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1 Abstracts of Invited Talks

Alfio Quarteroni

Mathematical and Numerical Modelling of the Cardiovascular System

Topic: 1.0

The interest in the use of mathematical modelling and numerical simulation in the study of the cardiovascular system (and its inherent pathologies) has greatly increased in the past few years. Blood flow interacts mechanically and chemically with vessel walls producing a complex fluid-structure interaction problem, which is practically impossible to simulate in its entirety.

Several reduced models have been developed which may give a reasonable approximation of averaged quantities, such as mean flow rate and pressure, in different sections of the cardiovascular system. They are, however, unable to provide the details often needed for understanding a local behavior, such as, e.g., the effect on the shear stress distribution due a modification in the blood flow consequent to a partial stenosis.

In this talk we address some mathematical issues arising from the modelling of the cardiovascular system through problems of different complexity. The most complex model is based on the coupling of the Navier-Stokes equations with structural models for the vessel walls. An intermediate model is derived from integrating these equations on a section of a vessel geometry, and it is formed by a system of hyperbolic equations for the evolution of mean pressure and flow rate. An even simpler model that will be considered is based on the solution of a system of ordinary differential equations which describe electrical networks.

The derivation of these models will be presented together with schemes for their numerical solution. Furthermore, we will specifically address the coupling problem, analyzing different possible strategies.

These techniques may be extended by including models for chemical transport. Some results in this direction are already available and will be presented.

The previous multi-scale approach looks a viable solution to obtain detailed numerical simulation of sections of the cardiovascular apparatus, while properly accounting for the presence of the global system. We expect that this technique will open new possibilities for the use of numerical modelling for medical research.

Michael S. Waterman

DNA Sequence Assembly Using Eulerian Graphs

Topic: 2.0

The standard approaches to assembling DNA sequence from randomly located and randomly oriented reads use “overlap-layout-consensus.” Existing algorithms make assembly errors and there is much difficulty with resolving repeats. The sequencing machine errors are easily mistaken for mutations or mutations mistaken for sequencing errors. In this talk I will give some historical perspective and then present the reduction of fragment assembly to a variation of the classical Eulerian path problem.

S. Jonathan Chapman

Models for Superconducting Thin Films

Topic: 3.0

Because of their relative ease of fabrication, many experiments on and applications of superconducting materials are performed with thin films. It is attractive mathematically to try and take advantage of the small aspect ratio of the sample by formulating a thin film model valid asymptotically in the limit as the thickness tends to zero.

In formulating this limit different models arise depending on the relative scaling of the aspect ratio with various other parameters present in the model for bulk superconductors. The talk will survey some of these different limits, showing where existing thin film models fit into the hierarchy and filling in some of the gaps.

If there is time, analogies with models of thin films of micromagnetic materials will be explored.

Andrew J. Majda

New Perspectives on Atmosphere/Ocean Science Through Modern Applied Mathematics

Topic: 4.0

Several important contemporary problems in atmosphere/ocean science for short term climate will be described as well as current emerging strategies to look at them through modern applied mathematics.

Michael Griebel

On the Numerical Simulation of the Material Properties of Nanotubes

Topic: 5.0

Carbon nanotubes are cylindrically rolled-up graphite sheets. Their diameter is about a few nanometers but their length can be in the micrometer range.

They show unique material properties: Their strength under tensile stress is about 200 times that of steel but their weight is substantially less. Furthermore, depending on their chiral angle, carbon nanotubes can show metallic or semi-conducting behavior. These properties make them interesting for a wide range of nano-technological applications. However, the investigation of the material properties of nanotubes in laboratory experiments is very difficult. To this end, large scale numerical simulations on parallel supercomputers are an important tool to gain further insight.

We study nanotubes on two different scales: On the quantum mechanical level we developed a parallel ab-initio code based on density functional theory with a plane wave basis set. Here, we report on the results of our experiments on the hydrogen storage properties of carbon nanotube bundles and on nanotubes and their caps made from boron-nitride. On the classical level we apply molecular dynamics to the nuclei. To obtain realistic results we use the bond-order potential due to Brenner. This is a generalization of the potential for silicon due to Abell and Tersoff which tries to take quantum effects for hydrocarbons as good as possible into account.

Based on it, we implemented a parallel algorithm for nanotube simulation. We present our results for different types of nanotubes. Depending on the chiral angle, nanotubes exhibit an elasticity modul of up to 1 TPa under tensile loading which is similar to that of diamond. Furthermore we show a comparison of the material properties of boron-nitride and carbon nanotubes. It turns out that boron-nitride tubes are even stronger by about a factor of two. We also consider fullerenes encapsulated in nanotubes, the so called peapods, and compare their material properties with standard nanotubes.

Finally, we study nanotubes as fibers to mechanically reinforce polymers. This leads to new and extremely durable composite materials. We investigate the load transfer mechanism between the polymer and the nanotube for model polyethylene matrices and epoxy matrices

Martin Grötschel

Designing Telecommunication Networks: Challenges for Integer Programming

Topic: 6.0

This talk will begin with a survey of mathematical challenges that arise in telecommunication. Mathematics is involved, e. g., in the design and manufacturing of chips, devices and network components, the choice of locations, the planning of the network topology, and the dimensioning of the equipment involved. Adequate cryptography, the need of fast data processing, demand routing and failure handling require efficient and reliable mathematical algorithms on the operational side.

The focus of the presentation will be on the problem of designing low-cost telecommunication networks that provide sufficient capacity to serve a given demand, are based on a certain technology mix, satisfy technical side constraints, and survive certain failure situations. This problem is difficult in theory and practice. It will be indicated how algorithms integrating polyhedral combinatorics, linear and integer programming, and various heuristic ideas can help solve real-world instances within reasonable quality guarantees in acceptable running times.

This talk is based on work of the telecommunications research group at ZIB, the examples discussed and the computational results reported are from joint projects with various telecommunication companies.

Kai Nagel

Large Scale Multi-Agent Transportation Simulations

Topic: 7.0

It is now possible to micro-simulate the traffic of whole metropolitan areas with 10 million travelers or more, “micro” meaning that each traveler is resolved individually as a particle. In contrast to physics or chemistry, these particles have internal intelligence; for example, they know where they are going. This means that a transportation simulation project will have, besides the traffic microsimulation, modules which model this intelligent behavior. The most important modules are for route generation and for demand generation. Demand is generated by each individual in the simulation making a plan of activities such as sleeping, eating, working, shopping, etc. If activities are planned at different locations, they obviously generate demand for transportation. This however is not enough since those plans are influenced by congestion which initially is not known. This is solved via a relaxation method, which means iterating back and forth between the activities/routes generation and the traffic simulation.

Benoit B. Mandelbrot

Prices, Fractals, and a Frontier of Applied Mathematics: Wild Variability

Topic: 8.0

The speaker will begin by sketching his new model of financial price variation, based on scale invariance and multifractals. He will continue by noting that one broad reason for this model's effectiveness and "creativity" resides in the fact that many of the basic limit theorems of probability are invalid. As a result, this and other fractal or multifractal models exemplify what the speaker calls the "wild state of randomness," a notion that he will describe. Wild fluctuations (e.g., "$1/f$ noises") are ubiquitous and play key roles in many fields of nature or culture. They prove difficult to reduce to other known facts, require new techniques of analysis, and altogether will be shown to represent a wide open and very attractive frontier of the sciences, therefore of applied mathematics.

Pietro Perona

Representation and Learning for Visual Object Recognition

Topic: 9.0

Recognizing objects in images is one of the most important functions of our visual system. Not only can we recognize individual objects, such as the Eiffel Tower or our grandmother's face, but also classes of objects, such as shoes, automobiles and frogs. I will first explore the key difficulties in visual recognition. I will then propose ideas on a class of 'constellation' models that may explain visual recognition. In the second part of my talk I will address the problem of how these models may be trained automatically in realistic conditions. Can a child, or a machine, learn to recognize 'faces' and 'cars' only by looking? Everyday images are cluttered and may not contain explicit information on the presence, location and structure of new objects making this a difficult problem.

I will propose a theory of how constellation models may be learned without supervision from collections of unsegmented cluttered images containing examples of a small number of object categories.

Thomas Y. Hou

Singularity Formation in Three Dimensional Vortex Sheets

Topic: 10.0

One of the classical examples of hydrodynamic instability occurs when two fluids are separated by a free surface across which the tangential velocity has a jump discontinuity. This is called Kelvin-Helmholtz instability. Kelvin-Helmholtz instability is a fundamental instability of incompressible fluid flow at high Reynolds number. The idealization of a shear layered flow as a vortex sheet separating two regions of potential flow has often been used as a model to study mixing properties, boundary layers and coherent structures of fluids. It is well known that small initial perturbations on a vortex sheet may grow rapidly due to Kelvin-Helmholtz instability. The problem is ill-posed in the Hadamard sense. Most analytical studies of vortex sheet singularity to date rely heavily on complexifying the interface variables. It is not clear how to generalize this technique to 3-D vortex sheets in a natural way.

In a joint work with G. Hu and P. Zhang, we study the singularity of 3-D vortex sheets using a new approach. First, we derive a leading order approximation to the boundary integral equation governing the 3-D vortex sheet. This leading order equation captures the most singular contribution of the integral equation. Moreover, after applying a transformation to the physical variables, we found that this leading order 3-D vortex sheet equation de-generates into a two-dimensional vortex sheet equation in the direction of the tangential velocity jump. This rather surprising result confirms that the tangential velocity jump is the physical driving force of the vortex sheet singularities. We show that the singularity type of the three-dimensional problem is similar to that of the two-dimensional problem. Moreover, we introduce a generalized Moore's approximation to 3-D vortex sheets. This model equation captures the same singularity structure of the full 3-D vortex sheet equation, and it can be computed efficiently using Fast Fourier Transform. This enables us to perform well-resolved calculations to study the generic type of 3-D vortex sheet singularities. We will provide detailed numerical results to support the analytic prediction, and to reveal the generic form of the vortex sheet singularity. We will also discuss the possible implication of our 3-D vortex sheet results on the shear flow instability in 3-D Euler and Navier-Stokes equations.

2 Abstracts of Minisymposia Talks

2.1 Medicine

MS38 Tissue Modelling - Simulation and Visualization
Organized by: Martin Brokate, Markus Gross, Hans-Christian Hege

Topic: 1 Medicine
Computer aided surgery planning and simulation is a rapidly evolving research field that is going to alter dramatically the way surgeons practice their art. One of the major challenges lies in the modeling of the behaviour of hard and soft tissue bringing together researchers from computer science, engineering, mathematics and medicine. Our minisymposium addresses issues related to biomechanical, in particular elastomechanical models for bones and soft tissues with some emphasis on craniofacial surgery applications. Topics include constitutive theory, the numerical solution of the corresponding partial differential equations, grid generation, and the design of surgical simulators. In addition, we discuss advanced visualization and 3D interaction methods that constitute an indispensible toolset for the management of all stages of complex surgical planning processes. This includes image segmentation, 3D reconstruction, numerical simulation and virtual surgery. The presentations will be given by a selection of experienced researchers in the field covering a broad range of the aforementioned topics.

Evgeny Gladilin, Stefan Zachow, Hans-Christian Hege, Peter Deuflhard

A Biomechanical Model for Soft Tissue Simulation in Craniofacial Surgery
In surgical planning postoperative appearance of the patient is an important criterion additional to functional aspects. This applies especially in craniofacial surgery. Reliable methods for realistic soft tissue prediction, sometimes including mimics, therefore are needed. Physically based models seem to be most suited for realistic results. However, the mechanical properties of biological tissues and anatomical structures are highly complex and scarcely investigated. Thus simplified models have to be applied. In this talk we describe our software frame work for cranio-maxillofacial surgery planning which offers 3D image segmentation, model creation, 3D planning and numerical simulation in an integrated way. Specifically we will describe our FE-based modeling approach for static soft tissue prediction and muscle simulation. First results of muscle-based simulations of facial mimics will be presented.

Andreas Hinz, Christian Clason, I. Hansen, R. Schreittmiller, H. Schieferstein, H. Deppe, A. Neff, H.-F. Zeilhofer

Simulation of the Mechanical Behavior of the Human Mandible
A mathematical model is developed to support planning in cranio-maxillofacial surgery. It takes into account the complex geometry of the individual mandible which has to be recovered from medical image data by segmentation and grid generation. The equations of linear elasticity are employed to determine displacement and stress under specific boundary conditions representing physiological situations arising from masticatory exercises. In addition to these boundary conditions, various assumptions are made for the material properties of the bone. Starting from a linear, homogeneous, isotropic behavior, several refinements leading to a composite of multiple, inhomogeneous, anisotropic materials have to be made in order to represent the genuine mechanical properties of living bone accurately. The resulting boundary value problem is numerically solved by the mathematical method of finite elements. For the implementation, the FE-environment FeliCs, developed at our research unit, was chosen because it provides the necessary flexibility. Special attention is paid to the experimental verification of the computational results. To this end, a special-purpose biomechanical test stand was designed and realized. It allows for contact-free measurements of arbitrarily defined dynamic load cases on plastic models or cadaveric human mandibles. Experiment and simulation are compared for a number of test cases.

Udo Nackenhorst

Constitutive Formulation and Numerical Simulation of Stress Adaptive Bone Remodeling
In this presentation existing theories of stress adaptive bone remodeling are compared and open questions are formulated first. Thereafter, a thermodynamically consistent constitutive theory for the stress adaptive bone remodeling in the sense of a mechanically - biologically two-field problem will be presented in detail. This theory of biomechanical equilibrium enables the restriction of constitutive parameters. Additionally, an extension of the constitutive model to an-isotropic bone remodeling will be given. For the numerical simulation the governing partial differential equations are discretized by finite element approximation. To avoid the well-discussed problem of checkerboard pattern super-convergent projection techniques are suggested, thus, stable and efficient algorithms are available today. Additionally, the performance of the simulation procedure can be increased by use of return

mapping algorithms, which are well known from the treatment of problems of plasticity. First results will illustrate the capability of the proposed approach. An outlook is given for future developments and tendencies of stress adaptive bone remodeling. As one example, here, the individual therapy by combining the simulation of stress adaptive more remodeling with image giving diagnosis will be discussed. Literature: 1. Nackenhorst, U.: Numerical simulation of stress stimulated bone remodelling, Technische Mechanik 17, 1, 1997, 31-40. 2. Krstin, N., Nackenhorst, U. und Lammering, R.: Zur konstitutiven Beschreibung des anisotropen beanspruchungsadaptiven Knochenumbaus, Technische Mechanik 20, 1, 2000, 31-40.

Martin Roth, Markus H. Gross

Technical Aspects in the Implementation of a Cranio-Maxillofacial Surgery Simulator

Computer assisted planning of cranio-maxillofacial surgical procedures aims at the prediction of changes on the facial surface prior to actual surgery. In the design of such a surgical simulator, various aspects have to be paid attention to: beside the choice of a mathematical model and the numerical solution of the inherent partial differential equations, the actual implementation of the prototype raises a great number of problems. In this talk, we will put emphasis on the practical aspects of simulator design. We will elaborate on topics concerning the implementation of a prototype used to evaluate the mathematical model, its discretization and the solution. This includes but is not restricted to the registration of datasets (e.g. CT volume data and laser range scans), the meshing of the tissue, bone cutting and realignment corresponding to actual surgery as well as the visualization and evaluation of simulation results.

MS33 Mathematical Models for Infectious Diseases

Organized by: Klaus Dietz, Horst Thieme

Topic: 1 Medicine

The minisymposium will present an overview of recent results in the field of mathematical epidemiology. Speakers and titles of their talks: Klaus Dietz, University of Tuebingen: Within-host models of malaria Andrea Pugliese, University of Trento: Models for competition among parasite strains and virulence evolution Michael Li, University of Alberta: Global stability problems in SEIR epidemic models Zhilang Feng and H. R. Thieme, University of Arizona: Endemic models with arbitrarily distributed periods of infection.

Klaus Dietz

Within-host models of malaria

Intra-host models of Plasmodium falciparum, one of mankind's main killers are reviewed. A new mathematical model of asexual parasitaemia is formulated and fitted to 35 spontaneously cured malariatherapy cases. The simulated courses of parasitaemia are more realistic than any previously published. The model uses a discrete time step of two days. Its realistic behaviour was achieved by the following combination of features: (i) intra-clonal antigenic variation; (ii) large variation of the baseline growth rates among variants within and between cases; (iii) innate case-specific regulation of the asexual parasite density; (iv) acquired variant-specific immunity; (v) acquired variant-transcending immunity, variable among cases. Some implications for pathogenesis and control are discussed.

A fraction of the asexual parasites develops into gametocytes. We present estimates of the conversion probability from asexual parasites to circulating gametocytes and of the gametocytes' sequestration and circulation times, obtained for the first time by fitting a dynamic model to the individual patients' histories (daily records of 113 neurosyphilitic patients undergoing malariatherapy). The model assumes that the conversion probability can vary among the successive waves of asexual parasitaemia of a patient, and that gametocytes die at an age-dependent rate which increases under high asexual parasite densities.

Andrea Pugliese

Models for competition among parasite strains and virulence evolution

Bremermann and Thieme proved that, if different parasite strains give hosts complete cross-immunity, only one could persist. If a trade-off is assumed between virulence and transmissibility of parasites, the surviving strain will be at an intermediate level of virulence. On the other hand, if it is assumed that a host already infected with one strain may become infected by another strain (superinfection), parasite coexistence becomes possible. I explore here the dynamical behaviour of different variants of these models, finding conditions for parasite coexistence at equilibrium and along periodic solutions. An important question concerns parasite evolution, when new strains may arise by mutation. In the approach of 'adaptive dynamics', mutations are assumed to be rare, and evolutionary dynamics can be understood through the 'invasibility' conditions; the existence and the properties of an evolutionary stable state depend on details of the function relating virulence to superinfection rates. In a different approach, mutations are described explicitly through a diffusion operator. One then obtains a reaction-diffusion equation in the space of viral types which has a unique stationary state (corresponding to the principal eigenfunction of a Schrödinger equation) the properties of which will be compared to the predictions of 'adaptive dynamics'.

Michael Li

Global stability problems in SEIR epidemic models

In this talk, I will present some recent methods and techniques for proving global stability of equilibria in general systems of ODE's and some applications to epidemic models.

Horst R. Thieme, Zhilang Feng

Endemic Models with Arbitrarily Distributed Periods of Infection

A model is developed and analyzed for the spread of an infectious disease which allows for arbitrarily many stages of infection all of which have general length distributions and disease mortalities. If the disease dynamics are much faster than the demographic dynamics, the different time scales make it possible to find explicit formulas for the inter-epidemic period (distance between peaks or valleys of disease incidence) and the local stability or instability of the endemic equilibrium.

It turns out that the familiar formula for the length of the inter-epidemic period of childhood diseases has to be re-interpreted when the exponential length distribution of the infectious period is replaced by a general distribution. The relevant parameter is not the average length but the average expectation of remaining sojourn. Using scarlet fever in England and Wales, 1897-1978, as an example, it is illustrated how different assumptions for the length distributions of the exposed and infectious periods (under identical average lengths) lead to quite different values for the minimum length of a quarantine period to destabilize the endemic equilibrium.

MS36 Cardiovascular and Respiratory Modelling

Organized by: Franz Kappel, J. T. Ottesen

Topic: 1 Medicine

The minisymposium is devoted to modeling efforts which consider the cardiovascular respectively respiratory system from a global point of view with special emphasis on the basic control mechanisms. A typical model considered in the presentations will be a compartment model for averaged quantities (pressures, concentrations etc.) over one heart beat resp. one breath.

Jerry Batzel, S. Timischl, F. Kappel

Modeling the Human Cardiovascular-Respiratory Control System with two State Delays: An Application to Congestive Heart Failure

In this paper we consider a model of the human cardiovascular-respiratory control system with one and two transport delays in the state equations of the respiratory system. The effectiveness of the respiratory control system is influenced by such transport delays. The interplay between heart rate, blood pressure, cardiac output, and blood vessel resistance in cardiovascular control is quite complex. Many physiologists assume that optimization is a basic concept in the evolution of biological systems (see, e.g., Swan 1984) and we will apply optimal control theory in the model control design. Short term cardiovascular control delays are not included.

We will first consider the combined cardiovascular-respiratory control using an optimal control approach with one transport delay between respiratory compartments. We will then consider the effects of a second delay in the state space by modeling the respiratory control via an empirical formula with delay. This second delay is associated with the sensory system of the respiratory control and plays an important role in respiratory stability. The cardiovascular control will still be modeled as an optimal control. Application of this model will include the transition from the quiet awake state to stage 4 sleep in congestive heart failure.

Johnny T. Ottesen, Gerrit J. Noordergraaf, Abraham Noordergraaf

Respiratory Mechanical Effects on Blood Circulation

Several investigators have reported observations in which the ration of the heart frequency to the respiratory frequency proved to be small integer numbers. These were found in humans as well as in warm blooded animals. They occurred primarily in healthy normal subjects during deep sleep. The ratio was reported to vary widely, from as low as 2 to as high as 7, with a preference for 3 and 4 in human [1].

Donders proposed in 1856 that the 'respiratory pump' assists the circulation of blood through a valveless mechanism [2], an idea that was debated for decades [3] without arriving at a firm conclusion.

To analyse the mechanical interaction between heart frequency and respiratory frequency a simple mathematical model of the central systemic venous system in conjunction with the right heart was developed. The model retains some of the basic properties in spite of its simplification. Hereby the impact of the integer ratio is analysed arriving at a fuller understanding of the respiratory pump issue.

Analysis of the results shows that in the steady state under the condition of an integer ratio, venous return flow, though modulated by the respiration mechanically, is on average not influenced by the presence or absence of respiration. This suggest that the Donders claim is not valid in the general formulation in which it was originally presented. However, if the condition of an integer ratio is eliminated, venous return is influenced by respiratory activity, both through modulation and in average value. This means that Donders' proposal would apply to the periods of wakefulness and activity.

Alternatively, another and more detailed mathematical model based on the Navier-Stokes equation and describing fluid flowing in a non-symmetric elastic and valveless torus is discussed. It turns out that some of the nonlinear terms may cause a unidirectional flow when the torus is rhythmically compressed in analogy with the respiratory mechanical effect.

References:

[1] G. Hildebrandt, M. Moser, M. Lehofer: Chronobiologie und Chronomedicine. hippocrates Verlag, Stuttgart, 1998.

[2] M. Moser, J.W. Huang, G.S. Schwarz, T. Kenner, A. Noordergraaf: Impedance defined flow. Generalization of William Harvey's concept of the circulation - 370 years later. Int. J. Cardiovascular Med. and Science 1:205-211, 1998.

[3] F.C. Donders: Physiologie des Menchen. hirzel, Leipzig, 1856.

[4] M. Olufson, J. Ottesen: Outflow conditions in human arterial flow. In Third international conference on computer simulations in biomedicine, BIOMED 95, edited by H. Power, R.T. Hart, C.A. Brebbia, Computional Mechanics Publications, Southamton, G.B., pp 249-256,1995.

MS31 Feedback and Dynamics for Early Visual Processing in the Cortex

Organized by: David McLaughlin

Topic: 1 Medicine

The Primary Visual Cortex (Area V1), located early in the visual pathway, is a region of the mammalian brain in which cortical processing of elementary visual information occurs. This cortical processing involves neurons working individually, and as members of a large-scale cortical network. This cortical network is a complex nonlinear feedback dynamical system consisting of a very large number of excitatory and inhibitory neurons.

Today, modern experimental and computational methods are beginning to unveil the mechanisms by which this large scale cortical network functions to detect and represent elementary features of the visual scene. This mini-symposium will summarize some recent theoretical and experimental progress toward understanding the feedback and dynamical mechanisms which underlie the functioning of the Primary Visual Cortex.

Lyle Borg-Graham, Yves Fregnac, Cyril Monier, Frederic Chavane, Pierre Baudot

Biophysical Dynamical Signatures in Visual Cortex

In addition to the topography of neuronal circuitry - feedback, feedforward, recurrent, etc. - a variety of biophysical mechanisms within each neuron underly the dynamics of spike responses in cerebral cortex. These include various stages of synaptic release at axons, integration of post-synaptic responses within dendritic trees, spike generation at various locations within the neuron, and eventually axonal spike transmission. In this talk I will discuss data from in vivo intracellular neuronal recordings made in visual cortex which shed light on these mechanisms in a functional context. A principle finding is that a neuron's conductance state in response to visual stimuli may be strongly and rapidly modulated by synaptic input, especially so by inhibitory synapses. This modulation has several implications for understanding the computational architecture of the brain: First, the integrative properties of neurons may be only weakly determined by the passive properties of the cell membrane. Second, the basic interaction between excitatory and inhibitory synaptic input is highly non-linear, independent of any voltage-dependent membrane properties. Third, periods of a high conductance state markedly reduce membrane voltage variance, which in turn has a direct effect on the probability of spike firing, thus suggesting important limitations of deterministic neuron models.

David McLaughlin

An Emergent Separation of Time Scales in Cortical Networks

This paper reports on the consequences of high, activity dependent synaptic conductances in a large-scale neuronal network model of input layer 4C of Area V1 in the Macaque Primary Visual Cortex. This high conductance network accounts for experimental observations about orientation selectivity, dynamics, and response magnitude (McLaughlin, Shapley, Shelley & Wielaard, PNAS, '00); and the linear dependence of simple cells on visual stimuli (Wielaard, Shelley, McLaughlin & Shapley, J. Neural Sci, '01.). The model's large conductances can be traced to inhibitory cortico-cortical synapses, and the model's predictions of large conductance changes are consistent with recent intracellular measurements (Borg-Graham, et al, '98; Hirsch, et al, '98; Anderson, et al, '00). During visual stimulation, large conductances emerge from network activity – producing significant decreases in the effective time constant of neurons within the model network. Consequences include a near instantaneous response, where (i) the intracellular membrane potential very closely tracks an "effective reversal potential" composed of synaptic inputs; and (ii) neurons respond very quickly to abrupt changes in the synaptic input. The separation of time scales which emerges from network activity makes the neurons better coincidence detectors and burst transmitters under stimulation than in background. (This is joint work with Robert Shapley, Michael Shelley, and Jacob Wielaard.)

Carl Van Vreeswijk, David Hansel

The Contribution of Noise to Contrast Invariance

The mechanism for contrast invariance is still vigorously debated. Due to the threshold non-linearity of the cells' response, it is thought that contrast invariant rate tuning implies that the tuning of the cells' input cannot be contrast invariant. Recently however it was shown that contrast invariance is also displayed by the tuning curves of the membrane potential of these neurons, implying contrast invariant input. Numerical simulation studies have suggested that the noise in the system could reconcile these findings.

In this study we investigate the role of noise analytically and explain how it might lead to contrast invariance. We find that it can only be approximate, requires that the rate is not too large and that there is an upper and lower limit for the noise variance. Within these constraints, the mechanism is quite general. This is confirmed by numerical simulations of a conductance based neuron that receives Poissonian synaptic inputs. With an appropriate setting of the noise,this input contrast invariance results in an approximate contrast invariance for the mean voltage as well as the mean firing rate.

Jack Cowan

Towards a Mathematically Tractable Model of the Action of the Visual Cortex

In 1952 Turing's paper on the chemical basis of morphogenesis initiated an important approach to the mathematical analysis of spontaneous pattern formation. In 1973 Wilson and Cowan introduced a similar formulation in nets of interacting neurons and in 1979 Ermentrout and Cowan developed the mathematical analysis of such nets using local bifurcation theory and symmetry groups. Recently Bressloff, Cowan, Golubitsky, Thomas and Wiener have further developed this approach to characterize and analyze some of the circuitry of the primate visual cortex. So far the symmetry group used is $E(2) \times Z_2$ under a novel rotation action. Such an action is related to the fact that the visual cortex is a network of oriented edge detectors. However it is clear that much more than the orientation of a local edge is detected in the visual cortex: movement, texture and surface information, color and depth, for example. In this talk I will describe our approach and how to extend it to more complex symmetry groups that incorporate some of these features, and apply the analysis to two topics: (a) how geometric visual hallucinations are formed, and (b) how the cortex responds to external stimuli.

Tai Sing Lee, Gustavo Deco

Computational Rationales and Physiological Evidence of Feedback Computation in Early Visual Cortex

We will discuss some theoretical ideas on the computational and functional rationales underlying feedback interaction in the visual cortex. Many of these ideas can be traced back to Ulf Grenander's Pattern theory. We will present neurophysiological evidence to show that early visual processing can be modulated by higher level processes and behavioral experience. We will present a neural dynamical model based on interactive biased competition that demonstrates how the early visual cortex can mediate the interaction of the dorsal stream and the ventral stream of the visual systems to localize and identify objects in a visual scene.

2.2 Biotechnology

MS05 Extracting Low Dimensional Effective Dynamics: Algorithms, Analysis and Applications

Organized by: Christof Schütte, Andrew Stuart

Topic: 2 Biotechnology

Simplified stochastic modeling of dynamical systems with large number of degrees of freedom is of great practical importance in many areas where the equations of motion are so complicated that practically their solutions cannot be computed, even numerically. Not much can be done about this problem unless some additional information about the dynamics allows us, e.g., to separate the modes into two subsets: one governing the effective dynamics of the system; the other representing some bath of modes evolving on a faster time scale. Typical examples arise from climate modeling, where the fast atmosphere is coupled to slow oceans, or from biomolecular dynamics where fast rotating or oscillating modes are super-imposed to the slow global motion of the molecule. In each case, the mere elimination of the fast modes would lead to a very bad approximation on the time scale of interest. The minisymposium will give an overview over recent developments in analysis and algorithmic realization of different stochastic approaches to this problem with applications to climate and biomolecular dynamics. Following this minisymposium Paul Tupper (page 50), Wilhelm Huisinga and Holger Kantz (page 65) will give their contributed talks.

Sean Meyn

Multiplicative Ergodicity, Spectral Theory, and Phase Transitions for Markovian Models

This talk begins with the observation that a spectral gap for a Markov operator is equivalent to geometric ergodicity, which is equivalent to V-uniform ergodicity. This provides a vector space setting, and a range of operator-theoretic tools for analysis. We will survey applications to large deviations, products of random matrices, and phase transitions in molecular models.

Eric Vanden-Eijnden, Andrew J. Majda, Ilya Timofeyev

Mathematical Strategy for Stochastic Modeling in Under-Resolved Systems

A strategy for stochastic modeling of a set of essential modes by elimination of unresolved modes is presented. The method is based on a simplification assumption of the dynamics of the unresolved modes which allows for rigorous elimination of these modes in a suitable asymptotic limit. We shall present the method and discuss some properties of resulting effective stochastic equations for the essential modes, including the emergence of both stable and unstable Langevin-type dynamics and the need to incorporate nonlinear corrections and multiplicative noises in these equations.

