The main concern of the Science Information (SI) is to reliably provide the scientific information required by the research groups. For this purpose, 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 to provide information for application-oriented research,
- 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).

Die Nutzungsmöglichkeiten sind aufgabenorientiert variabel gestaltet, z. B. ist die

The facilities for data retrieval are flexibly realized, depending on the respective tasks.

- 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 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 nicht-mathematischen Datenbanken aus Kostengründen 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) is expensive and requires a professional approach. Therefore, this service can be realized only via SI.

Außer dem Datenbank-Retrieval gab es die folgenden Aktivitäten seitens 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 on the WIAS server http://www.wias-berlin.de/publications/. The abstracts of these publications are indexed meta-linguistically 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 Nutzung des Science Citation Index mittels webbasierter institutsoffener Recherche WoS (Web of Science) von ISI/Thomsson Scientific ist realisiert.

- Implementation of the Web-based data-recall facility WoS (Web of Science) of ISI/Thomsson Scientific to facilitate the usage of the Sciences Citation.

- 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).

- Der Fachinformationsbeauftragte des WIAS arbeitet in der IuK-Kommission der Wissenschaftlichen Fachgesellschaften mit.

- The SI representative of WIAS is a member of the “IuK-Kommission” (commission for information and communication) of the scientific societies of Germany.

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).
Neben dem Einsatz immer leistungsfähigerer Workstations und PCs bestimmten folgende Projekte die Entwicklung der Rechentechnik des WIAS im Jahr 2001:

1. Corporate Network, GWIN

   Mit anderen Instituten des Forschungsverbundes Berlin e. V. wurde das Corporate Network aufgebaut. Kern ist eine 622 Mbit ATM-Verbindung der Standorte Berlin-Mitte und Berlin-Adlershof. Dadurch wurde es möglich, alle Institute des Forschungsverbundes über einen GWIN-Anschluss an das Internet mit einer Geschwindigkeit von 155 Mbit anzuschließen.

   Mit den Arbeiten zur Nutzung des Corporate Networks für ein gemeinsames Datensicherungskonzept wurde begonnen.

2. LAN

   In einigen Etagen wurden ältere Access-Switches durch neuere Geräte ersetzt.

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).
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 2001:

1. Corporate Network, GWIN

   Together with other institutes of Forschungsverbund Berlin e.V., the Corporate Network has been constructed. Its core is a 622 Mbit ATM connection between the sites Berlin center and Berlin Adlershof, thus making it possible to connect all institutes of the Forschungsverbund at a 155 Mbit rate to the internet via a GWIN connection.

   Work has been started to use the Corporate Network for a common data protection plan.

2. LAN

   On some of the floors, older access switches have been replaced by new ones.

Dadurch können nun alle Arbeitsplätze mit Fast-Ethernet-Anschlüssen versorgt werden.

3. Grafikserver

   Es wurde eine SGI Octane 2 mit zwei Prozessoren und Vpro 12 Grafik als Grafikserver in Betrieb genommen.

4. Vortragsraum

   Der Vortragsraum des WIAS wurde mit moderner Projektionstechnik ausgestattet.

5. SUNRays

   Die im Jahre 2000 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 dreißig alte CRT-Farbmonitore durch TFT-Flachbildschirme ersetzt. Dadurch konnte die Qualität vieler Arbeitsplätze wesentlich verbessert werden.

7. Farbdrucker

   Für den allgemeinen Gebrauch wurde ein neuer Farblaserdrucker beschafft und installiert. Dabei handelt es sich um einen Lexmark C720, der sich sehr bewährt hat.

Thus, all work-places were now provided with Fast Ethernet connections.

3. Graphics server

   An SGI Octane 2 with two processors and Vpro 12 graphics has been put into service as a graphics server.

4. Lecture room

   The lecture room of WIAS has been equipped with modern projective technique.

5. SUNRays

   The Thin Clients SUNRay1s purchased in 2000 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

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

7. Color printer

   For common use, a new color laser printer has been purchased and installed, a Lexmark C720 which has clearly proved its worth.

6 Publications, Scientific Life

6.1 Publications

6.1.1 Monographs

A. BOVIER, *Statistical Mechanics of Disordered Systems*, vol. 10 of MaPhySto Lecture Notes, Univ. of Aarhus, Aarhus, 2001, 192 p.

J. ELSCHNER, I. GOHBERG, B. SILBERMANN, eds., *Problems and Methods in Mathematical Physics, The Siegfried Prössdorf Memorial Volume*, vol. 121 of Oper. Theory Adv. Appl., Birkhäuser, Basel, 2001, viii+523 p.

K. HOFFMANN, R. HOPPE, V. SCHULZ, eds., *Fast Solution of Discretized Optimization Problems*, vol. 138 of Internat. Ser. Numer. Math., Birkhäuser, Basel, 2001, 292 p.

L. SHILNIKOV, A. SHILNIKOV, D. TURAEV, L. CHUA, *Methods of Qualitative Theory in Nonlinear Dynamics. Part II*, vol. 5 of World Sci. Ser. Nonlinear Sciences A, World Scientific, Singapore, 2001, 587 p.

6.1.2 Articles in Refereed Journals

B. ALBERS, *Dependence of adsorption/diffusion processes in porous media on bulk and surface permeabilities*, Arch. Mech., 53 (2001), pp. 303–320.

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E. BÄNSCH, *Finite element discretization of the Navier-Stokes equations with a free capillary surface*, Numer. Math., 88 (2001), pp. 203–235.

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J. BORCHARDT, *Newton-type decomposition methods in large-scale dynamic process simulation*, Comput. Chem. Engng., 25 (2001), pp. 951–961.

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W. DREYER, W.H. MÜLLER, *Modeling diffusional coarsening in eutectic tin/lead solders: A quantitative approach,* Internat. J. Solids Structures, 38 (2001), pp. 1433–1458.

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[697] Wolfgang Wagner: Stochastic, analytic and numerical aspects of coagulation processes.

[698] Jürgen Sprekels, Songmu Zheng: Global existence and asymptotic behaviour for a nonlocal phase-field model for non-isothermal phase transitions.

[699] Messoud Efendiev, Georg Hebermehl, Rupert Lasser: Generalized necessary scaling condition and stability of chemical reactors with several educts.

[700] Paolo Dai Pra, Pierre-Yves Louis, Sylvie Rœlly: Stationary measures and phase transition for a class of Probabilistic Cellular Automata.

[701] Gennadi A. Leonov: The time-varying stabilization of linear discrete control systems.

[702] Pavel Krejčí, Jürgen Sprekels, Ulisse Stefanelli: One-dimensional thermo-visco-plastic processes with hysteresis and phase transitions.

[703] Klaus Zacharias: A special reaction-diffusion system — The pseudo-steady-state case.

[704] Karl K. Sabelfeld, Irina Shalimova: Random walk on spheres methods for iterative solution of elasticity problems.

[705] Christian Engelhardt, Orazgeldi Kurbanmuradov, Karl K. Sabelfeld, Alexander Sukhodolov: Numerical study of the statistical characteristics of the mixing processes in rivers.

[706] Klaus Fleischmann, Jie Xiong: Mass-time-space scaling of a super-Brownian catalyst reactant pair.

[707] Bettina Albers, Krzysztof Wilmański: Relaxation properties of a 1D flow through a porous material without and with adsorption.

[708] Pascal Azerad, Eberhard Bänsch: Quasi-stability of the primary flow in a cone and plate viscometer.

[709] Wolfgang Dreyer, Michael Herrmann, Matthias Kunik: Kinetic solutions of the Boltzmann-Peierls-Equation and its moment systems.

6.2.2 WIAS Reports Series

Reports 2001[2]

[20] Jan Sieber: Longitudinal dynamics of semiconductor lasers.

6.2.3 WIAS Technical Reports Series

E. BÄNSCH, D. DAVIS, *An Operator-Splitting Finite-Element Approach to an 8:1 Thermal Cavity Problem*, Tech. Rep. no. 1, WIAS, 2001.

[2] http://www.wias-berlin.de/publications/index.pl?reports:2001

6.2.4 Preprints/Reports in other Institutions

E. BONETTI, P. COLLI, W. DREYER, G. GILARDI, G. SCHIMPERNA, J. SPREKELS, *On a model for phase separation in binary alloys driven by mechanical effects*, Preprint no. 1213, Università di Pavia, Istituto di Analisi Numerica del Consiglio Nazionale delle Ricerce, Italy, 2001.

O. SCHENK, K. GÄRTNER, *Sparse factorization with two-level scheduling in PARDISO*, Tech. Rep. no. 6, Swiss Federal Institute of Technology in Zurich, 2001.

S. JASCHKE, *The Cornish-Fischer expansion in the context of delta-gamma-normal approximations*, Disc. Paper no. 54, Humboldt-Universität zu Berlin, Sonderforschungsbereich 373, Berlin, 2001.

——, *Quantile-VaR is the wrong measure to quantify market risk for regulatory purposes*, Disc. Paper no. 55, Humboldt-Universität zu Berlin, Sonderforschungsbereich 373, Berlin, 2001.

O. KLEIN, C. VERDI, *A posteriori error estimates for a time discrete scheme for a phase-field system of Penrose-Fife type*, Preprint no. 29, Università degli Studi di Milano, Dipartimento di Matematica "Federigo Enriques", Italy, 2001.

W. WEISS, *A posteriori error estimates*, Preprint no. 105, Russian Academy of Sciences, Novosibirsk, Russia, 2001.

6.3 Membership in Editorial Boards

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, USA.

P. MATHÉ, Editorial Board, Monte Carlo Methods and Applications, VSP, Zeist, The Netherlands.

J. POLZEHL, Associate Editor, 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.

J. SPREKELS, Editorial Board, 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

Talks

B. ALBERS, *Über Stabilität von Strömungen in Böden*, Thermodynamisches Seminar, WIAS, Berlin, February 7.

——, *Linear stability analysis of some flow processes in soils*, Workshop on Methods of Applied Mathematics and Mechanics in an Environmental, Geophysical and Climatological Context, Conference on the Occasion of the 60th birthday of Prof. Kolumban Hutter, Seeheim-Jugenheim, March 20.

——, *Mass exchange and diffusion in porous materials*, Conference on Differential Equations and Related Topics, dedicated to the Centenary Anniversary of Ivan G. Petrovskii, Moscow, Russia, May 26.

——, *Linear stability analysis of adsorption/diffusion processes in porous materials*, XIth International Conference on Waves and Stability in Continuous Media (WASCOM), Porto Ercole, Italy, June 8.

——, *Modellierung von Erdrutschvorgängen*, Thermodynamisches Seminar, WIAS, Berlin, July 18.

——, *Continuum mechanics and thermodynamics*, exercises for a course for PhD students, 6 talks, Politecnico di Torino, Dipartimento di Ingegneria Strutturale e Geotecnica, Torino, Italy, April 23–27.

G. ALBINUS, *Bemerkungen zur Boxmethode bei gemischten Randwertproblemen für elliptische Gleichungen 2. Ordnung mit unstetigen Koeffizienten*, Seminar "Funktionalanalytische Methoden" (Langenbach-Seminar), WIAS, Berlin, May 2.

U. BANDELOW, *Erzeugung kurzer Pulse mit modegelockten Lasern*, Seminar "Halbleiterlaser", WIAS, July 19.

U. BANDELOW, H.-CHR. KAISER, *Simulation of multi quantum well lasers with* `WIAS-TeSCA`, First SIAM-EMS Conference "Applied Mathematics in our Changing World", Berlin, September 5.

E. BÄNSCH, *Finite element discretization for "nonstandard" boundary conditions for the Navier-Stokes equations*, University of Maryland, College Park, USA, January 25.

——, *Finite-Elemente-Verfahren bei der FZ-Kristallzüchtung*, DGKK Workshop "Angewandte Simulation in der Kristallzüchtung", Deutsche Gesellschaft für Kristallwachstum und Kristallzüchtung e. V., Aufseß, February 15.

——, *Freie Randwertprobleme für die Navier-Stokes-Gleichungen*, Technische Universität Dresden, February 16.

——, *An adaptive Uzawa FEM for Stokes: Convergence without the Inf-Sup*, Rheinisch-Westfälische Technische Universität Aachen, July 4.

——, *An adaptive Uzawa FEM for Stokes: Convergence without the Inf-Sup*, Universität Bremen, Zentrum für Technomathematik, November 1.

M. BARO, *Dilatation und Eigenfunktionen von eindimensionalen dissipativen Schrödinger-Operatoren*, Mathematisch-Physikalisches Kolloquium, Technische Universität Clausthal, November 21.

——, *Über das stetige Spektrum verallgemeinerter Schrödinger-Operatoren*, Seminar "Funktionalanalytische Methoden" (Langenbach-Seminar), WIAS, Berlin, December 12.

J. BORCHARDT, *Newton-type decomposition methods in parallel process simulation*, ICheaP-5, the 5th Italian Conference on Chemical and Process Engineering, Florence, Italy, May 21.

A. BOVIER, *Statistical mechanics of disordered systems*, Concentrated Advanced Course of 10 talks, MaPhySto Program, University of Copenhagen, Denmark, April 23–27.

——, *Aging in the random energy model*, Meeting "Phase Transitions", Mathematisches Forschungsinstitut Oberwolfach, May 2.

——, *Aging in the random energy model*, Universität Göttingen, May 5.

——, *Random Gibbs measures and the metastate formalism for disordered systems*, Workshop "Spin Glasses", Eindhoven, The Netherlands, May 16.

——, *Aging in the random energy model*, Università di Bologna, Italy, June 25.

——, *Glauber dynamics of the Ising model*, Università di Roma 2 "Tor Vergata", Italy, June 26.

——, *Aging in the random energy model*, Università de L'Aquila, Italy, June 28.

——, *Aging in the random energy model. I*, Miniworkshop "Aging and Glassy Systems", Mathematisches Forschungsinstitut Oberwolfach, August 21.

——, *Aging in the random energy model. III*, Miniworkshop "Aging and Glassy Systems", Mathematisches Forschungsinstitut Oberwolfach, August 23.

——, *Random walks on sequence space*, Workshop "Stochastic Genetic Processes", Greifswald, October 4.

——, *Le modèle de Hopfield: des reseaux de neurones aux verres de spins*, Journée commune des troisièmes Cycles de la Suisse Romande en Mathématiques et Statistique, Lausanne, Switzerland, November 30.

G. BRUCKNER, *On the inverse problem of diffractive optics. Reconstruction of 2-d gratings*, University of Kyoto, Japan, April 23.

——, *On the inverse problem of diffractive optics. Reconstruction of 2-d gratings*, University of Tokyo, Japan, April 27.

——, *Reconstruction of a perfectly conducting grating profile*, 3rd International ISAAC Congress, Freie Universität Berlin, August 29.

——, *On the reconstruction of a perfectly reflecting periodic grating profile*, WIAS Workshop "Inverse Problems in Applications", Berlin, September 10.

D. DAVIS, *Computational predictability of natural convection flows in enclosures*, First M.I.T. Conference on Computational Fluid and Solid Mechanics, Cambridge, Massachusetts, USA, June 15.

W. DREYER, *Keimbildung in der Phasenfeldtheorie*, Colloquium "Keimbildungsmechanismen", Freiberg, March 7.

——, *Industrial needs versus capabilities of phase field models*, Meeting "Phase Transitions", Mathematisches Forschungsinstitut Oberwolfach, May 5.

——, *Atomistische Motivationen von Phasenfeldgleichungen und die Rolle des Gibbs-Thomson-Gesetzes*, Thermodynamisches Seminar, WIAS, Berlin, June 20.

——, *Phasenübergänge in binären Legierungen und ihre thermomechanische Beschreibung innerhalb von Phasenfeldtheorien*, Technische Universität Dresden, June 21.

——, *The continuum limit and micro-macro transitions of microscopic systems*, Colloquium of the DFG Priority Program "Analysis, Modeling and Simulation of Multiscale Problems", Bonn, July 2.

——, *Phase transition in binary alloys*, International Conference on Continuum Mechanics & Thermodynamics, Potsdam, August 2.

——, *Towards rigorous micro-macro transitions*, WIAS Workshop on Multiscale Problems and Phase Transitions, Berlin, August 29.

——, *Atomistic motivations and a numerical study of a nonlocal model for phase separation*, WIAS Workshop on Multiscale Problems and Phase Transitions, Berlin, August 30.

——, *An atomistic study of extended Cahn/Hilliard systems*, First SIAM-EMS Conference "Applied Mathematics in our Changing World", Berlin, September 6.

——, *Metastabilität*, Workshop "Komposite Forschung in der Mechanik", Paderborn, December 4.

F. DUDERSTADT, *Kirchhoff versus Karman-Plattentheorie*, Thermodynamisches Seminar, WIAS, Berlin, July 5.

A. EIBECK, *Stochastic particle approximation of the coagulation equation and gelation phenomena*, Workshop "Methodes Particulaires de Simulation Numérique", Bourget-du-Lac, France, May 18.

——, *Stochastic algorithms for the coagulation equation*, Miniworkshop "Stochastic Models for Coagulation Processes", Mathematisches Forschungsinstitut Oberwolfach, August 24.

J. ELSCHNER, *Inverse scattering for periodic structures*, GAMM Workshop "Computational Electromagnetics", Kiel, January 27.

——, *Direkte und inverse Probleme der diffraktiven Optik*, BMBF Workshop "Moderne numerische Methoden zur Lösung der Helmholtzgleichung", Stuttgart, March 3.

——, *From Fredholm operators and stability of projection methods to inverse diffraction problems*, International Conference on Toeplitz Matrices, Pobershau, April 11.

——, *Inverse problems for scattering by periodic structures*, 3rd International ISAAC Congress, Freie Universität Berlin, August 24.

——, *Inverse problems for diffraction gratings*, University of Kyoto, Japan, November 22.

——, *On profile reconstruction for diffraction gratings*, University of Tokyo, Japan, November 26.

V. ESSAOULOVA, *Large deviations of L_1-error of kernel and histogram density estimators*, Centre International de Rencontres Mathématiques, Marseille, France, December 14.

K. FLEISCHMANN, *Cyclically catalytic super-Brownian motion*, Workshop "Stochastic Analysis: Geometric Aspects and Applications", Eindhoven, The Netherlands, January 9.

——, *Clumping of a super-Brownian reactant with a stable catalyst*, Workshop "Discrete and Continuous Stochastic Evolutions", Warwick, UK, March 20.

——, *A cyclically catalytic super-Brownian motion*, Technion Israel Institute of Technology, Haifa, April 24.

——, *Strong clumping of a super-Brownian reactant with a stable catalyst*, University of Knoxville, USA, October 30.

J. FUHRMANN, *Numerical simulation of coupled heat and mass transport in the North-East-German basin*, Sixth SIAM Conference on Mathematical and Computational Issues in the Geosciences, Boulder, Colorado, USA, June 11.

——, *Numerische Modellierung von Direktmethanolbrennstoffzellen*, Albert-Ludwigs-Universität Freiburg, Institut für Angewandte Mathematik, July 19.

——, *Numerical modelling of direct methanol fuel-cells*, MCEB 2001, Workshop on Modelling and Computation in Chemical Engineering and Biotechnology, Hohenwart, October 2.

——, *The FZ-Jülich-WIAS DMFC model: Species transport*, WIAS Workshop "Open Problems of Direct Methanol Fuel Cells (DMFC)", Berlin, November 23.

H. GAJEWSKI, *Über ein nichtlokales Phasenseparationsmodell*, Seminar "Funktionalanalytische Methoden" (Langenbach-Seminar), WIAS, Berlin, April 11.

——, *On a nonlocal model of phase separation*, WIAS Workshop "Multiscale Problems and Phase Transitions", Berlin, August 30.

——, *On a nonlocal model of phase separation*, First SIAM-EMS Conference "Applied Mathematics in our Changing World", Berlin, September 5.

——, *On parabolic equations with nonlocal drift term*, Conference on the occasion of an Honorary Doctorate for M.I. Vishik, Freie Universität Berlin, December 18.

K. GÄRTNER, *Sparse factorization with two-level scheduling in PARDISO*, University of California, Berkeley, USA, March 8.

——, *The FZ-Jülich-WIAS DMFC model: Reaction kinetics and energy transport*, WIAS Workshop on Open Problems of Direct Methanol Fuel Cells (DMFC), Berlin, November 23.

B. GENTZ, *Stochastic resonance in a double-well potential*, Meeting "Stochastics in the Sciences", Mathematisches Forschungsinstitut Oberwolfach, March 15.

——, *Stochastic resonance in a double-well potential*, Workshop "Stochastic Models from Statistical Physics", Blaubeuren, April 2.

——, *Singularly perturbed dynamical systems with additive noise*, Meeting on Stochastic Analysis, Berlin, July 2.

——, *Slowly time-dependent dynamical systems with additive noise: Synchronization, delay and hysteresis*, Second Workshop on Stochastic Climate Models, Chorin, July 9.

A. GLITZKY, *Neue Ergebnisse zur Analysis von Elektro-Reaktions-Diffusionsgleichungen (I)*, Seminar "Funktionalanalytische Methoden" (Langenbach-Seminar), WIAS, Berlin, May 16.

——, *Neue Ergebnisse zur Analysis von Elektro-Reaktions-Diffusionsgleichungen (II)*, Seminar "Funktionalanalytische Methoden" (Langenbach-Seminar), WIAS, Berlin, May 23.

F. GRUND, *Chemical process simulation on parallel computers*, 2001 SIAM Annual Meeting, San Diego, California, USA, July 13.

——, *Pivot strategies for direct linear solvers with sparse matrices*, 15th Congress, 2001 DMV Annual Meeting, Universität Wien, Austria, September 21.

——, *Solution of linear systems with sparse matrices*, Workshop "Modellierung, Simulation und Optimierung integrierter Schaltkreise", Mathematisches Forschungsinstitut Oberwolfach, November 29.

R. GUCKEL, *Über ein freies Randwertproblem in der Elektrostatik*, Seminar "Funktionalanalytische Methoden" (Langenbach-Seminar), WIAS, Berlin, April 18.

G. HEBERMEHL, *On the computation of eigen modes for open waveguide structures using artificial boundary conditions*, 2001 SIAM Annual Meeting, San Diego, California, USA, July 10.

——, *Perfectly Matched Layers in microwave transmission lines*, ENUMATH 2001, European Conference on Numerical Mathematics and Advanced Applications, Ischia Porto, Italy, July 27.

——, *Simulation of microwave and optoelectronic devices*, First SIAM-EMS Conference "Applied Mathematics in our Changing World", Berlin, September 4.

R. HENRION, *Optimierungsprobleme mit stochastischen Parametern*, Universität Dortmund, April 19.

——, *Subdifferentielle Charakterisierung der „calmness"-Eigenschaft mengenwertiger Abbildungen*, Universität Halle-Wittenberg, May 22.

——, *Stabilität in nichtlinearen Optimierungsproblemen*, Universität Erlangen-Nürnberg, July 5.

——, *Chance constrained programs: Theory and solution methods*, 9th International Conference on Stochastic Programming, Humboldt-Universität zu Berlin, August 25.

——, *Structure and stability of probabilistic storage level constraints*, 9th International Conference on Stochastic Programming, Humboldt-Universität zu Berlin, August 27.

——, *Steuerung eines kontinuierlichen Destillationsprozesses mit stochastischer Zuflussrate*, Final Colloquium of the DFG Priority Program "Real-time Optimization of Large Systems", Berlin, September 14.

——, *Einführung in Methoden der Stochastischen Optimierung*, DECHEMA continuation course "Optimierung verfahrenstechnischer Prozesse", 3 talks, Technische Universität Berlin, September 26.

——, *Optimierungsprobleme mit Wahrscheinlichkeitsrestriktionen und Bedingungen für Fehlerschranken*, Universität Hamburg, November 27.

M. HERRMANN, *Lösungen von kinetischen Gleichungen mit Relaxationszeiten*, Thermodynamisches Seminar, WIAS, Berlin, January 10.

D. HÖMBERG, *Ein mathematisches Modell für das Widerstandsimpulsschweißen*, Universität Bremen, May 7.

——, *Induction hardening – modeling, analysis and optimal design*, Auburn University, Alabama, USA, July 6.

——, *A mathematical model for capacitor resistance welding*, 2001 SIAM Annual Meeting, San Diego, USA, July 9.

——, *Optimal shape design of inductor coils*, Fifth SIAM Conference on Control and its Applications, San Diego, California, USA, July 14.

——, *Modeling and optimal control of the surface hardening of steel*, 4 talks, International School on Industrial Mathematics, Siena, Italy, July 23–28.

R. HÜNLICH, *Reaction-diffusion equations for electrically charged species*, Eötvös Loránd University, Budapest, Hungary, February 26.

——, *Simulation of semiconductor devices with* `WIAS-TeSCA`, Eötvös Loránd University, Budapest, Hungary, February 28.

S. JASCHKE, *Risk measures*, Seminar "Numerik stochastischer Modelle", Humboldt-Universität zu Berlin, June 18.

——, *Über die Approximation von Value at Risk durch Fourier-Inversion*, Humboldt-Universität zu Berlin, November 15.

H.-CHR. KAISER, *About Kohn-Sham systems arising from nanoelectronics*, Workshop "Wavelets and Electronical Structure Calculation", Technische Universität Chemnitz, January 26.

——, *Macroscopic current induced boundary conditions for Schroedinger-type operators*, 3rd International ISAAC Congress, Freie Universität Berlin, August 24.

——, *On an open quantum system driven by a macroscopic flow*, Workshop "Multiscale Problems in Quantum Mechanics and Averaging Techniques", DFG Priority Program "Analysis, Modeling and Simulation of Multiscale Problems", Universität Konstanz, October 26.

O. KLEIN, *Modellierung von Unterkühlung mit Phasenfeldsystemen und Stefanproblemen*, Seminar "Funktionalanalytische Methoden" (Langenbach-Seminar), WIAS, Berlin, May 9.

——, *Modeling and numerical simulation of induction heating of crucibles for sublimation growth of SiC*, International Conference on Continuum Mechanics & Thermodynamics (ISIMM), Potsdam, July 31.

——, *Anisotropic phase-field systems of Penrose-Fife type with general heat flux laws*, WIAS Workshop on Multiscale Problems and Phase Transitions, Berlin, August 31.

TH. KOPRUCKI, *Exact ground states for one-dimensional quantum many-body systems*, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, March 8.

——, *Exact ground states for one-dimensional quantum many-body systems*, Seminar "Funktionalanalytische Methoden" (Langenbach-Seminar), WIAS, Berlin, April 25.

——, *On eigenvalue problems arising from the modeling of semiconductor nanostructures*, 22. Norddeutsches Kolloquium "Angewandte Analysis und Numerische Mathematik", Christian-Albrechts-Universität Kiel, May 18.

——, *Envelope function approximation for electronic states in semiconductor nanostructures*, 2nd Colloquium of the DFG Priority Program "Analysis, Modeling and Simulation of Multiscale Problems", Andreas Hermes Akademie Bonn-Röttgen, July 4.

——, *On eigenvalue problems arising from the modeling of semiconductor nanostructures*, First SIAM-EMS Conference "Applied Mathematics in our Changing World", Berlin, September 4.

——, *Envelope function approximation for electronic states in semiconductor nanostructures*, Workshop "Multiscale Problems in Quantum Mechanics and Averaging Techniques", DFG Priority Program "Analysis, Modeling and Simulation of Multiscale Problems", Universität Konstanz, October 25.

——, *What can Wigner formalism based modelling learn from kp-Schrödinger equations?*, Workshop "Numerical and Asymptotic Methods for Kinetic Equations", Universität des Saarlandes, Saarbrücken, November 29.

C. KÜLSKE, *Gibbs or non-Gibbs: Joint measures of disordered spin systems*, Workshop "Stochastic Models from Statistical Physics ", Blaubeuren, April 6.

——, *Gibbs-Maße von ungeordneten Spin-Systemen*, Technische Universität Berlin, October 24.

——, *Selfaveraging of random diffraction measures*, EURANDOM, Eindhoven, The Netherlands, October 30.

——, *Ungeordnete Gitterspin-Modelle: Gibbsmaße und Phasenübergänge*, Universität Tübingen, December 17.

P. MATHÉ, *Anwendung der Wahrscheinlichkeitsrechnung*, Hans und Hilde Coppi-Gymnasium, Berlin, April 1.

——, *Approximation by Bernstein polynomials: A probabilistic approach*, Ukrainian Academy of Sciences, Kiev, April 25.

——, *Using ergodic Markov chains for numerical integration*, 3rd IMACS Seminar on Monte Carlo Methods, Salzburg, Austria, September 10.

——, *Markov chains for numerical integration*, Workshop "Numerical Integration and its Complexity", Mathematisches Forschungsinstitut Oberwolfach, November 22.

——, *Stable summation of noisy orthonormal series*, Centre International de Rencontres Mathématiques, Marseille, France, December 13.

G. MILSTEIN, *The simplest random walk for the general Dirichlet problem*, Stochastic Numerics Conference, University of Zurich, Switzerland, February 19.

——, *Symplectic integration of Hamiltonian systems with noise*, Workshop "Computational SDE", The University of Warwick, Coventry, UK, March 29.

——, *Transition density estimation for stochastic differential equations via forward-reverse representations*, Seminar of Probability and Statistics, Technische Universiteit Delft, The Netherlands, October 3.

——, *Transition density estimation for stochastic differential equations via forward-reverse representations*, Colloquium Probability, Statistics and Financial Mathematics, Korteweg-de Fries Institute, Vrije Universiteit Amsterdam, The Netherlands, October 8.

A. MÖLLER, *Robust optimal distillation control with stochastic inflow rate*, First SIAM-EMS Conference "Applied Mathematics in our Changing World", Berlin, September 3.

H.-J. MUCHA, *Stabilisierte modellbasierte Clusteranalyse und deren Anwendung in der Archäologie*, Annual Meeting of Gesellschaft für Klassifikation, München, March 15.

——, *Kern-Clustering Venezianischer Gläser*, Technische Universität Berlin, September 29.

——, *Clustering techniques accompanied by matrix recording techniques*, Technische Universität München, Iffeldorf, November 6.

——, *Data Mining mit Verfahren der Clusteranalyse*, Technische Universität Ilmenau, December 7.

H. NEIDHARDT, *On self-adjoint and dissipative Schrödinger-Poisson systems*, Academy of Sciences of the Czech Republic, Nuclear Physics Institute, Rez, January 24.