Christof Schütte

Extracting Macroscopic Stochastic Dynamics of Biomolecules

The function of many important biomolecules comes from their dynamic properties and their ability to make statistically rare switches between different conformations. Recent investigations demonstrated that (a) these conformations can be understood as metastable or almost invariant sets of certain Markov chains related with the dynamical behavior of the molecular system and that (b) these sets can efficiently be computed via the dominant eigenvectors of an appropriately defined transfer operator. Furthermore, these eigenvectors can be used to identify the essential degrees of freedom of the system. Hence, one can reformulate the effective dynamical behavior in two ways: (a) as a low-dimensional finite state space Markov chain which describes stochastic hops between the metastable conformation sets of the system, and (b) as a low-dimensional stochastic differential equation (SDE) in terms of the essential degrees of freedom. The Markov chain in (a) can explicitly be derived even for "real" biomolecules like peptides and RNA systems by means of novel algorithmic techniques, while the SDE in (b) is explicitly computable in some simple cases only.

Andrew Stuart

Macroscopic Stochastic Models from ODEs with Random Data

The problem of deriving stochastic differential equations (SDEs) from mechanical systems with random data has a long history going back to early work of Kac, Zwanzig and their co-workers in the 1960s and 1970s. The subject has recently been re-invigorated by the possibility of using such derivations to bench-mark a variety of different algorithms used in computational molecular dynamics. This possibility stems from the fact that, in many cases, the primary objects of interest in molecular simulations are macroscopic. Having some explicitly understood model problems, where the dynamics of macroscopic quantities are completely understood, is invaluable in evaluating computational algorithms.

I will describe generalizations of this basic framework which give derivations of various Langevin equations, including ones with memory, and a damped driven stochastic wave equation. I will show how these stochastic macroscopic model problems can be used to evaluate a variety of numerical algorithms.

2.3 Materials Science

MS24 Mathematical Modelling in Polymer Industry

Organized by: Vincenzo Capasso, Luis L. Bonilla

Topic: 3 Materials Science

Polymer industry raises a large amount of relevant mathematical problems with respect to the quality of manufactured polymer parts. These include in particular questions about polymerization and the nucleation/crystallisation kinetics of the polymer melt, the coupling of the crystallisation process with environmental heterogeneities (temperature, stresses, etc.).
In crystallization processes, the final morphology of the crystallized material is a fundamental factor in the physical properties of a solidified part. Also the long term behaviour of such properties (dimensional stability, physical ageing, ...) is strongly influenced by the microstructure of the crystallised material.
This mini-symposium is aimed at a unified presentation of some mathematical problems which arise in connection with the above mentioned processes. The group of speakers participate in the ECMI initiative of establishing an interdisciplinary and international Special Interest Group on the subject.

Luis L. Bonilla, D. Reguera, J. M. Rubí

Nucleation and Crystallization

We develop a statistical mechanical approach to describe processes of nucleation and growth. This approach is based upon Nonequilibrium Thermodynamics ideas and allows us to consistently derive kinetic equations of Fokker-Planck type. The methodology is presented for nucleation processes and then extended to deal with growth processes. Possible applications of this methodology include consideration of polymer crystalization in temperature gradients or shear flows.

Vincenzo Capasso, Martin Burger

Controlling the Crystallization Process of Polymers

Crystallization of polymers is composed of two processes, nucleation (birth) and subsequent growth of crystallites, which are in general both stochastic in time and space. If we assume that at points of contact between two growing crystallites they stop growing, a random division of the relevant region in a d-dimensional space is obtained, known as a random Johnson-Mehl tessellation, which has been studied in previous literature with homogeneous parameters. The coupling of the kinetic parameters of the birth-and-growth process with the underlying temperature field induces time and space heterogeneities (and stochasticity) of all parameters involved, thus motivating a more general analysis of the stochastic geometry of the crystallization process.
It is well known that mechanical properties of the final material strongly depend on the mean densities of the interfaces (n-facets: cells, faces, edges, vertices) of the random tessellation, at different Hausdorff dimensions, with respect to the usual d-dimensional Lebesgue measure. Thus optimization problems arise in terms of the temperature profile of cooling. In this respect an analysis of the above quantities in terms of the kinetic parameters of the process is presented here, coupled with the evolution equations of the underlying temperature field.

Flavius Guias

Coagulation-Fragmentation Processes

We construct a stochastic model for coagulation-fragmentation processes and analyze its convergence properties towards the solution of a deterministic infinite-dimensional system of reaction-diffusion equations. This type of processes arises in many fields of science, such as polymer chemistry, meteorology, astronomy. One considers a spectrum of particles of different sizes, which can merge (coagulate) or split at given rates. The time evolution of such a system can be modelled either by Markov processes based on a finite number of particles, or by differential equations involving the densities of each type of particle. In this contribution we analyze the consistency of these two models and give conditions under which the family of Markov processes approximates the deterministic system.

Alessandra Micheletti, Vincenzo Capasso

The Stochastic Geometry of Crystallization Processes

Stochastic Geometry and in particular Boolean models, under proper assumptions, are good instruments to represent and statistically analyse crystallization phenomena. The dynamics of this kind of processes enables the construction of Dynamical Boolean Models, or equivalently of birth-and-growth processes, in general heterogeneous both in space and time. The growth of crystals and the impingement phenomenon creates a final tessellation of the available space, whose geometric properties determine the final mechanical, chemical and physical properties of the product. Thus the statistical study of the shape of the final tessellation has a big industrial relevance. In this talk we will present models and statistical methods to analyse the stochastic shape features of crystallization processes, with particular attention to the estimate of the density of interfaces of the cells of a Johnson-Mehl tessellation.

MS40 Numerical Analysis in Materials Science

Organized by: Carsten Carstensen

Topic: 3 Materials Science

Smart materials or optimal design problems involve nonconvex energy densities to model phase transitions. The numerical analysis of which faces oscillations on every length scale of a finite element mesh. Four lecturers provide examples with emphasis on the effective simulation of macroscopic phenomena driven by microscopic microstructures, time evolution with microstructures, and the simulation of the microscopic phenomena with details on interior interfaces aud surfaces.

Carsten Carstensen

Macroscopic Finite Element Simulation of Micro-structures in Phase Transitions

The rapidly developing mathematical modeling of microstructure allows for important applications in material science (advanced materials), micromagnetism, homogenization and optimization. Typically, the variational problem (M) involves an energy density with more than one zero state (the wells or transition strains) and thereby is non-convex. Consequently, (M) lacks classical solutions and in applications, we see finer and finer oscillations on a length-scale that is determined by another mechanism such as interfacial energy.

There exist infimizing sequences in (M) that have a weak limit, but non-(quasi-)convexity implies, in general, that the weak limit u is *not* a solution of the problem (M).

In experiments, we observe oscillations of strains which form a macroscopic or averaged quantity u. The efficient numerical simulation on the macroscopic level aims to compute the weak limit u as a solution of a related *Relaxed Problem* (RP) while the microscopic mechanism can be detected by a direct finite element minimization of (P) or, more sophisticated, by a generalized formulation (GP).

The presentation will focus on efficient (adaptive) strategies for relaxed problems such as the double-well problem in one-dimension (Young's example), in higher dimensions, or in linearized elasticity and mention related topics in micromagnetism and homogenization problems.

C. Carstensen, P. Plechác: Numerical analysis of a relaxed variational model of hysteresis in two-phase solids. Preprint Nr. 80/2000. Publications of the Max-Planck-Institute for Mathematics in the Sciences 04103 Leipzig/Germany.

C. Carstensen, K. Hackl, A. Mielke: Nonconvex potentials and microstructures in finite-strain plasticity. Preprint Nr. 72/2000. Publications of the Max-Planck-Institute for Mathematics in the Sciences 04103 Leipzig/Germany.

C. Carstensen, A. Prohl: Numerical Analysis of Relaxed Micromagnetics by Penalised Finite Elements. Numerische Mathematik (2000) Accepted. Berichtsreihe des Mathematischen Seminars Kiel 99-9 (1999).

C. Carstensen, P. Plechác : Numerical analysis of compatible phase transitions in elastic solids. SIAM J. Numer. Anal. 37 (6) (2000) 2061-2081

C. Carstensen, T. Roubícek : Numerical approximation of Young measures in non-convex variational problems. Numer. Math. 84 (2000) 395-415

C. Carstensen, Petr Plechác : Numerical solution of the scalar double-well problem allowing microstructure. Math. Comp. 66 (1997) 997-1026.

C. Carstensen, Petr Plechác : Adaptive algorithms for scalar non-convex variational problems. Appl. Num. Math. 26/1-2 (1997) 203-216.

Alexander Mielke, Florain Theil

Convergence of Time Discretizations in Rate-Independent Problems

Many rate–independent models in continuum mechanics can be formulated in terms of an energy functional $\mathcal{E}(t,\cdot) : z \in P \subset X \to [0,\infty]$ and a dissipation norm Δ on the Banach space X. The solutions are described by imposing a stability condition (S) and an energy inequality (E):

(S) $\mathcal{E}(t,z(t)) \le \mathcal{E}(t,a) + \Delta(a-z(t))$ for all $a \in P$,

(E) $\mathcal{E}(T,z(T)) + \int_0^T \Delta(\dot{z}(t)), \mathrm{d}t \le \mathcal{E}(0,z(0)) - \int_0^T \partial_t \mathcal{E}(t,z(t)), \mathrm{d}t.$

The most natural time–discretization is obtained by solving the time–incremental minimization problem:

$$z_{k+1} \in \arg, \min\{\ \mathcal{E}(t_{k+1},z) + \Delta(z-z_k) \mid z \in P\ \}.$$

We discuss conditions on $\mathcal{E}$, P and Δ which guarantee the convergence of this time discretization. We obtain weak convergence to a solution under weak closedness of the set of stable states (i.e. those satisfying (S)), which has applications in phase transformation problems. Strong convergence can be obtained under the assumption of uniform convexity of $\mathcal{E}(t,\cdot)$, P being the full Banach space and technical smoothness conditions.

Zhiping Li

Computation of the Twin Width Scale of Laminated Microstructure with Surface Energy

The mesh transformation method is applied to a mathematical model to study how the twin width of the needle-like laminates is related to the twin length and the surface energy density in austenite-martensite phase transition. Numerical experiments are made to establish such a relationship for an elastic crystal model.

1. Z.-P. Li, *Rotational transformation method and some numerical techniques for the computation of microstructures.* **Math. Models Meth. Appl. Sci., 8**(1998), 985-1002.

2. Z.-P. Li, *Laminated microstructure in a variational problem with a non-rank-one connected double well potential*, **J. Math. Anal. Appl.,** **217**(1998), 490-500.
3. Z.-P. Li, *A periodic relaxation method for computing microstructures.* **Appl. Numer. Math.,** **32**(2000), 291-303.
4. Z.-P. Li, *Finite order rank-one convex envelopes and computation of microstructures with laminates in laminates.* **BIT Numer. Math.,** **40**(4)(2000), pp.745-761.
5. Z.-P. Li, *Computations of needle-like microstructures*, To appear in **Appl. Numer. Math.**.
6. Z.-P. Li, *Mesh Transformation and Regularization in Numerical Simulation of Austenitic-Martensitic Phase Transition.* To appear in **Comp. Mater. Sci.**.
7. Z.-P. Li, *A mesh transformation method for computing microstructures.* To appear in **Numer. Math.**.

Michel Chipot

Microstructures and Interfaces in Well-Problems

Let $M_{m,n}$ the space of $m \times n$ matrices. Let

$$\varphi : M_{m,n} \to \mathbb{R}^+$$

a continuous function such that

$$\varphi(W_1) = \varphi(W_2) = \cdots = \varphi(W_k) = 0, \quad q \quad \varphi(W) > 0 \quad \forall, W \neq W_k.$$

Let $A \in M_{m,n}$. If

$$\begin{aligned} W_A^{1,\infty}(\Omega) &= W_A^{1,\infty}(\Omega\, \mathbb{R}^m) \\ &= \{v : \Omega \to \mathbb{R}^m \mid \\ &\quad v_i \in W^{1,\infty}(\Omega)\forall, i \text{ and } v(x) = A \cdot x \text{ on } \Gamma\} \end{aligned}$$

we consider the model problem

$$\operatorname*{Inf}_{W_A^{1,\infty}(\Omega)} \int_\Omega \varphi(\nabla v(x)), dx \qquad (1)$$

with $\nabla v = (\frac{\partial v_i}{\partial x_j})_{i=1\ldots m,,j=1\ldots n}$. In order to achieve the infimum (1) the minimizing sequences use alternatively the different wells W_i creating different zones or phases where

$$\nabla v = W_i.$$

We analyse the appearance of these zones in different contexts.

MS18 Variational Modelling of Microstructured Materials

Organized by: Sergio Conti, Antonio DeSimone

Topic: 3 Materials Science

Formation of microstructure in materials is often a consequence of nonconvexity of the microscopic energy, and of its interplay with kinematic constraints. The techniques developed in mathematical analysis to deal with nonconvex functionals shed light on different problems in materials science. This minisymposium will present applications of the general mathematical framework to problems in micromagnetics, thin films and soft matter.

Sergio Conti, Hafedh Ben Belgacem, Antonio Desimone, Stefan Müller

Energy Scaling of Compressed Elastic Films

Debonding from the substrate and subsequent blistering is a mechanism by which a film can release compressive stresses. This happens for example upon cooling films deposited at high temperature on a substrate with a larger thermal expansion coefficient. Most studies of blistering are based on the Föppl-von Kármán theory of plates.

Typical observed configurations exhibit folds perpendicular to the boundary, which coarsen in the interior of the debounded region. We explain this phenomenon through energy minimization. Indeed, we show that in order to achieve minimal energy the displacement field develops fine-scale oscillations. The oscillation period decreases approaching the boundary, corresponding to branching of the observed folds. We also show that, for this purpose, the Föppl-von Kármán model is equivalent to the full three-dimensional elasticity theory.

Antonio Desimone, Sergio Conti, G. Dolzmann

Soft Elastic Response of Stretched Sheets of Nematic Elastomers: a Numerical Study

Stretching experiments on sheets of nematic elastomers have revealed soft deformation modes and formation of microstructure in parts of the sample. Both phenomena are manifestations of the existence of a symmetry-breaking phase transformation from a random, isotropic phase to an aligned, nematic phase. The microscopic energy delivers a continuum of symmetry-related zero-energy states, which can be combined in different ways to achieve a variety of zero-energy macroscopic deformations.

We replace the microscopic energy with a macroscopic effective energy, the so-called quasiconvexification. This procedure yields a coarse-grained description of the physics of the system, with (energetically optimal) small-scale oscillations of the state variables correctly accounted for in the energetics, but averaged out in the kinematics. Knowledge of the quasiconvexified energy enables us to compute efficiently with finite elements, and to simulate numerically stretching experiments on sheets of nematic elastomers.

Our numerical experiments show that up to a critical, geometry-dependent stretch, no reaction force arises. At larger stretches, a force is transmitted through parts of the sheet and, although fine phase mixtures disappear from most of the sample, microstructure survives in some pockets. We reconstruct from the computed deformation gradients the local orientation of the nematic director.

Huajian Gao

Modeling of Deformation Mechanisms in Metal Thin Films

Problems to be discussed in this talk include micromechanical modeling of diffusional creep in polycrystalline thin films and dislocation core spread along interfaces between crystalline and amorphous solids. Both problems are important for the interpretation of experimental observations of stress-temperature behavior of thin metal films on substrate. One mechanism that arises in the diffusional creep of polycrystalline thin films is the exchange of material between the free surface of the film and grain boundaries. Modeling of such process leads to singular integro-differential equations representing a strong coupling between stresses in the film and grain boundary diffusion. We consider a uniformly strained film with periodic grains and show that the traction along the grain boundary decays exponentially with time. This process leads to the formation of an array of crack-like grain boundary diffusion wedges at the junction between grain boundaries and substrate. The solution is used to explain the experimentally observed stress-temperature behaviors for unpassivated and passivated films. Dislocation core spreading is used to explain the effect of oxygen on the mechanical behaviors of such films.

Christof Melcher

Singular Perturbation in the Context of Néel Wall Transitions in thin Ferromagnetic Films

We are going to present the multiple scale problem of a parametrisized planar 180° rotation of magnetization states in a thin ferromagnetic film. In an appropriate scaling and when the diameter d is comparable to the Bloch line width w, the underlying variational principle has the form

$$\kappa^2, Q, \left|m\right|^2_{\dot{H}^1} + \left|u\right|^2_{L^2} + \left\{u\middle|\mathcal{S}_Q\middle|u\right\} \to \min$$
$$m = (u,v) : R \to \mathbb{S}^1 \text{ with } u(0) = 1$$

where the reduced strayfield operator $\mathcal{S}_Q$ approximates $(-\Delta)^{1/2}$ as the quality factor Q tends to zero. Limiting elliptic regularity methods on the basis of the associated Euler-Lagrange equation and symmetrization arguments on the basis of the variational principle yield a pointwise estimate and the renormalized limit behaviour of the associated Néel wall profile u as Q tends to zero. Our estimate exhibits the very long logarithmic tail of a Néel wall profile and its scaling laws in terms of all involved parameters.

Barbara Niethammer, Andreas Hoenig, Felix Otto

On the Scaling of the First Order Correction to The LSW–Model for Ostwald–Ripening

The last stage of a first order phase transformation is characterized by coarsening of particles of one phase in a background matrix, where particles interact by diffusional exchange to reduce the total surface energy.

The classical theory by Lifhitz, Slyozov and Wagner (LSW) describes coarsening in the limit of vanishing volume fraction of particles. We present a rigorous analysis in a stochastic setting which identifies the scaling of the first order correction of the coarsening rate to the one predicted by LSW. The scaling of the correction exhibits a cross–over between two different scales, which is due to screening effects.

Our proof relies on the fact that the evolution of the particles has the structure of a gradient flow and thus allows a variational formulation of the problem.

MS37 Industrial Problems Solved with Sharp Interface and Phase Field Models

Organized by: Wolfgang Dreyer, Wolfgang H. Müller

Topic: 3 Materials Science

Micromorphological changes are pertinent to many industrially relevant materials and directly linked to their material properties. Examples include alpha/gamma phase transitions in steel, phase separation in microelectronic solders, rafting in Ni-based superalloys, motion of grain boundaries and associated creep behavior in ductile metals, or development of mushy zones and concentration gradients during solidification of alloys. From a mathematical point of view these problems can be tackled by using free boundary value problems where phase boundaries are modeled by sharp interfaces or within the framework of phase field models where the transition between two adjacent phases occurs in a continuous manner.

The objective of this symposium is to open a forum for mathematicians, physicists and engineers to formulate suitable models for problems as mentioned above and to solve the corresponding equations quantitatively in a mathematically stringent manner.

James F. Blowey, J.W. Barrett

Finite Element Approximation of an Allen-Cahn/Cahn-Hilliard System

In this talk an overview of the work on an Allen-Cahn/Cahn-Hilliard system will be presented. The system arises in the modelling of phase separation and ordering in binary alloys. In particular for a non-degenerate mobility and either (i) a logarithmic free energy or (ii) a non-smooth free energy (the deep quench limit) the existence of a unique solution for sufficiently smooth initial data will be established. Furthermore, an error bound for a fully practical piecewise linear finite element approximation of (i) and (ii) in one and two space dimensions (and three space dimensions for constant mobility) will be presented. In addition to showing well-posedness and stability bounds for the approximation to (i) with a degenerate mobility there is convergence in one space dimension. Finally some numerical experiments will be presented.

Wolfgang Dreyer, Wolfgang H. Müller

An Atomistic Study of Extended Cahn/Hilliard Systems

This paper presents an atomic interpretation of the various parameters that occur in a phase field model, which is capable of predicting quantitatively the spinodal decomposition and coarsening observed in binary eutectic alloys (such as SnPb or SnAg solders). Parameters to be discussed include the Gibbs free energy of a binary alloy, the second gradient parameters introduced by Cahn and Hilliard, as well as (anisotropic) stiffness constants. Deviations to the classical theory as outlined in the seminal paper by Cahn and Hilliard are discussed, various other higher gradient terms for the extended diffusion flux are derived, and their influence on microstructural development is assessed. All steps and procedures involved are demonstrated explicitly and evaluated numerically for the special case of eutectic SnPb, by means of a comparison with its phenomenological Gibbs free energy (Redlich-Kisler Ansatz).

Evgeniy V. Radkevich

The Singular Limit of a Phase Field Model for the Eutectic Tin/Lead Alloy

Dreyer & Müller studied an extended Cahn/Hilliard phase field model for the description of phase separation processes in an eutectic tin/lead alloy. An observed strong coupling of diffusion and external mechanical loads is taken into account. Moreover, Dreyer & Müller consider strain gradient coefficients that depend on the (tin-) concentration.

In this paper we establish the singular limit of that model leading to sharp interfaces. We prove existence of solutions and convergence of the asymptotic expansions. In particular we show that the concentration dependence of the gradient coefficients leads to a normal dependence of the concentration field along the interface, which generalizes the classical common tangent construction.

Vanessa Styles

Numerical Simulations of Diffusion Induced Grain Boundary Motion

In this talk we consider the numerical approximation of models concerning the motion of grain boundaries in thin metallic films. The grain boundary is forced to move by the diffusion, into the thin film through the grain boundary, of atoms from an external metallic vapour. The first problem we consider couples equations for the diffusion and the motion of the grain boundary. We consider a phase field approach and a sharp interface approach. Formal asymptotics yield the sharp interface model as the limit of the phase field equations as the width of the associated diffuse interface tends to zero. A finite element approximation of the phase field model is presented and is shown to be convergent to a weak solution. Numerical simulations of both models are described and compared. We show that the two approaches are consistent.

The second problem we consider arises from an asymptotic approximation of the first in which the diffusion takes place very rapidly. As the grain boundary advances the concentration takes the value of the external concentration. Thus the forcing is history dependent. We present sharp interface, phase field and level set formulations of this problem and numerical discretizations are derived. Simulations with the three approaches are shown to be consistent displaying double seam configurations typical of experimental observations.

MS01 Mathematical Methods in Glass Manufacturing

Organized by: Axel Klar

Topic: 3 Materials Science

This minisymposium will present numerical and theoretical approaches to problems appearing in glass manufacturing. In particular, numerical solution and approximation of the radiative transfer equations for glass will be discussed.

Norbert Siedow

Spectral Remote Sensing for Temperature Reconstruction

Almost all production steps of glassmaking are influenced by the temperature within the glass. To determine the temperature behaviour of hot glass direct measurements as well as numerical simulation methods can be used. The direct measurement of temperature, e.g with thermocouples, inside the glass or glassmelt is in general not possible under production conditions. Thus, non-contact methods are required. In the paper we propose an inverse method to determine the temperature inside the glass using information about the spectral radiative intensity.

Guido Thömmes, Thomas Götz, Axel Klar, Edward W. Larsen, Mohammed Seaid

Diffusion Approximations to the RHT Equations in Glass Cooling

The Simplified-P_N approximations to the radiative heat transfer equations in glass for the optically thick, diffusive regime are presented. An asymptotic analysis is performed in order to derive the approximations. The boundary conditions can be obtained from variational arguments. Numerical studies for problems appearing in the simulation of RHT in glass cooling confirm the efficiency of the approach.

Oscar Lopez-Pouso, Maurizio Falcone

On two Classical Methods to Solve the Transient Diffusion Approximation of the Radiative Transfer Equations in the 1-D Slab

This talk is devoted to the analysis of some facts regarding numerical solution of the evolutive, gray, 1D radiative transfer diffusion equations in the slab with isotropic scattering. It is known that simple fixed point iteration does not work when the medium is optically thick, and that this difficulty can be overcome by using a Newton method. It is our aim to quantify the first observation, giving a criterion to decide "a priori" whether fixed point converges or not. We observe also that the Newton method can be implemented in a faster way (but this depends strongly on the particular discretization schemes used) than fixed point when the last one converges. Existence theorems for the discrete (nonlinear) problem are also proved.

Rene Pinnau, Guido Thömmes

Optimal Control of Glass Cooling Processes

An optimal control problem for glass cooling processes is considered. The temperature and radiation in the material is modelled via the SP_1 approximation, which yields a nonlinear parabolic system. We investigate various cost functionals of tracking type and consider the control problem as a constrained optimization problem. We derive the first order optimality system and and solve it numerically with a descent algorithm, where the gradient is computed via the adjoint equations. Numerical examples are presented.

MS26 Recent Progress in Superconductivity

Organized by: Daniel Phillips, Patricia Bauman

Topic: 3 Materials Science

This minisymposium will bring together mathematicians and materials scientists who will describe their latest research on various models for superconducting materials. The challenges they face in their work are specific versions of those that are highlighted as themes for the conference. Recent work in this area includes studies at various length scales, including the mezoscopic Ginzburg-Landau theory and macroscopic models for the distribution of current in the material. At present, many challenges remain, such as understanding the interrelationship of critical currents, magnetic flux, and pinning in the presence of applied electric and magnetic fields. The intended audience is mathematicians and scientists working on superconducting or electro-magnetic materials.

Patricia Bauman, Nelly Andre, Daniel Phillips

Mathematical Analysis of a Ginzburg-Landau System Related to Pinning

We investigate a mathematical model for vortex pinning for a Ginzburg-Landau system of PDE's in which a certain coefficient, $a(x)$, vanishes at a finite number of points in the domain. This model has been used to describe a nonhomogeneous superconducting material. We prove that the order parameter is nonvanishing except near the zeroes of $a(x)$ and describe a limiting problem, as the Ginzburg-Landau parameter tends to infinity, for the order parameter and the induced magnetic field with physically realistic natural boundary conditions.

Lia Bronsard, S. Alama, A.J. Berlinsky

On the Shape of the Vortex Lattice for a Layered Superconductor in a Parallel Field

We consider the Lawrence-Doniach model for a layered superconductor, and impose an external magnetic field parallel to the superconducting layers. We consider periodic configurations, using 't Hooft-type boundary conditions and study minimizers of the energy in the small coupling limit, corresponding to a "transparent" regime observed by physicists. Using a degenerate perturbation procedure we calculate the energy minimizers for an arbitrary period geometry and find an optimal shape for the Josephson vortex lattice among all possible geometries.

Daniel Phillips, Eunjee Shin

Thermoelectric Effects in Superconductivity

We investigate a thermoelectric model for superconductors based on the time dependent Ginzburg-Landau (TDGL) theory proposed by Zhou and Miya and by Maugin. The model accounts for Joule heating and the generation of thermoelectric currents due to temperature gradients.

The model is a parabolic system consisting of the TDGL equations, with temperature dependent coefficients,and a heat conduction equation such that the Clausius-Duhem inequality is valid. We establish existence, uniqueness, and large time behavior results for the system. Furthermore we show how large current densities or variations in the magnetic field initially can subsequently generate hot spots in the material causing the dissipation of superconductivity.

The model is examined numerically as well. In particular comparisons are made between this model and the isothermal TDGL model with the same initial and boundary conditions. It is shown that these two systems display markedly different large time current distributions.

Itai Shafrir, Nelly Andre

On a Class of Vector Valued Singular Perturbation Problems

We study the asymptotic behavior of the $\mathbb{R}^2$-valued minimizers u_ϵ, as $\varepsilon \to 0$, for energies of the form $E_\varepsilon(u) = \int_G |\nabla u|^2 + \frac{1}{\varepsilon^2}F(u)$ for a given boundary condition g on ∂G. Here $F(u)$ is a non-negative function on $\mathbb{R}^2$ which takes its minimal value 0 on a closed curve Γ and G is a smooth bounded domain in $\mathbb{R}^2$. It is proved that $u_\varepsilon \to u_*$ where u_* is a singular $\Gamma-$valued harmonic map. One of the variants that we study is motivated from models in Liquid Crystals and Ferromagnetism.

2.4 Environmental Science

MS19 Mesh Adaptation in Atmospheric Modelling

Organized by: Jörn Behrens, Tor Sørevik

Topic: 4 Environmental Science

In recent years, adaptive mesh refinement techniques found their way into applications of atmospheric modeling. In contrast to other fields of application, a lot of work remains to be accomplished before adaptively refined meshes can be considered a common tool in atmospheric simulation.

This minisymposium tries to give a snapshot of the current state in the field. It will investigate unstructured versus structured (blocked rectangular) mesh refinement strategies, and will try to quantify the gain of adaptive mesh refinement in terms of accuracy and computational cost. Asymptotically adaptive methods even go beyond pure mesh adaptivity. Some considerations on the feasibility of adaptive methods in the context of production codes are given. Finally, some real applications will be shown, demonstrating the benefit of adaptive techniques.

Tor Sørevik, Ragnhild Blikberg

Modeling the Savings and Costs of Adaptive Mesh Refinement

Adaptive routines usually offer a large variety of user defined parameters through which the user can influence the behavior of the algorithm. Examples might be: how often to regrid, which cells should be tagged for refinement, how many levels of refinement to use and many more. These choices may, or may not, have great influence on the computational cost as well as the accuracy of the computed solution.

The purpose of this paper is to quantify how these choices influence the computational costs and the accuracy in adaptive routines in general and AMRCLAW in particular. First we present some computational results on our test case, the shallow water equations. Next we develop a mathematical model for the computational cost and compare the theoretical estimates with the actual measurements. The model helps us to explain the behavior we observe. Combined the model an the experimental results provide assistance to the user in the choice of parameter, as well as being a tool for assessing the true savings of AMR.

Keywords: Adaptive Mesh Refinement, AMRCLAW, Shallow water equation

Rupert Klein, Nicola Botta

Towards Asymptotically Adaptive Numerical Methods for Atmospheric Flows

Atmospheric flows are characterized by a considerable variety of singular asymptotic limit regimes. This is evident from the large collection of simplified model equations to be found in contemporary textbooks on theoretical meteorology. The presence of such singular flow regimes induces multiple length and time scale solutions which call for adaptive grids and time steps. However, these regimes also involve dominant balances of selected terms within the governing equations. The associated numerical dynamic range problems lead to numerical stiffnesses and to amplifications of numerical truncation errors. This presentation will describe a generalized asymptotic framework for analysing these effects and will discuss first examples of numerical methods that overcome the numerical difficulties through “asymptotic adaptivity”.

Reinhold Hess

Feasibility of Adaptive Grid Refinement for Operational Weather Prediction

High–resolution numerical weather prediction requires enormous computing power in order to provide reliable and early weather forecasts. With mesh adaptation the computational costs can be distributed according to the actual requirements of the simulation. This can be done statically dependent e.,g. on orography or dynamically based on the weather conditions being simulated. Because of the potential of mesh adaptation to provide highly resolved simulation at reduced computational costs some operational weather models (e.,g. LM, MM5) already support static block–structured refinements.

Dynamically adaptive refinements, however, that exploit the potential of adaptivity to a higher degree, are not generally accepted yet, although some research has been performed and fundamental pre–requisites are available: e.,g. dynamically adaptive block–structured refinements have been implemented on parallel distributed memory computers for a two dimensional shallow water model including dynamical load balancing. Nevertheless, a number of open problems still exist: a refinement criterion has to detect the critical areas based on meteorological conditions. Interpolation at the boundaries of the refined blocks has to consider physical problems as the critical equilibrium of temperature and humidity. Also vertical discretization and refinement strategy is an open question.

Jörn Behrens

Triangular Mesh Refinement for Atmospheric Transport Problems

Triangular or tetrahedral mesh refinement offers high variability in constructing locally refined adaptive meshes. However, in the context of atmospheric simulation, there are still several unsolved problems related to this type of meshes.

We will address some of these issues. The adaptive mesh generator *amatos* will be introduced which is used in the simulation of tracer transport in the atmosphere. amatos forms the basis of a semi-Lagrangian advection method. The method is well suited for parallelization on high performance computers. However, it is not inherently conservative, posing new problems in constructing a conservative advection scheme.

MS23 Statistical Mechanics Models for Atmosphere and Ocean

Organized by: Marcus Grote, Andrew Majda

Topic: 4 Environmental Science

Long time weather and climate prediction remains a formidable challenge for current computers. Because of the vast disparity of scales present in geophysical flows, numerical methods require the modeling of unresolved eddy motion. In regimes of real physical interest, statistical mechanics models are able to represent the nonlinear behavior of the large scales without detailed resolution of the small scales. Hence, they can lead to subscale models with substantial improvement in model fidelity, without incurring the cost of eddy resolution. This minisymposium will provide both applied mathematicians and computational scientists with an opportunity to present recent advances in both mathematical and computational aspects of statistical mechanics models of large-scale ocean and atmosphere flows.

Joel Sommeria

Statistical Mechanics of the Shallow Water System in a Rotating Medium

We extend the statistical mechanics of vorticity, initially developed for the 2D Euler equation, to the case of the shallow water system. Slow motion in the presence of background rotation is assumed, to avoid shock effects. Relaxation equations towards the maximum entropy state are proposed, which provide a parametrization of sub-grid scale eddies in 2D compressible turbulence. Application to the Great Red Spot of Jupiter is discussed.

Dieter A. Wolf-Gladrow

Simulation of Ocean Circulation with Lattice Boltzmann Methods

Lattice Boltzmann (LB) is a relatively new method to solve hydrodynamic and other problems that are usually described by systems of nonlinear partial differential equations. Starting point of LB methods is an artificial microworld on a lattice with dynamics obeying certain conservation laws (mass and momentum in the case of hydrodynamics). The corresponding partial differential equations which describe the macroscopic behavior of the system can be derived by a Chapman-Enskog (multiscale) expansion. After introducing the principles of LB methods a simulation of ocean circulation will be presented. Finally I will discuss advantages and disadvantages of LB methods, open questions and future perspectives.

Bruce Turkington

Statistical Models and Coherent States in Geostrophic Turbulence and Jupiterś Winds

For many years geophysical fluid dynamicists have used Gibbsian statistical ensembles to represent the equilibrium states of oceanic or atmospheric flows. When these ensembles are based on the conservation of energy and potential entrophy, a simple Gaussian theory results, which successfully predicts some of the key features of quasi-geostrophic turbulence over topography. But, more modern theories based on non-Gaussian statistics are now available to capture the full range of phenomena exhibited by geophysical flows. In this talk we describe such a theory, and we apply it to the observed zonal jets and embedded vortices in the active weather layer on Jupiter. For a 1+1/2-layer equivalent barotropic model of the Jovian atmosphere, we impose a prior distribution on the small-scale potential vorticity having a nonzero, anticyclonic skewness, and we consider the microcanonical ensemble in energy and circulation. The effective topography determined by the flow of the deep lower layer is deduced in a manner suggested by Dowling. The most probable states in this statistical equilibrium model are zonal shear flows containing multiple prograding and retrograding jets, and monopolar anticyclonic vortices rolling in those jets. These predicted equilibrium states agree remarkably well with the observed Jovian wind fields. Moreover, the nonlinear stability of these steady flows follows from an extension of the Arnold method, which in its usual form is indefinite for these Jovian flows.

Marcus Grote, Andrew J. Majda, Mark DiBattista

Statistical Models and Prediction for Large-scale Geophysical Flows

The tendency of turbulent geophysical flows to display two-dimensional behavior and self-organize into coherent structures has been reported numerous times from physical observations and numerical simulations. Equilibrium statistical theories provide a mathematical framework underpinning the emergence of coherent structures in freely evolving two-dimensional flow. These theories apply to inviscid and unforced flow and attempt to predict the large time behavior as it approaches statistical equilibrium.

Here we quantitatively evaluate the success of the statistical theory in predicting the congregation of heat or potential vorticity in two distinct situations. First, we consider the recent statistical theory of DiBattista, Majda, and Marshall (J. Phys. Ocean. 1999, 2000) for open-ocean deep convection, which plays an important role in maintaining the poleward transport of heat in the ocean. This theory predicts the spread of heat and potential vorticity following cold-air outbreaks based just on a few large-scale parameters. Comparison with numerical simulations of two-layer geostrophic dynamics demonstrates the remarkable predictive capabilities of equilibrium statistical theories. Second, in the simpler context of purely barotropic flow over topography, we devise crude closure algorithms, which predict the large-scale dynamic behavior of damped flow driven by small-scale random forcing. Even under harsh conditions, where all assumptions underlying equilibrium statistical theories are clearly violated, the crude closure algorithms again display remarkably accurate and robust predictive ability - see Grote and Majda (Phys. Fluids 1997, Nonlinearity 2000).

Stefan Pickl, Gerhard Wilhelm Weber

On Earth Warming System Analysis The TEM-Model and the Optimal Control Problem of Heating

This paper is concerned with a mathematical analysis of the nonlinear time-discrete TEM model for environmental protection. Real-world data and numerical experience are presented. As the steady states are not attractive, the necessary introduction of control parameters in the dynamics of the TEM model leads to new results in the field of time-discrete control systems. Furthermore the results give new insights into a Joint-Implementation Program and herewith, they may improve this important economic tool. The steady states of the TEM model can be regarded as limiting values mentioned in Kyoto Protocol. In a second step, we regard the determined control parameters as candidates for influencing heating of the earth atmosphere (greenhouse effect). We consider the earth as a ball and look for an optimal control such that the temperature in the stratosphere remains within lower and upper bounds. Here, we utilize scientific experience from Krabs, Tichatschke and the authors on time-minimal control of heating and generalized semi-infinite optimization. We present a iteration procedure and first numerical results.

MS27 Turbulent Transport in the Presence of Large Scale Inhomogeneities

Organized by: Peter Kramer, Grigorios Pavliotis

Topic: 4 Environmental Science

The dynamical evolution of heat, pollutants, water vapor, and other substances immersed in the atmosphere and ocean are strongly influenced by the turbulent fluctuations present in these media. These turbulent fluctuations are however either difficult or impossible to model in detail in numerical simulations for environmental applications. An ongoing mathematical goal is to characterize the influence of these turbulent fluctuations on the immersed quantities, with the applied aim of capturing the effects of turbulence without the need to represent explicitly its complicated multiscale structure. The aim of this minisymposium is to present some recent work on the turbulent diffusion in applications which have large-scale inhomogeneities, which are abundantly present in environmental applications. For example, both the atmosphere and ocean have vertical density stratification and various climactic and seasonal mean flow patterns, and the turbulence in the atmospheric boundary layer varies with distance from the ground. The talks in this minisymposium will present theoretical developments, examples, and numerical simulations which illustrate some of the subtle and interesting ways in which large-scale inhomogeneities interact with turbulence in determining the transport and fluctuations of heat and material density in the total flow.

Richard McLaughlin

Scalar Transport: Some Properties of Anelastic Mixing, and Averaging in Time Varying Flow

We discuss enhanced mixing induced by complex fluid motion, first overviewing the importance of these problems from a general perspective in modelling turbulence with closure coefficients, and then focusing upon rigorous averaging theories in idealized contexts to try to explicitly quantify effective mixing coefficients.

We overview the idealized problem of calculating enhanced diffusivities for passive transport in steady periodic geometries, reviewing the poor dependence of these coefficients upon large scale flow parameters. Through the introduction of temporal variation into these models through rapid wind fluctuations, we present a theory which identifies regions in the Peclet-Strouhal plane for which fluctuation massages the poor coefficient dependence existing in the steady geometry, and regions with the mixing coefficients plagued by non-monotonic Peclet dependence.

We then consider applying similar averaging methods to divergent flows designed to respect large scale layered anisotropies (motivated by atmospheric density variation), and discuss various trapping phenomena arising in this theory.

Grigoris Pavliotis, Peter R. Kramer

Homogenized Transport by a Spatiotemporal Mean Flow with Small-Scale Periodic Fluctuations

The transport of a pollutant in the ocean or atmosphere is influenced strongly by both the prevailing large-scale mean flow structure and disordered turbulent motion prevalent on smaller scales. To obtain some insight into the effects of turbulent transport, various authors over the last decade have studied the transport of passive material in model flows which have a periodic structure. For such flows, one can develop a rigorous homogenization theory to describe the effective transport on large scales and long times. We will present an extension of these homogenization studies to a class of model flows which consist of a superposition of a large-scale mean flow with a small-scale periodic structure (both of which can depend on space and time). Using the two-scale convergence method, we rigorously derive homogenized equations for these models, in which the mean flow and periodic structure are shown to interact nonlinearly. Different kinds of homogenized equations can emerge, depending on the spatio-temporal relationships between the mean flow and periodic fluctuations and the relative magnitude of the molecular diffusivity. The physical manifestations of the interaction between the mean flow and the periodic fluctuations are illustrated through some simple examples.

Karl Sabelfeld

Monte Carlo Evaluation of the Footprint Function Over Inhomogeneous Forest

Forward and backward stochastic Lagrangian trajectory simulation methods are developed to calculate the footprint function for the concentration and its fluxes in the case when the ground surface is inhomogeneous along the mean wind direction. The input data to the stochastic model are calculated from a closure model for the mean flow in the atmospheric boundary layer. We analyse the impact of the roughness change and thermal inhomogeneity on the footprint function.

Guido Boffetta

Relative Dispersion in Fully Developed Turbulence

The statistics of relative dispersion in fully developed turbulence is studied by means of direct numerical simulations. The results are compatible with the original Richardson description based on a diffusion equation. By using an exit time statistics small deviation from self-similarity are detected. These deviations, signature of Lagrangian intermittency, are found to be well described by a simple extension of the multifractal model to Lagrangian statistics.

2.5 Nanoscale Technology

MS09 Nanoscale Semiconductor Devices: Mathematical Modelling and Numerical Simulation

Organized by: Angelo Marcello Anile, Armando Majorana

Topic: 5 Nanoscale Technology

Recent advances in mathematical modeling, numerical algorithms and computer performances allow to simulate in a reasonable CPU time:

- implantation processes at the atomistic level
- electron transport described by the semiclassical semiconductor Boltzmann equation
- quantum transport in nanostructures
- oscillations in superlattices semiconductors

Aim of the minisymposium is to bring present a review of some recent work in these areas with talks given by experts. In particular:

- Sub-lattice kinetic Monte-Carlo modeling of the nanostructural evolution of dopants and intrinsic point and extended defects in silicon (A. La Magna and M. Srobel, IMETEM-CNR, Catania)
- Deterministic numerical solution of the semiclassical semiconductor Boltzmann Transport equation; recent advances and comparison with stochastic simulation (A. Majorana, Catania)
- Electron transport in nanostructures: Quantum phenomena and hybrid models (N. Ben Abdallah, Toulouse)
- Nonlinear Charge Transport, Wave Propagation and Self-oscillations in Semiconductor Superlattices (L. Bonilla, Madrid)

Armando Majorana, C. Milazzo, O. Muscato

A Comparison Between Numerical Solutions to the Boltzmann-Poisson System and Monte Carlo Results for Silicon Devices.

Two models describing charge transport in semiconductors are considered. The first is the Boltzmann transport equation for an electron gas, coupled to the Poisson equation for the electric field. The other is the direct Monte Carlo simulation of the electron gas. Numerical results of the Boltzmann-Poisson system have found in the case of one-dimensional $n^+ - n - n^+$ device and compared with Monte Carlo simulations. In the case of spatially homogeneous solutions for constant doping, Boltzmann-Poisson and Monte Carlo results are compared with experimental data.

Naoufel Ben Abdallah

Hybrid Models for Electron Transport in Nanostructures

We present in this talk some models and numerical simulations for electron transport in nanostructures. The models account for quantum ballistic phenomena which take place in the active zone of the device. This is done via the Schrödinger equation with open boundary conditions. We also present some hybrid models which simultaneously account for quantum and classical effects. This is done in two situations. The first concern the coupling of a classical model in the reservoirs and a quantum model in the active region (like the double barrier in a resonant tunneling diode) and the second concerns partially confined systems like 2D electron gases where both classical and quantum effects coexist. Indeed, in the confined direction, the description relies on the Schrödinger equation while transport is classical in the nonconfined directions. Simulations in one dimensional and multidimensional cases for resonant tunneling diodes and quantum waveguides are shown.

"This work has been partially supported by the TMR project ERB FMRXCT970157 run by the European Commission"

Luis L. Bonilla

Nonlinear Charge Transport, Wave Propagation and Self-oscillations in Semiconductor Superlattices

Nonlinear charge transport in semiconductor superlattices under strong electric fields parallel to the growth direction results in rich dynamical behavior including formation of electric field domains, pinning or propagation of domain walls, self-sustained oscillations of the current and chaos. Theories use reduced descriptions of transport in terms of average charge densities, electric fields, ... This is simpler when the main transport mechanism is resonant tunneling of electrons between adjacent wells followed by fast scattering between subbands. In this case, we will derive microscopically appropriate discrete models and boundary conditions. Their analyses reveals differences between low field behavior where domain walls may move opposite or parallel to electrons, and high field behavior where they can only follow the electron flow. Dynamics is controlled by the available charge in the superlattice and doping at the injecting contact. For large charge inside the wells, boundaries between electric field domains are pinned resulting in multistable stationary solutions. Lower charge inside wells results in self-oscillations of the current due to recycling and motion of domain walls, which form kinks (high contact doping) or pulses (low contact doping). We also explain how controlling parameters such as voltage, doping or temperature affect self-oscillations.

MS06 Quantum Semiconductor Modelling and Simulations

Organized by: Ansgar Jüngel, Rene Pinnau

Topic: 5 Nanoscale Technology

The ongoing miniaturization of semiconductor devices reached nowadays a length scale at which quantum effects play a dominant role. Therefore, standard models like the classical drift-diffusion equations are physically inaccurate and have to be replaced by models which incorporate the relevant quantum effects. The state of the art in quantum semiconductor modeling ranges from microscopic models, like the kinetic Wigner equation, to macroscopic equations, like quantum hydrodynamic models.

This minisymposium presents some recent results on the modeling and numerical simulation of modern quantum semiconductor devices, for instance resonant tunneling diodes or heterostructure hot-electron diodes, using both the Wigner formalism and quantum hydrodynamic (or density gradient) models. Furthermore, spatio-temporal dynamics and pattern formation in layered nanostructures are discussed.

Hans Kosina, R. Kosik, M. Nedjalkov

A Hierarchy of Kinetic Equations for Quantum Device Simulation

A hierarchy of transport models describing quantum effects at different levels of approximation is presented. Approximations are introduced in the electron-phonon interaction only, while the influence of the device potential on the coherent transport is taken fully into account. The hierarchy is derived from the generalized Wigner function, which depends on position and momentum of one electron and two sets of phonon occupation numbers. Introducing the weak scattering limit and assuming an equilibrium phonon system yields an equation set consisting of a main equation for the reduced Wigner function and two auxiliary equations. From this set several quantum kinetic equations can be derived. Assuming a space homogeneous electric field the set reduces to the Levinson equation, which allows quantum effects in the electron-phonon interaction to be studied, such as collision broadening, collision retardation due to the memory character of the kernel, and the intra-collisional field effect. Solutions of the Levinson equation obtained by a backward Monte Carlo method will be discussed. By taking the classical limit in the phonon interaction the equation set reduces to a Wigner equation including a Boltzmann scattering operator. This equation is considered a feasible model for far from equilibrium transport in nano structures.

Rene Pinnau

Numerical Methods for the Quantum Drift Diffusion Model

We present numerical methods for the solution of the quantum drift diffusion model. The stationary equations are treated via a generalized Gummel iteration, which proves to be convergent. For the spatial discretization we propose a new exponentially fitted scheme. The transient equations are fully implicitly discretized in time, which ensures the strict positivity of the discrete density. The scheme converges with optimal rate. Numerical experiments are presented.

Eckehard Schöll

Spatio-Temporal Instabilities in Semiconductor Quantum Structures

This paper focusses on modeling and simulation of nonlinear charge transport in semiconductor quantum structures resulting in complex spatio-temporal dynamics and self-organized pattern formation [1]. Current filamentation and further secondary bifurcations are common phenomena in those systems. In particular, I present a model describing transport in layered nanostructures such as the double barrier resonant tunneling diode or the heterostructure hot electron diode. Complex dynamics including spatio-temporal chaos and spiking is found on one- and two-dimensional spatial domains.

[1] E. Schöll: *Nonlinear spatio-temporal dynamics and chaos in semiconductors*, Cambridge University Press (2001).

Andreas Wettstein, Oleg Penzin, Eugeny Lyumkis

Implementing the Density Gradient Method into a Classical Device Simulator

We describe the implementation of the Density Gradient Model into the device simulator Dessis. The basic prerequisite for the implementation is a robust discretisation scheme applicable for multi-dimensional problems. We also present a generalisation of Density Gradient model made necessary by the special handling of insulators in DESSIS. The implementation is evaluated for a couple of examples and shows excellent agreement to results obtained by the Schrödinger equation.

MS11 Current Problems and New Approaches in Circuit Simulation

Organized by: Roswitha Maerz, Robert M.M. Mattheij

Topic: 5 Nanoscale Technology

Recently, good progress was made concerning the recognition and utilization of mathematically and, in particular, numerically relevant structural properties of DAEs in circuit simulation.First of all this refers to the monitoring of the DAE-index and adapted numerical integrators.

The increasing miniaturization of circuits and the related high-performance require to take into account factors that have been neglected so far, as e.g. the noise of a circuit, the interaction between thermal and electrical effects, parasitic effects due to short channels of transistors, etc. The resulting necessary complex modelling of circuits leads to systems that are a great challenge to applied mathematics not only because of their size complexity, but mainly because of the coupling effects when coupling different components (classical DAEs, PDEs, stochastic DAEs).

The minisymposium shall reflect the progress made in this respect as well as provide the opportunity for discussing open problems.

Caren Tischendorf

Structure and Index for DAEs and PDAEs in Circuit Simulation

The simulation of integrated circuits requires the inclusion of special models describing the voltage-current or charge-current characteristics of semiconductor elements. Depending on the model level, the resulting equation system may represent a differential-algebraic equation (DAE) or a coupled system of first order PDEs, second order PDEs and DAEs. Such coupled systems are sometimes denoted as PDAEs, but we will consider them as abstract DAEs with unbounded operators.

The different resulting systems may provide solutions with a different qualitative behaviour. This will be illustrated for the NAND gate simulated by different MOSFET models. Finally, we present detailed structural informations and index criteria for (usual) DAEs and abstract DAEs in this field.

Stephan Houben, Joseph M. Maubach, E.J.W. ter Maten

Time-Domain Simulation Techniques for Voltage Controlled Oscillators

Voltage Controlled Oscillators (VCOs) form an important building block of electrical circuits. However, simulating VCOs is still problematic. There is great interest in better simulation techniques for VCOs.

A new time-domain method is presented for simulating VCOs. The new method is robust and can also be used to compute phase noise in the VCO. The method is being implemented in Pstar, the in-house circuit simulator of Philips. Numerical results will be presented.

Renate Winkler

Stochastic DAEs in Transient Noise Simulation

The increasing scale of integration, high tact frequencies and low supply voltages cause smaller signal-to-noise-ratios. In several applications linear noise analysis is no longer satisfactory and thus transient noise analysis becomes necessary. We deal with the thermal noise of resistors as well as the shot noise of semiconductors modeled by additional sources of additive or multiplicative white noise currents. The resulting system is described by a stochastic differential algebraic equation (SDAE) of the form

$$A(x(t)-x(t_0)) + \int_{t_0}^{t} f(x(s),s)ds + \int_{t_0}^{t} G(x(s),s)dw(s) = 0 \quad ,$$

where A is a constant singular matrix which is determined by the topology of the electrical network and w is a k-dimensional Wiener process. One has to deal with a large number of equations as well as of noise sources. Using techniques from the theory of DAEs as well as of the theory of SDEs we analyze such systems and present suitable discretization schemes.

Roland Pulch

PDE Techniques for Finding Quasi-Periodic Solutions of Oscillators

The steady state response of an electric circuit often characterises its physical behaviour. Hence circuit simulation aims at the determination of periodic or quasi-periodic solutions of the corresponding ODE models. In radio frequency applications, oscillatory signals with widely separated time scales arise due to the coupling of analogue and digital components. Thus transient analysis becomes costly, since the fastest rate restricts the integration step size. We present a PDE model, which yields more efficient techniques in these applications. This quite new approach decouples time scales by a special multidimensional signal representation. Accordingly, we apply this strategy to compute the quasi-periodic steady state response of source driven oscillators. The special structure of the PDE system and the resulting information transport leads to a method of characteristics. We discuss the practicability of the corresponding numerical methods. Test with LC-oscillators and the ring modulator are presented.

MS20 Numerical Methods for Wave Propagation in Unbounded Media

Organized by: Frank Schmidt, Marcus Grote

Topic: 5 Nanoscale Technology

The minisymposium covers recent results on theoretical and numerical aspects of wave propagation in unbounded media. The talks deal with the analysis and application of the PML method, both for time-dependent and time-harmonic problems, the construction and analysis of high-order transparent boundary conditions as well as a new concept called pole condition. Applications of these methods range from integrated optics and microwave technology to acoustics, oceanography and quantum mechanics.

Eliane Bécache, P. Joly, S. Fauqueux

Stability and Instability Results for PML Models

In this talk we investigate the question of stability of the Perfectly Matched Layers (PML) introduced by Bérenger in order to design efficient numerical absorbing layers for the computation of time dependent solutions of Maxwell's equations in unbounded domains. Previous works aimed essentially at proving the well-posedness of such models. The corresponding results do not exclude a possible exponential blow up of the solutions for large time. We think that for the applications, a more pertinent concept is the one of stability: one wishes to get uniform estimates in time. We first show that such a stability result is valid for isotropic Maxwell and acoustic equations, for which the result can be obtained by Fourier analysis and energy estimates. Then we show that the stability properties can be lost in case of anisotropy. We illustrate in particular this on the case of anisotropic elastic waves. We show that a necessary condition of stability can be interpreted in terms of group velocities and geometrical properties of the slowness curves. This applies for showing instability results for the classical PML models for linearized Euler equations and anisotropic Maxwell's equations.

Marcus Grote

Nonreflecting Boundary Conditions, High-order Methods, and Energy Decay

The simulation of waves in unbounded media usually requires an artificial boundary, which truncates the unbounded exterior domain and restricts the region of interest to a finite computational domain. To avoid any spurious reflection from the artificial boundary, we have devised exact nonreflecting boundary conditions for the wave equation, Maxwell's equations, and the elastic wave equation. These boundary conditions are local in time and involve only first derivatives of the solution. Therefore, they are easy to use with standard numerical methods. Clearly, in the absence of forcing the wave energy initially present inside the computational domain should decay with time. Starting from a new energy equality, which explicitly relates the initial energy to that at later time and thus identifies the energy loss through the artificial boundary, we are able to establish this result rigorously. Recent numerical simulations of wave scattering from complex geometry, which were obtained with a high-order finite element method, are also presented to demonstrate the expected faster convergence and improved accuracy.

Thorsten Hohage, Lin Zschiedrich

Analysis of Time-Harmonic Scattering Problems Based on the Pole Condition and Convergence of the PML Method

In this talk we outline the theoretical foundations of our approach to solve time-harmonic scattering problems. We consider equations of Helmholtz-type with a radially symmetric potential. It turns out that the far-field behavior of solutions is determined by the singularities of their Laplace transforms in radial direction. Singularities in the upper half of the complex plane correspond to outgoing waves and singularities in the lower half to incoming waves. The pole condition excludes singularities in the lower half of the complex plane. A new representation formula based on the pole condition is derived and used to establish existence, uniqueness and asymptotic properties of solutions. The well-known asymptotic formulas of the Hankel and the Matthieu-Hankel functions drop out naturally as special cases from our analysis. Moreover, we show that for our class of problems the pole condition is equivalent to Sommerfeld's radiation condition. Our results also shed new light on the PML method and can be used to establish exponential convergence as the thickness of the sponge layer tends to infinity.

Frank Schmidt

Pole Condition: A New Approach to Solve Scattering Problems

We derive exact transparent boundary conditions for time-harmonic scattering problems modeled by the Helmholtz equation. This talk covers the essential aspects of our approach. First, the entire space is decomposed into an interior domain containing the scatterer and an exterior domain. The basic idea is to consider the Laplace transform of the field in the exterior domain. We characterize the exterior fields by the poles of their Laplace transforms and say that a field satisfies the pole condition if its Laplace transform has no pole in the lower half of the complex plane. Fields which satisfy the pole condition are outgoing fields. This enables us to formulate scattering problems based on the pole condition rather than on Sommerfeld's radiation condition. Moreover, the pole condition leads in a direct way to new numerical algorithms which allow to solve some types of practically relevant problems with variable coefficients and infinite obstacles.

Achim Schädle, Christian Lubich

A Fast Convolution Algorithm for Non-Reflecting Boundary Conditions

Non-reflecting boundary conditions for problems of wave propagation are non-local in space and time. While the non-locality in space can be efficiently handled by Fourier or spherical expansions in special geometries, the arising temporal convolutions still form a computational bottleneck. We present a new algorithm for the evaluation of these convolution integrals based on local approximation on fast growing time intervals and on the numerical inversion of Laplace transforms. To compute a temporal convolution over N_t successive time steps, the algorithm requires $O(N_t \log N_t)$ operations and $O(\log N_t)$ memory. In the numerical examples, this algorithm is used to discretize the Neumann-to-Dirichlet operators arising from the formulation of geometries for Schrödinger and wave equations.

2.6 Communication

MS21 Mathematical Modelling of Semiconductor Lasers

Organized by: Klaus Schneider, Bernd Krauskopf

Topic: 6 Communication

The Minisymposium concerns recent developments and results in semiconductor laser modeling. The main objects are multiquantum well lasers and multisection DFB (distributed feedback) lasers, two types of optoelectronic devices which are of great importance for current and future optical communication nets, and effects of external feedback phenomena on their performance.The mathematical models are boundary value problems for systems of nonlinear ordinary and partial differential equations (drift diffusion equations, Schrödinger equations, wave equations, delay differential equations and others) and corresponding numerical tools.

Uwe Bandelow, Hans–Christoph Kaiser

Simulation of Multi Quantum Well Lasers with WIAS–TeSCA

Semiconductor lasers are, due to their miniature shape and their efficiency, a potentially attractive and already widely used source of coherent optical radiation. The modelling of semiconductor lasers has to cope with the electronic behaviour of the semiconductor, the optical field, mechanical stress in the composite material, and the warming up of the device. The question is, how all these influences intertwine. That leads to coupled systems of partial differential equations on the device domain including Poisson's equation for the electrostatic potential generated by free roaming electrons and holes and ionized dopants, current continuity equations for electrons and holes, some derivative of Maxwell's equations for the optical field, and eventually an energy balance equation. Moreover, quantum effects are an important feature of the semiconductor laser, the active zone of which is a nanostructure, often formed by a stack of strained quantum wells. Quantum effects require the incorporation of an appropriate (matrix) Schrödinger equation for the description of individual electronic states into the model. We report on a semiconductor device modelling strategy with WIAS–TeSCA in the framework of the above set of coupled equations.

Michael Pfeiffer, B. Witzigmann, A. Witzig, W. Fichtner

Laser-DESSIS: A Comprehensive Multidimensional Microscopic Simulation Tool for Quantum Well Lasers

Understanding the critical performance parameters of quantum-well laser diodes is a challenging task. Device simulation supports this process, however, the number of physical models, and their strong numerical coupling involve complex computations. In this contribution, a commercial simulation tool [1] is presented which allows for microscopic simulation of semiconductor lasers in one to three spatial dimensions. In the framework of a hydrodynamic model, it solves the carrier drift-diffusion equations and the energy flux equations together with photon rate equations and the Helmholtz equation for the optical field [2]. Quantum wells are treated as scattering centers, which enables explicit treatment of quantum carrier capture. The equations are solved in a self-consistent fashion applying robust and efficient numerical methods. Both static and dynamic properties can be calculated. Geometric modeling, mesh generation and visualization is provided by tools widely established in silicon TCAD. As simulation example, a 980nm ridge waveguide laser is investigated and the application of multidimensional simulation for device design is discussed. Comparisons of simulations and measurements show excellent agreement.

[1] DESSIS-ISE 7.0, ISE Integrated Systems Engineering AG. [2] B. Witzigmann, A. Witzig, W. Fichtner, "A Multidimensional Laser Simulator for Edge-Emitters Including Quantum Carrier Capture", IEEE TED, 47/10, pp. 1926-1934, October 2000.

Mindaugas Radziunas, Jan Sieber

Simulation and analysis of dynamics in multi-section semiconductor DFB laser

Edge emitting multi-section semiconductor lasers are of great interest in the process of developing all optical data transmission in optical communication systems. When designing lasers with required dynamical behaviour, modelling plays a crucial role.

Different nonlinear dynamical effects, such as different kinds of self pulsations, bistability and excitability, observed experimentally in multi-section DFB semiconductor laser, can be described and recovered by the traveling wave (TW) model. This model is given by a hyperbolic system of PDE's for counter-propagating optical fields coupled with ODE's for carrier densities. We reduce the model by applying center manifold theory and arrive to a low dimensional system of ODE's. Being in good qualitative and quantitative agreement with the TW model, the ODE model can be analyzed with well known numerical tools for bifurcation analysis such as AUTO.

This analysis allows us to identify different types of bifurcations leading to switching on and switching off of the self pulsations. Now we can explain the origin of observed bistability, as well as the mechanisms of excitable behaviour of lasers, demonstrated experimentally and theoretically by the "full" TW model.

Bernd Krauskopf, Kirk Green

Routes to Chaos in a Semiconductor Laser Subject to Phase-Conjugate Feedback

We explain and demonstrate a new numerical technique for delay differential equations, namely the computation of unstable 1D unstable manifolds of a saddle-type periodic orbit as intersection curves in a suitable Poincaré section. While this method is useful in quite some generality, we illustrate its power with the example of a semiconductor laser subject to phase conjugate optical feedback.