——, *On dissipative Schrödinger-Poisson systems*, XVth Max Born Symposium "Schrödinger Operators, (Random) Potentials and Singular Perturbations", Wroclaw, Poland, June 29.

——, *Über das eindimensionale dissipative Schrödinger-Poisson-System: Vom Spektralparameter unabhängige Randbedingungen (I)*, Seminar "Funktionalanalytische Methoden" (Langenbach-Seminar), WIAS, Berlin, July 4.

——, *Über das eindimensionale dissipative Schrödinger-Poisson-System: Vom Spektralparameter abhängige Randbedingungen (II)*, Seminar "Funktionalanalytische Methoden" (Langenbach-Seminar), WIAS, Berlin, July 18.

——, *Operator inequalities and Trotter-Kato product formula*, International Conference on Functional Analysis, National Academy of Sciences of Ukraine, Kiev, August 22.

——, *Sturm-Liouville operators: Dilations and currents*, Workshop "Extensions of Symmetric Operators and Indefinite Matrices", Technische Universität Berlin, November 16.

M. PETZOLDT, *Regularität für Laplace-Interface-Probleme in 2D und 3D*, Seminar "Funktionalanalytische Methoden" (Langenbach-Seminar), WIAS, Berlin, February 7.

——, *Singularities in Laplace interface problems in 2d and 3d*, PRISM2001, University of Nijmegen, The Netherlands, May 22.

——, *Probleme mit unstetigen Diffusionskoeffizienten: Regularität und Fehlerschätzer*, Institutskolloquium, WIAS, Berlin, July 7.

P. PHILIP, *Zeitabhängige Simulation der Züchtung von SiC-Einkristallen durch Sublimation*, DGKK Workshop "Angewandte Simulation in der Kristallzüchtung", Deutsche Gesellschaft für Kristallwachstum und Kristallzüchtung, Aufseß, February 14.

——, *Stationäre und zeitabhängige Simulation*, WE-HERAEUS Summer Course "SiC und GaN – Materialien für die Leistungs- und Optoelektronik", Cottbus, September 3.

J. POLZEHL, *Structural adaption in non-parametric smoothing*, Departamento de Estadistica y Econometria, Universidad Carlos III de Madrid, Spain, March 2.

——, *Structural adaption — A method to estimate the effective dimension reduction space*, Closed Meeting of SFB 373, Wulkow, May 18.

——, *Can structural assumptions be used to improve nonparametric estimates?*, University of Minnesota, School of Statistics, Minneapolis, USA, May 31.

——, *Structural adaptation in nonparametric regression*, WIAS Workshop on High-Dimensional Nonlinear Statistical Modelling, Wulkow, September 16.

——, *Structural adaptive estimation*, Bayer AG, Leverkusen, November 29.

——, *Angewandte Statistik*, Continuation Seminar for Engineers, 8 talks, Haus der Technik, Essen, November 12–13.

M. RADZIUNAS, *Traveling wave model and its approximations simulating and analysing multisection semiconductor lasers*, Seminar "Mathematische Modelle der Photonik", WIAS, Berlin, July 12.

——, *Simulation and analysis of dynamics in multi-section semiconductor DFB laser*, First SIAM-EMS Conference "Applied Mathematics in our Changing World", Berlin, September 3.

——, *Travelling wave model and its mode approximations analyzing and designing semiconductor lasers*, WIAS Workshop "Dynamics of Semiconductor Lasers", Berlin, September 14.

——, *Locking properties of self-pulsations in multi-section semiconductor lasers*, Seminar "Mathematische Modelle der Photonik", WIAS, Berlin, December 6.

A. RATHSFELD, *Polynomial collocation for integral equations with fixed singularities*, Università della Basilicata, Potenza, Italy, January 30.

——, *Approximative Approximation, ein anderes Konzept zur Näherung von Funktionen und Operatoren*, Technische Universität Chemnitz, June 21.

J. REHBERG, *Existence, uniqueness and regularity of solutions to Kohn-Sham systems*, Workshop "Wavelets and Electronical Structure Calculation", Technische Universität Chemnitz, January 26.

——, *Verformung von Würfeln in Kugeln*, Berlin Day of Mathematics, Humboldt-Universität zu Berlin, May 19.

——, *Spectral theory for non-Hermitian Schrödinger operators arising from open quantum systems*, Workshop "Ellipticity and Asymptotics in Spaces with Singularities", The Mathematical Conference Center, Będlewo, Poland, September 4.

O. REISS, *Efficient computation of option price sensitivities using homogeneity and other tricks*, Technische Universiteit Delft, The Netherlands, May 8.

——, *Risk measures and value at risk*, Technische Universiteit Delft, The Netherlands, May 8.

S. RŒLLY, *Equilibrium states for different classes of infinite-dimensional Brownian diffusions*, Berliner Kolloquium Wahrscheinlichkeitstheorie, WIAS, Berlin, November 11.

K. SABELFELD, *Stochastic Lagrangian model for spatially inhomogeneous Smoluchowski equation*, Fourth St. Petersburg Workshop on Simulation, St. Petersburg, Russia, June 19.

——, *Backward and forward stochastic Lagrangian models for transport of scalars in turbulent flows*, Fourth St. Petersburg Workshop on Simulation, St. Petersburg, Russia, June 20.

——, *Lagrangian stochastic models for turbulence simulation*, N.N. Yanenko Conference on Numerical Simulation in Mechanics of Fluids, Novosibirsk, Russia, June 25.

——, *Monte Carlo evaluation of the footprint function over inhomogeneous forest*, First SIAM-EMS Conference "Applied Mathematics in our Changing World", Berlin, September 3.

——, *Stochastic Lagrangian method for solving spatially inhomogeneous Smoluchowski equation*, First SIAM-EMS Conference "Applied Mathematics in our Changing World", Berlin, September 4.

——, *Stochastic models of coagulation processes governed by a class of Smoluchowski equations*, First SIAM-EMS Conference "Applied Mathematics in our Changing World", Berlin, September 5.

——, *Valuation of natural resources deposits*, First SIAM-EMS Conference "Applied Mathematics in our Changing World", Berlin, September 6.

——, *A Lagrangian stochastic model for transport in a statistically homogeneous porous medium*, 3rd IMACS Seminar on Monte Carlo Methods, Salzburg, Austria, September 14.

——, *Lagrangian stochastic models for transport of interacting and diffusing particles*, 3rd IMACS Seminar on Monte Carlo Methods, Salzburg, Austria, September 14.

——, *On a variance reduction technique in the particle simulation governed by SDEs*, 3rd IMACS Seminar on Monte Carlo Methods, Salzburg, Austria, September 14.

——, *Stochastic Lagrangian footprint calculations over inhomogeneous surface*, 2nd INTAS Footprint Workshop, Schloss Turnau, Turnau, September 30.

J. SCHEFTER, *Berechnung des Umkugelmittelpunktes eines Tetraeders mittels MATHEMATICA*, 2nd Workshop "Computeralgebra MATHEMATICA", WIAS, Berlin, April 26.

I. SCHMELZER, *Grid generation and geometry description with COG*, 17th GAMM Seminar Leipzig on Construction of Grid Generation Algorithms, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, February 3.

G. SCHMIDT, *Zum optimalen Entwurf optischer Beugungsgitter*, Universität Stuttgart, January 30.

——, *Asymptotische Entwicklung von Randintegraloperatoren*, Universität Stuttgart, February 6.

——, *Untersuchungen zur Randpunktmethode*, BMBF Workshop "Moderne numerische Methoden zur Lösung der Helmholtzgleichung", Stuttgart, March 2.

——, *Optimal design of diffraction gratings*, First SIAM-EMS Conference "Applied Mathematics in our Changing World", Berlin, September 6.

——, *On the optimal design of diffraction gratings*, University of Tokyo, Japan, November 26.

——, *Zu mathematischen Problemen der diffraktiven Optik*, Technische Universität Chemnitz, December 6.

K.R. SCHNEIDER, *Canards und Kalziumoszillationen*, WIAS Colloquium "Mathematical Modeling of Biochemical Processes", Berlin, February 22.

——, *Vibrational control of singularly perturbed systems*, Technische Universität Ilmenau, May 11.

——, *Oszillationen und Erregbarkeit von Halbleiterlasern*, Universität Würzburg, June 22.

——, *Forced canards*, Conference "Nonlinear Dynamics", Nizhny Novgorod, Russia, July 3.

——, *A method to determine the dimension of long-time dynamics in multi-scale systems*, First SIAM-EMS Conference "Applied Mathematics in our Changing World", Berlin, September 3.

——, *Eine Methode zur Abschätzung der Dimension der Langzeitdynamik in Mehrskalensystemen*, GAMM Expert Committee Meeting "Dynamik und Regelungstheorie", Universität Karlsruhe, November 19.

J. SCHOENMAKERS, *Term structure dynamics endogenously induced by multi-asset markets*, Conference Risk 2001 Europe, Paris, France, April 10.

——, *Correlation structure in LIBOR market models, calibration to caps and swaptions*, Technische Universiteit Delft, The Netherlands, May 8.

V. SCHULZ, *Parameterschätzung und Formoptimierung bei Bingham-Fluiden*, Universität Augsburg, March 6.

——, *Multigrid optimization in applications*, FORTWIHR Conference, Erlangen, March 13.

——, *Multigrid optimization in applications*, University of Tokyo, Japan, April 21.

——, *Mehrgittermethoden für Sattelpunktprobleme*, Universität Potsdam, May 4.

——, *Parameterschätzung und Formoptimierung bei Bingham-Fluiden*, Institutskolloquium, WIAS, May 7.

——, *Parameter estimation in flow problems*, Workshop "Schnelle Löser für partielle Differentialgleichungen", Mathematisches Forschungsinstitut Oberwolfach, May 30.

——, *Parameter estimation and shape optimization for Bingham fluids*, Fifth SIAM Conference on Control and its Applications, San Diego, USA, July 11.

N. SCURTU, *Taylor-Couette-System für Newton'sche Fluide mit asymmetrischen Randbedingungen*, Workshop "Strukturbildung und Stabilität in rotierenden Systemen", Brandenburgische Technische Universität Cottbus, March 12.

J. SIEBER, *Dynamik in longitudinalen Modellen von Halbleiterlasern*, Research Seminar "Algebro-Differentialgleichungen", Humboldt-Universität zu Berlin, January 31.

——, *Dynamics of semiconductor lasers*, Senior Seminar "Nichtlineare Dynamik", WIAS, Berlin, July 12.

——, *Numerical bifurcation analysis of lasers with short external cavity using mode approximations*, WIAS Workshop "Dynamics of Semiconductor Lasers", Berlin, September 14.

——, *Bifurcations in lasers with short external cavity*, Seminar "Mathematische Modelle der Photonik", WIAS, Berlin, October 25.

——, *Bifurcation analysis for lasers with delayed feedback*, WIAS Colloquium "Excitability in lasers", Berlin, December 14.

V. SPOKOINY, *Structure adaptive methods for dimension reduction*, Université Catholique de Louvaine, Louvain-la-Neuve, Belgium, February 7.

——, *Struktur adaptiver Methoden der Bildverarbeitung*, Universität Bremen, March 22.

——, *Structure adaptive methods in dimension reduction*, Institut Henri Poincaré, Paris, France, May 20.

——, *Varying coefficient modelling with applications to volatility estimation*, Colloque Dystoch, Institut Henri Poincaré, Paris, France, June 14.

——, *Realized volatility and covariance forecasting for stock returns*, WIAS Workshop on High-Dimensional Nonlinear Statistical Modelling, Wulkow, September 16.

——, *Varying coefficient modelling by adaptive weights*, Universidad Carlos III de Madrid, Spain, October 5.

——, *Structural adaptive estimation*, Bayer AG, Leverkusen, November 29.

——, *Adaptive methods in nonparametric estimation*, 4 talks, Université Catholique de Louvaine, Louvain-la-Neuve, Belgium, February 6–17.

J. SPREKELS, *Hysteresis operators in phase-field systems*, University of Warsaw, ICM, Poland, January 5.

——, *Mathematik — Schlüsseltechnologie des 21. Jahrhunderts*, URANIA, Berlin, March 16.

——, *Mathematik — Schlüsseltechnologie des 21. Jahrhunderts*, Walther-Rathenau-Oberschule, Berlin-Wilmersdorf, April 5.

——, *Hysteresis operators in phase-field modelling*, Workshop "Phasenübergänge", Mathematisches Forschungsinstitut Oberwolfach, May 1.

——, *Mathematik — Schlüssel für neue Technologien*, Forum Adlershof e. V., Berlin, May 8.

——, *Laudatio anlässlich der Verleihung der Ehrenpromotion an Herrn Prof. Dr. K.-H. Hoffmann durch die Universität Augsburg*, Augsburg, June 18.

——, *On nonlocal phase transition models for non-conserved order parameters*, Università di Pavia, Dipartimento di Matematica, Italy, September 19.

J. SPREKELS, P. KREJČÍ, *Phase-field systems with multidimensional Prandtl-Ishlinskii operators*, The Third International Symposium on Hysteresis and Micromagnetics Modeling (HMM'01), The George Washington University, Virginia Campus, Ashburn, Virginia, USA, May 22.

H. STEPHAN, *Wie kann man 4 Liter mit 8-, 5- und 3-Litergefäßen abmessen?*, Berlin Day of Mathematics, Humboldt-Universität zu Berlin, May 19.

——, *Lyapunov-Funktionen für eine Klasse von Fokker-Planck-Gleichungen*, Seminar "Funktionalanalytische Methoden" (Langenbach-Seminar), WIAS, Berlin, May 30.

——, *Modellierung und Simulation von Bauelementen für Schaltkreise der Leistungselektronik*, DFG Colloquium "Halbleiterbauelemente hoher Leistung", Bremen, September 26.

A. STURM, *About convergence to the heat equation with colored noise*, Berliner Kolloquium Wahrscheinlichkeitstheorie, WIAS, Berlin, November 21.

D. TIBA, *On the optimization of arches*, First SIAM-EMS Conference "Applied Mathematics in our Changing World", Berlin, September 6.

D. TURAEV, *Complicated dynamics in the Newhouse regions*, Georgia Tech, Atlanta, USA, February 6.

——, *Smooth approximations to scattering billiards*, University of Georgia, Atlanta, USA, May 18.

——, *Elliptic periodic orbits near homoclinic bifurcations*, SIAM Conference "Dynamical Systems – VI", Snowbird, Utah, USA, May 21.

——, *On dynamics of laser models*, The Israeli Mathematical Union, Applied Mathematics Meeting, Rehovot, Israel, June 7.

——, *Dimension estimates and homoclinic bifurcations*, The Weizmann Institute, Rehovot, Israel, June 10.

——, *On homoclinic and superhomoclinic orbits*, Workshop "Numerical Methods in Homoclinic Bifurcations", University of Utrecht, The Netherlands, June 21.

——, *Elliptic periodic orbits near homoclinic bifurcations*, Conference "Nonlinear Dynamics", Nizhny Novgorod, Russia, July 4.

——, *Dimension estimates and homoclinic bifurcations*, ICTP School and Workshop on Dynamical Systems, Trieste, Italy, August 17.

W. WAGNER, *Diffusion, coagulation, and stochastic numerics*, Conference "Stochastic Numerics 2001", Zürich, Switzerland, February 2.

——, *A new kinetic equation for dense gases*, Meeting "Asymptotic and Numerical Methods for Kinetic Equations", Mathematisches Forschungsinstitut Oberwolfach, April 16.