Specifically, we are able to explain in detail transitions to chaos as the feedback strength is increased, including the break-up of a torus and a sudden transition via a boundary crisis. This allows us to make statements on properties of the ensuing chaotic attractor, such as its dimensionality. Information of this sort is important for applications of chaotic laser signals, for example, in communication schemes.

2.8 Market and Finance

MS16 Qualitative Aspects and Economic Applications of Hysteresis Modelling

Organized by: Martin Brokate, Rod Cross, Alexei Pokrovskii

Topic: 8 Market and Finance

Standard neoclassical economic analysis has microeconomic foundations in which some representative economic agent responds continuously to economic shocks. This yields economic equilibria that do not contain a memory of the past shocks. Since the '70s it has become reasonably clear that some important economic phenomena are not well described by such models. For example, expansionary shocks (e.g. the UK departure from the ERM in 92, the buoyant US stock market of the '90s) have reduced unemployment rates without leading to the rising rates of inflation predicted by standard models. Thus, many economists have proposed that hysteresis effects are at work in labour markets. Other examples include habit formation and the excess smoothness of aggregate consumption, sunk costs and irreversibilities in investment and market entry decisions, lasting effects of temporary exchange rate changes on international trade flows.

The mathematical theory of hysteresis contributes to the analysis of such situations in several respects. It provides a toolbox of simple and complex models for hysteretic dependence. Combined with dynamical systems theory, it yields qualitative insights into the short-term and long-term behaviour of such processes, and it forms the basis for their reliable numerical simulation.

This minisymposium aims at fostering this connections by bringing together scientists from mathematics and economics who work on these models.

Richard Hule, Martin Brokate

Solow Type Economic Growth with Labor Market Hysteresis

Neoclassical growth models have problems in explaining and describing the behavior of labor market variables, especially the persistence of unemployment and the asymmetric reaction of several labor market variables to shocks. On the other hand, microeconomic investigations of the labor market focus on hysteresis effects as one of the crucial features in describing peculiar characteristics of the labor market because of unions, insider-outsider behaviour, search or loss of skill. The hysteretic behavior is also supported by empirical evidence. It is therefore natural to investigate growth models modified by unemployment and hysteresis in the labor markets.

In this paper, we discuss a stochastic Solow-type growth model augmented by an endogenous determination of the labor input whose formal description includes a hysteresis operator. We assume the technology to be a time-dependent random variable and study, by means of numerical simulation, the dependence of the mean values of and correlations between capital, labor and output upon the strength of the hysteresis (that is, the width of the hysteresis loop) and the initial conditions.

Matthias Göcke, Trond-Arne Borgersen

Exchange Rate Overshooting and Hysteresis in Foreign Trade

The paper integrates a Dornbusch exchange rate overshooting model with a macro-economic model of hysteresis in foreign trade based on a Preisach aggregation approach. This combined framework shows how a situation with sticky prices and short run exchange rate overshooting results in long run persistence in exchange rates. Monetary shocks can lead to hysteresis in both foreign trade and exchange rate processes, invalidating the long run neutrality of money hypothesis of the conventional overshooting model.

Oleg Rasskazov, A. Pokrovskii

Hyperbolic Behaviour in Systems with Normal Hysteresis Nonlinearities.

The concept of normal hysteresis nonlinearity was suggested by M. Brokate and A. Pokrovskii in [1]. As examples of normal nonlinearities we mention von Mises model of plasticity, Giltay-Preisah and Mayergoyz-Fridman models of ferromagnetism and similar models used recently in mathematical macroeconomics [2,3].

We consider the problem of robustness of phase diagram of an ordinary differential equation with respect to small normal hysteresis perturbations. For instance we prove that a robustness of hyperbolic auto oscillations and forced oscillations. Also robustness of chaotic behaviour is considered.

Proofs are based on the method of split-hyperbolicity [4,5].

[1] M. Brokate, A.V. Pokrovskii, Asymptotically stable oscillations in systems with hysteresis nonlinearities, JDE, 150 (1998), 98-123.

[2] R. Cross, On the foundation of hysteresis in economic systems, Economics and Philosophy, n. 9 (1993), 53-74.

[3] L. Piscitelli, R. Cross et al., A test for strong hysteresis, Computational Economics, 15(1/2), 59-78, April 2000

[4] A.V. Pokrovskii, Topological shadowing and split-hyperbolicity, Functional Differential Equations, special issue dedicated to M.A. Krasnosel'skii Vol. 4, No3-4 (1997), 335-360.

[5] O. Rasskazov, Forward and backward stable sets of split-hyperbolic mappings, Reports of INS 00-009. July 2000

Ansgar Belke

On the Role of Hysteresis Models in Giving Policy Advice

This paper strengthens the case for hysteresis models in giving policy advice with respect to path-dependent variables by focusing on the debate about European Monetary Union from a public choice perspective. The main focus is on the 'two-handed approach' to economic policy. This approach can be traced back to the hysteresis approach and alludes to the fact that a combination of supply-side and demand-side measures is the most efficient way to tackle the bad performance of economic variables which exhibit path-dependence. The application of supply-side measures lowers the magnitude of the demand shock necessary to reverse the effect of an adverse shock in the past. Demand-side measures enhance the probability of supply-side reforms. Since supply-side measures are often proposed by politicians adhering to neoclassical theory and demand-side measures are favoured by those who are advised by Keynesian economists, policy advice derived from a hysteresis model typically has a high chance to lead to a political consensus. Moreover, politicians are rewarded for reform efforts with long-lasting benefits. Given the reduction in polarisation of the political parties' programs in Western Europe, the mathematical theory of hysteresis contributes to progress in a non-mathematical area, i.e. to a more efficient policy advice giving.

A.M. Krasnoselskii, D.I. Rachinskii

Hopf Bifurcation in Systems with Preisach Hysteresis

In the talk we study autonomous systems with complex hysteresis nonlinearities (Preisach hysteresis). We give sufficient conditions of existence of small cycles in the vicinity or the curve of equilibria, these conditions are close to classical conditions of Hopf bifurcations for systems of ODE with a parameter. The existence of such cycles is defined by internal properties of Preisach nonlinearities.

MS39 Aspects of Financial Time Series and Portfolio Problems

Organized by: Claudia Klüppelberg

Topic: 8 Market and Finance

Financial risk management is very much model dependent. Risk measures like Value-at-Risk and expected shortfall are sensitive to extreme behaviour and dependence of the underlying financial time series. This minisymposium studies time series aspects like dependence in one- and multivariate setting as well as consequences for the portfolio optimization problem.

Andreas Kunz

Extremes of Multidimensional Diffusion Processes

In risk management the extreme behavior of diffusion processes is of natural interest as for example interest rates are modeled by stationary diffusions. In the one dimensional case, the extreme behavior of stationary diffusion processes is well known. In this talk I will present some results in the multidimensional case. It turns out that the extreme behavior of a diffusion process can be described by characterizing the asymptotic decay of eigenvalues of an eigenvalue problem associated with the generator of the process.

Alexander Lindner

Angles and Linear Reconstruction of Missing Data

We characterize a class of stationary time series for which the linear reconstruction of missing data is uniformly bad in a certain sense. This involves angles between Hilbert subspaces. It is shown that most ARMA-models belong to this class. Also, time series with better reconstruction properties are considered and examples are given.

Ross Maller, D. A. Turkington

New Light on the Portfolio Allocation Problem

The basics of the mean-variance portfolio optimisation procedure have been well understood since the seminal work of Markowitz in the 1950's. A vector x of asset weights, restricted only by requiring its components to add to 1, is to be chosen so that the linear combination $\mu_p = x'\mu$ of the expected asset returns μ (or, expected excess returns), which represents the expected return on a portfolio, is maximised for a specified level of "risk", σ_p, the standard deviation of the portfolio. The efficient frontier is the curve traced out in (μ_p, σ_p) space by portfolios whose return/risk tradeoff is optimal in this sense. The portfolio with the maximum *Sharpe ratio* is the portfolio with the highest return/risk tradeoff achievable from the assets, and under some conditions can be obtained as the point of tangency of a line from the origin to the efficient frontier, as is well known. But when the tangency approach fails, which it commonly can, the question arises as to the maximum Sharpe ratio achievable from the assets. This problem, which has not been dealt with before, is solved explicitly in this paper, and the corresponding optimal portfolio found. The suggested procedure is easily implemented when the usual inputs – estimates of mean excess returns and their covariance matrix – are available.

Catalin Starica, Clive Granger

Non-Stationarities in Stock Returnd

The assumption of stationarity is hard to defend when modelling financial return s on longer time intervals, given the pace at which new technological tools and financial instruments have been introduced on the financial markets. Relinquishing the global stationarity hypothesis, this paper conducts a data analysis focused on the size of the returns, i.e. the absolute values of returns, under the assumptions that, at least locally, the $S\&P500$ daily return series can be modelled by stationary processes. The challenging task when working under the assumption of local stationarity is to define the intervals on which stationary processes provide a good approximation. This task is accomplished by using a goodness of fit test based on the integrated periodogram. The conclusion of the paper is that almost all the dynamics of return time series seem to be concentrated in the shifts of the variance. More concretely, the $S\&P500$ absolute returns, $|r_t|$ can be described by the following

$$|r_t| = h(t)\exp(\epsilon_t), \quad t = 0, 1, \ldots$$

where (ϵ_t) is a sequence of iid random variables, $E(\epsilon) = 0$, $E(\epsilon)^2 = \sigma^2$ and $h(t)$ a function of t which can be well approximated by a step function, yielding a model with piecewise constant variance.

MS35 Credit Risk

Organized by: Ludger Overbeck

Topic: 8 Market and Finance

Mathematical modelling for the measurement, management and trading of credit risk is the topic of an increasing number of academic research papers and is also in the focus of the financial industry. The symposium will cover therefore academic research as well as an insight into recent questions in the applications.

Michael Kalkbrenner

Economic Capital for Credit and Market Risk: An Integrated Approach

This talk is on the quantification of portfolio risk in a mark-to-market framework. We consider portfolios which consist not only of traditional credit products and fixed income instruments but also of market-driven instruments subject to counterparty default. For those portfolios no clear distinction exists between credit and market risk and therefore a realistic quantification of portfolio risk has to be based on an integrated approach. The main obstacle in applying integrated credit and market risk models is the inherent computational complexity of this approach. In this talk we focus on the development of efficient models and algorithms which can be applied to large portfolios.

William Morokoff

Risk Analysis of CDOs with Multi-Step Monte Carlo Simulations

Collaterized Debt Obligations (CDOs) are financial structures that direct cash flows from an underlying collateral portfolio (typically high yield bonds and corporate loans) to tranches of varying credit quality. The waterfall of payments to the tranches depends on various collateral tests intended to protect the tranches in the event of substantial deterioration of the credit quality of the collateral. While the market for CDOs continues to grow, the associated risks are often not clearly understood.

This talk will address the use of multi-step Monte Carlo simulations over the life of a CDO deal to describe these risks, focusing on the stochastic models for credit migration as well as on the effects of diversification in CDO collateral portfolios.

Ludger Overbeck

Credit Risk Capital Allocation Based on Expected Shortfall

In the talk we first present the basic probabilistic concepts in modeling the credit risk in portfolios. We present first a simple one period model for large portfolios. Then a model of multivariate asset-values that are consistent with the market is constructed. Finally a capital allocation scheme based on the notion of expected shortfall risk is introduced and compared with classical approaches based on variance/covariance analysis.

Eckhard Platen, Mark Craddock

Benchmark Pricing of Credit Derivatives under a Standard Market Model

The paper exploits an integrated benchmark modelling framework, which allows to consistently model and price credit risk. It will be demonstrated how to price contingent claims under the historical probability measure in a benchmarked world. Furthermore, put and call options on an index are studied that measure the creditworthiness of a firm.

MS10 Applications of Stochastic Simulations

Organized by: Wesley Petersen, Denis Talay

Topic: 8 Market and Finance

Numerical simulations of stochastic differential equations are of increasing interest in finance, solutions of partial differential equations in high dimensions, polymer physics, and quantum statistical mechanics. In this mini-symposium, I would like to cover several topics: stochastic delay differential equations, solutions of the Dirichlet problem, and stochastic partial differential equations.

Fabian Buchmann

Solving Dirichlet Problems of Laplace Type Using a Random Walk with Bounded Increments

We propose an algorithm for solving Dirichlet problems for equations of Laplace type in a bounded domain D in Euclidean n-space. Using a probabilistic approach, we approximately solve a system of stochastic differential equations using weak Taylor approximations. This approach requires the approximation of both exit time and exit point of a standard Wiener process from the domain D. We construct a weak one-step approximation of the Markov process to 3nd order of accuracy. In order that every step until exit remains in the closure of D, we use bounded random variables to approximate the Ito integrals appearing in the stochastic Taylor expansion of the SDEs to the desired order.

We show numerous numerical tests for the Poisson equation that confirm the order of convergence as predicted by theory. Especially in higher dimensions (n¿4) we find good agreement with theory. The resulting algorithm is easy to implement: grid-free and ideally suited for cluster architectures as it parallelizes embarrassingly well with negligible communication overhead.

Evelyn Buckwar

Strong Approximation Schemes for Stochastic Functional Differential Equations

We discuss some strong approximation schemes for evolutionary stochastic delay differential equations. We give emphasis to the Euler-Maruyama method for equations with discrete, variable and distributed time-lag, and we take into account the properties of the initial data. We will present some of our recent results on convergence and the order of convergence and on stability in p-th mean, and illustrate the theory with the outcomes of numerical experiments. The talk is based on joint work with Christopher T.H. Baker (Manchester, UK).

Wesley Petersen

Some Distribution Functions from Weak Approximations of Diffusion Processes

In this talk I discuss models for multi-dimensional stochastic integrals that appear in Wagner-Platen expansions of stochastic differential equations. In one dimension, these integrals can be reduced to Hermite polynomial representations. In multiple dimensions, there is no closure in the space of multivariate Hermite polynomials so cruder models must be constructed. I will review various models, their distribution functions, and inner correlations for both conditional (exit time problems) and unconditional expectations.

Karl Sabelfeld

Stochastic Models of Coagulation Processes Governed by a Class of Smoluchowski Equations.

A stochastic model is constructed for a system of diffusing and coagulating particles in a host gase flow. The main result concerns the probabilistic representation of the solution in the inhomogeneous case via an expectation over stochastic Lagrangian solutions to homogeneous Smoluchowski equation. This drastically decreases the cost of Monte Carlo numerical simulations.

Tony Shardlow

Numerics for Dissipative Particle Dynamics

Dissipative Particle Dynamics is a particle method for modelling fluids and polymers. The model features a simple pairwise interactions between particles arising from a conservation law plus fluctuation and dissipation terms. The model is used to simulate flows in equilibrium. I will discuss numerical issues, especially the widely used Verlet method and splitting methods.

MS44 Recent Progress in Levy Process Driven Ornstein-Uhlenbeck Type Stochastic Volatility Models: Pricing, Hedging, Estimation

Organized by: Walter Schachermayer, Peter Imkeller

Topic: 8 Market and Finance

Recently Barndorff-Nielsen and Shephard proposed a class of models that combine Levy processes and stochastic volatility to allow more realistic modelling of financial time series, and that is analytically very tractable.
Four young researchers present at this minisymposium their recent results for pricing, hedging, estimation, and related mathematical problems based on such models.

Elisa Nicolato, Emmanouil Venardos

Derivative Asset Analysis in Stochastic Volatility Models Based on Levy Driven Ornstein-Uhlenbeck Processes

Stochastic volatility models using L'evy driven processes of the Ornstein-Uhlenbeck type possess authentic capability of capturing some stylized features of financial time series. In this talk we investigate this class of models from the viewpoint of derivative asset analysis. We discuss topics related to the incompleteness of this type of markets. In particular, for structure preserving martingale measures, we derive the price of European calls, puts and simple exotic options in closed form. Furthermore, the range of viable prices is determined.

Friedrich Hubalek, Elisa Nicolato

On multivariate extensions of Levy process driven Ornstein-Uhlenbeck type stochastic volatility models and multi-asset options

We introduce a continuous-time multivariate stochastic volatility model, such that the univariate marginal proceses capture well-known stylized features of financial time series, such that the various asset price processes display an interesting stochastic (realistic?) dependence structure, and that is analytically very tractable.

In particular the univariate marginal processes are following a stochastic volatility model recently proposed by Barndorff-Nielsen and Shephard, with the instantaneous variance processes a superposition of non-Gaussian Ornstein-Uhlenbeck type processes.

Our approach is a continuous-time extension of a multivariate factor modelling popular for discrete time-modelling of time series.

Equivalent martingale measures are studied, explicit formulae (in terms of multivariate Laplace or Fourier inversion) for option pricing and multivariate probability densities resp. distributions, and numerical illustratins are given.

2.9 Speech and Image Recognition

MS29 Harmonic Analysis and Statistics for Signal and Image Processing

Organized by: Peter Maaß, Ludwig Cromme, Yehoshua Zeevi

Topic: 9 Speech and Image Recognition

The goal of this minisymposium is to stimulate interactions between theoretical and applied research in the field of multiscale signal- and image processing.

From the mathematical point of view, the main areas involved are:

- Harmonic analysis, in particular time-frequency and time-scale analysis,
- numerical analysis for signal processing applications.

The minisymposium consists of theoretical talks and presentations of successful applications.

Otmar Scherzer, C.W. Groetsch

Inverse Scale Space Theory for Inverse Problems

We derive scale space methods for inverse problems which satisfy the fundamental axioms of fidelity and causality and we provide numerical illustrations of the use of such methods in deblurring. These scale space methods are asymptotic formulations of the Tikhonov-Morozov regularization method. The analysis and illustrations relate diffusion filtering methods in image processing to Tikhonov regularization methods in inverse theory.

Gerd Teschke

Constructing Wavelets via Generalized Uncertainty Principles

The representations in L_2 of the affine, Weyl-Heisenberg or affine Weyl-Heisenberg group and the corresponding integral tranformations are well known. We extended this setting to (anisotropic) Sobolev spaces and ask for adequate wavelets. The search for outstanding quality of localization in phase-space or scale-angle-space representation leads to uncertainty principles. Naturally one has several uncertainties and minimizing them simultaneously is in general not possible. Hence, we propose to define generalized uncertainties. Under some assumptions we combine different infinitesimal operators by linear combinations and create therewith a new uncertainty principle. The resulting minimizing wavelets may be used in signal and image processing. One promisingly application is the generation of a continuous H^s multiscale analysis via minimizing wavelets.

Ludwig Cromme

Quality Checks of Colored Boxes in the Packaging Industry

Quality checks are an important part of product control in the packaging industry. Not only is the quality of the enclosing box often taken by the consumer as representative of the product itself, but it also carries important information about the product. This is in some cases so essential that correctness of warning labels, readability of product information, correct language etc must be guaranteed 100% by the manufacturer. At the same time packing which is normally done at speeds of a few (up to more than a hundred) per second should not be slowed down much.

In this presentation we analyze existing and discuss new image processing methods meeting the demands of high speed visual inspection applications as good as possible. The algorithms are compared with respect to their convergence, time complexity, and parallelization potential. The proposed approach was realized with dedicated hardware.

Peter Maaß, Y. Zeevi

Two Perspectives of Multiscale Analysis: A Relation Between Differential Operators and Wavelets

The latest developments in the field of mathematical morphology are almost entirely based on non-linear diffusion equations. The starting point of this development is the well-known connection between filtering a signal with a scaled Gaussian and the solution of the heat-transfer equation.

Since then many different types of linear Fourier-filters and non-linear operations like erosion and dilation have been investigated in terms of their related differential equation.

The aim of this talk is to present some preliminary results on adapting this approach to filtering with wavelet methods and defining their related differential equations.

MS15 Partial Differential Equations and Variational Methods in Image Analysis

Organized by: Joachim Weickert, Luis Alvarez

Topic: 9 Speech and Image Recognition

Many recent image analysis techniques use methods that are based on nonlinear partial differential equations and variational techniques. These approaches are mathematically well-founded, they have led to the unification of existing methods and the discovery of novel techniques, and the continuous modeling allows to study rotationally invariant models. In this minisymposium we present four approaches that illustrate the use of PDE methods and variational techniques for shape representation, image enhancement, and motion analysis.

Luis Alvarez, Carmelo Cuenca, Luis Mazorra, Francisco Santana

Applications of Morphological Multiscale Analysis to Shape Representation

In the last years, a lot of attention has been devoted to the morphological multiscale analysis (MMA) provided by geometric partial differential equations. The MMA satisfy very interesting invariances like the morphological invariance (invariance under non-decreasing histogram modifications) or the invariance under geometric transformations like Euclidean, similarity or affine transformations. In this paper we explore the applications of the MMA to shape representation. The first application that we study is the extraction of characteristic points (corners) of a shape. We will show that, by using MMA, we can extract corners in the image with a high accuracy. The proposed method is robust and independent of the contrast of the corner. We will present the application of this technique to the problem of multiple camera calibration. The second application of MMA that we present in this paper is a new geometric invariant representation of shapes. The geometric invariance is based on a normalized surface and/or perimeter evolution of the shape under the action of a MMA. We analyze the cases of Euclidean invariant, similarity invariant, and affine invariant geometric representations. We also present some numerical results to evaluate the performance of the proposed models.

Matteo Novaga, G. Bellettini, V. Caselles

The Total Variation Flow

I consider the minimizing total variation flow in R^n, discussing existence and uniqueness results. Bounded finite perimeter sets in R^2 which evolve without distortion of the boundary are completely characterized.

As an application, I discuss explicit solutions of the denoising problem in image processing.

Otmar Scherzer, Walter Hinterberger, Joachim Weickert

Analysis of Optical Flow Models in the Framework of Calculus of Variations

In image sequence analysis, variational optical flow computations require the solution of a parameter dependent optimization problem with a data term and a regularizer. In this paper we study existence and uniqueness of the optimizers. Our studies rely on quasiconvex functionals on the spaces $W^{1,p}(\Omega, \mathbb{R}^d)$, with $p > 1$, $BV(\Omega, \mathbb{R}^d)$, $BD(\Omega)$. The methods that are covered by our results include several existing techniques. Experiments are presented that illustrate the behavior of these approaches.

Joachim Weickert

Diffusion and Regularization Methods for Tensor-Valued Images

In recent years, many nonlinear diffusion and regularization methods for image restoration have been developed. Hardly any attention, however, has been paid to the development of nonlinear filters for matrix-valued image data. Such matrix-valued images arise e.g. in medical applications using diffusion tensor magnetic resonance imaging (DT-MRI), but also in motion analysis in image sequences. In this talk we will present nonlinear regularization functionals for such matrix-valued images, and we will describe corresponding nonlinear diffusion filters. Isotropic as well as anisotropic methods are derived.

2.10 Engineering Design

MS02 Shape Calculus and Relaxation Methods in Domain Optimization

Organized by: Karsten Eppler, Thomas Slawig

Topic: 10 Engineering Design

Shape optimization is mainly concerned with the optimal choice of geometrical domains for systems described by partial differential equations. It covers various aspects of application in structural engineering design, progress in computational methods, and the theoretical foundation. In this minisymposium, the further development of a differential calculus is discussed for the case of smooth shapes. Effects of degeneration are sketched for more irregular situations. Moreover, special properties such as symmetry and additional regularity of optimal shapes are considered. The applicability of different numerical methods is another important issue.

Sergei Belov

Symmetry in Shape Optimization and its Applications

The class of planar elliptic shape optimization problems which possess a high degree of symmetry is under consideration. It turns out that a circle (an annulus in the class of doubly-connected domains, or a sphere in R^3) is always a “critical point” in these optimization problems, which may or may not provide optimum.

The sufficient conditions for a circle (an annulus, a sphere) to be optimal have been established. It turns out also that these sufficient conditions of optimality can be formulated in terms of monotonicity and convexity of the integrand in a problem formulation.

These results have been applied for solving various shape optimization problems in elasticity theory and infiltration theory.

Marc Dambrine

Variations of the Shape Hessian for Neumann Boundary Condition

To prove stability for critical shapes is a difficult task. The stability of a critical shape is connected to the hessian of the shaping function at the critical shape. It turns out that usually the norms of differentiability and of coercivity are not equivalent. In previous works, I have proposed a method based on a precise estimate of the variations of the hessian around the critical points. This was achieved for problems where the state function solves an elliptic problem with Dirichlet boundary conditions. We present here the corresponding estimate for Neumann boundary data.

Helmut Harbrecht, Karsten Eppler

Application of Wavelet-Based BEM-Methods for the Study of Shape Optimization Problems in Elasticity

We consider the problem of maximizing the bending rigidity of an elastic cylindrical bar under given inequality constraints on their torsional rigidity and volume. Numerical results for gradient type and Quasi-Newton type algorithms are presented. The state equation (related to torsional rigidity) is solved by wavelet-based BEM-methods. In particular, we discuss the complexity of these methods, applied to the optimization algorithms.

Maciej Smolka

Relaxation in Shape Optimization Problems Described by Hyperbolic Equations

We consider the shape optimization problem

$$\min_{G \in \mathcal{A}(\Omega)} J(G, u_G)$$

with u_G satisfying the hyperbolic equation

$$\begin{cases} u_G'' + Au_G = f \\ u_G(0) = u^0, \quad u_G'(0) = u^1 \\ u_G = 0 \quad \text{on } (0,T) \times (\Omega \setminus G). \end{cases}$$

As the class of admissible shapes we take $\mathcal{A}(\Omega)$, i.e., the family of all open subsets of a fixed open and bounded $\Omega \subset \mathbf{R}^N$. It can be shown that such a problem in general does not admit a solution, so we need to apply the procedure of relaxation. This method consists of two parts. First we extend, in a sense, the class of admissible shapes and introduce the notion of relaxed hyperbolic problem. This extended admissible set is a suitable family of Borel measures on Ω. Then we find the relaxation of J on this greater space. The theory of relaxed functionals ensures the existence of solutions for such problems. Finally, we provide some necessary conditions for optimality for relaxed problems.

MS41 Sensitivity Analysis for PDEs and Dynamical Systems by Automatic Differentiation
Organized by: Andreas Griewank, Christian Bischof

Topic: 10 Engineering Design

On nonlinear models parameter identification, design optimization, numerical integration, optimal control and other computational tasks can usually only be performed effectively when accurate sensitivity is available. For problems defined in terms of procedural computer programs this can be achieved by the chain-rule based technique of automatic differentiation. It has been implemented in various packages for codes written in Fortran or C or their extensions.

The four talks in this minisymposium report numerical results on large scale problems and discuss various challenges. These are in particular: the differentiation of state of the art CFD solvers, the reduction of the memory requirement for adjoint calculations by checkpointing, the integration of AD into a large package for parallel scientific computing, and the evaluation of higher derivatives for the calculation and analysis of singular points.

Paul Hovland

Truly automatic Automatic Differentiation: Coupling AD and PETSc

Despite its name, automatic differentiation (AD) is often far from an automatic process. Often one must specify independent and dependent variables, indicate the derivative quantities to be computed, and perhaps even provide information about the structure of the Jacobians or Hessians being computed. However, when AD is used in conjunction with a toolkit with well-defined interfaces, many of these issues do not arise. We describe recent research into coupling the ADIC, ADIFOR, and ADOL-C automatic differentiation tools with PETSc, a toolkit for the parallel numerical solution of PDEs. This research leverages the interfaces and objects of PETSc to make the AD process very nearly transparent.

Hubert Schwetlick, Gerd Pönisch, Uwe Schnabel

Calculation of Higher Order Singularities by Using AD

When modeling a real world process by a nonlinear parameter dependent nonlinear system of equations, singular points on the solution manifold where the Jacobian with respect to the state variables is singular, are of special interest. At such points the underlying process changes its qualitative behavior. For the classification as well as for the calculation of singular points not only the Jacobian but also also higher order derivatives with respect to low dimensional subspaces are needed. The latter ones are used for defining and evaluating some auxiliary functions and their derivatives. These auxiliary functions depend on the type of the singularity considered and have low dimension but they are in general rather complex.

It will be demonstrated how techniques from nonlinear analysis can be combined with techniques from Automatic Differentiation as, e.g., computation of Taylor coefficients so that an efficient calculation also of higher order singularities is possible. Several numerical examples confirm the expected results.

Andrea Walther, Michael Hinze

Memory-reduced Calculation of Adjoints

A control problem based on the Navier-Stokes-Equations and the corresponding adjoint equations is considered. Appropriate discretization for both the direct and the adjoint equations are presented. Then two approaches for calculating an approximation of the adjoint equations are studied.

The usual method calculates an approximation of the Navier-Stokes-Equations. During this forward integration all intermediate results needed for the adjoint computation are stored. Hence, the memory requirement of the usual method is proportional to the runtime of the forward integration.

An alternative method stores only a limited number of intermediate states. Then the forward integration is started repeatedly from these suitable placed checkpoints in order to provide the data required by the adjoint calculation. Using this technique the memory requirement can be reduced drastically in comparison to the usual approach.

The storage needed by both methods is discussed. Then the memory reduction that is achievable for several numbers of checkpoints is presented. Furthermore the increase in runtime caused by the repeated forward integration is illustrated and analyzed.

Christian Bischof, Martin Bücker, Arno Rasch, Bruno Lang

Experiences with the automatic differentiation of large CFD Codes

We are involved in several engineering projects in aerodynamics and chemical process control to provide the derivatives needed for inverse and optimization problems around CFD solvers. The CFD codes employed are large Fortran codes, employing a wide class of numerical modelling techniques, and have been developed over the years without AD in mind.

In this context, we report on our experiences in applying the ADIFOR tool to the SEPRAN and FLUENT codes. SEPRAN is a general-purpose finite-element based CFD solver developed by Guus Segal at TU Delft (see http://ta.twi.tudelft.nl/sepran/sepran.html). The total SEPRAN package consists of about 3000 subroutines, comprising overall approximately 800,000 lines of Fortran 77 code. The FLUENT V4.52 package (see www.fluent.com) consists of approximately 1.6 mio. lines of Fortran 77/F90 code in roughly 2500 files.

In applying AD to those codes, we encountered various difficulties such as legacy and non-standard Fortran coding practices and numerical difficulties arising from an ill-posed choice of differentiation variables for a noisy time-dependent problem. In addition, the sheer size of the codes posed an organisational challenge. However, in the end these difficulties could be overcome and the sensitivity-enhanced versions of these CFD packages now provide a robust and efficient method for computing the derivatives desired by the users of these codes.

MS04 Applications of Optimal Shape Design

Organized by: Dietmar Hoemberg, Jan Sokolowski

Topic: 10 Engineering Design

The goal of this minisymposium is to demonstrate that shape optimization and shape calculus can be a powerful tool in various fields of application.

The topics considered range from a more theoretical application in a level set approach for for state-constrained optimal control problems to the optimal design of diffraction gratings.

Further applications concern the optimization of arches and problems of dynamic contact for viscoelastic bodies.

Michael Hintermüller

A Level Set Approach for the Solution of State-Constrained Optimal Control Problems

State constrained optimal control problems for linear elliptic partial differential equations are considered. The corresponding first order optimality conditions in primal-dual form are analyzed and linked to a free boundary problem resulting in a novel algorithmic approach with the boundary (interface) between the active and inactive sets as optimization variable. The new algorithm is based on the level set methodology. The speed function involved in the level set equation for propagating the interface is computed by utilizing techniques from shape optimization. Encouraging numerical results attained by the new algorithm are reported on.

Andrzej Myslinski

Shape Optimization of Dynamic Contact Problems for Viscoelastic Bodies

This paper deals with formulation of a necessary optimality condition and a numerical solution of a shape optimization problem of a viscoelastic body in unilateral dynamic contact with a rigid foundation. It is assumed that the contact with friction, described by Coulomb law, occurs at a portion of the boundary of the body. The contact condition is described in velocities. The equilibrium state of this contact problem is described by an hyperbolic variational inequality of the second order. The shape optimization problem for the elastic body in contact consists in finding, in a contact region, such shape of the boundary of the domain occupied by the body that the normal contact stress is minimized. It is assumed that the volume of the body is constant. In this paper, using material derivative method as well as the results of regularity of solutions to the dynamic variational inequality we calculate the directional derivative of the cost functional and we formulate the necessary optimality condition for this optimization problem. The finite element method is employed as a discretization method. The Augmented Lagrangian Technique combined with conjugate gradient method are employed to solve the discretized optimization problem numerically. Numerical examples are provided.

Gunter Schmidt

Optimal Design of Diffraction Gratings

In the talk we consider optimal design and inverse problems for diffraction gratings. These devices are modelled by Helmholtz equations in $\mathbb{R}^2$ with piecewise constant periodic coefficients. The non-smooth interfaces between different materials lead to strong singularities of solutions near corner points.

Based on the concept of material derivatives we obtain analytic formulas for gradients of the reflection and transmission coefficients with respect to the variation of interfaces. These formulas can be used to perform the sensitivity analysis for diffraction gratings, to study local stability estimates for the reconstruction of grating profiles from far-field data and gradient-based minimization algorithms.

Dan Tiba, J. Sprekels

On the Optimization of Arches

We develop a new approach for the solution of the Kirchhoff-Love model of elastic arches based on control theory and valid even for Lipschitzian arches.We obtain explicit integration rules for the corresponding fourth order equation and o decomposition of it related to the classical Pontryagin principle.This allows as well a complete study of shape optimization problems associated to arches.We derive existence of the optimal arch and the first order optimality conditions and we compute several numerical example without imposing differentiability assumptions on the geometry of the arches.

MS07 Computer Aided Control Systems Design I

Organized by: Volker Mehrmann

Topic: 10 Engineering Design

Systems and control theory are disciplines widely used to describe, control, and optimize industrial and economical processes. There is now a huge amount of theoretical results available which has lead to a variety of methods and algorithms used throughout industry and academia. Although based on theoretical results, these methods often fail when applied to real-life problems, which often tend to be ill-posed or of high dimension. This failing is frequently due to the lack of numerical robustness when implemented in a finite-precision environment. Moreover, the users of these methods are often not aware of new algorithmic developments and rely on available software. In this minisymposium some new developments in software for computer aided control system design will be presented that will be integrated in the SLICOT package for computer-aided control system design (CACSD).

Peter Benner

Numerical Solution of Linear-Quadratic Optimal Control Problems for Parabolic PDEs

The space discretization of point or boundary control problems for parabolic PDEs, like., e.g., convection-diffusion equations, with a quadratic performance index leads to the computational task of solving large-scale symmetric algebraic Riccati equations (AREs). These are nonlinear matrix equations of the form

$$0 = \mathcal{R}(X) := Q + A^T X + XA - XGX, \qquad G = G^T, Q = Q^T,$$

where A, G, Q are real $n \times n$-matrices. Here, A is sparse and G, Q usually have very low rank. We will discuss a numerical method based on Newton's method for AREs that makes use of the special structure of the coefficient matrices. If embedded in a direct updating technique for the feedback solution of the optimal control problem, this approach can be used to tackle very large problems.

Heike Fassbender

A Hybrid Method for the Numerical Solution of Discrete-Time Algebraic Riccati Equations

The numerical solution of discrete-time algebraic Riccati equations is discussed. We propose to compute an approximate solution of the discrete-time algebraic Riccati equation by the (butterfly) SZ algorithm. This solution is then refined by a defect correction method based on Newton's method. The resulting method is very efficient and produces highly accurate results.

Michael Karow

Computation of Structured Spectral Value Sets for Block Diagonal Matrices

Given a matrix triple (A, B, C), a set of matrices $\mathbf{\Delta} \subseteq \mathbb{C}^{\ell \times m}$ and a norm $\| \cdot \|$ on span($\mathbf{\Delta}$), the spectral value sets $\sigma_{\mathbf{\Delta}}(A, B, C, \delta)$ are defined as the sets of all eigenvalues of all matrices of the form $A + B\Delta C$, where $\Delta \in \mathbf{\Delta}$ and $\|\Delta\| < \delta$. These sets are known to be the super level sets of the function $s \mapsto \mu_{\mathbf{\Delta}}(C(s-A)^{-1}B), s \in \mathbb{C}$, where $\mu_{\mathbf{\Delta}}(M) := (\inf\{\|\Delta\| \, : \Delta \in \{\mathbf{\Delta}\}, \, \det(I - \Delta M) = 0\})^{-1}$.

Here we investigate spectral value sets which occur in stability analysis of composite linear systems with prescribed interconnection structure. More precisely: we consider the sets $\sigma_{\mathbf{\Delta}_{\mathcal{I}}}(A, B, C, \delta)$ where A, B, C are block diagonal and $\mathbf{\Delta}_{\mathcal{I}}$ is the set of all block matrices $\Delta = (\Delta_{jk})_{j,k \le r}$ with $\Delta_{jk} = 0$ for all (j, k) in the index set $\mathcal{I} \subseteq \mathbb{N}^{r \times r}$. Explicit formulas for the corresponding $\mu_{\mathbf{\Delta}}$-functions are given with respect to various norms. The eigenvalue inclusion theorems of Gershgorin, Brauer and Brualdi are shown to be special cases of our results.

Daniel Kressner

Software for Structured Matrix Factorizations

Structured matrix problems play an important role in many areas of systems and control. Identification techniques for linear time-invariant state-space models often require the solution of problems involving block Toeplitz or Hankel matrices. The presented toolbox implements direct (least squares) solvers, Cholesky and QR factorizations for such matrices. All algorithms are based on the generalized Schur algorithm using new reliable and efficient methods for semi-definite block Cholesky downdating. Additional structure, as in the case of banded matrices, is exploited.

The routines form an integral part of the FORTRAN library SLICOT whereas a Matlab interface provides convenient accessibility to the complete functionality of the toolbox.

MS42 Computer Aided Control Systems Design II

Organized by: Volker Mehrmann

Topic: 10 Engineering Design

Systems and control theory are disciplines widely used to describe, control, and optimize industrial and economical processes. There is now a huge amount of theoretical results available which has lead to a variety of methods and algorithms used throughout industry and academia. Although based on theoretical results, these methods often fail when applied to real-life problems, which often tend to be ill-posed or of high dimension. This failing is frequently due to the lack of numerical robustness when implemented in a finite-precision environment. Moreover, the users of these methods are often not aware of new algorithmic developments and rely on available software. In this minisymposium some new developments in software for computer aided control system design will be presented that will be integrated in the SLICOT package for computer-aided control system design (CACSD).

Ivan Markovsky, Sabine Van Huffel, Bart De Moor

H2-Optimal Linear Parametric Design

The paper considers an LTI parameter dependent model $\tilde{H}(z,p)$, where the parameter p is a design variable. The $\mathcal{H}_2$-optimal parametric design aims to minimize $||\tilde{H}(z,p)||_2$. The solution depends critically on the function $\tilde{H}(z,\cdot)$. Affine function $\tilde{H}(z,\cdot)$ corresponds to an open-loop design and leads to a convex quadratic optimization problem. An analytic solution is given in this case. Affine-fractional function $\tilde{H}(z,\cdot)$ corresponds to a closed-loop design and leads to a non-convex optimization problem. In this case the solution remains an open problem.

Volker Mehrmann, Peter Benner, Hongguo Xu

Robust Numerical Methods for Robust Control

In this talk we discuss the numerical solution of H_∞ control problems. It is well known that the numerical methods for the computation of the optimal γ often suffer from the ill-conditioning of the Riccati equations. We show how numerical methods via Hamiltonian eigenvalue problems can be designed that also work satisfactory near the optimum.

Diana Maria Sima, Vasile Sima, Sabine Van Huffel

Recent Developments in SLICOT Library for System Identification

Advanced computer aided control systems design techniques use mathematical models of the processes to be controlled. Frequently, these models are state space representations, obtained by system identification procedures. In contrast to the first principles model building, based on physical laws, system identification uses available process data measurements and mathematical or statistical methods to find the structure and the coefficients of a model best fitted to the data. Since many measurements should be used for getting a model accurate enough, it is of paramount importance to have efficient, as well as reliable identification techniques, and associated numerical software.

This paper summarizes the results obtained in the framework of the Thematic Networks Programme NICONET for developing a new system identification toolbox, SLIDENT, based on the freely available Fortran 77 Subroutine Library in Control Theory (SLICOT). SLIDENT uses subspace-based techniques for linear multivariable system identification. Both advanced computational kernels, and user-friendly interfaces have been implemented. SLIDENT combines the efficiency of the Fortran routines and fast, structure-exploiting algorithms, with the easy of use and graphical abilities of the widely used environments Matlab and Scilab. The numerical results show that the SLIDENT toolbox is reliable and highly performant, significantly more efficient than the previously available Matlab codes.

Recent developments address the identification of Wiener-type systems, containing both a linear part and a static nonlinearity. The linear part is identified in the usual manner, and then the parameters of both the linear and nonlinear parts are optimized using a neural network approach, based on a Levenberg-Marquardt algorithm.

Tatjana Stykel

Numerical Solution and Perturbation Theory for Generalized Lyapunov Equations

We study generalized continuous-time Lyapunov equations that arise in stability analysis and control problems for descriptor systems. We present a generalized Schur-Bartels-Stewart method and a generalized Schur-Hammarling method for computing a solution of the generalized Lyapunov equation with a special right-hand side. Perturbation theory and error estimates for this equation are discussed.

MS32 Power Systems Optimization
Organized by: Werner Roemisch, Ivo Nowak

Topic: 10 Engineering Design

Many issues motivate a growing interest in mathematical modeling and optimization techniques for the design and the operation of power systems and for trading electricity. They are related to the complex nature of mathematical models (mixed-integer decisions, nonlinearities, data uncertainty, huge dimensions), to the ongoing liberalization of electricity markets and to the necessity for designing and building new power plants. The talks report on recent developments in mathematical modeling and on algorithmic approaches for solving relevant nonlinear mixed-integer programs (under uncertainty).

Nicole Groewe-Kuska, Werner Roemisch

Modeling of Uncertainty for the Real-Time Management of Power Systems

A major issue in the application of multistage stochastic programming to model the cost-optimal generation and trading of electric power is the approximation of the underlying stochastic data processes by tree-structured schemes. We present a methodology for the generation and optimal reduction of scenario trees for the electric load (demand) and for electricity prices from simulation scenarios.We report on numerical results for a German power utility.

Ivo Nowak, Hernan Alperin

A MINLP Heuristic with Application to Energy Conversion Systems

We present an approximation algorithm for mixed-integer nonlinear programming (MINLP) problems and study the application of the method to the design of an energy conversion plant. The MINLP-method is based on the following steps: (i) reformulating the MINLP-problem using quadratic forms and convex non-quadratic functions; (ii) constructing an all-quadratic lower bounding program (QQP); (iii) solving the dual of QQP (approximately) by a proximal bundle algorithm; (iv) retrieving primal solutions from dual solutions.

Werner Roemisch, Nicole Groewe-Kuska, K.C. Kiwiel, M.P. Nowak

Decomposition of Multistage Stochastic Integer Programs and Power Management in Hydro-Thermal Systems

We consider a stochastic power management model for a hydro-thermal generation system. The corresponding multistage stochastic mixed-integer program is solvable by Lagrangian decomposition approaches combined with heuristics. We present numerical results based on real-life data of a German power utility.

MS17 Numerical Methods in Shape Optimization
Organized by: Thomas Slawig, Karsten Eppler

Topic: 10 Engineering Design

Shape (or domain) optimization problems deal with finding the optimal geometrical form of a physical or technical system with respect to some given cost function. One typical application is the design of airfoils or whole airplanes to minimize the drag at a desired lift. Mathematically speaking the aim is to find the optimal shape of a domain to minimize a cost function under the constraint of a (partial) differential equation. Typical features of such problems are the highly non-linear dependency of the solution of the state equations with respect to the domain variations. Moreover there are technical difficulties concerning the numerical solution of the state equations on the varying domain during an iterative optimization algorithm, and of the optimization method itself. Crucial points are the parameterization of the domain (or boundary) variation, the treatment of local minima, and the efficient solution of high-dimensional technical applications. The Minisymposium tries to present some of the modern numerical methods used in this area.

Nicolas R. Gauger

Aerodynamic Shape Optimization Using Adjoint Method

Numerical shape optimization will play a strategic role for future aircraft design. It offers the possibility of designing or improving aircraft components with respect to a pre-specified figure of merit subject to geometrical and physical constraints. However, the extremely high computational expense of straightforward methodologies currently in use prohibits the application of numerical optimization for industry relevant problems. Optimization methods based on the calculation of the derivatives of the cost function with respect to the design variables suffer from the high computational costs if many design variables are used. However, these gradients can be efficiently obtained by solution of the continuous adjoint flow equations. DLR is actively developing and validating hand-coded adjoint solvers based upon the work of A. Jameson. The talk will outline the potential of the adjoint method for aerodynamic design optimization and will give a review of the work which has been done at DLR in this field.

Tomas Kozubek

A Fictitious Domain Method for the Numerical Realization of Bernoulli's Free-Boundary Value Problems

This contribution deals with an efficient method for the numerical realization of exterior and interior Bernoulli's free-boundary problems which is based on a shape optimization approach. The respective state problem is solved by a fictitious domain solver using boundary Lagrange multipliers.

Mohamed Masmoudi

The Topological Asymptotic and its Application to Some Industrial Problems

Classical shape optimization tools start with an initial design provided by the user and arrive to a final shape with a same topology as the initial one.

The aim of topological optimization is to find an optimal shape without any textita priori information about the topology of the structure.

Main contributions in this field are concerned with structural analysis and in particular the optimization of the compliance (external work) subject to a volume constraint. Most of the authors considered composite material optimization and the homogenization theory.

The range of application of this approach is quite restricted. For this reason global optimization techniques like genetic algorithms and simulated annealing are used in order to solve more general problems. Unfortunately, these methods are very slow.

The notion of topological asymptotic gives an interesting alternative: - its range of application is very large, - using topological sensitivity information, we can build fast algorithms.

More exactly, a shape optimization problem consists in minimizing a functional $j(\Omega) = J(\Omega, u_\Omega)$ where u_Ω is the solution to a Partial Differential Equation defined in the domain Ω. Let us consider $\Omega_\varepsilon = \Omega \backslash B(x, \varepsilon)$ where $B(x, \varepsilon)$ is the ball of radius ε about the center x. An asymptotic expansion of the functional j can be obtained in the following form:

$$j(\Omega_\varepsilon) = j(\Omega) + f(\varepsilon)g(x) + o(f(\varepsilon))$$

$$\lim_{\varepsilon \to 0} f(\varepsilon) = 0, f(\varepsilon) > 0.$$

We call this expansion the **topological asymptotic** . It can be obtained if the solution $u_\varepsilon := u_{\Omega_\varepsilon}$ converges to u_0 in a sense to be defined later.

No such condition holds for one-dimensional problems. This can be explained by the potential theory: only manifolds of dimension less or equal to $n-2$ have null capacity with respect to a manifold of dimension n.

Wolfram Mühlhuber

Optimal Design of Industrial Components

The industrial application of our work consists in minimizing the mass of a frame used for an injection moulding machine. This frame has to compensate the forces acting on the mould inside the machine and has to fulfill certain critical constraints concerning e.g. geometry, maximal stresses or deformations. The deformation of that frame with constant thickness is described by the plain stress state equations for linear elasticity. If the thickness varies then we use a generalized plain stress state with piecewise constant thickness.

We consider two problems: Either vary the shape of the 2D cross section keeping the thickness constant, or vary the thickness keeping the cross section constant respectively.

This mass minimization problem leads to a constrained minimization problem for a non-linear functional which will be solved by some standard optimization algorithm which requires the gradients with respect to design parameters.

In the case of optimal sizing we combine Automatic Differentiation (AD) and the hand-coded adjoint method. This means, that we handle derivatives with respect to the differential equations by the adjoint method and all remaining derivatives by AD. This combination of hand-coded gradient routines and AD results in a very powerful and efficient tool.

MS28 Recent Advances in Krylov Subspace Methods I

Organized by: Eric De Sturler, Jörg Liesen

Topic: 10 Engineering Design

Krylov subspace methods are among the most popular iterative methods for solving large linear systems and eigenvalue problems. Their broad range of applications includes basically every branch of scientific computation. In this minisymposium we will focus on recent advances in the theory of Krylov subspace methods. While it seems that these methods have been around for a long time, some major developments have only occurred in recent years. These include progress in the areas of convergence and finite precision analysis, improved stopping criteria, and a better understanding of the geometry behind Krylov subspace methods.

Eric De Sturler

Fast and Robust Short Recurrence Methods

It is well-known that no optimal short recurrence methods exist for general matrices. This leaves, broadly speaking, two approaches. Economize on optimal methods like full GMRES or improve the robustness and convergence of short recurrence (non-optimal) methods like BiCG and the methods derived from it. Optimal truncation, restarting while keeping the basis of a selected subspace, may provide significant improvements in efficiency for methods like GMRES with near optimal convergence rates. How to improve the convergence and robustness of short recurrence methods is still an open question. Our lecture will focus on this question.

One link between the two approaches is understanding the effects of oblique projections. We will derive some basic theorems to analyze the effect of oblique projections and provide a brief analysis of BiCG. We will then derive ways to improve the convergence and robustness of BiCG and the methods derived from it (such as CGS, BiCGSTAB, and TFQMR).

Oliver Ernst, Michael Eiermann, Olaf Schneider

A Numerical Study of Accelerated Restarted Minimal Residual Methods

This talk reviews recent joint work with Michael Eiermann and Olaf Schneider which introduced a framework for analyzing some popular techniques for accelerating restarted Krylov subspace methods for solving linear systems of equations. Such techniques attempt to compensate for the loss of information due to restarting methods like GMRES, the memory demands of which are usually too high for it to be applied to large problems in unmodified form. We summarize the basic strategies which have been proposed and present both theoretical and numerical comparisons.

Anne Greenbaum

Generalizations of the Field of Values Useful in the Study of Polynomial Functions of a Matrix

Given a matrix A and a positive integer k, we identify the largest set Ω in the complex plane such that

$$\|p(A)\| \geq \max_{z\in\Omega} |p(z)|$$

for all polynomials p of degree k or less. We refer to this as the *effective spectrum of A for degree k* since, under the action of kth degree polynomials, A behaves like a normal matrix with eigenvalues throughout this set. For $k = 1$, this set is just the field of values of A, and for $k \geq m$, where m is the degree of the minimal polynomial of A, it is the spectrum of A. For $1 < k < m$, these sets are intermediate between the field of values and the spectrum and sometimes resemble pseudospectra.

MS43 Recent Advances in Krylov Subspace Methods II

Organized by: Eric De Sturler, Jörg Liesen

Topic: 10 Engineering Design

Krylov subspace methods are among the most popular iterative methods for solving large linear systems and eigenvalue problems. Their broad range of applications includes basically every branch of scientific computation. In this minisymposium we will focus on recent advances in the theory of Krylov subspace methods. While it seems that these methods have been around for a long time, some major developments have only occurred in recent years. These include progress in the areas of convergence and finite precision analysis, improved stopping criteria, and a better understanding of the geometry behind Krylov subspace methods.

Martin H. Gutknecht, Stefan Roellin

Variations of Zhang's Lanczos-Type Product Method

Among the Lanczos-type product methods, which are characterized by residual polynomials $p_n t_n$ that are the product of the Lanczos polynomial p_n and another polynomial t_n of exact degree n with $t_n(0) = 1$, Zhang's algorithm GPBiCG has the feature that the polynomials t_n are implicitly built up by a pair of coupled two-term recurrences whose coefficients are chosen so that the new residual is minimized in a 2-dimensional space. There are several ways to achieve this. We discuss here alternative algorithms that are mathematically equivalent (that is, produce in exact arithmetic the same results). The goal is to find one where the ultimate accuracy of the iterates x_n is guaranteed to be high and the cost is at most slightly increased.

Joerg Liesen, Miro Rozložník, Zdeněk Strakoš

The Choice of the Basis in Minimal Residual Methods

We study Krylov subspace methods for solving unsymmetric linear algebraic systems that minimize the norm of the residual in each step of the iteration (MR methods). We show that the norm of the MR residual is strongly related to the conditioning of different bases of the same Krylov subspace.

The choice of the basis leads to different implementations which are mathematically equivalent. However, as we will explain, the choice of the basis is fundamental for the numerical stability of the implementation. We will demonstrate that the best orthogonalization technique used for computing the basis does not compensate for the loss of accuracy due to an inappropriate choice of the basis. Our theoretical results will be illustrated by comparing the implementations MINRES (for symmetric matrices), classical GMRES and simpler GMRES.

Gerard Sleijpen, Henk van der Vorst

Residual Expansion for Subspace Methods

In iterative numerical solution methods, such as FOM and GMRES, for linear systems and, Arnoldi for eigenvalue problems, an approximate solution is efficiently extracted from a low-dimensional search subspace by projecting the high dimensional problem onto this search subspace. For more accurate approximations, the search subspace is expanded in each step. In Arnoldi's approach, the new basis vector for the search subspace is obtained by orthonormalizing the image under the operator of the previous basis vector. As an alternative, the search subspace can also be expanded by the residual associated with the present approximate solution. In exact arithmetic and when starting with a one dimensional search subspace, then both approaches are equivalent. In methods such as inexact Shift-and-Invert Arnoldi, the expansion will not be exact. With perturbed expansion vectors, the differences may be dramatic: the residual expansion is much more stable than Arnoldi's approach. This may explain the success of methods that rely on residual expansion, for instance GMRESR for linear systems and Jacobi–Davidson for eigenvalue problems.

In this presentation, we will explain the differences between the stability for Arnoldi's approach and for the residual expansion.

Zdeněk Strakoš, Petr Tichy

On Error Estimation in the Conjugate Gradient Method

Numerical estimation of the A-norm and the Euclidean norm of the error in the conjugate gradient method (CG) has been studied in many papers. All published estimates known to us assume exact arithmetic. Their derivations are based on global orthogonality among the residuals and/or the direction vectors. In finite precision arithmetic, the computed residuals as well as direction vectors become typically non-orthogonal (and even linearly dependent) after a few iterations, and convergence is significantly delayed. Still, the exact precision estimates seem to be confirmed by finite precision numerical experiments, though in finite precision computations they estimate quantities which can be orders of magnitude different from their exact precision counterparts!

Our goal is to extend previous results of Golub and Strakoš and to explain that without a proper rounding error analysis there is no justification of using exact precision CG error estimates in finite precision computations. We concentrate on the lower bound for the A-norm of the error, and show that the simplest possible bound, which is equivalent to the Gauss quadrature estimate, can essentially be found in the original paper by Hestenes and Stiefel. We describe its relationship to other existing estimates and provide its detailed rounding error analysis.

MS25 Homogenization and Fluid Dynamics for Complex Flows

Organized by: Nils Svanstedt

Topic: 10 Engineering Design

The minisymposium is devoted to various aspects of theoretical and computational modeling of fluid dynamics for complex flows by means of e.g. homogenization and LES techniques.

Björn Birnir

Homogenization of Jet Engine Flow

We present a homogenization of the Euler equation producing the viscous Moore-Greitzer equations that have been very successful in modeling the flow through a jet engine. The viscous term is produced by eddy viscosity that is computed explicitly in the homogenization limit. Numerical comparison of the homogenized equations with the eddy viscosity terms and the Moore-Greitzer equations is presented.

Christer Fureby

New Trends in Large Eddy Simulation of Complex Flows

We aim at presenting a recent update on the wide field of LES focusing on complex flows. The general principles and issues will be discussed based on incompressible flows, but, when necessary, extensions will be made both to compressible and reacting flows. A number of examples will be presented as to facilitate the discussion and to highlight both the advance of LES and the pacing items still to be addressed. As a background for the discussion practical problems relevant to the industry needs will be provided.

Bernd R. Noack

A Hierarchy of Low-Dimensional Models for Shear-Flows

Low-dimensional modelling of flows plays an increasing role in industrial research for a quick exploration of actuation concepts and for the mathematical analysis. Thus, expensive high-fidelity simulations and experiments may be physically explained and new actuations may be suggested. In the present talk, modelling efforts for wakes, mixing layers and other free- and wall-bounded shear-flows are discussed. Results of a hierarchy of models including simulations, models with few to several hundred degrees of freedom, and mean-field models with only three modes are presented and compared.

Nils Svanstedt

Two-Scale Asymptotics for the Vorticity and Vector Potential Fields for Incompressible Oscillatory Fluids

We consider the incompressible Navier-Stokes equation in the vorticity and vector potential formulations and prove two-scale asymptotics for these systems in the sense of Nguetseng's two-scale convergence.

MS12 Analysis, Numerics and Applications of Magnetohydrodynamics

Organized by: Manuel Torrilhon, Rolf Jeltsch

Topic: 10 Engineering Design

The equations of magnetohydrodynamics (MHD) describe the flow of plasmas in interaction with a magnetic field. MHD equations are relevant in investigations in several areas of engineering and astrophysical research. For example they are necessary to predict space weather caused by solar winds or to simulate thermonuclear plasma in fusion experiments.

The MHD equations form a system of hyperbolic partial differential equations. The analysis and numerical modelling of these equations became an ever growing research field in the last years.

The minisymposium will be devoted to the analysis and numerics of MHD-equations as well as to applications to physical problems. Special interests are, for instance, the div(B)-constraint in numerical methods or the existence of non-evolutionary waves in the results of MHD.

Hans De Sterck

Multi-Dimensional Upwind Constrained Transport (MUCT) of Divergence-Free Fields on Unstructured Grids

Novel Multi-dimensional Upwind Constrained Transport (MUCT) schemes on unstructured triangular grids are described. Constrained Transport (CT) discretizations conserve the divergence-free nature of divergence-free vector fields on the discrete level.

Multi-dimensional Upwind (MU) schemes generalize the concept of dimensionally split upwind schemes for hyperbolic systems to truly multidimensional upwind discretizations on unstructured grids with compact stencils consisting of nearest neighbors. In the present paper the concept of Constrained Transport, generalized to unstructured triangular grids using face elements, is combined with the concept of Multi-dimensional Upwind advection schemes. The resulting MUCT schemes are applied to the numerical solution of Faraday's law of induction in the Magnetohydropdynamic (MHD) approximation, which describes the dynamical evolution of a divergence-free magnetic field, and to the numerical solution of the the system of full MHD equations.

In the MUCT schemes the Constrained Transport approach is generalized to multi-dimensional methods on unstructured grids. As an application of the Multi-dimensional Upwind schemes, MHD bow shock flow simulations are discussed in which overcompressive (or 'non-evolutionary') intermediate shocks occur.

Dietmar Kröner, A. Dedner, F. Kemm, C.-D. Munz, M. Wesenberg, T. Schnitzer, I. Sofronov

Divergence Cleaning and Absorbing Boundary Conditions for the MHD Equations

The mathematical model for the flow of electrical currents conducting fluids consists of the system of magnetohydrodynamics (MHD), which itself follows from the Euler equations of gas dynamics and the Maxwell equations. It describes the complex couplings between the flow variables, the magnetic and the electric fields.

In this talk we will concentrate on two main problems which will appear in numerical simulations. Firstly the problem of transparent or artificial boundary conditions, if the system has to be solved on an unbounded outer domain and secondly the discretization of the divergence-free property of the magnetic field.

On unbounded domains we derive suitable boundary conditions on the basis of the linearized problem, to avoid that perturbations will be reflected at the artificial boundary. The accuracy of this result will be demonstrated by several numerical examples.

Usually the initial data for the magnetic field are divergence free and the exact solution will keep this property for all times. But due to numerical errors the numerical magnetic field will lose this property for later times. For the discretization of the divergence-free property of the magnetic field many attempts can be found in the literature. In this lecture we will discuss a new method which generalizes previous ideas of Munz and Sonnendruecker to the MHD equation. Roughly speaking the system is extended and perturbations of the divergence of the magnetic field will be transported away to the boundary.

Rho Shin Myong

Riemann Solutions and Solvers for MHD

Regardless of degree of nonequilibrium, the magnetohydrodynamic waves have to satisfy the certain conservation principle. Three degrees of freedom are in general required for its description so that the problem becomes three-dimensional. This property plays a critical role in the construction of solutions of the MHD Riemann problem.

In this talk, by considering the MHD system and a model system that exactly preserves the hyperbolic singularities, issues in Riemann solutions and solvers for MHD will be discussed. In particular, a new method of exploring the rotational symmetry of the MHD system will be proposed.

Gabor Toth

The div B=0 Constraint in Numerical Magnetohydrodynamics

Numerical modeling of space and laboratory plasmas is carried out routinely with various numerical schemes. Still there are some unresolved issues regarding the numerical enforcement of the divergence free nature of the magnetic field. I will review some of the more popular divergence B control methods: (i) the "8-wave" scheme by Powell, (ii) the "constrained transport" scheme by Evans and Hawley, and its newer conservative variants by Dai and Woodward, Ryu et al., Balsara and Spicer, and Toth, and (iii) the "projection" scheme first suggested by Brackbill and Barnes. I will present a new non-staggered finite volume interpretation of the constrained transport type schemes, and also prove that the projection scheme gives correct weak solutions. On the other hand the 8-wave scheme is shown to yield incorrect weak solutions in some cases.

I will also discuss some very recent ideas, which are not yet published: The diffusive divergence B control scheme by Linde and Malagoli, the generalization of the conservative constrained transport schemes to AMR grids by Toth and Roe, and a new hyperbolic-parabolic scheme by Dedner et al.