——, *The limiting kinetic equation of the Consistent Boltzmann Algorithm for dense gases*, Workshop "Computational Kinetic Theory: Mesoscale Applications", Lyon, France, May 28.

——, *Gelation phenomena: Conjectures and numerical observations*, Miniworkshop "Stochastic Models for Coagulation Processes", Mathematisches Forschungsinstitut Oberwolfach, August 22.

——, *Stochastic, analytic and numerical aspects of coagulation processes*, Third IMACS Seminar on Monte Carlo Methods, Salzburg, Austria, September 13.

——, *Stochastic algorithms and their limiting kinetic equations*, Yokohama National University, Japan, October 10.

——, *Stochastic algorithms and their limiting kinetic equations*, Kyoto University, Japan, October 22.

——, *Stochastic algorithms for coagulation processes*, TMR Workshop "Numerical and Asymptotic Methods for Kinetic Equations", Saarbrücken, November 30.

W. WEISS, *An upper bound for the critical Mach number in the calculation of shock waves with the moment theory*, International Conference on Continuum Mechanics & Thermodynamics (ISIMM), Potsdam, July 30.

K. WILMANSKI, *Asymptotic solutions of dynamical problems for porous and granular materials*, 2nd Euroconference "Mathematical Foundations of Geomechanics", Innsbruck, Austria, February 14.

——, *Interfaces in porous materials*, Workshop on Methods of Applied Mathematics and Mechanics in an Environmental, Geophysical and Climatological Context, Seeheim-Jugenheim, March 20.

——, *Modeling of drainage in poroelastic materials*, Università di Milano, Italy, April 20.

——, *Hyperbolic field equations for porous bodies*, Conference on Differential Equations and Related Topics, dedicated to the Centenary Anniversary of Ivan G. Petrovskii, Moscow, Russia, May 24.

——, *Some problems of surface and nonlinear waves in porous materials*, XIth International Conference on Waves and Stability in Continuous Media (WASCOM), Porto Ercole, Italy, July 8.

——, *Propagation of sound and surface waves in porous materials*, International Symposium on Structured Media, Poznan, Poland, September 17.

——, *Rheologische Zustandsgleichungen von Hantellösungen*, Thermodynamisches Seminar, WIAS, Berlin, November 9.

——, *Thermodynamics of immiscible mixtures*, 12 talks, Università di Torino, Italy, April 24–27.

M. WOLFRUM, *A new criterion for heteroclinic connections in scalar parabolic PDE*, EQUADIFF 10, Prague, Czech Republic, August 31.

——, *Hopf instabilities of lasers with short external resonator*, WIAS Workshop “Dynamics of Semiconductor Lasers”, Berlin, September 14.

——, *Dynamische Effekte in integrierten Halbleiterlaser-Bauelementen*, Institutskolloquium, WIAS, Berlin, October 15.

K. ZACHARIAS, *Geometrie für schlechte Zeiten oder was Napoleon aus Italien mitbrachte*, Berlin Day of Mathematics, Humboldt-Universität zu Berlin, May 19.

Posters

B. ALBERS, *Linear stability of flows in porous materials*, (poster), International Conference on Continuum Mechanics & Thermodynamics (ISIMM), Potsdam, July 30 – August 3.

W. DREYER, *Mathematische Modellierung und Simulation der Entstehung, des Wachstums und der Auflösung von Arsenausscheidungen in einkristallinem Galliumarsenid*, (talk), DGKK Workshop “Angewandte Simulation in der Kristallzucht”, Deutsche Gesellschaft für Kristallwachstum und Kristallzüchtung, Aufseß, February 14–15.

W. DREYER, R. GUCKEL, M. KUNIK, J. SPREKELS, *Towards rigorous micro-macro transitions*, (poster), International Conference on Continuum Mechanics & Thermodynamics (ISIMM), Potsdam, July 30 – August 3.

W. DREYER, M. HERRMANN, M. KUNIK, *Kinetic treatment of selected initial and boundary value problems for hyperbolic systems and kinetic equations*, (poster), International Conference on Continuum Mechanics & Thermodynamics (ISIMM), Potsdam, July 30 – August 3.

J. ELSCHNER, A. RATHSFELD, G. SCHMIDT, *Accurate FEM simulation and optimization of diffraction by polygonal profile gratings*, (poster), EOS Topical Meeting on Diffractive Optics, Budapest, Hungary, October 9–11.

H. GAJEWSKI, U. BANDELOW, H. STEPHAN, K.R. SCHNEIDER, M. RADZIUNAS, M. WOLFRUM, J. SIEBER, L. RECKE, F. JOCHMANN, *Modellierung von Halbleiterlasern — Strukturbildung in Raum und Zeit*, (poster), April 5, Evaluation of SFB 555 "Complex Nonlinear Processes", Humboldt-Universität zu Berlin.

H. GAJEWSKI, K. GÄRTNER, *Domain separation by means of sign changing eigenfunctions of p-Laplacians*, (poster), Tenth SIAM Conference on Parallel Processing for Scientific Computing, Portsmouth, Virginia, USA, March 12–14.

M. HERRMANN, *Kinetic solutions of the Boltzmann-Peierls equation and its moment systems*, (poster), International Conference on Continuum Mechanics & Thermodynamics (ISIMM), Potsdam, July 30 – August 3.

O. KLEIN, *Modeling and numerical simulation of induction heating of crucibles for sublimation growth of SiC*, (poster), WE-HERAEUS Summer Course "SiC und GaN — Materialien für Leistungs- und Optoelektronik", Cottbus, September 3–14.

I. SCHMELZER, *Grid generation and geometry description with COG*, (poster), 17th GAMM Seminar Leipzig on Construction of Grid Generation Algorithms, February 1–3.

K. WILMANSKI, *Surface waves in porous media*, (poster), International Conference on Continuum Mechanics & Thermodynamics (ISIMM), Potsdam, July 30 – August 3.

Contributions to Exhibitions

U. BANDELOW, *`WIAS-TeSCA`, LDSL and KPLIB count in semiconductor lasers*, (fair), 15th International Trade Fair "Laser 2001, World of Photonics", München, June 18–22.

D. HÖMBERG, W. WEISS, *Numerical simulation of laser and electron beam surface hardening of steel*, (fair), Hannover Messe 2001, April 23–28.

TH. KOPRUCKI, *TeSCA, LDSL and KPLIB count in semiconductor lasers*, (fair), 15th International Trade Fair "Laser 2001, World of Photonics", München, June 20–22.

M. RADZIUNAS, *Presentation of different softwares of WIAS*, (fair), 15th International Trade Fair "Laser 2001, World of Photonics", München, June 16–20.

6.5 Visits to other Institutions

B. ALBERS, Politecnico di Torino, Dipartimento di Ingegneria Strutturale e Geotecnica, Italy, April 23–27, in the framework of the project “Flows and transport problems in continua”.

E. BÄNSCH, University of Maryland, College Park, USA, January 11–26, in the framework of a DAAD-NSF grant.

A. BOVIER, Dipartimento di Matematica, Università di Roma 2 “Tor Vergata”, Italy, June 17–30.

——, Charles University Prague, Faculty of Mathematics and Physics, Czech Republic, July 28 – August 2.

——, École Polytechnique Fédérale de Lausanne, Département de Mathématiques, Switzerland, September 16 – October 1.

——, École Polytechnique Fédérale de Lausanne, Département de Mathématiques, Switzerland, October 7–20.

G. BRUCKNER, University of Tokyo, Department of Mathematics; University of Kyoto, Department of Mathematics, Japan, April 17 – May 1, in preparation of the DFG project “Scientific cooperation with Japan: Inverse problems in electromagnetics”.

J. ELSCHNER, University of Tokyo, Department of Mathematics, Japan, November 19 – December 1, in the framework of the DFG project “Scientific cooperation with Japan: Inverse problems in electromagnetics”.

K. FLEISCHMANN, University of Warwick, Mathematics Institute, UK, April 1–6.

——, Technion Israel Institute of Technology, Faculty of Industrial Engineering and Management, Haifa, April 18 – May 3.

——, University of Knoxville, Department of Mathematics, USA, October 14 – November 9.

K. GÄRTNER, Compaq Computer Corporation, Nashua, USA, March 15–17, in the framework of the project “Parallel sparse direct solvers”.

——, University of California, Berkeley, USA, March 7–11, in the framework of the project “Parallel sparse direct solvers”.

B. GENTZ, Eidgenössische Technische Hochschule Zürich, Forschungsinstitut für Mathematik, Switzerland, February 11 – March 11.

——, Eidgenössische Technische Hochschule Zürich, Forschungsinstitut für Mathematik, Switzerland, December 11–22.

R. HENRION, Universität Halle-Wittenberg, Institut für Optimierung und Stochastik, visiting professorship (C4), summer semester 2001 and winter semester 2001/2002.

D. HÖMBERG, Auburn University, Department of Mathematics, Alabama, USA, July 3–8.

R. HÜNLICH, Eötvös LoràND University, Department of Numerical Analysis and Department of Applied Analysis, Budapest, Hungary, February 26 – March 1.

S. JASCHKE, LADSEB Institute for Systems Science and Biomedical Engineering of the Italian National Research Council (CNR), Padova, Italy, June 18–30.

TH. KOPRUCKI, Universität des Saarlandes, Fakultät für Mathematik und Informatik, Saarbrücken, November 26 – December 1, in the framework of the project "Envelope function approximation of electronic states in semiconductor nanostructures".

P. MATHÉ, Ukrainian Academy of Sciences, Institute of Mathematics, Kiev, Russia, April 20–27.

H. NEIDHARDT, Academy of Sciences of the Czech Republic, Nuclear Physics Institute, Rez, January 22–27, in the framework of the project "Coupling between van Roosbroeck system and a Schrödinger-Poisson system including exchange of carriers".

——, Centre de Physique Théorique, Marseille, France, March 26 – April 3, in the framework of the project "Coupling between van Roosbroeck system and a Schrödinger-Poisson system including exchange of carriers".

J. POLZEHL, Universidad Carlos III de Madrid, Departamento de Estadistica y Econometria, Spain, March 1–4.

——, University of Minnesota, School of Statistics, Minneapolis, USA, May 22 – June 22.

A. RATHSFELD, Università della Basilicata, Dipartimento di Matematica, Potenza, Italy, January 22 – February 1.

K. SABELFELD, Russian Academy of Sciences, Institute for Physics of the Atmosphere, Moscow, February 5–26.

——, Russian Academy of Sciences, Institute for Applied Mathematics and Mathematical Geophysics, Novosibirsk, July 2 – August 31.

G. SCHMIDT, Universität Stuttgart, Mathematisches Institut A, January 15 – February 15.

——, University of Tokyo, Department of Mathematics, Japan, November 19 – December 1, in the framework of the DFG project "Scientific cooperation with Japan: Inverse problems in electromagnetics".

K.R. SCHNEIDER, Moscow State University, Faculty of Physics, Russia, February 8–17, in the framework of the DFG cooperation project "Singularly perturbed systems and exchange of stability" of German and Russian scientists within *Memorandum of Understanding* between DFG and RFFI.

——, Moscow State University, Faculty of Physics, Russia, July 7–11, in the framework of the DFG cooperation project "Singularly perturbed systems and exchange of stability" of German and Russian scientists within *Memorandum of Understanding* between DFG and RFFI.

V. SCHULZ, Universität Augsburg, Institut für Mathematik, March 5–8.

——, University of Tokyo, Department of Mathematics, Japan, April 18–23, in the framework of the DFG project “Scientific cooperation with Japan: Inverse problems in electromagnetics”.

V. SPOKOINY, Université Catholique de Louvaine, Institute de Statistiques, Louvain-la-Neuve, Belgium, January 28 – February 23.

——, Université Paris VII, Laboratoire de Probabilité, France, May 10–18.

——, Universidad Carlos III de Madrid, Departamento de Estadistica y Econometria, Spain, October 4–7.

J. SPREKELS, Università di Pavia, Dipartimento di Matematica, Italy, September 17–23.

J. TSENG, Hong Kong Polytechnic University, Department of Applied Mathematics, China, February 1–28.

D. TURAEV, The Weizmann Institute of Science, Department of Mathematics, Rehovot, Israel, May 30 – June 18.

W. WAGNER, University of Cambridge, Department of Chemical Engineering, UK, June 27 – July 4.

——, Yokohama National University, Department of Applied Mathematics, Japan, October 3–19.

——, Kyoto University, Department of Aeronautics and Astronautics, Japan, October 19–26.

K. WILMANSKI, Università di Milano, Italy, April 20–23, in the framework of the project “Flows and transport problems in continua”.

——, Politecnico di Torino, Dipartimento di Ingegneria Strutturale e Geotecnica, Italy, April 24–27, in the framework of the project “Flows and transport problems in continua”.

6.6 Academic Teaching[1]

E. BÄNSCH, *Theorie und Numerik für die Navier-Stokes-Gleichungen* (lecture), Freie Universität Berlin, 2 SWS, summer semester 2001.

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.

A. BOVIER, *Extrema stochastischer Folgen und Prozesse* (lecture), Technische Universität Berlin, 2 SWS, winter semesters 2000/2001 and 2001/2002.

I. BREMER, *Grundlagen der elektronischen Datenverarbeitung* (exercises), Technische Fachhochschule Berlin, 4 SWS, winter semester 2000/2001.

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.

W. DREYER, K. WILMANSKI, *Mikro- und makroskopische Modellierung in der Kontinuumsmechanik* (lecture), Technische Universität Berlin, 2 SWS, winter semester 2000/2001.

H. GAJEWSKI, *Nichtlineare partielle Differentialgleichungen — Analysis und Numerik* (lecture), Freie Universität Berlin, 2 SWS, winter semester 2000/2001 and summer semester 2001.

B. GENTZ, *Lineare Algebra für Ingenieure* (lecture), Technische Universität Berlin, 2 SWS, winter semester 2001/2002.

——, *Stochastik für Informatiker* (lecture), Technische Universität Berlin, 2 SWS, summer semester 2001.

A. GLITZKY, *Analytische Behandlung von Reaktions-Diffusionsgleichungen* (lecture), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2000/2001.

J.A. GRIEPENTROG, *Lebesgue- und Sobolev-Räume* (lecture), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2001/2002.

——, *Maß und Integration auf Mannigfaltigkeiten* (lecture), Humboldt-Universität zu Berlin, 2 SWS, summer semester 2001.

R. HENRION, *Stochastische Optimierung II* (lecture), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2000/2001.

[1] SWS = semester periods per week

R. HENRION, W. RÖMISCH, *Numerik stochastischer Modelle* (seminar), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2000/2001.

C. KÜLSKE, *Gibbsmaße und Phasenübergänge* (lecture), Technische Universität Berlin, 2 SWS, summer semester 2001.

——, *Stochastik für Informatiker* (lecture), Technische Universität Berlin, 2 SWS, winter semester 2000/2001.

J. REHBERG, *Analysis für Informatiker* (lecture), Hasso-Plattner-Institut für Softwaresystemtechnik, Potsdam, 4 SWS, summer semester 2001.

K.R. SCHNEIDER, *Qualitative Theorie gewöhnlicher Differentialgleichungen* (lecture), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2000/2001.