3 Abstracts of Contributed Talks

3.1 Medicine

Fredrik Andersson

Doppler Tomography, a Mathematical Approach

Topic: 1.0

As an alternative to radiation based tomography, a non-invasive tomography method based on continuous ultrasonic measurements has been investigated. In such application measurements of a velocity distribution of the projection of the flow along each tomographic line can be made. Thus each line is characterized by a spectrum instead of a single value. Here we introduce a new mathematical transform, the $\mathcal{M}$-transform, as a tool in the reconstruction process of flows from such spectras. The transform opens up several new possibilities of field reconstruction. Some interesting properties of the transform are also discussed. Several different areas of mathematics are used, such as PDE, optimization, image analysis, algebraic equations, and algebraic geometry. A Doppler tomography based method might be useful in routine investigations in mammography.

Andriy Borisyuk

Application of Methods of Spectral and Correlation Analysis to Modelling of an Acoustic Field of a Human Blood Vessel

Topic: 1.0

An acoustic field in the human chest due to turbulent flow in blood vessel is modelled. The thorax is represented by a finite cylinder filled with an acoustic medium and surrounded by air. A vessel is simulated by a coaxial pipe with an inner turbulent flow. Random wall pressure fluctuations at the vessel surface radiate sound into the body. This sound can be analysed in order to diagnose the vessel state.

The problem is solved by taking a Fourier transform and expanding the random sound field into an infinite series of the acoustic modes of the volume between the cylinders, with subsequent transition to statistical characteristics of the sound field. Turbulent pressure is described in terms of the wavenumber-frequency spectrum. The cases of normal and stenosed vessels are considered.

The analysis of the acoustic field reveals the characteristic signs of a stenosis. These are a general increase in the sound level and the production of new frequency components in the acoustic power spectrum. The components are determined by the mean flow velocity in and the diameter of the stenosis. Another important result is that the stenosis generated acoustic power is approximately proportional to the fourth power of the stenosis severity and the same power of the flow Reynolds number.

Christian Bourdarias, S. Gerbi, J. Ohayon

A Finite Element Method for an Active Soft Tissue

Topic: 1.0

We present a finite element modeling for large deformations response of active incompressible nonlinear elastic and transversely isotropic soft tissue. The functional form of the strain energy function describes the mechanical properties of the active muscle during the whole cardiac cycle.

We derive the finite element equations for the active soft tissue. A very good agreement between analytic solutions and the numerical ones for free active contractions, uniaxial and equibiaxial extensions of a rectangular sample is obtained.

Volker Dicken

Tikhonov Regularization in Electrical Impedance Tomography

Topic: 1.0

In Electrical Impedance Tomography the nonlinear ill-posed problem of reconstructing a conductivity distribution inside an object (e.g. medical patient or geological/archeological site) from boundary potential measurements arises. We present convergence results on a Tikhonov regularization approach and numerical results based on an adaptive FEM simulation of a geological unbounded domain problem.

Inga Hansen, R. Schreittmiller, H. Wawrzyn, W. Hauck, R. Sader, H.-F. Zeilhofer, Martin Brokate

Modelling of a Human Skull — Relative Importance of Influence Factors

Topic: 1.0

The development of models for maxillo-facial surgery makes up a main focus of our research topics. In this context the relative importance of three factors (geometry, material parameters, anisotropy) is studied based on a clinical example. For this purpose several load cases are defined and combined with different geometries derived from CT-scans; material parameters and anisotropy vary depending on measurements. The resulting pde's are solved under the above boundary conditions and the results analyzed.

Evgueni Haroutunian, Harutyun Shahumyan

Statistical Analysis of Epidemiologial Indices of Tubercolosis in Armenia During Last 20 Years

Topic: 1.0

Special online parametrical and non-parametrical methods are presented which were applied for statistical analysis of the main epidemiologial indicees of tubercolosis in Armenia. The epidemiologial characters of tubercolosis in 1980, 1990 and 2000 are compared. Then we analyzed the time series of morbidity prevalence and mortality of tubercolosis from 1980 to 2000. The change points of these time series are estimated by online methods using several parametrical and non-parametrical statistics. We have also developed a computer program for time series investigations which allows to choose several online and offline and also parametrical and non-parametrical methods.

Juri M. Rappoport, Arkadii A. Kasparov, Nikolai V. Ermakov

Computational Assistance of Therapy Planning after Penetrating Keratoplasty
Topic: 1.0

The dynamics of the changes of the endocelium cells count in the donor cornea after penetrating keratoplasty is investigated. The protective influence of the endothelium bioprotectors to the transplant in the reconstructive surgery of front parts of the eye is studied on the computer by means of statistical methods. The therapy planning is conducted on the basis of the operation's kind, endothelial protector, diagnosis, donor transplant's diameter and percent of the endothelial cell's loss.

Teresa Reginska

Numerical Regularization of Ill-Posed Problems
Topic: 1.0

There are problems in medicine which lead to an ill-posed equation $Au = f$ with $A \in L(X,Y)$ and $A^{-1} \notin L(Y,X)$. As discretization of the problem we consider a family of finite dimensional equations which should be regularized since corresponding condition numbers tends to infinity with the dimension. Therefore, the problem of choosing regularization parameters arises. Analysis of this choice will be given by means of a family of L-curves parametrized by the dimension of approximate equation.

Nikolaos Myridis, Christodoulos Chamzas

Assumptions of K-Angularly and Radially Bandlimited 2-D Functions in Medical Imaging
Topic: 1.1

In many applications ranging from Computerized Tomography to MRI, the samples of a 2-D function do not lie onto a rectangular grid, but on a polar raster. Reconstruction of such a function from its samples is usually based on the additional assumption, that it is also K-angularly bandlimited. In this contribution, we prove that a 2-D (radially) bandlimited function does not imply that it is K-angularly bandlimited too. We also examine classes of functions being simultaneously radially and angularly bandlimited.

Constantin Popa, Marcus Mohr, Ulrich Rüde

Iterative Solvers for Inverse Problems in Bioelectromagnetic Field Computations
Topic: 1.1

The localization of bioelectromagnetic signals is of major importance in the fields of cardiology, neurology and neurosurgery. With standard analysis techniques (electroencephalogram or electrocardiogram) we usually get only qualitative results whose correct interpretation requires considerably expertise. In this paper we present numerical simulation techniques and experiments for the reconstruction of the electromagnetic activity from the measured data. They are based on iterative solution of finite-differences discretization of an associated differential inverse problem.

Andreas Rieder

On Reconstruction Filters in 2D-Tomography
Topic: 1.1

The filtered backprojection algorithm is probably the most often used reconstruction method in computerized tomography. The quality of the reconstructed images depend heavily on the chosen filter function. For the different scanning geometries we investigate how to scale the filter in relation to the discretization step size to avoid artefacts. Numerical experiments illustrate the theoretical findings.

Thomas Schuster

Mollifier Design and Reconstruction in 3D Vector Field Tomography
Topic: 1.1

In vector field tomography we are interested in reconstructing a velocity field f from line integrals over certain components of the field

$$y(L) = \int_L \langle f, \omega(L) \rangle \, d\sigma \, .$$

The mapping $f \mapsto y(L)$ is called *Doppler transform*. Using the method of approximate inverse, we compute moments of the searched for field f with so called mollifiers E_γ. In the talk we present suitable mollifiers, which are adjusted to the Doppler transform as well as some numerical results for a straight flow.

Christian Clason

Simulation of the Elastic Behaviour of the Human Mandible and Experimental Validation: A Method for Material Parameter Identification
Topic: 1.2

A simulation of the elastic behaviour of the mandible via the finite element method is based on a mathematical model which contains several simplifying assumptions. To test the validity of these simplifications, carefully chosen in vitro experiments are done on a special-purpose biomechanical test stand. Based on this validation procedure, a method for identifying the material properties of the mandible can be implemented by solving a nonlinear inverse problem. First results are discussed.

Cornelia Kober, R. Sader, H.-F. Zeilhofer, S. Prohaska, Stefan Zachow, Peter Deuflhard

Individual Biomechanics of the Human Mandible: Simulation and Modeling
Topic: 1.2
By computed tomography data (CT), the individual geometry of the mandible is quite well reproduced, also the separation between cortical and trabecular bone. Using anatomical knowledge about the architecture and the functional potential of the masticatory muscles, realistic situations were approximated.Computed tomography measures tissue density, the inherent three dimensional information concerning the highly anisotropic material law is lost. The authors present an alternative ansatz for an anisotropic material description. By this, fully anisotropic simulations can be performed.

Luis M. Abia, Juan Carlos Lopez-Marcos

A Numerical Method for a Model for the Cell Kinetics in Tumour Growth
Topic: 1.4
A numerical method for a model for the cell kinetics in tumour growth, proposed by A. Bertuzzi and A. Gandolfi in J. Theor. Biol. (2000) 204, is analyzed. The model describes the age structure of the cell population and its spatial dependence in a tumour cord at the stationary state, and it is discretized using several finite differences schemes. Extensions of the numerical method for variations of the model equations are also considered.

Michael Friger, B. Sarov, I. Karakis, L. Naggan

Parallel Capture-Recapture Analysis: An Estimate of the "True" Size of Historic Cohort of HbsAg Carriers
Topic: 1.6
Our research deals with spreading and controlling Hepatitis B Virus(HBV). One of the objectives of our study is to estimate persistent HbsAg-carriage over time and the number of those who developed antibodies to HBV. For solving this problem it is very important to estimate "true" number of HBV-carriers. For this proposes we propose an original model based on n-sources Capture-Recapture Model(CRM). The proposed model allows obtaining more accurate estimates than those based on standard CRM.

Pascal Azerad, Eberhard Baensch

Quasi-Stability of the Basic Flow in a Cone-Plate Device
Topic: 1.7
We investigate the flow between a rotating cone and a stationary plate. This device is used in haemostasis to study properties of blood flow w.r.t. shear stress. Physical experiments show that close to the apex the flow is approximately azimuthal and the wall shear-stress is constant within the device, the approximation being controlled by Reynolds number and thinness of the cone-plate gap.newline We establish this by means of boundary-layer analysis, energy estimates and numerical simulations.

Linda Ingebrigtsen, Aslak Tveito, Hans-Petter Langtangen

Moving Mesh Techniques for Fluid Flow Simulations
Topic: 1.7
Our aim is to develop a numerical simulator enabling an analysis of the relation between the stiffness of the wall and pressure gradients in the left heart during diastole. In order to develop such a simulator, we need to solve the incompressible Navier-Stokes equations on a moving domain. Hence, the purpose of this study is to compare three moving grid methods for the Navier-Stokes equations. The methods are compared on a test problem where we have an analytical solution, thus allowing a comparison of CPU-effort vs. the error for the three methods.

Peter R. Kramer, Charles Peskin

A Simulation Method for Microphysiological Fluid Systems with Thermal Fluctuations
Topic: 1.7
I present a new computational method for simulating microscopic processes in physiology which accounts for stochastic thermal fluctuations and a dynamically evolving fluid environment. This latter feature is a principal advantage of our method relative to Brownian or Stokesian particle dynamics methods. Our approach builds on the "Immersed Boundary Method" of Peskin, which simplifies the coupling between the fluid and the immersed particles and membranes so as to avoid complex boundary problems.

Glenn Terje Lines, Joakim Sundnes, Kent Andre Mardal, Aslak Tveito

On Numerical Techniques for the Bidomain Model
Topic: 1.7
The solution of the Bidomain equations, modeling the electrical activity of the heart, requires a very fine spatial resolution. For realistic geometries this leads to a large number of grid points and consequently large linear systems to be solved for each time step. We present a fully implicit time discretization of the equations, leading to a block structured linear system for which efficient preconditioners may be constructed using operator splitting and multigrid.

Karstein Sorli, Chris A. Toomer

Numerical Solution of Inverse Problems of Fluid Flow in Shrinking Domains

Topic: 1.7

A numerical procedure for inverse problems of non-steady fluid flow in shrinking domains is described. Numerical solutions of corresponding direct problems are performed to produce "measurements". Those are used in the procedure, aiming at recreating the "a priori unknown" behaviour of the moving boundary. A least squared approach is applied. The boundary is represented by spline curves, whose control points are optimization parameters.

Some simulation results are given, and comments on the application to cardiovascular dynamics are given.

3.2 Biotechnology

Theodore Nikitopoulos, Ioannis Z. Emiris

An Efficient Approach for Computing Molecular Conformations

Topic: 2.0

We present a way to formulate molecular conformational problems in terms of geometric or kinematic constraints. Our approach is conceptually simple and geometric, in that it applies structured rank-reducing perturbations on symmetric (i.e. distance) matrices. We focus on conformations lying on the same manifold, hence topological close to each other. Results of a MATLAB implementation are reported, including computational performance with respect to speed and correctness, for molecules of up to 20 atoms or more.

A.K. Prykarpatsky, N.K. Prykarpatska

Quantum Chaos and its Testing

Topic: 2.0

Since 1963 when V.K. Melnikovdeveloped an analytical tool for testing the transition of classical weakly perturbed planar dynamical systems to homoclinic due to A. Poincare chaotic motion via the Birkhoff-Smale scenario, a lot of new results and generalizations were obtained by many researchers worldwide. Especially there were devised new techniques for studying the chaotic motion both in multidimensional and adiabatically (slowly) perturbed Hamiltonian systems. On the other hand a great deal of results both theoretical and computational were produced by mathematical physicists concerning the related problem of describing so called quantum chaos in finite dimensional quantum dynamical systems, especially weakly perturbed. Our study here deals with developing some physically reasonable quantum analog of the above mentioned Melnikov theory and its application to studying transition to quantum chaotic motion in weakly perturbed quantum completely integrable Hamiltonian systems.

Klaus Schneider, S. Handrock-Meyer, Leonid V. Kalacev

A Method to Determine the Dimension of Long-Time Dynamics in Multi-Scale Systems

Topic: 2.0

Modeling reaction kinetics in a homogeneous medium usually leads to stiff systems of ordinary differential equations the dimension of which can be large. The problem of determination of the minimal number of phase variables needed to describe the characteristic behavior of large scale systems is extensively addressed in current chemical kinetics literature from different point of views. Only for a few of these approaches there exists a mathematical justification.
In this paper we describe and justify a procedure allowing directly to determine how many and which state variables are essential in a neighborhood of a given point of the extended phase space. This method exploits the wide range of characteristic time-scales in a chemical system and its mathematical justification is based on the theory of invariant manifolds. The procedure helps to get chemical insight into the intrinsic dynamics of a complex chemical process.

Paul Tupper

Long Term Statistics for Random ODEs Approximating SDEs

Topic: 2.0

Previous work has shown that SDEs can be derived as the limit of series of ODE systems with random data. In particular, weak convergence of trajectories on finite intervals of time has been shown. Here we examine whether the ODEs also correctly approximate long-term statistical behaviour of the SDEs. We offer analytical and numerical evidence that empirical distribution functions of trajectories converge appropriately, whereas other statistical properties may not.

A.R. Tzafriri, H. Parnas, M. Bercovier

Reaction Diffusion Modeling of Enzymatic Erosion of Collagen Matrices

Topic: 2.0

Collagen and gelatin are widely used in biomedical applications. A crucial aspect in these applications is the degradation of these bio-materials in the body, by collagenases and nonspecific proteolytic enzymes. We model this process as a reaction diffusion model. The resulting equations are highly nonlinear and stiff. The equations were solved over a parallelepiped domain, using the FEM. Using realistic parameter values we find a moving front solution, in agreement with the experimental observation of surface erosion.

Holger Kantz, Wolfram Just

Stochastic Modelling: Replacing Fast Chaotic Degrees of Freedom by Noise

Topic: 2.2

For systems with timescale separation, fast chaotic degrees of freedom are replaced by suitable stochastic processes. We employ a projection operator technique to derive equations of motion for the phase space density of the slow variables by eliminating the fast ones. The resulting equations can be approximated by Fokker-Planck equations, which can be turned into Lagevin equations for the slow variables.

Markus Kirkilionis

The Cell Cycle, Division Mechanisms and Population Dynamics

Topic: 2.2

I will investigate the population dynamics of unicellular bacterial populations growing in a continuous culture. This is a common setting in industrial fermentation processes, or more generally the situation when cells are used as factories for certain products. Cell division mechanisms lead to different population behaviour, and this connection will be discussed in detail. For this investigation the framework of physiologically structured population will be used, moreover different analytical and numerical procedures will be introduced.

Karin Gatermann

Symbolic Computations for Systems in Chemistry

Topic: 2.3

Differential equations in chemistry are often given by the so-called mass action kinetics. That means that the ordinary differential equations are given by a directed graph and a weighted bipartite graph. Depending on the discrete structure the system may have several stable steady states. We will explain how symbolic computation enables the exploitation of the structure of the system. First, Hermite normal form computation enables the reduction of the problem. Secondly, we use deformed toric varieties computed by Groebner bases.

Darko Veljan, Tomislav Doslic

Enumerative Aspects of Secondary Structures

Topic: 2.3

Secondary structures play an important role in biology and their graph-theoretic models are also interesting in mathematics itself. In this talk we shall show how to enumerate these structures in terms of their size, rank and order. We shall also establish asymptotic and logarithmic behavior of their numbers. We also emphasize their connections with some well known combinatorial objects, such as Motzkin and Dyck paths, matchings and permutations with forbidden patterns.

Klaus Neymeyr

Preconditioned Eigensolvers

Topic: 2.5

Several applied problems, e.g. in electronic structure theory, structural mechanics and reactor physics, require the solution of eigenvalue problems for self–adjoint and coercive elliptic partial differential operators. Preconditioned gradient type eigensolvers can be used to determine a modest number of the smallest eigenvalues/vectors with multigrid efficiency; they are conceptionally simple, robust, easy to implement and computationally cheap. We present some new short and sharp convergence estimates and illustrate the efficiency of preconditioned eigensolvers for mesh eigenvalue problems.

3.3 Materials Science

Herbert Gajewski

On a Nonlocal Model of Phase Separation

Topic: 3.0

A nonlocal model of non–isothermal phase separation in binary alloys is presented. The model is deduced from a free energy with a nonconvex part taking into account nonlocal particle interaction. The model consists of a system of second order parabolic evolution equations for heat and mass, coupled by nonlinear drift terms and a state equation which involves a nonlocal interaction potential. The negative entropy turns out to be Lyapunov functional of the system and yields the key estimate for proving existence and uniqueness results and for analyzing the asymptotic behaviour as time goes to infinity.

Alexandre Kolpakov, L. Berlyand

Net Model for a System of the Dense Packing Particles

Topic: 3.0

The Laplace equation in the domain with the large number of small absolutely conducting fillers can be approximated with a finite-dimensional ("net") model if the distances between the neighbor fillers are small. The novelty of the result is that it can be used for discontinuous composites (mixtures).

W.G. Litvinov, R.H.W. Hoppe

Model and Problems on Flow of Electrorheological Fluids

Topic: 3.0

Electrorheological fluids are smart materials whose rheological properties dramatically changes in response to electric fields. We introduce a constitutive equation of electrorheological fluids such that a fluid is considered as a viscous one with the viscosity depending on the second invariant of the rate of strain tensor, on the module of the vector of electric field strength, and on the angle between the vectors of velocity and electric field. We study the general problem on the flow of such fluids at nonhomogeneous mixed boundary conditions, wherein values of velocities and surface forces are given on different parts of the boundary. We consider the cases where the viscosity function is continuous and singular, equal to infinity, when the second invariant of the rate of strain tensor is equal to zero. In the second case the problem is reduced to a variational inequality. The singular viscosity function is approximated by a continuous bounded one with a parameter of regularization. By using the methods of a fixed point, monotonicity, and compactness we prove the existence of a solution of the regularized problem and that the solutions of the regularized problems converge to the solution of the variational inequality as the parameter of regularization tends to zero. We also address efficient methods for numerical solution of the problems under consideration. Then we consider a problem on modelling and optimization of electrorheological shock absorber.

Leonid Manevitch

Solitons in Polymer Physics

Topic: 3.0

A wide class of physical processes in polymer systems is considered in framework of unified approach based on analysis of localized soliton-like excitations. We consider different types of localized excitations which are specific for polymers. On this basis a series of physical processes are discussed. It is shown how understanding of experimental data can be attained if using theoretical representations related to solitons.

Thomas Pohl, Claus Hammerl, Bernd Rauschenbach, Ulrich Rüde

Simulation of Ostwald ripening using Multigrid Methods

Topic: 3.0

Ostwald Ripening (OR) is essential for many applications in material science. Accurate models are needed to predict and better control this process. One mayor disadvantage common to most models concerning OR is the simplification of the diffusion process due to the high computational demands. The new simulation algorithm uses a 3D multigrid method and a predictor–corrector like strategy to integrate the evolution equations for ensembles of up to several ten thousands of precipitates which are coupled via the material diffusion.

Eugenia Radzikowska

Macroscopic Theory of Micropolar Superconductors

Topic: 3.0

The micropolar continuum theory is applied to type II superconductors containing a vortex network. Quantum-mechanical quantities describing the phenomenon of superconductivity supplement the classical electrodynamics of micropolar continua. The generalized variational principle for dissipative processes taking place in type II superconductors is formulated. Finally, the complete system of equations describing the interactions of electromagnetic, mechanical and thermal fields in microelastic high T_C superconductors is obtained together with the constitutive relations and the jump conditions on the discontinuity surface.

Christian Reichert, Jens Starke, Markus Eiswirth

Stochastic Model of CO Oxidation on Platinum Surfaces and Deterministic Limit

Topic: 3.0

We present a stochastic model for the oxidation of CO on low-index platinum single crystal surfaces. A corresponding deterministic limit for large particle numbers can be derived rigorously. The dynamical behaviour of the reaction kinetics is investigated by means of a numerical bifurcation analysis of the deterministic limit and stochastic simulations. The computed bifurcation diagrams for Pt(110) and Pt(100) are in good agreement with experimental results.

Malin Siklosi, Gunilla Kreiss

Elimination of Numerical Errors in Time Dependent Shock Calculations

Topic: 3.0

In many cases, numerical solutions of hyperbolic conservations laws are only first order accurate downstream of shock layers, even though computed by a formally higher-order numerical method. However, it is possible to avoid this degeneracy in order of accuracy. Often, a numerical solution can be viewed as a solution of a corresponding slightly viscous system with a scalar viscosity coefficient. We construct a matrix viscosity coefficient which gives a truly higher-order method. Numerical calculations verify the improved accuracy.

Jens Starke, Jürgen Vollmer

Relaxation Oscillations in Droplet Merging Driven by Wetting

Topic: 3.0

Starting with a randomly chosen initial distribution of droplets on a surface, we analyze the wetting kinetics upon a gradual spreading of the droplets. Consequently droplets collide and merge, thus releasing part of the covered surface. In contrast to thermodynamical expectations, this negative feedback leads to relaxation oscillations in the temporal evolution of the mean droplet size and the fraction of surface covered by the droplets.

Josip Tambača

A Numerical Procedure for Solving the Curved Rod Model

Topic: 3.0

In this work a numerical procedure for the solution of the one dimensional equilibrium model of elastic curved rods is derived. The middle curve of the curved rod is approximated by a piecewise linear curve and applied loads by a piecewise constant function. The difference in sup norm of the solutions of the boundary value problem of curved rods for the smooth and piecewise linear curve is estimated. The constants in the estimate are explicit.

Omur Umut

Transverse Impact to the Flexible Elastic Membranes with a Rigid Hole
Topic: 3.0

In this study, the problem of transverse impact to the flexible elastic membranes possessing a hole is investigated. This problem has no a similarity solution like the problems studied previously and hence one deals with the nonlinear initial and boundary value problem for a set of partial differential equations in regions with a priori unknown boundaries.

The algorithm for the numerical solution to the problem is worked out. This algorithm is based on the characteristics method of solution of the hyperbolic type of systems by making use of the jump conditions on the unknown boundary of regions.

Kees Verhoeven

Modelling Laser Induced Melting
Topic: 3.0

In simulating a laser drilling process, melting is one of several physical phenomenae that have to be modelled. Two different mathematical formulations of this laser induced melting are derived. For every formulation we give a specific numerical recipe. Special attention is paid to problems where 'mushy regions' occur and to extensions to 2D. Finally, the numerical results of these different recipes are discussed.

Giovanna Carcano, Victoria Rosca

Analysis of Wave Propagation in Composite Laminate Using Wavelets
Topic: 3.1

The paper studies the application of wavelet transform in the analysis of transient waves propagation in the graphite/epoxy laminates. It will be shown that by using the peak of the magnitude of the wavelet transform,the arrival times of group velocity at each frequency can be extracted.Also,we discuss the problem of planar source location for anisotropic laminates using frequency-dependent,arrival times and the directional dependence of flexural mode velocities.

Alina Fedossova

About Equalities Constraints in the Stochastic Outer-Approximation Algorithm for Convex Semi-Infinite Programming Problems
Topic: 3.1

Many variational problems have been reduced to semi-infinite programming problems using some approximations. The propose of this paper is to register some boundary conditions of these problems with the help of infinite number of equalities. Then we have convex semi-infinite programming problems with constraints of equalities and inequalities. This paper presents a stochastic algorithm which incorporates mechanisms for active search of relevant constraints. Numerical experiments have been made for elastic-plastic torsion of hollow bars.

Mårten Gulliksson

Some Models for Material Properties and Light Scattering in Paper
Topic: 3.1

Paper is a fascinating and very complicated material difficult to model in a realistic way. In our talk we will give two examples. Firstly, we describe how to determine material characteristics from measured displacements when the paper is considered to be linearly elastic. Secondly, a light scattering model for paper is presented with emphasis on computational stability and efficiency. Finally, the extension of our models to a more complicated setting are given together with some related research.

Thomas Götz

Asymptotic Methods for Melt Spinning Processes
Topic: 3.1

An asymptotic method for determining the interaction of air flow around slender fibers in a melt spinning process is presented. The model results in an integral equation relating the air flow to the force that is exerted onto the fibers. Besides theoretical and numerical aspects, the application of this model to industrial melt spinning processes is discussed.

Iavor Hristov

Model of Deformations of a Double Emulsion Drop Subjected in an Uniform Electric Field
Topic: 3.1

The model of finite deformations of a double emulsion drop in an uniform electric field is studied. The drop consists of two homogenous, incompressible and Newtonian fluids of different properties. The Reynolds number is assumed small enough and the hydrodynamic problem is solved in quasi-steady Stokes approximation. The initial forms of the drops are considered spherical. The electric and hydrodynamic problems are separated and the electric field has influence on the hydrodynamic one by the Maxwell stress tensor appearing in the boundary conditions at the fluid surfaces. Using semianalytical-seminumerical method based on boundary elements and the kinematic condition, the forms of the fluid particles are obtained at each time step.

The influence of some fluid parameters and the electric field intensity on the deformation of the double emulsion drop is represented in figures.

Cornelia Kober

Simulation of Shape Memory Alloy Reinforced Composite Material
Topic: 3.1

A micromechanical mathematical model is presented. The system of partial differential equations is similar to a layered media concept with the SMA-fibers between the layers. The embedded fibers become sub wave guides interacting with the ambient matrix. We restrict ourselves to a one dimensional formulation of the fibers, the contact forces between the matrix and the fibers are realised by jump terms. For the dynamics of the SMA, we refer to Landau-Ginzburg-Devonshire-theory. Numerical test cases demonstrate the ability of the model to capture the dynamical behaviour of the composite structure.

Joachim Linn

On the Characterization of the Phase Space of the Folgar-Tucker-Equation

Topic: 3.1

The Folgar-Tucker-Equation (FTE) is the model most frequently used for the prediction of fiber orientation (FO) in the simulation of the injection molding process for short-fiber reinforced thermoplasts. The dependent variable (2nd order FO-tensor) is a symmetric matrix with certain constraints on its coefficients. We report recent results on the characterization of the phase space of the FTE and discuss implications for the numerical solution of the coupled free surface flow and FO equations in full 3D.

Julia Orlik, S.E. Mikhailov

Homogenization Techniques and Prediction of Strength and Fatigue Strength for Periodically Reinforced Composites

Topic: 3.1

The asymptotic homogenization is applied for calculation of homogenized macro-stresses and first approximation to the micro-stress field, from properties of the components, applied macro-loads and micro-geometry. A non-local approximate macro-strength condition, defined on homogenized stress-field, is derived from the micro-strength conditions and their convergence to the approximate macro-strength condition, as the structure period tends to zero, is proved using the two-scale convergence for the micro-stresses. The same was obtained and proved for the macro-fatigue strength.

Cristian Petre, V. Anghel

Finite Element Formulation for Piezoelectrically Actuated Composite Plates

Topic: 3.1

A finite element formulation for static and dynamic analysis of composite laminated plates integrated with piezoelectric layers is presented. Available from literature finite elements, with three or four nodes, for thin or thick plates, are adapted in order to model the coupled electroelastic behaviour. Some elements are derived using the discrete Kirchhoff technique. Then the transverse shear effects are added, which can be significant for thick multilayered plates. The models are validated using published data and results. Displacements induced by the actuated piezoelectric layers produce results which show good agreement with those obtained using other methods. Natural frequencies of plates are also in excellent agreement with other models.

Sergei Sinchilo, J. Rushchitsky

Energy of Plane Harmonic Waves in Composite Materials (Analytical and Computer Analysis)

Topic: 3.1

Composite materials are described by two microstructural models of the quadratic nonlinear deformation – the classical model (model of the 1st order) and the mixture model (model of the 2nd order). Within the framework of the first model, the influence of nonlinearity on the parameters of wave energy is analyzed. The second model permits to take into account simultaneously the influence of a microstructure and nonlinearity of materials on the velocity of energy propagation. Obtained three – dimensional plots are analyzed and commented.

Katya Terletska, J. Rushchitsky

Modelling of Solitary Waves in Composite Materials

Topic: 3.1

The solitary wave means as the wave with a specific profile, which should be practically with a compact support and have one or a few humps. In our computer modelling we deal with profiles, which are described by Whittaker functions.

Waves in composites are studied within the framework of the microstructural theory of mixtures. Two approaches to a wave evolution study are realized: 1. when Fourier series approximation (200-300 harmonics) is used; 2. when the propagating profile is assumed to be described by the initially given Whittaker function. New wave effects are detected and will be discussed.

Michael Wulkow

Numerical Solution of 2D Population Balances in Polymer Chemistry and Material Science

Topic: 3.1

Population balances describing particle properties play an important role in the modeling of disperse systems (e.g. production of polymers, crystals, bio pellets). A particular complexity is given by the appearance of integrals and sums in the respective partial or countable systems of differential equations and the increasing interest in models with more than one property coordinate (dimension). The talk will describe the extension of the well-accepted discrete Galerkin h-p-method to higher dimensions and present some recent applications.