K.R. SCHNEIDER, B. FIEDLER, *Nichtlineare Dynamik* (seminar), Freie Universität (FU) Berlin, 2 SWS, winter semesters 2000/2001 and 2001/2002 at FU Berlin, summer semester 2001 at WIAS.

K.R. SCHNEIDER, L. RECKE, H.-J. WÜNSCHE, *Mathematische Modelle der Photonik* (seminar), Humboldt-Universität zu Berlin, 2 SWS, winter semesters 2000/2001 and 2001/2002, summer semester 2001.

V. SCHULZ, *Praktische mathematische Modellierung* (seminar), (together with S.B. Hazra, Universität Heidelberg), Technische Universität Berlin, 2 SWS, winter semester 2000/2001.

V. SPOKOINY, *Statistik der Finanzmärkte* (lecture), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2000/2001.

V. SPOKOINY, O. BUNKE, *Kurvenschätzung und Resampling* (seminar), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2000/2001 and summer semester 2001.

V. SPOKOINY, O. BUNKE, W. HÄRDLE, *Mathematische Statistik* (research seminar), Humboldt-Universität zu Berlin, 2 SWS, winter semesters 2000/2001 and 2001/2002, summer semester 2001.

J. SPREKELS, *Funktionalanalysis* (lecture), Humboldt-Universität zu Berlin, 4 SWS, winter semesters 2000/2001 and 2001/2002.

H. STEPHAN, *Anfänge der Zahlentheorie und Analysis* (lecture), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2001/2002.

G. TELSCHOW, *Einführung in die Datenverarbeitung I* (lecture), Technische Fachhochschule Berlin, 6 SWS, winter semester 2000/2001.

——, *Einführung in die Datenverarbeitung II* (lecture), Technische Fachhochschule Berlin, 6 SWS, summer semester 2001.

——, *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 2001.

W. WAGNER, *Grundlagen der Monte-Carlo-Methode* (lecture), Humboldt-Universität zu Berlin, 2 SWS, winter semester 2001/2002.

K. WILMANSKI, *Dynamik von mehrkomponentigen Körpern* (exercises), Technische Universität Berlin, 1 SWS, summer semester 2001.

——, *Dynamik von mehrkomponentigen Körpern* (lecture), Technische Universität Berlin, 2 SWS, summer semester 2001, winter semester 2001/2002.

K. WILMANSKI, I. MÜLLER, *Thermodynamisches Seminar* (seminar), WIAS/Technische Universität Berlin, 2 SWS, winter semester 2000/2001, summer semester 2001.

6.7 Ph.D. Theses, Habilitations, Calls, Awards, and Distinctions

Ph.D. Theses

J. NIEBSCH, *Zur numerischen Lösung von Evolutionsgleichungen mit nichtlokalen Operatoren auf der Basis approximativer Approximationen*, Universität Bremen, supervisor: Dr. G. Schmidt, April 4.

R. GUCKEL, *Einige freie Randwertaufgaben aus der Elektrostatik und Hydrodynamik*, Universität Leipzig, supervisor: Prof. Dr. M. Günther, January 23.

M. PETZOLDT, *Regularity and error estimators for elliptic problems with discontinuous coefficients*, Freie Universität Berlin, supervisor: Prof. Dr. E. Bänsch, May 30.

J. SIEBER, *Longitudinal dynamics of semiconductor lasers*, Humboldt-Universität zu Berlin, supervisor: PD Dr. K.R. Schneider, July 23.

Habilitations

A. GLITZKY, *Elektro-Reaktions-Diffusionssysteme mit nichtglatten Daten*, Humboldt-Universität zu Berlin, December 17.

C. KÜLSKE, *Gibbs-Maße von ungeordneten Spin-Systemen*, Technische Universität Berlin, October 24.

A. RATHSFELD, *On wavelet algorithms for boundary element methods*, Technische Universität Chemnitz, June 21.

Calls

V. SCHULZ, C4 professorship, Universität Trier, February 26.

V. SPOKOINY, C4 professorship, Universität Wien, Austria, August 28.

——, C4 professorship, Humboldt-Universität zu Berlin, April 9.

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).*

6.8 WIAS Conferences, Colloquiums, and Workshops

COLLOQUIUM "MATHEMATICAL MODELING OF BIOCHEMICAL PROCESSES"
Berlin, February 22
Organized by: WIAS (FG[2] 2)
Sponsored by: WIAS

The main focus of this colloquium was on the role of calcium oscillations in the cellular information process. Different mathematical models have been presented including a qualitative and quantitative investigation of their behavior. Some contributions addressed the problem of model reduction. About 15 people attended the colloquium.

COLLOQUIUM "SINGULARLY PERTURBED PROBLEMS"
Berlin, April 24
Organized by: WIAS (FG 2)
Sponsored by: WIAS

This international colloquium was devoted to the 75th birthday of Prof. A.B. Vasilieva (Moscow State University, Russia). The contributions demonstrated the influence of the work of Prof. Vasilieva on recent research not only in Russia but also at the WIAS and the Free University of Berlin. New trends in the field of singularly perturbed systems and important applications in modern technology have been presented. About 30 people attended the colloquium.

INTERNATIONAL CONFERENCE ON CONTINUUM MECHANICS & THERMODYNAMICS
Potsdam, July 29 – August 3
Organized by: Technische Universität (TU) Berlin (FB 6), WIAS (FG 7)
Sponsored by: WIAS, TU Berlin

The meeting was held under the auspieces of The International Society for the Interaction of Mechanics and Mathematics (ISIMM). There were 35 invited lecturers on the subjects of Granular Matter, Kinetic Theory, Extended Thermodynamics, and Phase Transitions. In addition to the invited lecturers, there were about 30 members of the Society who participated in the discussions and presented posters.
The meeting was financially supported by the Weierstrass Institute and by the Technical University of Berlin. This made it possible to organize the meeting without a conference fee. By merging on its last day with a workshop of the European network on Phase Transitions in Crystalline Bodies, the meeting was enriched by the participation of some 30 scientists working within this network. In total, 76 scientists participated in the conference.

WORKSHOP ON MULTISCALE PROBLEMS AND PHASE TRANSITIONS
Berlin, August 29–31
Organized by: WIAS (FG 7)
Sponsored by: WIAS, DFG, BMBF

Binary alloys that are in use in industrial processes frequently consist of two coexisting phases. When these alloys are subjected to thermo-mechanical loads, the interface boundaries start to move, and there arise drastic changes of the morphology on the μm scale.
There were about 30 participants including 20 invited speakers.

[2] research group

The application of continuum phase-field models to the evolution of the morphology in modern alloys has become very popular. Phase-field models are motivated by atomic considerations of diffusion and order-disorder transitions both of which are strongly influenced by local mechanical stress fields.
Rigorous treatments of micro-macro transitions can, however, only be done for very simple systems, like the atomic chain and related microscopic systems whose evolution is described by a large number of ordinary differential equations. The understanding of the transition to a small number of partial differential equations is crucial for a serious development of phase-field models.
The objective of this workshop has been to open a forum for mathematicians, physicists, and engineers to discuss both categories of problems and their relationships.

WORKSHOP "INVERSE PROBLEMS IN APPLICATIONS"
Berlin, September 10–12
Organized by: Universität Linz, Austria, Universität Bremen, WIAS (FG 4)
Sponsored by: DFG, WIAS

Inverse Problems play a major role in the mathematical modeling and optimization of physical, technical, and biological systems. The fields of application encompass the elasticity modal analysis for turbines, the material identification of pastes, and also the characterization of chemical processes—to name only a few from the spectrum of applications discussed in this workshop. Despite of the multiplicity of applications, usual meetings often cover only the theoretical aspects of inverse problems. Therefore, this workshop was planned as an application counterpart.
It was organized at the WIAS by Prof. Dr. Schulz (since 10/2001 University of Trier) together with Prof. Dr. Maaß (University of Bremen) and Prof. Dr. Engl (University of Linz). The aim was to discuss the state of the art in this industrially relevant topic, mainly from an application point of view and therefore emphasizing numerical aspects.
Since the topic of the workshop is currently of high interest, the resonance to its announcement was enthusiastic. Therefore, 35 participants have been registered for the workshop. Although the atmosphere of the workshop was inevitably influenced by the events of September 11, still mathematical discussions on the subject of the workshop have been initiated, so that it can be considered a success.

WORKSHOP "DYNAMICS OF SEMICONDUCTOR LASERS"
Berlin, September 13–15
Organized by: Heinrich-Hertz-Institut für Nachrichtentechnik Berlin (HHI), Humboldt-Universität zu Berlin (HU), WIAS (FG 2)
Sponsored by: HHI, HU (SFB 555), WIAS

The international workshop addressed challenging problems in modern technology of communication networks. Modeling, simulation, analysis, and experiments of and with semiconductor lasers formed the main focus of the workshop. The contributions demonstrated the possibility to design semiconductor lasers with special properties needed for the signal regeneration in transparent optical networks. Self-pulsations, synchronization (also of chaotic lasers), delayed feedback, short external resonators, excitability, and ultrafast effect formed important topics of the workshop. Discussions and a visit to the laser labs in the Heinrich Hertz Institute contributed also to the success of the workshop, which was attended by 47 people, among them

outstanding scientists from Europe and the USA.

WORKSHOP ON HIGH-DIMENSIONAL NONLINEAR STATISTICAL MODELLING
Wulkow, September 15–19
Organized by: Humboldt-Universität zu Berlin (HU), WIAS (FG 6)
Sponsored by: HU (SFB 373), Seminar Berlin–Paris, WIAS

The conference continued a series of conferences held under the title Seminar Berlin–Paris (Seminaire Paris–Berlin) since 1993. The focus of this year's conference was on methods for the analysis of complex high-dimensional data structures. Methods to address these problems are developed and investigated separately in the statistics and machine learning community. The conference included a lecture series by Klaus-Robert Müller (FHG FIRST) on Vector Support Machines and Boosting methods and several lectures from both communities on new methods and applications. Young scientists were especially encouraged to present their results.
Approximately 50 participants attended the workshop.

WORKSHOP ON GRANULAR MATERIALS IN GEOTECHNICS
Berlin, November 22–23
Organized by: WIAS (FG 7)
Sponsored by: WIAS

The workshop was devoted to experimental and theoretical results essential for the description of land slides processes. The following scientists delivered lectures on their recent research: I. Herle (Czech Academy of Sciences, Prague, on memory effects in granular materials; due to illness the lecture was delivered by D. Kolymbas), K. Hutter (TU Darmstadt, two lectures: On observations and on the theory of avalanches and debris), V.A. Kolodko (Russian Academy of Sciences, Novosibirsk, on the localisation of strains in consolidation), D. Kolymbas (TU Innsbruck, Austria, on hypoplasticity of soils), P. Lade (Aalborg University, Denmark, on laboratory experiments on instability, shear banding, and failure in granular materials), R. Lancellota (TU Turin, Italy, on nondestructive testing of soils), F. Rackwitz (TU Berlin, on shear band formation in cohesionless soils). In addition to scientists from Weierstrass Institute, some 15 scientists from the Technical University (TU) of Berlin and Bundesanstalt für Materialforschung und -prüfung have participated in the Workshop.

WORKSHOP ON OPEN PROBLEMS OF DIRECT METHANOL FUEL CELLS (DMFC)
Berlin, November 23–24
Organized by: WIAS (FG 3)
Sponsored by: WIAS

The goal of the workshop was to address all problems related to modeling the membrane electrode assembly (MEA) of a Direct Methanol Fuel Cell (DMFC) and the individual processes, especially: transport models for fluids and gases, reaction kinetics, and boundary conditions. Within the present cooperation with IWV3, Forschungszentrum Jülich, we observed different activities in Germany, hence we tried (based on the progress reached) to bring together different groups in a first, informal meeting centered around the simulation possibilities, problems, and future perspectives.
30 participants contributed 14 talks during the first day of the workshop. These talks have been grouped around mathematics and modeling, membrane chemistry, and reaction kinetics. The

second day has been devoted to a discussion resulting in different agreements to exchange data, models, and enhance the collaboration. The workshop ended with the suggestion to meet again at WIAS in November 2002.
Further details can be found at http://www.wias-berlin.de/dmfc/workshop/workshop-prog.html.

COLLOQUIUM "EXCITABILITY IN LASERS"
Berlin, December 14
Organized by: Humboldt-Universität zu Berlin (HU), WIAS (FG 2)
Sponsored by: HU (SFB 555), WIAS

Semiconductor lasers play a fundamental role in transparent optical communication networks to increase the data transmission rate. For the regeneration of the degraded signals, special devices are required, acting like a neuron: They respond only to impulses above some threshold. The symposium was devoted to the problem of designing semiconductor lasers which exhibit this threshold property (also called excitability). In this design process, the interaction between simulations and experiments is crucial. About 35 persons attended the colloquium.

6.9 Visiting Scientists

H.W. ALT, Rheinische Friedrich-Wilhelms-Universität Bonn, Institut für Angewandte Mathematik, October 7–13.

T. ARENS, Brunel University, Department of Mathematical Sciences, Uxbridge, UK, July 30 – August 20.

G. BAO, Michigan State University, Department of Mathematics, East Lansing, USA, August 15–19.

I. BELOPOLSKAIA, St. Petersburg State University for Architecture and Civil Engineering, Russia, April 30 – May 14.

N. BERGLUND, Eidgenössische Technische Hochschule, Forschungsinstitut für Mathematik, Zürich, Switzerland, August 20 – September 20.

M. BROKATE, Technische Universität München, Zentrum Mathematik, March 26–30.

——, August 27–31.

V. BUTUZOV, Moscow State University, Faculty of Physics, Russia, April 1–30.

K. CHEN, University of Liverpool, Department of Mathematical Sciences, UK, September 2–10.

J. CHENG, Fudan University, Department of Mathematics, Shanghai, China, August 15 – September 14.

A. DALALYAN, Université Le Mans, France, June 23–28.

P. DEGOND, Université Paul Sabatier, Laboratoire de Mathématiques pour l'Industrie et la Physique (MIP), Toulouse, France, December 2–7.

D. DEREUDRE, Université Lille 1, Laboratoire de Statistique et Probabilités, France, November 5–9.

E. DUDNIKOV, Russian Academy of Sciences, International Research Institute for Management Sciences, Moscow, June 11–15.

Y. DUMONT, IREMIA-Université de La Réunion, Saint Denis, Ile de La Réunion, France, December 1–18.

M.A. EFENDIEV, Universität Stuttgart, Fakultät Mathematik, February 12–26.

——, May 17–31.

——, August 14–28.

——, December 17–21.

V. ESSAOULOVA, St. Petersburg State University, Russia, July 18–22.

L. FONTES, Universidade de São Paulo, Instituto de Matemática e Estatística, Brazil, August 13–19.

M. FRIED, Albert-Ludwigs-Universität Freiburg, Institut für Angewandte Mathematik, June 5–9.

V. GAYRARD, Ecole Polytechnique Fédérale de Lausanne, Département de Mathématiques, Switzerland, February 11 – March 11.

——, July 1–31.

O. GILSON, Université de Liège, Département de Mathématiques, Belgium, October 15–25.

I. GOLDSHEID, University of London, Queen Mary and Westfield College, UK, January 8–11.

S. GONCHENKO, Institute for Applied Mathematics and Cybernetics, Nizhny Novgorod, Russia, November 5 – December 1.

S.B. HAZRA, Universität Heidelberg, Interdisziplinäres Zentrum für Wissenschaftliches Rechnen, July 18–25.

A. HEEMINK, Technische Universiteit Delft, The Netherlands, December 17–21.

W. HOFFMANN, Fa. Braun GmbH, Friedrichshafen, August 29 – September 2.

J.T. JENKINS, Cornell University, Department of Theoretical and Applied Mechanics, Ithaca, USA, June 13–16.

A. JOURANI, Université de Bourgogne, Département de Mathématiques, Dijon, France, February 25 – March 25.

A. JUDITSKI, Université Grenoble, France, May 30 – June 5.

L. KALACHEV, University of Montana, Department of Mathematical Sciences, Missoula, USA, August 1–8.

A.M. KHLUDNEV, Russian Academy of Sciences, Lavrentyev Institute of Hydrodynamics, Novosibirsk, December 3, 2000 – January 31, 2001.

——, December 1–31.

A. KLENKE, Friedrich-Alexander-Universität Erlangen-Nürnberg, Mathematisches Institut, October 1–7.

W. KNOBLOCH, Universität Würzburg, Mathematisches Institut, February 20–23.

A. KOLODKO, Russian Academy of Sciences, Institute for Applied Mathematics and Mathematical Geophysics, Novosibirsk, February 25 – June 30.

M. KONIK, Technische Universität Chemnitz, Fakultät für Mathematik, July 16–20.

M. KRAFT, University of Cambridge, Department of Chemical Engineering, UK, March 26 – April 7.

——, July 18 – August 31.

——, December 10–22.

P.S. KRASILNIKOV, Moscow State Aviation Institute, Department of Differential Equations, Russia, December 3–6.

B. KRAUSKOPF, University of Bristol, Department of Engineering Mathematics, UK, September 2–16.

P. KREJČÍ, Academy of Sciences of the Czech Republic, Institute of Mathematics, Prague, July 23 – August 8.

——, October 1 – November 11.

O. KURBANMURADOV, Turkmenian Academy of Sciences, Scientific Center Climate, Ashkhabad, March 10 – May 11.

I. KURKOVA, Université Paris VI "Pierre et Marie Curie", Laboratoire de Probabilités et Modèles Aléatoires, France, August 25 – September 16.

C. LECOT, Université de Savoie, Le Bourget-du-Lac, France, April 1–8.

T. LEDWINA, Technical University of Warsaw, Mathematical Institute, Poland, May 20–27.

G. LEONOV, St. Petersburg University, Department of Mathematics and Mechanics, Russia, December 3–8.

O. LEPSKI, Université AIX-Marseille, France, October 21–28.

A. LEVYKIN, Russian Academy of Sciences, Institute for Applied Mathematics and Mathematical Geophysics, Novosibirsk, April 19 – May 26.

——, November 1 – December 1.

P.-Y. LOUIS, Université Lille 1, Laboratoire de Statistique et Probabilités, France, October 20 – December 20.

A. LUSHNIKOV, Karpov Institute of Physical Chemistry, Moscow, Russia, August 25 – September 2.

Y. MAISTRENKO, National Academy of Sciences of Ukraine, Institute of Mathematics, Kiev, October 9–13.

M. MALIOUTOV, Northeastern University, Mathematical Department, Boston, USA, June 30 – July 30.

M. MASCAGNI, Florida State University, Tallahassee, USA, May 30 – June 2.

V.G. MAZ'YA, Linköping University, Department of Mathematics, Sweden, February 14–28.

——, July 31 – August 26.

K. MIKULA, Slovak University of Technology, Department of Mathematics, Bratislava, November 11 – December 7.

P. MORIN, Universidad Nacional del Litoral, Facultad de Ingenieria Quimica, Departamento de Matemática, Santa Fe, Argentina, June 20 – July 18.

P. MÖRTERS, University of Bath, Department of Mathematics, UK, December 16–23.

C. MUELLER, University of Rochester, Department of Mathematics, USA, August 4–11.

W.H. MÜLLER, Heriot-Watt University, Department of Mechanical and Chemical Engineering, Edinburgh, UK, March 16 – April 13.

L. MYTNIK, Technion Israel Institute of Technology, Faculty of Industrial Engineering and Management, Haifa, August 11 – September 3.

N. NEFEDOV, Moscow State University, Faculty of Physics, Russia, April 1–30.

C. NEWMAN, New York University, Courant Institute of Mathematical Sciences, USA, August 13–19.

R.H. NOCHETTO, University of Maryland, Department of Mathematics, USA, June 15 – July 4.

J. OUTRATA, Czech Academy of Sciences, Institute of Information Theory and Automation, Prague, March 4–17.

S.V. PEREVERZEV, National Academy of Sciences of Ukraine, Institute of Mathematics, Kiev, September 1–30.

——, October 1 – November 17.

A. PUCHALSKII, University of Colorado at Denver, Mathematical Department, USA, May 20 – June 20.

D. RACHINSKII, Institute for Information Transmission Problems, Moscow, Russia, May 20 – June 18.

E. RADKEVICH, Moscow State University, Faculty of Mechanics and Mathematics, Russia, June 10 – August 10.

Ü. RANNIK, University of Helsinki, Department of Physics, Finland, May 5–11.

S. RJASANOW, Universität des Saarlandes, Fachbereich Mathematik, February 7–10.

V. ROM-KEDAR, Weizmann Institute of Science, Faculty of Mathematics and Computer Science, Rehovot, Israel, November 5–9.

A. SAMAROV, Massachusetts Institute of Technology, Department of Computer Science, Cambridge, USA, June 10–20.

B. SCHMITHÜSEN, Swiss Federal Institute of Technology Zurich, Integrated Systems Laboratory, Switzerland, January 20 – February 2.

G. SELL, University of Minnesota, School of Mathematics, Minneapolis, USA, March 8–21.

I. SHALIMOVA, Russian Academy of Sciences, Institute for Applied Mathematics and Mathematical Geophysics, Novosibirsk, May 20 – June 17.

——, September 2 – December 2.

E. SHCHEPAKINA, Samara State University, Department of Differential Equations and Control Theory, Russia, October 8 – November 4.

K. SHCHETININA, Samara State University, Department of Differential Equations and Control Theory, Russia, January 22 – February 1.

K.G. SIEBERT, Albert-Ludwigs-Universität Freiburg, Institut für Angewandte Mathematik, March 28–31.

N. SIMONOV, Russian Academy of Sciences, Institute for Applied Mathematics and Mathematical Geophysics, Novosibirsk, May 20 – June 17.

I.V. SKRYPNIK, National Academy of Sciences of Ukraine, Institute of Applied Mathematics and Mechanics, Donetsk, July 1–31.

A.L. SKUBACHEVSKII, Moscow State Aviation Institute, Department of Differential Equations, Russia, March 24–31.

——, December 3–6.

O. SMIDTS, Université Libre de Bruxelles, Belgium, October 29 – November 21.

F. SMITH, University College London, UK, August 25 – September 3.

V. SOBOLEV, Samara State University, Department of Differential Equations and Control Theory, Russia, October 8 – November 4.

J. SOKOŁOWSKI, Université de Nancy I, Laboratoire de Mathématiques, Vandœuvre-les-Nancy, France, April 1–7.

S. SPERLICH, Universidad Carlos III de Madrid, Spain, January 2–14.

——, December 20, 2001 – January 8, 2002.

D. STEIN, University of Arizona, Department of Physics, USA, August 13–19.

G. STOYAN, Eötvös Loránd University, Department of Numerical Analysis, Budapest, Hungary, July 9–13.

T. SZÁNTAI, Technical University of Budapest, Department of Differential Equations, Hungary, January 13 – February 12.

F. THEIL, University of Warwick, Mathematics Institute, Coventry, UK, August 26–29.

M. THIEULLEN, Université Paris VI, Laboratoire de Probabilités et Modèles Aléatoires, France, November 15–30.

J. TÓTH, Budapest University of Technology and Economics, Institute of Mathematics, Department of Analysis, Hungary, February 19–25.

M. TRETYAKOV, University of Wales, Department of Mathematics, Swansea, UK, August 2 – September 1.

L. TRUSKINOVSKI, University of Minnesota, Department of Aerospace Engineering and Mechanics, Minneapolis, USA, August 3–17.

C.J. VAN DUIJN, Technical University of Eindhoven, Department of Mathematics and Computer Sciences, The Netherlands, June 1–31.

A. VASILIEVA, Moscow State University, Faculty of Physics, Russia, April 8–28.

O. VASSILIEVA, Moscow State University, Faculty of Mechanics and Mathematics, Russia, June 10 – July 10.

V.A. VATUTIN, Steklov Institute of Mathematics, Moscow, Russia, November 17 – December 16.

C. VIAL-ROGET, ENSAI, Rennes, France, December 9–21.

G. WEI, Hong Kong Baptist University, China, November 24 – December 24.

S. WIECZOREK, Free University of Amsterdam, Faculty of Sciences, Department of Physics and Astronomy, The Netherlands, December 11–14.

J. XIONG, University of Tennessee, Department of Mathematics, Knoxville, USA, May 25 – June 23.

M. YAMAMOTO, University of Tokyo, Department of Mathematical Sciences, Japan, May 5–10.

——, August 15–27.

S. YANCHUK, National Academy of Sciences of Ukraine, Institute of Mathematics, Kiev, November 22–25.

M. YOUSEFI, Free University of Amsterdam, Department of Theoretical Physics, The Netherlands, November 7–11.

M. ZAHRADNÍK, Charles University Prague, Faculty of Mathematics and Physics, Czech Republic, November 1 – December 14.

S. ZELIK, Moscow State University and Russian Academy of Sciences, Institute for Problems of Transmission, Russia, April 23 – May 20.

S. ZHENG, Fudan University, Institute of Mathematics, Shanghai, China, July 4 – August 3.

S. ZWANZIG, Uppsala University, Sweden, December 17–21.

Scholarship Holders

I. EDELMAN, Russian Academy of Sciences, Institute of Physics of the Earth, Moscow, Humboldt Research Fellowship, September 1 – December 31, 2001.

A. KADOYA, Hiroshima Shudo University, Faculty of Economic Sciences, Japan, Fellowship of Visiting Professor Program sponsored by the Hiroshima Shudo University, August 31, 2000 – August 31, 2001.

A. KOLODKO, Russian Academy of Sciences, Institute for Applied Mathematics and Mathematical Geophysics, Novosibirsk, Humboldt Research Fellowship, May 4, 2001 – April 30, 2002.

L. SHILNIKOV, Institute for Applied Mathematics and Cybernetics, Nizhny Novgorod, Russia, Humboldt Research Award, October 18 – December 14, 2001.

Doctoral Candidates and Post-docs supervised by WIAS Collaborators

M. GIURCANU, Graduate College "Stochastic Processes and Probabilistic Analysis", Technische Universität Berlin, doctoral candidate, January 1, 2001 – December 31, 2002.

F. MANZO, Graduate College "Stochastic Processes and Probabilistic Analysis", Technische Universität Berlin, post-doc, January 1 – September 30, 2001.

D. MERCURIO, Graduate College "Applied Microeconomics", Humboldt-Universität zu Berlin, doctoral candidate, September 1, 2000 – August 31, 2003.

H. ZÄHLE, Graduate College "Stochastic Processes and Probabilistic Analysis", Technische Universität Berlin, post-doc, January 1 – December 31, 2001.

6.10 Guest Talks

H.W. ALT, Rheinische Friedrich-Wilhelms-Universität Bonn, *On the entropy principle for surface diffusion*, August 29.

I. ANDRIANOV, Universität Köln, *Asymptotic approaches and Pade approximations in nonlinear mechanics*, January 11.

T. ARENS, Brunel University, Uxbridge, UK, *Integral equation formulations and numerical solution for scattering from diffraction gratings*, August 9.

H. BALTRUSCHAT, Rheinische Friedrich-Wilhelms-Universität Bonn, Institut für Physikalische und Theoretische Chemie, *Eine Durchfluss-Dünnschichtzelle für den elektrochemischen Produktnachweis: Anwendung auf die Methanoloxidation*, July 19.

——, *Ideal and real catalysts for methanol oxidation: A quantitative product analysis using differential electrochemical mass spectrometry*, November 23.

G. BAO, Michigan State University, East Lansing, USA, *Maxwell's equation in nonlinear periodic structures: L^p estimates*, August 16.

V. BELYKH, Institute for Applied Mathematics and Cybernetics, Nizhny Novgorod, Russia, *Synchronization*, November 20.

——, *Homoclinic bifurcation in slow fast systems*, November 21.

P. BINKELE, Universität Stuttgart, Staatliche Materialprüfungsanstalt (MPA), *Atomistic Monte-Carlo simulations of the formation of precipitates*, August 29.

T. BLESGEN, Universität Leipzig, *A generalization of Navier-Stokes equations to two-phase flows*, August 31.

T. BLEY, Technische Universität Dresden, *Metabolic Modelling und Bioprocess Engineering — Stand und Perspektiven bei der Anwendung mathematischer Modelle in der Bioverfahrenstechnik*, November 12.

J. BLOWEY, University of Durham, UK, *Numerical analysis of a coupled pair of Cahn-Hilliard equations*, August 30.

E. BONETTI, Università di Pavia, Italy, *Some mathematical results on a model for phase separation in binary alloys driven by mechanical effects*, August 30.

ST. BONSS, Fraunhofer-Institut für Werkstoff- und Strahltechnik, Dresden, *Schweißen und Härten mit Hochleistungslasern*, October 29.

A.S. BORMANN, Technische Universität Berlin, *Über die Problematik der Boussinesq-Approximation beim Rayleigh-Bénard-Problem*, April 4.

T. BOROWSKI, Technische Universität Berlin, *Reaktions-Diffusionsmodelle in Verfahrenstechnik und Biologie*, May 16.

Z.Y. CAI, Technische Universität Berlin, *Shear band formation in cohesionless soils*, November 23.

C. CERCIGNANI, Università di Milano, Italy, *Kinetic theory of granular materials*, July 30.

P. CIZEK, Humboldt-Universität zu Berlin, Institut für Wirtschaftswissenschaften, *Robust estimation with discrete explanatory variable*, October 24.

S. CLEMENCON, Université Paris X, France, *Adaptive estimation of the transition density of a regular Markov chain by wavelet methods*, January 10.

P. COLLET, École Polytechnique de Lausanne, Switzerland, *Some extensive entropies and dimensions for extended dynamical systems*, May 29.

P. COLLI, Università di Pavia, Italy, *Generalized systems for irreversible phase changes and supercooling*, August 1.

A. DALALYAN, Université Le Mans, France, *Trend coefficient estimation for ergodic diffusion*, June 27.

P. DEGOND, Université Paul Sabatier, Toulouse, France, *Quantum/classical coupling in the time-dependent case*, December 5.

M. DELECROIX, ENSAI, Bruz, France, *Optimal smoothing in M-Estimators for S.I. and P.P. regression*, February 7.

F. DIETSCH, Ebinger Prüf- und Ortungstechnik GmbH, Köln, *Sensorik und mathematische Modelle in der computergestützten Munitionssondierung. Stand der Technik, Probleme und Tendenzen*, December 10.

J. DIVISEK, Forschungszentrum Jülich, IWV-3, *Beeinflussung der DMFC-Leistungskurven durch die Elektrodenkinetik*, November 23.