Dmitry Zakharov

Modelling of Edge Bending Waves in Anisotropic Composites

Topic: 3.1

On the basis of 2D long-wave asymptotic theory of thin anisotropic laminates a model of edge localized waves is considered. Characteristic timescale is chosen in accordance with dynamic bending. Existence and properties of Rayleigh type waves are investigated. As shown, the propagation of waves along the stress-free edge under exponential decay at the distance from the edge is essentially different from the case of isotropy. Some principal new effects are revealed: exponential decay is realized with oscillations, velocity of waves is not a minimal between bending waves, energy flux may contradict to the direction of phase velocity, and may be equal to zero. A few numerical examples with parametrical analysis of dispersion curves and energy flux are presented and discussed.

Dmitry Zakharov

Asymptotic Simulation of Laminates with Highly Anisotropic Directions

Topic: 3.1

Using multiple scale method an average 2D asymptotic theory of thin elastic laminates with high difference of modulii in different directions is obtained. Two classes of laminates are considered: - first class presumes different asymptotic orders of modulii in different directions, but there is no asymptotic difference between layers in the laminate (only combinations of soft/rigid directions in layers); - second class contains laminates, constructed of soft/rigid groups of sub laminates, and each of them belongs to the first class. A a set of dynamic models are obtained, classified and discussed. Coincidence and difference with existing engineering models are analysed. Statement of main boundary value problems and their properties are considered.

Pavel Dubovski

New kinetic models in the coagulating two-phase systems and their fluid dynamic limit

Topic: 3.1

We consider coagulation processes for two-phase systems and construct two one-parameter families of the models of coagulation (merging) of particles. The maximal parameter of the first family leads to the celebrated M. Smoluchowski coagulation equation, meanwhile the maximal parameter of the second family yields a new discrete kinetic coagulation model. It turns out that this new model is the discrete version of V.S. Safronov continuous coagulation equation. We compare analytically and numerically new and Smoluchowski coagulation models and conclude that the structural stability (gel transition) of a coagulation system is closely connected with the property of the coagulation front to be finite. The coagulation front can be estimated from Safronov model.

Also, we consider spatially inhomogeneous coagulation-fragmentation equation, pass to the fluid dynamic limit and obtain a new model of dynamics of two-phase systems.

Thomas Apel

Computation of 3D Vertex Singularities for Linear Elasticity

Topic: 3.2

The stress distribution at the top of a polyhedral corner or at a crack tip has the typical r^α-singularity. Mathematically, the exponent α is an eigenvalue of a quadratic operator eigenvalue problem. The finite element method is sufficiently flexible to solve the problem numerically, such that also anisotropic or composite materials can be treated. In the talk we present new approximation results, strategies for the solution of the corresponding matrix eigenvalue problem and numerical tests.

Rolf Krause, Ralf Kornhuber, Barbara Wohlmuth

A Nonlinear Dirichlet Neumann Algorithm for Contact Problems with Friction

Topic: 3.2

We present a new nonlinear method for solving contact problems with friction. It is based on the combination of monotone multigrid methods and mortar methods. The basic idea is to use a fixed point iteration in the normal stress. To do so, we introduce the normal stress as an additional unknown. It plays the role of the Lagrange multiplier in the mortar setting. In each step, we solve a nonlinear unilateral contact problem using monotone multigrid methods and a linear problem with given stress. The transfer of the boundary data is realized in terms of a scaled mass matrix. It turns out that our non linear fixed point iteration can be interpreted as a Dirichlet Neumann algorithm. Numerical results illustrate the performance of our algorithm.

Gerardo Oleaga

A Variational Principle for Dynamic Crack Propagation

Topic: 3.2

A basic law of motion for a dynamic crack propagating in a brittle material is derived in the case of two space dimensions. The only basic assumptions for this purpose are the energy conservation law and a variational inequality following the well known Hamilton's principle. Our study is developed within Griffith's framework, that is under the assumption that crack surface energy is proportional to crack length. It is shown that the speed and direction of the crack can be found without further assumptions. Moreover, the corresponding law is local, and if expressed in terms of the stress intensity factors yields the principle of local symmetry previously proposed for quasi-static evolution.

Arkadi Berezovski

Thermomechanical Modeling of Martensitic Phase-Transition Front Propagation

Topic: 3.3

Recently developed wave-propagation algorithm for conservation laws is modified for the simulation of martensitic phase-transition front propagation in solids. Instead of kinetic relation between the driving force and the velocity of the phase boundary, the thermodynamic consistency conditions are satisfied at the phase boundary. Results of computations are compared with experimental data.

Heike Emmerich

Front Capturing Versus Front Tracking for Thin Film Epitaxial Growth

Topic: 3.3

I address the problem of thin film epitaxial growth on the basis of a front capturing as well as a front tracking method. The particular problem arising in this context is the correct handling of the discontinuities of transport fields as well as the asymmetric properties of the two phases separated by the interface. Here I present two numerical procedures to overcome technical as well as modelling related questions resulting from the above.

Eryk Infeld

Theoretical Confirmation of Feynman's Hypothesis on the Creation of Circular Vortices in Superfluid Media

Topic: 3.3

The changes observed in the typology of superfluid helium vortices have intrigued people for some time now [1]. They either extend from wall to wall, or else are roughly circular and move freely in the fluid. Here we describe how the one create the other. See also [2].

[1] R J Donnelly, Quantized vortices in Helium II, CUP, 1991. [2] A Senatorski and E Infeld, Ohys Rev E57, 6050 (1998).

Teresa Lenkowska-Czerwińska, Dominik Rogula

Alternating States in Layered High-Tc Superconductors

Topic: 3.3

The coupling between lattice distortion modes and the superconducting order parameters for the layered, high temperature superconductors of La214 class is considered. The set of structural micro-order parameters is determined on the ground of a model of coupled quasi-rigid CuO_6 octahedra. The admissible combinations of the superconducting micro-order parameter components are presented. Possible phase diagrams taking into account the structural micro-order are discussed on the ground of an appropriately generalized Ginzburg-Landau free energy functionals.

Alexander A. Nepomnyashchy, Alexander A. Golovin, S.H. Davis, M.A. Zaks

Convective Cahn-Hilliard Models: from Coarsening to Roughening

Topic: 3.3

Convective Cahn-Hilliard models are suggested for the description of phase separation of driven systems and instabilities of crystallization fronts. With the increase of the driving force, a transition from the coarsening regime to a chaotic behavior takes place via a plethora of stable patterns characterized by a complex spatial structure but simple time dynamics. The relation of the dynamic transitions to the phenomenon of kinetic roughening of interfaces is discussed. A comparison with the dynamics governed by a convective Allen-Cahn equation is presented.

Dmitry Ofengeym, M. Bogdanov, S. Kochuguev, A. Kulik, M. Ramm, A. Zhmakin

Using Virtual Reactor Simulator for Crystal Shape Prediction at SiC Sublimation Growth

Topic: 3.3

A Virtual Reactor Simulator has been developed for numerical analysis and optimization of growth processes. The Virtual Reactor approach allows one to simulate time evaluation of the crystal shape and can be very useful to design an environment for growth process providing optimal growth conditions. The software is based on modern programming approaches (object-oriented programming, unstructured nonmatched grids) and hides all the numerics while has an easy-to-learn and easy-to-use interface thus providing an inexperienced user means to solve real-life problems. Some results obtaining by the Virtual Reactor Simulator will be presented.

Dominik Rogula

Dislocations and Superconducting Vortices. Fluxoid Compatibility Law in Electrodynamics of Superconductors

Topic: 3.3

Structured material media containing dense distributions of linear, string-like objects are considered in terms of continuum field theory.The strings are assumed to carry a quantized abelian topological charge, such as the Burgers vector or magnetic flux. The concept of incompatible distortions is transplanted from dislocation theory into the realm of type-II superconductivity. Starting from the multivalued phase description of the Ginzburg-Landau order parameter in type-II superconductors, the fluxoid compatibility equation is derived. As a result, one obtains an appropriate generalization of the classic Londons' equation. The resulting macroscopic setting of electrodynamics of type-II superconductors is discussed.

Malgorzata Sztyren, Dominik Rogula

Directional Instability of Quantized Flux Lines in Strongly Anisotropic Superconductors

Topic: 3.3

The equilibrium configurations of magnetic vortices pinned to an anisotropic superconducting material are described in terms of the anisotropic string model. Contrary to the isotropic case, the string tension is not tangent to the flux line. In these circumstances, for sufficiently strong anisotropy of the material, there exist extremals exhibiting spontaneous sharp bends, energetically more favourable than straight lines. This phenomenon is complementary to the known helical instability in isotropic superconductors with background current. It is, however, governed by entirely different physical mechanism. The question of degeneracy and the dynamical aspects of the directional instability are discussed.

Alexander A. Golovin, T.V. Savina, Alexander A. Nepomnyashchy, S. Brandon, D.R. Lewin

Feedback Control of Morphological Instabilities in Directional Solidification

Topic: 3.4

Feedback control of morphological instabilities in directional solidification by means of adjustable melt heating is investigated theoretically. Linear stability analysis of the problem taking into account thermal diffusion in the solid and liquid phases, constitutional and kinetic undercooling and crystal-melt interfacial tension is performed. It is shown that the feedback control can substantially increase the critical morphological number above which the instability occurs. Effect of the feedback control on both monotonic and oscillatory instabilities is analyzed.

George Makrakis, Stathis Filippas

High Frequency Energy Densities via Wigner Transform

Topic: 3.5

High frequency fields near caustics for the Schrödinger equation are computed through the Wigner equation. In the simplest case of caustics generated from the initial data, explicit computations show that Wigner transform can capture the singularities of the Lagrangian manifold. In the presence of a potential, we show that Wigner's equation retrieves the WKB method for regular fields, and provides a way for understanding the caustic formation and the evolution of Lagrangian singularities

3.4 Environmental Science

Oscar Angulo, Juan Carlos Lopez-Marcos

An Efficiency Study of Numerical Methods for the Dynamics of Population Models with Nonlinear Growth Rate

Topic: 4.0

We consider the numerical integration of the nonlinear size-structured population model, which is an extension of the model proposed by Murphy,

$$u_t + (g(x,t,I_g(t)),u)_x = -\mu(x,t,I_\mu(t));u, \quad 0 < x < 1,$$

$$g((x,0,I_g(0)),u(0,t) = \int_0^1 \alpha((x,t,I_\alpha(t))\, u(x,t)\, dx\ ,$$

$$u(x,0) = \phi(x), \quad 0 \le x \le 1,$$

where

$$\begin{aligned} I_g(t) &= \int_0^1 \gamma_g(x)\, u(x,t)\, dx, \\ I_\mu(t) &= \int_0^1 \gamma_\mu(x)\, u(x,t)\, dx, \\ I_\alpha(t) &= \int_0^1 \gamma_\alpha(x)\, u(x,t)\, dx, t > 0. \end{aligned}$$

The independent variables x, y, t denote, respectively, size and time, and the function $u(x,t)$ is the size specific density of individuals of size x at time t. The population dynamic is determined by the size-dependent growth rate g, the mortality rate μ and the fertility rate α. These vital functions depend on the total amount of individuals of the population by means of the functions $I_g(t)$, $I_\alpha(t)$ and $I_\mu(t)$, which represent a way of weighting the size distribution density to model the different influence on the condition of life due to individuals of different size.

Alexander Avdeev, Elder V. Goryunov, Mikhail M. Lavrentiev, Renato Spigler

Simultaneous Identification of Two Coefficients in a Diffusion Equation

Topic: 4.0

An algorithm for the simultaneous determination of it two coefficients in an inverse problem for equations of the parabolic type is presented. The model under investigation has been proposed in the literature to describe the long–time coastal profile evolution. The iterative inversion procedure is based on the minimization of a suitable cost functional. Such a functional is considered in terms of Laplace transforms of the solution to the original dynamical problem. As have been proved, in the simplest case of constant equation coefficients, the Laplace transform is correct. Results of numerical tests also shown to illustrate the performance of the algorithm. Finally, the measured real data of the coastal profile evolution have been numerically processed to validate the aforementioned diffusion type model.

Ludek Benes, Karel Kozel, Ivo Sladek

Numerical Simulation of the Pollution Dispersion over a Complex Terrain

Topic: 4.0

The work deals with a numerical solution of viscous turbulent flows in the atmospheric boundary layer including pollution propagation. Mathematical model is based on the system of RANS equations with an algebraic turbulent model. This system is completed by two transport equations for the concentration of passive pollutants and the potential temperature. Numerical solution is based on a finite volume method and the artificial compressibility method. Numerical results over 2D and 3D single hill and over complex topography are presented.

Aijie Cheng, Shmulik P. Friedman, Yakov Krasnov

Mathematical Model and Numerical Simulation for Controlled-Release and Spread of Agrochemicals in Soil

Topic: 4.0

The optimal design and application of controlled-release agrochemical requires an understanding of the process of spread of the agrochemical, which includes two consecutive processes, the release into the surrounding soil and its subsequent dispersion, uptake and degradation in the soil profile.

The problem of transient release of an agrochemical from a membrane-controlled formulation into a spherical soil volume with stagnant water was analyzed by Friedman and Mualem [1994]. Friedman [1997] analyzed the problem of simultaneous controlled-release and vertical spread of the agrochemical in the soil profile by artificial decoupling of diffusive release and vertical, convection-dispersion transport processes at each time step of simulation. Namely, for calculating the release rate at each depth, he neglected the effect of the vertical water flow, assuming also an approximate quasi-steady state diffusion process. The calculated release rate served as a source term in the one-dimensional, convection-dispersion transport equation. In order to avoid the decoupling approximation applied by Friedman [1997], we established and analyzed the full (not decoupled) three-dimensional (axisymmetric) model of controlled-release and convection-dispersive transport of the agrochemical in the soil. Finite difference model and finite element scheme were established and some numerical simulation were performed for practical application. The main objective of this study is to find the role of different factors affecting the release rate and distribution of agrochemical for more realistic scenarios.

Dan Emanuel Popovici, Adriana Popovici

Models for Stochastic Stationary Processes and their Prediction

Topic: 4.0

The prediction of a (two-time parameter) stationary process $f = f_{n_{n\in\mathbb{Z}^2}}$ consists in finding information about the process in the next moment using all the facts already known and represented by $\mathcal{K}_n^f$, the past and present up to the moment $n \in \mathbb{Z}^2$.

In the model proposed by I. Suciu and I. Valuşescu the structure of f can be related to the properties of the commuting isometric pair $U_f^* \mid \mathcal{K}_{(0,0)}^f$, U_f being the bi-shift operator associated to the process. A result of Berger, Coburn and Lebow shows that every completely non-unitary bi-isometry can be modeled in terms of a unitary operator U and an orthogonal projection P, called its unitary invariants. As a consequence we can state that any purely non-deterministic stationary process f is equivalent with a stationary process g, the bi-shift operator associated to it $[\ell_Z^2(\mathcal{K}_{(0,0)}^f \ominus \mathcal{K}_{(-1,-1)}^f), U_g = (U_g^{(1)}, U_g^{(2)})]$ having the matrix structure $U_g^{(k)} = (U_{ij}^{(k)})_{i,j\in\mathbb{Z}}$, $U_{ii}^{(k)} = (2-k)(I-P)U^* + (k-1)UP$, $U_{i,i+1}^{(k)} = (2-k)PU^* + (k-1)U(I-P)$ and $U_{ij}^{(k)} = 0$ for $j - i \notin \{0,1\} (k = 1, 2, i, j \in \mathbb{Z})$. Moreover $\mathcal{K}_{(0,0)}^g = \ell_{Z+}^2(\mathcal{K}_{(0,0)}^f \ominus \mathcal{K}_{(-1,-1)}^f)$.

Finally we characterize some particular classes of purely non-deterministic processes (such as white noises, moving averages for maximal white noises, horizontal or vertical non-deterministic processes) and compute the prediction-error operator in terms of U and P. Corresponding results can also be obtained for the so-called harmonizable processes by using the dilation of such a process to a stationary one.

Budi Nurani Ruchjana

The Space Time Autoregressive Model Case Study on Selenium Pollution in Water

Topic: 4.0

Many places in the world have a serious problem on an environmental, especially in water pollution. It gives a dangerous influence for people. Also for fish or another animal and plant in water habitat. One of a pollutant for fisheries is selenium. It can come from industry or household's rubbish, which it is thrown away to a river. The concentration of selenium in water can be measured both in time and space.

There are many models can be used in analysis of selenium pollution in time or in space. This paper present the model to describe the effect of time on a series of observations made at a particular location, together with the effect of spatial correlation of neighbouring locations. It is called *the space time autoregressive* (STAR) model. One of the characteristics of the STAR model is a matrix consisting of weights that reflect the dependence on neighbouring locations.

The paper addresses two issues, viz:

1. Study on the space time autoregressive model order one both in time and space, it is noticed STAR(1_1).
2. Apply the STAR(1_1) model using the uniform weights to selenium concentration data from several stations at The Saguling Lake.

Checking diagnostic model will be done through examination of the residuals between the observations and the fitted values using the conditional least squares.

Key Words: autoregressive, space time, uniform weight

Tatjana V. Samodourova, Julia V. Fedorova

Mathematical Modeling of Air Pollution within a Roadside Strip in Winter Period

Topic: 4.0

The method of mathematival simulation is used to study the conditions of ice formation on road surfaces, average over-all speed and traffic pollution for different states of road pavements in winter period.

The mathematical models are based upon the calculating analysis of the pavement temperature (the heat conductivity equation), the logical modules describing the conditions for the ice formation, the equation of motion for traffic stream, and the empirical equations for traffic pollution. Practical application the results defined is discussed.

I. Selezov, V. Moskovkin

Evolution of Shore Zone Due to Water Wave Impact

Topic: 4.0

Shoaling water waves of large amplitudes strongly interact with the near shore sediment and granular structure. As a result, a shore layer is strongly reformed and destroyed. Formerly gradual and last time more and more intensive accumulation of negative ecological factors approximates the structure levels close to the critical levels. In these cases the ecological state is subjected to significantly growing disturbances and can pass from this state to the new states, which can be stable or unstable, including catastrophic states.

This paper presents the analysis of the above phenomena on the basis of the theory of bifurcation. The ecological model of reformation of shore line is governed by the strongly coupled nonlinear differential equations

$$\frac{dW'}{dt'} = -\kappa_1 W' + \kappa_2 B' W' + \kappa_5 B' + \kappa_3$$

$$\frac{dB'}{dt'} = B'\left(1 - B'\right) - \kappa_4 W'$$

where W is the clastic beach-forming material volume per unit length of the shore-line, B is the biomass of the bottom biocenose per unit width of abrasion shelf, $\kappa_m \left(m = \overline{1,4}\right)$ are the coefficients depending on physical parameters.

Following [1] the singular points are determined and the conditions of bifurcation are established. Analysing the corresponding eigenvalue problem and the limit circle stability allows to establish the existence of periodic solutions. The possibilities of transition from the initial ecological state to new ones are analysed. One of the real example is considered showing that for some concrete data the vibration period 50-100 years is predicted.

[1] Poston T. and Stewart I. Catastrophe theory and its applications. Pitman, London - San Francisco - Melbourne, 1978.

V.P. Stulov

Inverse Problems in Meteor Physics

Topic: 4.0

The ballistic coefficients and ablations parameters of Prairie Network (United States) fireballs are determined by the best fitting in velocity-height variables. It is given by the model of successive destruction and the model of a single body, both with ablation. Our analysis of the trajectory indicates that either there is no fragmentation or it affects only slightly the trajectory. The solution of inverse problem for bolide Beneshov (Czech Republic 07.05.1991) has shown that the trajectory is good described by a model of a single body with ablation. It conforms to observations, according to which the fragmentation of the bolide consists in separation of small-sized fragments from the massive parental body.

Enrique Thomann, R. Bhattacharya, S. Dobson, R. Guenther, L. Chen, C. Orum, M. Ossiander, Edward Waymire

Stochastic Cascades and the Navier Stokes Equations

Topic: 4.0

The representation of weak solutions of the incompressible Navier Stokes equations using a stochastic cascade introduced by Le-Jan and Snitzman (Prob Theory and Related Fields, 1997) will be related to a fixed point iteration scheme establishing the existence of global solutions of the Navier Stokes equations under appropriate restrictions on the initial data and forcing. Examples and applications of similar solution representation to other nonlinear differential equations, e.g. Burgers and KPP, will be presented.

Paula Budu

Stability Results of Thawing Subsea Permafrost Model

Topic: 4.1

Penetrative convection is investigated in a porous medium bounded above by the ocean bed and below by the interface of the thawing permafrost ground. Such convection flow is observed off the coast of Alaska. The physical model for the thawing subsea permafrost is that of Harrison and Swift hs§84, with field variables: the brine velocity, the temperature and the salinity. We simplify the problem by imposing a temperature field that is linear in the depth variable. For this simplified model values are obtained for the critical Rayleigh number, for both linear and nonlinear stability. From the mathematical point of view the analysis reduces to studying convection in a porous medium with a nonlinear boundary condition. Initially we consider the linear instability analysis which provides us with a linear critical Rayleigh number. If the linear critical Rayleigh number boundary is exceeded, this ensures instability. It does not preclude the possibility of subcritical instabilities. In order to complete the stability analysis, we use the energy method to determine a nonlinear critical Rayleigh number below which convection cannot develop. This critical value is found to be close to that of linear theory. The nonlinear critical Rayleigh number guarantees *unconditional nonlinear stability.*

Michael Friger, Yelena Novack

Quasi-Fourier Modeling in Climate Impact Research

Topic: 4.1

This paper presents a modeling approach based on time-series technique for investigating the impact of meteorology and pollution on health outcome. This approach assumes that health, as well, as meteorology and pollution belong to a multivariate hierarchical system. All connections in this system are mathematically formalized by means of trigonometric and polynomial functions. The model is simulated on the data of daily mortality and a set of meteorological and pollution measurements in Philadelphia during 1974-1980.

Bakhtiyor Abdurakhimov, M. Aripov

Numerical Modelling of the Atmospheric Processes Over Central Asia

Topic: 4.2

On the basis of 15 leveled regional of non-adiabatic model, the modeling of winter dynamic processes over Central Asia is executed. Besides, the model intended for modelling of large-scale processes is used for the diagnosis of such mezo-scale phenomena as fronts. As such models do not reproduce the structure of front sharply, as the parameter, on which it is possible to judge about presence of developing front, the frontogenetic function was chosen.

Yuri Skiba, Ismael Pérez-García

The Linear Stability Study of Barotropic Atmosphere Flows

Topic: 4.2

The linear stability study of a 2D incompressible flow on a rotating sphere is considered. For a viscous fluid, the spectral approximation problem is examined. For an ideal fluid, a necessary instability condition is obtained for a Legendre-polynomial (LP) flow, Rossby-Haurwitz (RH) wave, Wu-Verkley (WV) wave, and modons. By this condition, Fjortoft's average spectral number of the amplitude of an unstable mode must be equal to a specific number that depends on the basic flow degree (LP flow and RH wave) and also on the spectral distribution of the mode energy in two basic flow regions (WV wave and modon). The maximum growth rate of the modes is estimated. The new instability condition is useful in testing a numerical linear stability study algorithm. Numerical results are discussed.

Chris A. Toomer

Numerical Flow Simulations over Highly Mountainous Terrain for Wind-Potential and Pollution Studies

Topic: 4.2

Conventional industrial approaches for modelling boundary layer atmospheric flows produce poor results when applied to highly mountainous terrains. A computational fluid dynamics package has been suitably extended & produces good estimations. Results will be presented for the estimation of power from wind farms and its optimisation through the relative positioning of the mills, and for pollution studies. Comparison with in-situ measurements is made and comments given on the sensitivity to initial conditions.

Alina Fedossova

Minimization of Costs for Air Pollution Control

Topic: 4.3

We present a mathematical model that reaches compliance with air quality standards for the every ground level point while minimizing the control costs which thereby occur. These air quality standards give rise to an infinite number of restrictions and this is semi-infinite programming problem. This paper presents a stochastic outer approximations algorithm for air pollution problems which incorporates mechanisms for active search of relevant constraints and for dropping of irrelevant constraints.

Andreas Keese, Hermann G. Matthies

Efficient Solution of Stochastic Groundwater Flow

Topic: 4.3

When simulating ground water flow, incomplete knowledge of the soil's permeability can be modeled by stochastic fields, yielding a stochastic partial differential equation. We discretize the stochastic part of the resulting system by the Karhunen–Loève expansion and expand the unknown solution in tensor products of finite elements and Wiener chaos polynomials. We present efficient solvers for the resulting large system of equations and present adaptive methods for choosing the stochastic ansatz functions.

Nikolai Larkin, Doronin Gleb

Kuramoto-Sivashinsky Model for Two-Phase Media

Topic: 4.3

There is a lot of mathematical models describing non-stationary flows of multi-phase media. But for existing models there are not theorems that prove their mathematical correctness: existence, uniqueness solutions for formulated problems, stability of solutions. Here we present the model based on the K-S equation for the liquid phase and nonlinear transport equations for the solid particles phase. We prove the existence and uniqueness of global strong solutions and the exponential decay of them.

Joseph M. Maubach

Rapid Numerical Modelling of Pollution Transport Problems

Topic: 4.3

Numerical solvers for pollution transport problems tend to become more and more complex: More accurate solutions are obtained at the expense of for instance using multi-phase media models, mixed finite elements and Lagrange flux-multipliers.

We present a rapid interactive visual construction method for the related numerical solvers, based on data-flow oriented networks and adapted finite element methods.

Yuri Skiba, Valentina Davydova-Belitskaya

Air Pollution Estimates
Topic: 4.3
Solutions to a pollution transport model and its adjoint are used for estimating the impact of vehicular emissions (CO) in an urban area. Unique solvability and continuous dependence of the solution on the forcing and initial condition are proved. Compatible, balanced and stable difference schemes based on splitting method are developed. Direct and adjoint pollution estimates are derived for ecological zones. The sensitivity of these estimates to emission rates of various parts of the main city roads, as well as to the wind and initial pollutant distribution is examined using adjoint problem solutions. Carbon monoxide transport in Guadalajara City is considered as application.

Ralph Lehmann

Determination of Dominant Pathways in Chemical Reaction Systems: An Algorithm and its Application to Stratospheric Chemistry
Topic: 4.4
The analysis of complex chemical reaction systems is frequently complicated because of the coexistence of fast cyclic reaction sequences and numerous slower pathways that yield a net production or destruction of a certain species of interest. An algorithm that finds the most important ones of these pathways (by solving a linear optimization problem for each of them) is presented. It is applied to examples in stratospheric chemistry, including the determination of catalytic ozone destruction cycles.

Lasha Ephremidze, G. Janashia, E. Lagvilava

A New Multivariate Spectral Factorization Algorithm
Topic: 4.5
A new effective factorization algorithm of positive definite matrix-function of all order is proposed. The volume of calculations is reduced to the minimum and its size can be estimated in advance for any given accuracy.

The algorithm is based on the methods of complex analysis and it looks very simple for creating the corresponding software.

This kind of factorization algorithm is useful in many areas of applied sciences including the linear prediction theory of stationary processes developed by Wiener and Kolmogorov.

Afet Golayoglu Fatullayev

Numerical Solution of an Inverse Problem for the Hydraulic Properties of Porous Media
Topic: 4.5
A nonlinear parabolic equation arising in modeling flow in homogeneous and isotropic porous media is considered in which coefficients representing water capacity and hydraulic conductivity are unknown and to be determined from overspecified data measured on the boundary. By using polygonal approximation for the unknown coefficients and their eliminating in the equation using overspecified data, the problem is transformed into the standard nonlinear initial boundary value problem. A numerical procedure for the solution of this problem and numerical examples are presented.

Frank Koster

Adaptive Solution of the Navier-Stokes equations with Wavelets
Topic: 4.5
In this talk we present a technique for the numerical solution of PDEs which is based on wavelets on adaptive sparse grids. This method combines the efficiency of finite differences with the remarkable approximation power of anisotropic tensor product wavelets. We present some numerical simulations of two- and three-dimensional shear flows which show the efficiency of our approach.

Frank Koster

Turbulence, Wavelets and Numerical Simulation
Topic: 4.5
In this talk we focus on the approximation of homogeneous turbulent flows. For a linear approximation using uniform splines or Fourier modes we get from Kolmogorov's K41 theory: 1) That, the convergence rate is very low, if the number of degrees of freedom (DOF) is less than $O(Re^{9/4})$. 2) That, the convergence rate is limited by the order of the splines only, if DOF $> O(Re^{9/4})$. We show that an adaptive approximation already leads to optimal convergence rates, if DOF $> O(Re)$ only.

3.5 Nanoscale Technology

Georg Hebermehl, Friedrich-Karl Huebner, Rainer Schlundt, Thorsten Tischler, Horst Zscheile, Wolfgang Heinrich

Simulation of Microwave and Optoelectronic Devices
Topic: 5.2
Basic elements of microwave and optoelectronic devices are the transmission lines. The electromagnetic properties can be calculated by applying Maxwell's equation to

the infinitely long homogeneous transmission line structure. In the presence of losses or Perfectly Matched Layers (PML) the matrix of the eigenvalue problem becomes complex. A method is presented which finds the interesting propagation constants solving a sequence of eigenvalue problems. Non physical PML modes are detected.

Thomas Koprucki

On Eigenvalue Problems Arising from the Modeling of Semiconductor Nanostructures.
Topic: 5.2

The kp-method in combination with envelope function approximation is a widely used tool for the near-bandage modeling of electronic states in one-dimensional semiconductor nanostructures like Quantum Wells. Within the nanostructure the wave function is represented in terms of envelope functions, which are eigenfunctions of matrix-valued kp-Schrödinger operators with discontinuous coefficients. We present results on the spectral properties of the kp-Schrödinger operators and on the electronic states for some Single and Multi Quantum Well structures.

Hsinchih Frank Liu

Nanoscale Couette Flow Simulation with Artificial Moving Wall Technique in Boundary Condition Control
Topic: 5.3

Artificial Moving Wall (AMW) technique is presented to handle the boundary interface existing at the tangential direction of a nanoscale Couette flow. Due to the small amount of the inward number flux in Direct Simulation of Monte Carlo (DSMC) method, the convergence rate becomes very slow that limits the boundary condition's effects. AMW technique is using an artificial wall on the interface and directly providing needed information for the boundaries to improve the convergence rate.

3.6 Communication

Götz Pfander, Werner Kozek, Georg Zimmermann

Perturbation Stability of Coherent Riesz Systems Under Convolutions
Topic: 6.0

We study the orthogonal perturbation of various coherent function systems (Gabor systems, Wilson bases, and wavelets) under convolution. This problem is of key relevance in the design of modulation signal sets for digital communication over time–invariant channels. Upper and lower bounds on the orthogonal perturbation are formulated in terms of spectral spread and temporal support of the prototype. The orthogonal perturbation of these coherent function systems is illustrated in a DMT/OFDM relevant setting.