L. DÜMBGEN, Medizinische Universität zu Lübeck, *P-Werte für Klassifikation*, May 30.

Y. DUMONT, IREMIA-Université de La Réunion, Saint Denis, France, *Dynamics of an impacting cantilever beam moving vertically at its clamped end and constraint at its free end*, December 13.

C. ECK, Friedrich-Alexander-Universität Erlangen-Nürnberg, Lehrstuhl für Angewandte Mathematik, *Ein Zweiskalenmodell für Phasenübergänge*, January 25.

——, *A two-scale phase field model for liquid-solid phase transitions with equiaxed dendritic microstructure*, August 31.

M.A. EFENDIEV, Universität Stuttgart, Fakultät Mathematik, *How symmetry properties of domains inherited to the attractors*, June 21.

C. EGBERS, Brandenburgische Technische Universität Cottbus, Lehrstuhl für Aerodynamik und Strömungslehre, *Instabilitäten in rotierenden Systemen*, October 25.

G. EHLEN, Rheinisch-Westfälische Technische Hochschule Aachen, Gießerei-Institut, *Simplified two-phase-flow model for the simulation of convection effects during solidification with free surfaces*, August 31.

C.M. ELLIOTT, University of Sussex, Falmer, UK, *Phase field and sharp interface models for diffusion-induced grain boundary motion*, August 30.

H. ENGEL, Technische Universität Berlin, *Über rückkopplungsgesteuerte Musterbildung in Reaktions-Diffusionssystemen*, June 26.

M. FRIED, Albert-Ludwigs-Universität Freiburg, Institut für Angewandte Mathematik, *Ein niveauflächenbasierter Finite-Elemente-Algorithmus zur Simulation dendritischen Wachstums*, June 7.

R. GATIGNOL, Université Pierre et Marie Curie, Paris, France, *Kinetic description of a two-phase dispersed medium*, July 31.

K. GELFERT, Université Paris Sud, France, *Abschätzungen der BOX-Dimension invarianter kompakter Mengen auf Mannigfaltigkeiten*, July 26.

V. GELFREICH, Freie Universität Berlin, *Exponential averaging for a singularly perturbed Hamiltonian system*, April 24.

O. GILSON, Université de Liège, Belgium, *A boundary value problem for the Lamé system*, October 22.

I. GOLDSHEID, University of London, UK, *Eigenvalues of non-self-adjoint random Schrödinger operator*, January 10.

S. GONCHENKO, Institute for Applied Mathematics and Cybernetics, Nizhny Novgorod, Russia, *Homoclinic bifurcations and generalized Henon-maps*, November 27.

R. HAHN, Fraunhofer-Institut für Zuverlässigkeit und Mikrointegration, Berlin, *Miniature fuel cell development at Fraunhofer society, simulation challenges*, November 23.

J. HART, Texas A & M University, USA, *Testing the fit of a mixture model using nonparametric density estimation*, July 18.

J. HÄRTERICH, Freie Universität Berlin, *Singularly perturbed boundary value problems and a class of global attractors*, April 24.

C. HENKEL, Universität Potsdam, *Probleme numerischer Elektrodynamik aus der Nahfeldoptik*, July 26.

M. HINTERMÜLLER, Karl-Franzens-Universität Graz, Austria, *Level Set Methoden für zustandsbeschränkte Optimalsteuerungsprobleme*, February 14.

A. HOENIG, Rheinische Friedrich-Wilhelms-Universität Bonn, *A cross-over for the scaling law of the first order correction to the LSW theory of Ostwald ripening*, August 29.

W. HOFFMANN, Braun GmbH, Friedrichshafen, *Strömungssimulation in der Keramik-Industrie*, February 19.

R. HOLLERBACH, Brandenburgische Technische Universität Cottbus, Lehrstuhl für Aerodynamik und Strömungslehre, *Numerische Lösung der Navier-Stokes-Gleichung in sphärischer Geometrie*, October 25.

K. HUTTER, Technische Universität Darmstadt, *Avalanching flows of snow, debris and mud — Geophysical systems between order and disorder of matter*, November 23.

K. JOHANNSEN, Ruprecht-Karls-Universität Heidelberg, Interdisziplinäres Zentrum für Wissenschaftliches Rechnen, *The Elder problem — Solution branches and asymptotic behaviour*, October 11.

A. JOURANI, Université de Bourgogne, Dijon, France, *Conditioning and upper Lipschitz subdifferentials*, March 15.

A. KADOYA, Hiroshima Shudo University, Japan, *Numerical results for the behavior of solutions of a parabolic variational inequality associated with the total variation functional*, January 31.

R. KAISER, B. HÜTTL, Heinrich-Hertz-Institut für Nachrichtentechnik Berlin, *Development of monolithic 40 GHz mode-locked lasers*, November 22.

A. KARAU, Degussa-Hüls AG, Hanau, *Biokatalyse — Neue Perspektiven für die chemische Produktion sowie deren verfahrenstechnische Herausforderungen*, December 3.

A. KELLER, Universität Kaiserslautern, Fachbereich Informatik, *Monte-Carlo- und Quasi-Monte-Carlo-Methoden in der Computergraphik*, October 8.

H. KLEINE, Technische Universität München, Fachbereich Physik, *RuSe als methanoltolerantes Kathodenkatalysatormaterial für die DMFC*, November 23.

H. KNOBLOCH, Universität Würzburg, *Der Herzrhythmus: Verständnis durch mathematische Modellierung*, February 22.

J. KOHLMORGEN, Gesellschaft für Mathematik und Datenverarbeitung First and Universität Potsdam, *Analysis and modeling of non-stationary time series using adaptive methods*, November 14.

N. KOKSCH, Technische Universität Dresden, *Inertiale Mannigfaltigkeiten für nichtautonome Systeme*, December 4.

G. KOLIOS, Universität Stuttgart, Institut für Chemische Verfahrenstechnik, *Modellierung und Simulation mehrphasiger verfahrenstechnischer Systeme*, February 15.

V.A. KOLODKO, Russian Academy of Sciences, Novosibirsk, *Localization of deformation in the soil under the influence of an embedded element*, November 23.

D. KOLYMBAS, Universität Innsbruck, Austria, *Hypoplasticity*, November 27.

M. KONIK, Technische Universität Chemnitz, *Wavelet analysis of discrete data in traffic regulation*, July 19.

S. KOOPMAN, Vrije Universiteit Amsterdam, The Netherlands, *A simple and efficient simulation smoother for state space time series analysis*, May 9.

W. KÖSSLER, Humboldt-Universität zu Berlin, Institut für Informatik, *Nichtparametrische Lokationstests bei eingeschränkten Alternativen*, November 21.

P.S. KRASILNIKOV, Moscow State Aviation Institute, Russia, *On the integration of n-dimensional Monge-Ampere equation*, December 5.

G. KREMER, Federal University of Parana, Curitiba-Parana, Brazil, *Thermodynamic problems with slip and jump boundary conditions*, July 30.

A. KULIKOVSKY, Forschungszentrum Jülich, IWV-3, *The model of water transport in membrane of PEFC, including DMFC*, November 23.

P. LADE, Aalborg University, Denmark, *Instability, shear banding, and failure in granular materials*, November 23.

R. LANCELLOTA, Politecnico di Torino, Italy, *Soil porosity from wave propagation*, November 22.

T. LEDWINA, Technical University of Warsaw, Poland, *On data driven Neyman's tests*, May 23.

G. LEONOV, St. Petersburg University, Russia, *The Brockett stabilization problem for linear discrete control systems*, December 6.

E. LIEBSCHER, Technische Hochschule Ilmenau, *Mischungsbedingungen und geometrische Ergodizität von Zeitreihen*, May 16.

B. LINDNER, Humboldt-Universität zu Berlin, *Resonance phenomena in excitable systems driven by noise*, December 14.

M. LIPPI, Università di Roma, Italy, *Dynamic factor models: Representation, estimation, and forecast*, June 6.

W.G. LITVINOV, Universität Augsburg, Lehrstuhl für Angewandte Analysis mit Schwerpunkt Numerische Mathematik, *Problems on the flow of electro-rheological fluids*, July 11.

P.-Y. LOUIS, Université des Sciences et Technologies de Lille, France, *Parallel Markovian dynamics on lattice stationary measures, Gibbs measures and phase transition*, November 28.

S. LUCKHAUS, Universität Leipzig, *Nicht isotherme Phasenübergänge*, February 14.

S. LUDING, Universität Stuttgart, *Dense granular gases: Phase transitions, shock-waves and clustering*, July 31.

Y. MAISTRENKO, National Academy of Sciences of Ukraine, Kiev, *Stability of periodic clusters in globally coupled logistic maps*, October 11.

M. MALIOUTOV, Northeastern University, Boston, USA, *Estimation of parameters of the protein motion over the membranes, and the Multi Trajectory Estimation*, July 25.

C. MASCIA, Università di Roma, Italy, *Singular limits for conservation laws with source*, July 10.

R.M.M. MATTHEIJ, Technical University of Eindhoven, The Netherlands, *Mathematical problems inspired by glass modelling*, November 26.

K. MATTHIES, University of Oxford, UK, *Exponential homogenization of elliptic systems*, May 15.

F. MEIER, Universität Stuttgart, Institut für Chemische Verfahrenstechnik, *Modellierung des transmembranen Stofftransports in der DMFC und experimentelle Bestimmung von Modellparametern*, November 23.

D. MERCURIO, Humboldt-Universität zu Berlin, *Modelling the distribution of stock returns for Value-at-Risk purposes*, December 12.

F. MERKL, Universität Bielefeld, *Reconstructing a random scenery seen along a random walk path with bounded jumps*, December 5.

A. MIELKE, Universität Stuttgart, *Derivation and analysis of macroscopic, rate independent models for phase transformations in solids*, August 29.

K. MIKULA, Slovak University of Technology, Bratislava, *A direct method for solving an anisotropic mean curvature flow of plane curves with an external force*, December 6.

A. MOLINARI, Université de Metz, France, *Modeling of the dynamic response of porous viscoplastic materials*, July 31.

P. MORIN, Universidad Nacional del Litoral, Facultad de Ingenieria Quimica, Departamento de Matemática, Santa Fe, Argentina, *An adaptive Uzawa finite element method for Stokes: Convergence without the Inf-Sup*, July 10.

P. MÖRTERS, University of Bath, UK, *Eine multifraktale Analysis der super-Brownschen Bewegung*, December 19.

I. MÜLLER, Technische Universität Berlin, *Untersuchungen an CuAlNi-Einkristallen. Teil I*, May 30.

K.R. MÜLLER, Gesellschaft für Mathematik und Datenverarbeitung First and Universität Potsdam, *Techniken der Independent Component Analyse*, April 18.

W.H. MÜLLER, Heriot-Watt University, Department of Mechanical and Chemical Engineering, Edinburgh, UK, *Physikalische Begründung höherer Gradiententerme in Phasenfeldgleichungen und über den Ursprung von Oberflächenspannungen*, April 11.

——, *Toward quantitative modeling of microstructural changes by means of the phase field theory*, August 2.

W.H. MÜLLER, Technische Universität Berlin, *Atomistic determination of parameters of an extended Cahn-Hilliard model*, August 30.

A. MUSOLFF, Technische Universität Berlin, *Untersuchungen an CuAlNi-Einkristallen. Teil II*, May 30.

N. NEFEDOV, Moscow State University, Russia, *On new spectral problems arising in singularly perturbed reaction-diffusion systems*, April 24.

T. NEUMANN, Universität Dortmund, Fachbereich Chemietechnik, Lehrstuhl Energieprozesstechnik und Strömungsmechanik, *Modellierung von Mehrphasenströmungen mit Phasenwechsel in porösen Medien*, November 23.

H.-P. NOLTING, Heinrich-Hertz-Institut für Nachrichtentechnik Berlin, *Fast Equalizer, ein neues Bauelement für die optische Signalverarbeitung*, January 11.

T. OGAWA, Osaka University, Japan, *Mode interaction of periodic waves/patterns*, May 29.

M. OHLBERGER, Universität Freiburg, Institut für Angewandte Mathematik, *3D-Modellierung von PEM-Brennstoffzellen (Vorstellung eines geplanten Projekts)*, November 23.

R. OSER, Bayer AG, Krefeld, *Optische Datenspeicher: Speicherprinzipien und Materialeigenschaften*, April 2.

B. PARK, Seoul National University, Statistical Research Institute, Corea, *Local polynomial estimation of smooth boundaries*, July 11.

D. PELINOVSKY, McMaster University, Hamilton, Canada, *Matrix stability criterion for multicomponent optical solitons*, May 22.

M.F. PEREIRA, Universidade Federal da Bahia, Brazil, *Applications of a many body theory to optical properties of semiconductors*, April 9.

S.V. PEREVERZEV, National Academy of Sciences of Ukraine, Kiev, *Self-regularization of projection methods with a posteriori discretization level choice for severely ill-posed problems*, October 29.

——, *Adaptive inverse estimation of linear functionals from random noisy observations in Hilbert scales*, October 31.

A. POLITI, Humboldt-Universität zu Berlin, *Calcium oscillations in gap functions coupled cells*, February 22.

D. RACHINSKII, Institute for Information Transmission Problems, Moscow, Russia, *On existence of periodic solutions for autonomous ODEs*, June 5.

E. RADKEVICH, Moscow State University, Faculty of Mechanics and Mathematics, Russia, *On asymptotic solutions of phase field models*, June 11.

——, *Sharp interface limits of extended Cahn-Hilliard models*, August 31.

M. RAMASWAMY, Tata Institute of Fundamental Research, Bangalore, India, at present Universität Kaiserslautern, *Improved Hardy-Sobolev inequality and application to PDE*, July 19.

D. REITEBUCH, Technische Universität Berlin, *Reflexionen zur Relativitätstheorie*, January 31.

A. REUSKEN, Rheinisch-Westfälische Technische Hochschule Aachen, Institut für Geometrie und Praktische Mathematik, *Navier-Stokes equations in rotation form: A robust multigrid solver for the velocity problem (joint work with M.A. Olshanskii, Moscow State University)*, February 22.

D. REZNIK, J. KROPP, Infineon Technologies/Fiber Optics, Berlin, *Infrarot VCSEL für optische Nachrichtentechnik*, June 11.

M. RHEINHARDT, Astrophysikalisches Institut Potsdam, *Magnetfeldzerfall in massiven Sternen unter dem Einfluss des Hall-Effekts*, April 19.

R. RICHTER, MPI Halbleiterlabor, München, *Entwicklung von Silizium-Strahlungsdetektoren für Hochenergie- und Astrophysik*, June 25.

U. RODEMERCK, Institut für Angewandte Chemie Berlin Adlershof e.V., *Katalysatorscreening, -charakterisierung, Mechanismus und Kinetik der anodischen Umsetzung von Methanol*, November 23.

V. ROM-KEDAR, The Weizmann Institute of Science, Rehovot, Israel, *Chaotic fluid mixing*, November 6.

J.-U. SCHEER, Johannes Gutenberg-Universität Mainz, *A new beginning approach for fast kernel smoothing*, December 5.

G. SCHIMPERNA, Università di Pavia, Italy, *Existence and asymptotic results for some nonlinear Cahn-Hilliard-like equations*, August 30.

S. SCHMAUDER, Universität Stuttgart, *Hierarchische Werkstoffmodellierung am Beispiel der schädigungsmechanischen Auswirkung von Cu-Ausscheidungen in Stählen*, February 12.

B. SCHMITHÜSEN, Swiss Federal Institute of Technology in Zurich, Integrated Systems Laboratory, Switzerland, *Gitter-Adaption basierend auf lokalen Fehler-Abschätzungen der Dissipationsrate für die Halbleiter-Bauelement-Simulation*, February 1.

T. SCHULTZ, Max-Planck-Institut für Dynamik komplexer technischer Systeme, Magdeburg, *Steady-state and dynamic process behaviour of DMFCs — A concept for systematic modeling*, November 23.

A. SCHUPPERT, Bayer AG, Leverkusen, *Structured hybrid modelling — Mathematics as key technology for process analysis and optimization*, January 22.

G. SELL, University of Minnesota, Minneapolis, USA, *WIAS SPECIAL GUEST LECTURE: What is this attractor we call climate modelling?*, March 9.

——, *WIAS SPECIAL GUEST LECTURE: Systems of delay equations with feedback: Longtime dynamics and numerical computation. Part I*, March 13.

——, *WIAS SPECIAL GUEST LECTURE: Systems of delay equations with feedback: Longtime dynamics and numerical computation. Part II*, March 16.

M.J. SETZER, Universität-Gesamthochschule Essen, *Die Mikro-Eislinsen-Pumpe — Das Stabilitätskriterium für 3 Phasen in porösen Medien und damit verbundene Transportphänomene*, March 19.

T. SHAPOSHNIKOVA, University of Linköping, Sweden, *Sobolev multipliers and their applications to nonsmooth elliptic theory*, February 21.

——, *Pointwise interpolation inequalities for derivatives and their applications in analysis*, August 15.

E. SHCHEPAKINA, Samara State University, Russia, *Canards and black swans in combustion*, October 25.

K. SHCHETININA, Samara State University, Russia, *One problem on the change of stability of the integral manifolds*, January 25.

L. SHILNIKOV, Institute for Applied Mathematics and Cybernetics, Nizhny Novgorod, Russia, *Mathematical problems of synchronization*, November 29.

K.G. SIEBERT, Albert-Ludwigs-Universität Freiburg, Fachbereich Mathematik, *Konvergieren adaptive Finite-Elemente-Methoden?*, March 29.

A. SIEBKE, Universität Stuttgart, DLR-ITT, *Modellbildung und Simulation von Stofftransport und Reaktion in der l-DMFC*, November 23.

I.V. SKRYPNIK, National Academy of Sciences of Ukraine, Donetsk, *On a topological approach to nonlinear equations with strong growth of coefficients*, July 25.

A. SKUBACHEVSKII, Moscow State Aviation Institute, Russia, *Nonlocal elliptic problems*, March 28.

——, *Feller semigroups*, December 6.

F. SMITH, University College, Department of Mathematics, London, UK, *Fluid flows through branching tubes*, August 30.

J. SOKOŁOWSKI, Université de Nancy I, France, *Optimality conditions for simultaneous topology and shape optimization*, April 2.

M. STERNBERG, Universität Paderborn, *Tight-Binding-Lösungen zur Dichtefunktionaltheorie*, May 16.

A. STEVENS, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, *Stochastische und deterministische Modelle für die Bewegungsdynamik selbstorganisierender Mikroorganismen*, May 21.

G. STOYAN, Eötvös Loránd University, Department of Numerical Analysis, Budapest, Hungary, *Auf dem Weg zu einer algebraischen Vektoranalysis*, July 12.

H. STRUCHTRUP, University of Victoria, Canada, *Heat transfer in the transition regime: Temperature jumps and boundary layers computed with Grad's moment method*, July 30.

V. STYLES, University of Sussex, Falmer, UK, *Numerical simulations of diffusion induced grain boundary motion*, August 30.

J. SWART, Technische Universität Berlin, *Renormalization of models with catalytic resampling*, January 24.

J. SYMANZIK, Utah State University, USA, *A course on web-based statistics*, July 11.

T. SZÁNTAI, Technical University of Budapest, Hungary, *Probabilistic constrained programming and AMPL*, February 5.

P. TAKAĆ, Universität Rostock, *Langzeitverhalten positiver Lösungen von analytischen Gradientensystemen*, May 8.

F. THEIL, University of Warwick, Warwick, UK, *From atomistic to continuum models: The Cauchy-Born rule*, August 29.

L. TRUSKINOVSKI, University of Minnesota, Minneapolis, USA, *Elastic crystals with a triple point*, August 2.

——, *Mathematical models of sceletal muscles: Stability and hysteresis*, August 8.

——, *Self heating in a bi-stable chain*, August 10.

J. TÓTH, Budapest University of Technology and Economics, Hungary, *Kinetic properties and lumping*, February 22.

Ł. TURSKI, Polish Academy of Sciences, Warsaw, *On metriplectic dynamics with Dirac-like constraints*, August 2.

C. VAN DUIJN, Technical University of Eindhoven, The Netherlands, *Application of Caffarelli's regularity theory to a two-phase free boundary problem*, July 25.

E. VERBITZKIY, EURANDOM, Technical University of Eindhoven, The Netherlands, *Mathematical modelling of rechargeable batteries: Simulation, optimisation and model reduction: Part I*, November 22.

——, *Mathematical modelling of rechargeable batteries: Simulation, optimisation and model reduction: Part II*, November 23.

M. VISHIK, University of Texas, Austin, USA, *Incompressible flows of an ideal fluid with unbounded vorticity*, July 24.

A. VISINTIN, Università di Trento, Italy, *Vector ferromagnetic hysteresis and Maxwell's equations*, August 1.

H.J. WAGNER, Universität Paderborn, FG 6 — Theoretische Physik, *Das inverse Problem der Variationsrechnung in der Hydrodynamik*, March 15.

N.J. WALKINGTON, Carnegie Mellon University, Department of Mathematical Sciences, Pittsburgh, USA, *Mathematical models of fluids with structure*, June 26.

U. WEIKARD, Rheinische Friedrich-Wilhelms-Universität Bonn, *Finite element approximation of the Cahn-Hilliard equation*, August 30.

W. WENDLAND, Universität Stuttgart, *Mathematical models for the solid-liquid separation of suspensions*, July 31.

A. WERWATZ, R. SCHULZ, Humboldt-Universität zu Berlin, Institut für Wirtschaftswissenschaften, *A space model for Berlin house prices*, January 24.

S. WIECZOREK, Free University of Amsterdam, The Netherlands, *Multipulse excitability in a diode laser with optical injection*, December 14.

M. WOLFF, Universität Bremen, *Zur Thermoelasto-Plastizität mit Phasenumwandlungen und Umwandlungsplastizität bei Stählen*, June 6.

H.-J. WÜNSCHE, Humboldt-Universität zu Berlin, *Two-mode excitability: Theory and experiment*, December 14.

J. XIONG, University of Tennessee, Knoxville, USA, *Stochastic differential equations in infinite dimensional spaces*, June 20.

M. YAMAMOTO, University of Tokyo, Japan, *Some uniqueness results for inverse elliptic problems*, May 9.

——, *Identification of coefficients in Maxwell's equations and the Lamé system*, August 17.

S. YANCHUK, National Academy of Sciences of Ukraine, Kiev, *Loss of synchronization in coupled Rossler systems*, November 23.

M. YOUSEFI, Free University of Amsterdam, The Netherlands, *Laser with filtered feedback*, November 8.

S. ZELIK, Moscow State University and Russian Academy of Sciences, Institute for Problems of Transmission, *Temporal averaging of regular attractors associated with reaction-diffusion equations with rapidly oscillating terms*, May 5.

J. ZHENG, Humboldt-Universität zu Berlin, Institut für Wirtschaftswissenschaften, *Implied binomial trees*, October 24.

S. ZHENG, Fudan University, Shanghai, China, *The Cahn-Hilliard equation with dynamic boundary condition*, July 18.

S. ZWANZIG, University of Uppsala, Sweden, *On the application of nonlinear error-in-variables models in astronomy*, December 19.

6.11 Membership in Organizing Committees of non-WIAS Meetings

E. BÄNSCH, member of the Local Organizing Committee, *First SIAM-EMS Conference "Applied Mathematics in our Changing World"*, Berlin, September 2–6.

A. BOVIER, member of the Organizing Committee, *Meeting "Stochastics in the Sciences"*, Mathematisches Forschungsinstitut Oberwolfach, March 11–17.

——, member of the Organizing Committee, *Meeting "Stochastic Models from Statistical Physics"*, Blaubeuren, April 1–6.

——, member of the Organizing Committee, *Miniworkshop: Aging and Glassy Systems*, Mathematisches Forschungsinstitut Oberwolfach, August 19–25.

R. HENRION, co-organizer, *DECHEMA continuation course "Optimierung verfahrenstechnischer Prozesse"*, Technische Universität Berlin, September 24–26.

R. HENRION, A. MÖLLER, member of the Local Organizing Committee, *9th International Conference on Stochastic Programming*, Humboldt-Universität zu Berlin, August 25–31.

K.R. SCHNEIDER, organizer of the minisymposium "Mathematical Modelling of Semiconductor Lasers" (together with B. Krauskopf, University of Bristok, UK), *First SIAM-EMS Conference "Applied Mathematics in our Changing World"*, Berlin, September 2–6.

J. SPREKELS, member of the Steering Committee, *Symposium on Hysteresis and Micromagnetics Modeling (HMM'01)*, The George Washington University, Virginia Campus, Ashburn, Virginia, USA, May 21–23.

——, member of the Local Organizing Committee, *First SIAM-EMS Conference "Applied Mathematics in our Changing World"*, Berlin, September 2–6.

——, member of the Advisory Board, *Research Symposium "Energiebedarf, Energieeffizienz und Energiebereitstellung"*, Haus der Deutschen Wirtschaft, Berlin, October 1–2.

W. WAGNER, member of the Organizing Committee, *Miniworkshop: Stochastic Models for Coagulation Processes*, Mathematisches Forschungsinstitut Oberwolfach, August 19–25.

6.12 Software

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/research/groups/nummath/projects/project1

`ClusCorr98`® (contact: H.-J. Mucha, phone: +49 30/20372-573)
The statistical software `ClusCorr98`® performs exploratory data analysis mainly by using adaptive methods of cluster analysis, classification, and multivariate graphics. Typically it aims at the extraction of knowledge from huge samples of numerical and alpha-numerical data. Some of the methods are: model-based cluster analysis, hierarchical clustering, principal components analysis, correspondence analysis.
The software `ClusCorr98`® is written in Visual Basic for Applications (VBA), formerly Excel's exclusive programming language. Meanwhile VBA is based on object models of various Microsoft Office applications. `ClusCorr98`® runs under Microsoft Windows taking advantage of the Excel environment.
Please find further information under: http://www.wias-berlin.de/products/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/cog.

DiPoG, Direct and Inverse Problems for Optical Gratings (contact: G. Schmidt, phone: +49 30/20372-456)
The program package 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. 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/research/projects/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/~gltools.

LDSL-tool (Longitudinal Dynamics in Semiconductor Lasers) (contact: M. Radziunas, phone: +49 30/20372-441)
LDSL 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 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.

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/~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 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/~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 2-d 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. 163) supported by the BMBF.
Please find further information under: http://www.wias-berlin.de/research/projects/sic#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.

`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/products/tesca.

WIAS-QW and **WIAS-KPLIB** (contact: U. Bandelow, phone: +49 30/20372-471)
WIAS-QW in combination with *WIAS-KPLIB* 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, KPLIB 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, 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.

6.13 Third-party Funds

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)

Deutsche Forschungsgemeinschaft (German research association), Bonn

- 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, FG 1, 2)

  "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)

[1] research group

- 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)

  “Stochastische Partikelsysteme als numerische Verfahren für Probleme der Aerosoldynamik” (Stochastic particle systems as numerical tools for problems in aerosol dynamics, 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: “Echtzeitoptimierung großer Systeme” (Real-time optimization of large systems)

  “Optimierung integrierter Kolonnensysteme unter stochastischen Echtzeitbedingungen” (Real-time optimization of distillation columns under probabilistic constraints, FG 4)

- Priority Program: “Analysis und Numerik von Erhaltungsgleichungen” (Analysis and numerics for conservation laws)

  “Kinetische Behandlung von ausgewählten Anfangs- und Randwertproblemen” (Kinetic treatment of selected hyperbolic initial and boundary value problems, FG 7)

  “Randbedingungen sowie Mehrdeutigkeit und Stabilität von Lösungen in der Erweiterten Thermodynamik” (Boundary conditions, ambiguities and stability of solutions in extended thermodynamics, FG 1)

- 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)

  “Mehrskalenmodelle thermomechanischer Körper” (Multiscale models of thermomechanical bodies, 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 system and a Schrödinger-Poisson system 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)

"Inverse Modellierung von Strömungs- und Transportvorgängen im heterogenen Untergrund auf der Basis von Mehrgitterverfahren" (Inverse modeling of flow and transport in a heterogeneous subsurface with multigrid methods, FG 4)

"Finite-Integrations-Methode mit Tetraedergitter zur elektromagnetischen Simulation von Mikrowellenschaltungen" (Electromagnetic simulation of microwave circuits using finite integration technique with tetrahedral grids, FG 3)

- Graduate College, Technische Universität Berlin
  "Stochastische Prozesse und Probabilistische Analysis" (Stochastic processes and probabilistic analysis, FG 5, 6)
- Graduate College, Humboldt-Universität zu Berlin
  "Angewandte Mikroökonomik" (Applied microeconomics, FG 6)
- 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)
- Scientist exchange with Turkmenistan (FG 6)

Alexander von Humboldt-Stiftung (Alexander von Humboldt Foundation)

- 1 Humboldt Laureate (FG 2) and 2 scholarship holders (FG 6, 7), see page 222

International Projects

- **(EU) HCM:** "Stochastic Analysis" (FG 5)
- **(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)
- **(EU) TMR:** “Breakthrough in the control of nonlinear systems” (FG 2)
- **NATO Linkage Grant:** “Stochastic modelling of aerosol particle transport and reacting pollutants in the atmosphere” (FG 6)

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, Baden, Switzerland: “Prozesssimulation bei Kraftwerksanlagen” (Power plant process simulation, FG 3)
- Bankgesellschaft Berlin AG: “Monte Carlo Simulation” (FG 6)
- BAYER AG, Leverkusen: Expert opinion “Optimale Stützstellenwahl bei multivariaten Problemen” (Optimal design points for multivariate problems, FG 6)
- Bundesanstalt für Materialforschung und -prüfung, Berlin: “Statistisch-methodische Verfahrensentwicklung zur Zertifizierung von Referenzmaterialien” (Statistical methods for certification of reference materials, FG 6)
- Carl Zeiss, Oberkochen: Study (FG 4)
- 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)
- 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)
- MergeOptics GmbH, Berlin: “Simulation und Optimierung von MQW-Lasern” (Simulation and optimization of MQW lasers, FG 1)
- Science & Tec, Paris, France: “Sur la methode CIRCÉ” (FG 5)
- Technical University of Delft, The Netherlands, Project NWO: “LIBOR interest rate models, interest rate derivatives and model calibration” (FG 6)

- a South German software company for production planning: “Bahnplanung für Industrieroboter und Menschmodelle” (Path planning for robots and human models, FG 4)

Advanced training courses

- Haus der Technik, Essen: “Seminar Angewandte Statistik” (Seminar on applied statistics, for engineers, FG 6)
- 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)

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