Akiyoshi Shioura

Quasi M-convex and L-convex Functions: Quasi-Convexity in Discrete Optimization
Topic: 6.0

We introduce two classes of discrete quasiconvex functions, called quasi M-convex and L-convex functions, by generalizing the concepts of M-convexity and L-convexity due to Murota (1996, 1998). We investigate the structure of quasi M-convex and L-convex functions with respect to level sets, and show that various greedy algorithms work for the minimization of quasi M-convex and L-convex functions.

Anjan Biswas

Perturbation of non-Kerr Law Soliutons
Topic: 6.1

The perturbation of solitons with non-Kerr law nonlinearity, that is governed by the generalized nonlinear Schrödinger's equation, is studied. The adiabatic parameter dynamics of the solitons is obtained by the soliton perturbation theory. Some special case of the non-Kerr law nonlinearity is considered with some specific perturbations.

Joachim Linn

Semiclassical Theory of High Bit Rate Optical Soliton Propagation in Distributed Fiber Amplifiers
Topic: 6.1

The stable propagation of sub-picosecond optical solitons in single mode fibers requires distributed amplification, as provided by active (rare earth doped) fibers. Recent research has been focussed exclusively on the propagation of single soliton pulses in active fibers. Starting from the semiclassical Lamb/Scully theory of the laser amplifier we present a model for the propagation of high bit rate signals consisting of ultrashort optical pulses in active fibers and show some results of numerical simulations.

Zouhair Ben Jemaa, Belghith Safya

Generaring Kneading Sequences for CDMA Application
Topic: 6.4

The theoretic studies done to analyse the performances of the DS-CDMA system has shown that spreading sequences must present particular correlation functions and be easy to generate. Kneading sequences was considered and it was shown that selected ones allow performances better than classical sequences. In this paper, performances of kneading sequences are presented and compared to those of Gold-like ones, moreover, the problem of determining and generating them is evoked, it is shown that it is easy to generate kneading sequences although they are generated by chaotic transformation.

Andreas Eisenblätter

Adapting GSM Frequency Plans Optimally
Topic: 6.4
From the variety of tasks called frequency planning, we focus on the one which is carried out the most often in GSM frequency planning practice. This is the adaption of an already existing frequency plan to local changes in the network setup. In contrary to general frequency planning, adoption planning can be solved (almost) optimally in many practical cases. We describe a branch-and-bound algorithm and present computational results for realistic planning cases.

Christoph Helmberg, Andreas Eisenblätter

Lower Bounds for Frequency Assignment in GSM Networks via Semidefinite Relaxations
Topic: 6.4
We present computational results for a semidefinite relaxation of the frequency assignment problem in GSM networks. The relaxation is based on the max-k-cut relaxation of Jerrum and Frieze. Our experiments on real-world instances yield bounds on the minimal interference that are within 50% of the best solutions known. This is a considerable improvement in comparison to LP-based approaches, where, to the best of our knowledge, no reasonable bounds have been obtained so far.

3.7 Traffic

Thorsten Materne, M. Günther, Axel Klar, R. Wegener

Multivalued Fundamental Diagrams and Stop and Go Waves
Topic: 7.0
In this talk a kinetic model for vehicular traffic leading to multivalued fundamental diagrams is developed and investigated. For this model phase transitions can appear depending on the local density and velocity of the flow. A derivation of associated macroscopic traffic flow equations from the kinetic equation is given. Moreover, numerical experiments show the appearance of stop and go waves for highway traffic with a bottleneck.

Mehdi Radjabalipour, Mehdi Ahmadinia

Application of Wavelets to Optimal Control Problems
Topic: 7.0
The paper presents a method for solving optimal control problems as well as differential equations with boundary conditions using wavelets. The method needs no knowledge of a bound on the trajectory and the approximate solutions satisfy the exact boundary conditions imposed on $x(t)$ or $x'(t)$ at the boundary points. The errors are compared with those of similar problems and in almost all cases are found smaller.

Leonid Safonov, Elad Tomer, Vadim V. Strygin, Yosef Ashkenazy, Shlomo Havlin

Chaos in a Traffic Flow Model
Topic: 7.0
We study the presence of chaos in a car-following traffic model based on a system of delay differential equations. We find that for sufficiently large delay the system may pass to chaos according to the Ruelle-Takens-Newhouse scenario (steady states – limit cycles – two-tori – three-tori – chaotic attractors) with changing the density towards intermediate values. Exponential decay of the power spectrum and non-integer correlation dimension suggest the existence of chaos. It is also found that the attractor is multi-fractal.

Michael McGettrick

Partial Synchronicity and the (max,+) Semiring
Topic: 7.2
In this paper we illustrate how non-stochastic (max,+) techniques can be used to describe partial synchronization in a Discrete Event Dynamical System. Our work uses results from the spectral theory of dioids and analyses (max,+) equations describing various synchronization rules in a simple network. The network in question is a transport network consisting of two routes joined at a single point, and our Discrete Events are the departure times of transport units along these routes.

We calculate the maximum frequency of circulation of these units as a function of the synchronization parameter. These functions allow us further to determine the waiting times on various routes, and here we find critical parameters (dependent on the fixed travel times on each route) which dictate the overall behaviour. We give explicit equations for these parameters and state the rules which enable optimal performance in the network (corresponding to minimum waiting time).

Sven Krumke, Jörg Rambau

Online Dial-a-Ride Problems: Theory and Practice
Topic: 7.4
In an online dial-a-ride transportation problem objects are to be transported between the vertices of a given network. Transportation requests arrive online, specifying the objects to be transported and the corresponding source and target vertex. We present theoretical results about the performance of online algorithms and discuss the application to real-world problems such as elevator control and dispatchinng of service vehicles.

Jörg Rambau, Sven O. Krumke, Luis Miguel Torres

Real-Time Dispatching of Automobile Service Units
Topic: 7.4
Given a set of service requests (events), a set of guided servers (units), and a set of unguided service contrac-

tors (conts), the vehicle dispatching problem VDP is the task to find an assignment of events to units and conts as well as tours for all units starting at their current positions and ending at their home positions (dispatch) such that the total cost of the dispatch is minimized. The cost of a dispatch is the sum of unit costs, cont costs, and event costs. Unit costs consist of driving costs and overtime costs; cont costs consist of a fixed cost per service; event costs consist of late costs linear in the late time, which occur whenever the service of the event starts later than its deadline. The program ZIBDIP based on dynamic column generation and set partitioning yields solutions on heavy-load real-world instances (215 events, 95 units) in less than a minute that are no worse than 1% from optimal.

3.8 Market and Finance

Elena Desyatirikova, V.G. Khromykh, A.I. Anissimov

Case Design of Integrated Information Manager System

Topic: 8.0

The "entity-relationship" conception of equipment-program complex TOPAZ-DBMS synthesis is proposed. The characteristics of TOPAZ-DBMS exceeds those ones of the second generation standard CASE-software; provides automatic design medium integration; makes sure the elaboration and accommodation of various data bases structures in the limits of unified integrated information system (IIS). The modeling of macroeconomics' complexes was performed by semantic with natural language at formation stage of IIS and by modification of SQL-language at the stage of IIS exploitation.

Hong Seo Ryoo

Large-Scale Portfolio Optimization with Skewness Consideration and Its Application to the NYSE

Topic: 8.0

This paper develops an efficient portfolio optimization model based upon the first three moments of the distribution of the rate of return. The efficiency of algorithm owes to our new measure of skewness and the compact factorization scheme, which allow fast solution of the model via traditional optimization techniques. We demonstrate the merits of the proposed model on the daily NYSE data collected since January 2001. In short, the proposed model allows construction of a portfolio with superb characteristics in less than 30 seconds on a standard Linux workstation.

Karl Sabelfeld, Maxim Osadchii

Valuation of Natural Resources Deposits

Topic: 8.0

The value of natural resources deposits is simulated through a diffusion process of a Wiener-Poisson type. Opportunity of termination of deposit's exploitation is assumed under adverse price conjuncture. The price of the right to terminate the production is determined. Discounted profit flow is equal to the discounted value of options flow that give a company the right to choose whether to extract resources or not, after discounted fixed costs. An explicit analytical approximation is compared with the numerical solution obtained by the Monte Carlo method. Numerical results suggest different strategies of the process under study.

Vadim Shmyrev, Maxim Osadchii

Leasing Payments Optimization by Complementary Variables

Topic: 8.0

The specific class of optimization problems arising from modeling of leasing in view of taxation and budget constraints of parties to a contract is investigated. Initial problem of leasing payments optimization is reduced to linear programming problem with additional condition of complementarity of assigned pairs of variables characterising lessor's profits and losses. It was shown that the problem admits solution by means of linear programming.

Enrique Thomann, Ellen Burnes, Edward Waymire

Valuation of Natural Resource Contracts

Topic: 8.0

A model for the valuation of contracts on assets that due to a cost conversion, c, can take negative values will be presented. By introducing the notion of localized non arbitrage condition, it is possible to derive the PDE

$$\frac{\partial \pi}{\partial t} + rs\frac{\partial \pi}{\partial s} + \frac{1}{2}\sigma^2 s^2 \frac{\partial^2 \pi}{\partial s^2} - r\pi = rc\frac{\partial \pi}{\partial s}$$

with a prescribed payoff at T and knock out boundary at $s = c$. Relations with Asian options will also be presented.

Ari Belenkiy

Inner Market as a "Black Box"

Topic: 8.1

Each market has its singular characteristic. Its inner structure is directly responsible for the observed distributions of returns though this fact is widely overlooked. Big orders lead to doubling the tails. The behavior of a market maker with many or few "friends" who can reliably loan money or stock to him is quite different from the one without. After representing the inner market "case" we suggest how to analyze its structure.

Alexander Szimayer, Taras Beletski, Angelika May

Testing for Conditional Heteroscedasticity in Financial Time-Series

Topic: 8.1

In this paper, we survey time-series models allowing for conditional heteroscedasticity and autoregression.

These models reduce to white noise when the autoregression and some of the conditional heteroscedasticity parameters take their boundary value of zero. We reproduce the asymptotic distribution of pseudo-log-likelihood ratio statistic for testing the presented models for reduction to white noise. The theoretical results are applied to financial data. We estimate the parameters for all models presented and further on, we test on reduction to white noise. The impact of these results on risk measurement is discussed by comparing Value-at-Risk calculations under alternative model specifications.

Ana Bermudez

A General Characteristics/Finite Element Approach for PDE Derivatives Pricing Models. Valuation of Convertible Bonds.
Topic: 8.2
This work presents a general approach for solving two factor (two-dimensional) option-pricing problems. Constraints in the solution are treated in a uniform manner using a Lagrange multiplier method. This approach can easily accommodate constraints such as early-exercise opportunities, conversion provisions, call and put provisions and barriers. Besides, discrete dividends and coupons can easily be incorporated into a numerical PDE framework. As illustrative example the pricing of Convertible Bonds with Stochastic Interest Rates is considered.

Joerg Kampen

On Pricing of Options on Multiple Assets in the Presence of Transaction Costs
Topic: 8.2
The extension of the Leland approach for pricing options on n assets in the presence of transaction costs leads to a fully nonlinear parabolic PDE with gauge function term. We provide a condition for replication of options in terms of correlations of assets and transaction cost numbers. Connecting to a Hamilton-Jacobi-Bellman equation we obtain an expectation value formula for the price via dynamic programming and numerically explore the differences to the Black-Scholes pricing.

Heinz Sorge

Stress Testing in Portfolio Management - Taking Lessons from Extreme-Value Theory
Topic: 8.3
There are two complementary methods to determine the capital adequacy of financial institutions in modern risk management, Value at risk and stress testing. The latter method may be more suitable to assess the dangers lurking from “abnormal events”. However, the usual approach in constructing the stress events is quite arbitrary. Here it is discussed how to construct these events based on results from extreme-value theory.

3.9 Speech and Image Recognition

Algis Garliauskas

Solution of Bifurcation Equations for Formation of Patterns - Form Contants in the Visual Cortex
Topic: 9.0
The layered structures in the celeberal and cerebellar cortices of the brain are attributed to most animals while the human and some primate neostriatum neurons are laid out as clustered higher and lower cell density mosaics. These ordered structures are formed by a self-organizing mechanism based on a solution of bifurcation equations. Considering theoretical principles and neuronal networks, the N-shaped current-voltage relation was included in the model and its influence on the stability and conditions of self-organization discussed. The formation of ordered structures was founded in vicinity of the equilibrium point. Based on the group and bifurcation theories, the self-organized topological structures for the visual cortex were grounded. The concomitant computational experiments with illustrations of the ordered structures - form constants - are presented. In the discussion the experimentally registered ordered structures and computational ones have been roughly compared.

Adriana Popovici, Dan Emanuel Popovici

Image Recognition with Cellular Automata
Topic: 9.0
Image enhancement is the processing of images to improve their appearance to human viewers or to enhance the performance of other image processing system. In most applications involving images or image processing one of the most common problems is the presence of noise. This fact often requires the application of some kind of smoothing procedure in order to attenuate noise and quantization error. Two-dimensional cellular automata can be applied to the problem of noise removal in digital images. A simple dynamical rule for the cellular automata is proposed that maps an initial configuration representing the original noisy image, to other configuration corresponding to an image with diminished noise. The proposed method is compared with a classical method.

Holger Kantz, Rainer Hegger, Lorenzo Matassini

Noise Reduction for Human Voice by Local Projections in a Reconstructed Phase Space
Topic: 9.1
A local projective noise reduction scheme, originally developed for low-dimensional deterministic chaotic signals, is successfully applied to human speech. This is possible by exploiting properties of the speech signal which mimic structure exhibited by deterministic dynamical systems. In high dimensional embedding spaces, the strong inherent non-stationarity is resolved

as a sequence of many different dynamical regimes of moderate complexity.

Olga Starikova, P.V. Golubtsov

Invariance Considerations in Problems of Synthesis and Optimal Calibration of Measurement Computer Systems

Topic: 9.1

Many modern measurement systems, producing a large amounts of data, are invariant with respect to a certain group of transformations. This work solves the problem of synthesis of invariant measurement computer system for the case of imprecise information about measurement system. If precise description of a measurement system is not available, then, usually, this leads to an uncontrolled error of source signal restoration. In this work impreciseness is described by parametric information about the measurement.

Note, that if a priori information about a measurement system is too rough then the inaccuracy of the constructed measurement computer system can be big enough. In such situations problem of an optimum calibration is stated. It consists in generating of a calibration map, converting calibration data (i.e. results of measurements of known signals) to processing map in an optimum way.

The work shows that the proper allowance for invariance can significantly simplify the solutions both for the problem of synthesis of optimal measurement computer system and for the calibration problem.

Najet Arous, Noureddine Ellouze

Self-Organizing Map Based on Different Metrics for Phoneme Recognition

Topic: 9.2

Any recognition system involve measures of distance, such systems are based on acoustic measures. We are interested in self-organizing map (SOM) for phoneme recognition. SOM is based only on the minimal distance to update its prototype vectors. In spite that input space is particular we focus in this paper on the study of SOM by means of different acoustic metrics. We conclude that the knowledge on the perception should also be useful to define metrics.

Dorra Ben Ayed, Noureddine Ellouze

Fuzzy C-Means Clustering for Phoneme Classification in Continuous Speech

Topic: 9.2

Fuzzy logic allows effective decision making in the presence of uncertainty. Classifying speech phoneme, even in ideal environment, is a complex task filled with uncertainty The speech waveform is nonlinear and variant, removing the possibility of simple analysis. the presented work focus on speech fuzzy clustering based on fuzzy C-means algorithm applied to phoneme classification. The developed classifier provides good classification rate. The speech database used is the DARPA TIMIT acoustic-phonetic continuous speech corpus.

Claudia Landi, Patrizio Frosini, Massimo Ferri

Geometrically Invariant Image Recognition by Size Functions

Topic: 9.2

Size functions are a mathematical transform for shape description. It is well known that it is possible to impose invariance properties to size functions. This is important in image analysis, where one studies shape properties independently of object appearance due to geometric transformations. So far, search of invariant size functions was not organized. Here we present 2-parameter families of size functions allowing recognition of closed contours up to scale transformation, rigid motions and similarities, respectively.

Maxim V. Shamolin

Pattern Recognition in the Model of the Interaction of a Rigid Body with a Resisting Medium

Topic: 9.2

In this work, we touch upon some qualitative questions of the theory of ordinary differential equations are arising in manufacturing of a rigid body interacting with a resisting medium in a jet flow under the assumptions of quasi-stationarity.

We shall review such problems as a bifurcation of the occurrence of the limit cycle from a weak focus, the existence of the so-called monotonic limit cycles, the existence of closed trajectories contractible to a point along two-dimensional surfaces, the existence of closed trajectories not contractible to a point along a phase cylinder, qualitative problems of the theory of topographical Poincare systems and more general systems for comparison with dynamical systems on a plane, the existence and uniqueness of trajectories which have infinitely remote points as limit sets for systems on a plane, elements of the qualitative theory of monotonic vector fields, and the existence of long-period trajectories stable in the Poisson sense. New families of the phase portraits and the cases of integrability in dynamics of a rigid body interacting with a medium are obtained.

Anders Vestbo, Ulrich Frankenfeld, Dieter Rohrich, Bernhard Skaali

Fast Pattern Recognition in Heavy Ion Experiments

Topic: 9.2

Real-time pattern recognition of tracking detectors in heavy ion experiments are key tasks in the operation of such experiments. In the ALICE-experiment at the upcoming LHC about 20,000 particles per interaction each produce about 100 clusters in the detectors. These signals have to be readout, processed, recognized and grouped into track segments within a time budget of about 5 milliseconds. An algorithm for fast pattern recognition using the adaptive generalized Hough transform will be presented.

3.10 Engineering Design

Dejan Bojovic

Fractional-Order Convergence Rates Estimates for Difference Method on non-Uniform Mesh

Topic: 10.0

In this paper we show how the theory of interpolation of function spaces can be used to establish convergence rate estimates for finite different schemes on non-uniform meshes. As a model problem we consider the first boundary value problem for the Poisson equation. We assume that the solution of the problem belongs to the Sobolev space. Using the interpolation theory we construct a fractional-order convergence rate estimate which is consistent with the smoothness of data.

Marc-Olivier Czarnecki

Asymptotic control and stabilization of nonlinear oscillators with non isolated equilibria

Topic: 10.0

Let $\Phi : H \to \mathbb{R}$ be a $\mathcal{C}^1$ function on a real Hilbert space H and let $\gamma > 0$ be a positive (damping) parameter. For any control function $\varepsilon : \mathbb{R}_+ \to \mathbb{R}_+$ which tends to zero as $t \to +\infty$, we study the asymptotic behavior of the trajectories of the damped nonlinear oscillator

$$(HBFC) \quad \ddot{x}(t) + \gamma\dot{x}(t) + \nabla\Phi(x(t)) + \varepsilon(t)x(t) = 0.$$

We show that, if $\varepsilon(t)$ does not tend to zero too rapidly as $t \to +\infty$, then the term $\varepsilon(t)x(t)$ asymptotically acts as a Tikhonov regularization, which forces the trajectories to converge to a particular equilibrium. Indeed, in the main result of this paper, it is established that, when Φ is convex and $S = \arg\min \Phi \neq \emptyset$, under the key assumption that ε is a "slow" control, i.e., $\int_0^{+\infty} \varepsilon(t)dt = +\infty$, then each trajectory of the $(HBFC)$ system strongly converges, as $t \to +\infty$, to the element of minimal norm of the closed convex set S. As an application, we consider the damped wave equation with Neumann boundary condition

$$\begin{cases} u_{tt} + \gamma u_t - \Delta u + \varepsilon(t)u(t) & = & 0 & \text{in} & \Omega \times \mathbb{R}_+, \\ \dfrac{\partial u}{\partial \mathbf{n}} & = & 0 & \text{on} & \partial\Omega \times \mathbb{R}_+. \end{cases}$$

Boris Epstein

Accuracy and Robustness of Flow Computations in Engineering Design of Air Vehicles

Topic: 10.0

Numerical flow simulation is used in engineering design prior to wind-tunnel and flight tests. High accuracy solutions for the Navier-Stokes equations are needed in order to attain realistic estimates of the aerodynamic coefficients. In a transonic regime high-order methods are often unstable and the robust low-order methods are insufficiently accurate.

In the present method, a low-order scheme is employed for multigrid relaxation in combination with a higher order scheme which supplies a correction to the discrete equations in the way ensuring the overall accuracy and robustness of the solution. The application to the aircraft design problems is discussed and compared with other methods.

Decan Ivanovic, Viktor Saljnikov

On PDE Analysis of Unsteady Incompressible MHD Boundary Layer on Porous Contour and its Application in Laminar-Turbulent Transition

Topic: 10.0

The MHD boundary layer theory has a significant place in the development of the magnetic hydrodynamics. The results of this theory have a wide application in technical practice, especially in nuclear reactors, MHD-generators, as well as in different devices in chemical technology etc.

We shall discuss the behaviour of a boundary layer in the presence of a positive or negative pressure gradient along the surface, which is particularly important for the calculation of the drag on as well as for the understanding of the processes which take in a diffuser, because there is transition from laminar to turbulent flow which determines the dividing line between a region with low drag and one where drag is dramatically increased. So one can control laminar-turbulent transition by fluid which has been injected or ejected through the porous contour or by use the magnetic field. Apart from skin friction we are interested in knowing whether the boundary layer will separate under given circumstances and if so, we shall wish to determine the point of separation. As the present time these very complicated phenomena are far from being understood completely but there are in existence several methods of calculation which lead to comparatively satisfactory results.

In this paper, the unsteady plane MHD boundary layer on a porous surface, has been studied. The fluid, flowing past the surface, is incompressible and its electroconductivity is constant. The present magnetic field is homogenous and perpendicular to the surface and through the porous contour also in perpendicular direction, the fluid of the same properties as incompressible fluid in basic flow, has been injected or ejected with velocity who is a function of the contour longitudinal coordinate and time. In order to study this problem, a polyparametric method known as generalized similarity method has been established.

The corresponding equations of this unsteady boundary layer, by introducing the appropriate variable transformations, momentum and energy equations and three similarity parameters sets, being transformed into so-called universal, i.e. generalized form. These parameters are expressing the influence of the outer flow velocity, the injection or ejection velocity, magnetic induction and the flow history in boundary layer, on the boundary layer characteristics. The numerical integration of the universal equation with boundary conditions has been performed by means of the difference schemes and by using Tridiagonal Algorithm Method with iterations in the four parametric and twice localized approximation, where the first unsteady, dynamic, magnetic and porous parameters will remain, while all others will be let to be equal to zero, and where the derivatives with respect to the first porous and magnetic parameters will be considered equal to zero. The obtained results can be used in the withdrawing of general conclusions on the development of boundary layer model and in the calculation of particular problems. A part of the obtained results is given in the form of diagrams from which one can see that the unsteady parameter has a significant influence on the friction distribution and especially on the location of separation point, ie. laminar-turbulent transition, of the MHD boundary layer. When this parameter is increasing the friction magnitude is increasing and the separation point location is removing toward the greater absolute values of the negative dynamic parameter. It means, that the positive local acceleration leads to the postponing of the separation of the MHD boundary layer in the diffuser region. The local deceleration favors the occurring of the separation of flow: in comparison with the steady flow, the separation is occurring at lower absolute values of the negative dynamic parameter. Also, for both in confuser and in diffuser regions as well as for both the accelerating and decelerating flows, the ejection of fluid increases the friction and postpones the separation of boundary layer, and vice versa the injection of fluid reduces the friction and favours the separation of flow. Magnetic field, for both acceleration and deceleration of flow, and for both injection and ejection of the fluid, increases the friction and postpones the separation of boundary layer.

A. Konrad Juethner

The hp-Discontinuous Galerkin FEM Applied to Transient Heat Diffusion Problems

Topic: 10.0

This thesis discusses the application of the hp-Discontinuous Galerkin algorithm for transient heat diffusion problems. The presentation will touch on strong and weak formulations of the heat diffusion equation. Furthermore, approximation spaces and convergence characteristics are discussed. Several exact solutions are used to investigate the convergence behavior and efficiency of several finite difference and finite element methods. Separately, spatial and temporal error control methodologies are investigated and demonstrated. For this purpose, custom software code was written in Matlab(R) to demonstrate the practical application for one- and two-dimensional transient problems. It is shown that the hp-Discontinuous Galerkin method converges exponentially. The superior convergence of this method is likely to find application in the time domain of many technical challenges.

Andris Möller

Robust Optimal Distillation Control with Stochastic Inflow Rate

Topic: 10.0

We will consider a feed tank coupled with a distillation system where the inflow rate to the feed tank is stochastic. The aim is to determine a control which is not only energy minimal but also fulfills the stochastic feed tank level constraints with a given probability. For this reason probabilistic constraints will be applied to two different models for the inflow profile. Numerical results will be reported.

Andreas Muench, Andrea Bertozzi, Michael Shearer, Xavier Fanton, Anne-Marie Cazabat, Kevin Zumbrun

Stability of Marangoni-Driven Thin Films

Topic: 10.0

This talk deals with the mathematical modelling and investigation of an experiment, where a film of silicon oil climbs a silicon wafer under the action of a temperature induced Marangoni shear stress. At certain ranges of inclination angles, this film gives rise to undercompressive shock profiles. We develop a theory to explain the unusual experiments, and compare it to the experimental results.

Tadeusz Nadzieja

Steady States for Energy-Transport Models of a Cloud of Self-Gravitating Particles

Topic: 10.0

We study the steady states of energy-transport models which describe the evolution of the density and temperature of a cloud of self-gravitating particles. These models extend the classical drift-diffusion systems of parabolic-elliptic equations for self-interacting charged particles (Nernst-Planck-Debye-Huckel models in electrolytes, semiconductors and plasma physics).

Mohammed Seaid, Axel Klar

Relevant Applications of Relaxation Methods for Unsteady Incompressible Flow Problems

Topic: 10.0

We present an overview of some unsteady incompressible flow problems where relaxation methods can offer attractive attributes to yield a procedure for either viscous or inviscous flows.

Numerical investigations are carried out on Euler and Navier-Stokes equations and these relaxation methods also made it possible to compute laminar flow at high Reylonds number as well as on refined grid at a reasonable cost.

Amandos Souranchyiev

Optimal Control of Steam Injection in Oil Extraction

Topic: 10.0

It was considered the boundary optimal control problem of the one-dimensional 3-phases non-isothermal filtration process governed by Baklee-Leverett equations. It was taken the algorithm of design of optimal pressure on the bound of domain which minimize the given cost functional.

Miodrag M. Spalevic

A Method of Constructing of Quadrature Formulae with Multiple Nodes

Topic: 10.0

As is well known the problem of finding the extremal nodes reduces to a nonlinear system of equations, described firstly by L. Tschakaloff about 50 years ago. The standard numerical methods have failed in the numerical treatment of this particular system. So, the construction of an appropriate algorithm became a challenge in the field of numerical integration. We propose a stable numerical procedure for solving the system.

Barbara Wagner, Andrea Bertozzi, Laurens Howle

Controlled Rayleigh-Benard Convection

Topic: 10.0

We consider the problem of active control of Rayleigh-Benard convection via shadowgraphic measurements. We consider the nonlinear dynamics of the system, both in the case of negative feedback (suppression of convection) and positive feedback, near the critical value of the gain, and show via numerical simulation, linear and weakly nonlinear stability analysis, that a simple reduced Galerkin model can capture much of the dynamics.

Martin Weiser, Peter Deuflhard

Central Path Methods for Optimal Control Problems

Topic: 10.0

The talk advocates a unified approach to optimal control problems combining ideas of direct and indirect methods. Our approach is based on the complementarity formulation of IP methods in infinite dimensional function space. A nested reduction of mesh size and duality gap parameter is realized via an adaptive multilevel scheme used for continuation along the central path.

The effectivity of the method is documented by the successful solution of the intricate windshear problem.

Gunilla Wikstrom, Per-Åke Wedin

Error Propagation for Linear Least Squares Studied with the Singular Value Decomposition

Topic: 10.0

Discrete inverse problems often result in linear least squares problems, $Ax \approx b$, e.g. overdetermined, underdetermined or rank-deficient. The singular value decomposition of A can then be used to investigate how changes in both matrix A (New results!) and vector b affect the solution x. For many problems of this type the condition number may be large even if the solution is insensitive to realistic perturbations in A and b and our proposed experimental error analysis should then be preferable.

Yuri Menshikov

Inverse Problem for Stream of Liquid with Free Surface

Topic: 10.1

The problem of profile of bottom definition by stream of ideal liquid by help the experimental measurements of free surface profile was considered this paper. The problem was reduced to solution of linear integral equation of first kind with kernal which is defined in terms of improper integral. By natural assumptions about properties of solution the initial problem belongs to the class of ill-posed problems. The Tichonov regularization was used for obtain the stable approximate solution with application of special mathematical models of researched process. The parameters of this mathematical models have been find. The test calculation was executed. This problem is actual and important for sea research and for check of submarines motion.

Hans-Görg Roos

Layer Adapted Meshes for Heat Transfer Problems in Flows

Topic: 10.1

The transfer of heat in a flow is described by a linear convection-diffusion equation, which is often convection dominated. Analytically the problem is a singular perturbation problem with strong parabolic boundary layers. Therefore it is natural to use layer adapted meshes for the discretization.

We discuss the question to prove optimal robust error estimates as well for finite difference as for finite element methods. (so far there is a strong gap between the existing theory and the convergence rate observed in numerical experiments)

Emine Can Baran, Afet Golayoglu Fatullayev

Determination of an Unknown Source Parameter in Two-Dimensional Heat Equation

Topic: 10.2

Numerical procedure for the solution of an inverse problem of determining unknown source parameter in heat equation is considered. In [1] by introducing some transformation this problem is written in the canonical, suitable form for the finite difference solution. In [2] we apply another method to the solution of same problem which based on the trace type functional (TTF) formulation of a problem. In [2] these two different procedures are studied and their comparison analysis is presented. Results observed indicated that method presented in [1] is more stable. On the other hand method based on TTF formulation is more effective on the solution of some problems and less sensitive to artificial errors than method presented in [1]. In this paper we examine the method based on TTF formulation to the solution of same problem in two-dimensional case.

1. J.R. Cannon, Y. Lin, S. Xu, Numerical procedures for determination of an unknown coefficient in semi-linear parabolic differential equation. Inverse problems, 10(1994)227-243.

2. A. Fatullayev, E. Can, Numerical procedures for determining unknown source parameter in parabolic equations. Mathematics and Computers in Simulation, 54(2000)159-167.

Roderick Melnik

Modelling Dynamics of Coupled Electromechanical Systems Embedded into Acoustic Fluid Media: Aspects of Numerical Approximation

Topic: 10.2

This paper is devoted to modelling issues of electromechanical systems embedded into fluid media. We consider the case where both the coupling between elastic and electric fields of such systems and matching conditions between acoustic media with different properties are important in describing the dynamics of such systems. Effective numerical procedures are discussed and results of numerical experiments are presented.

Marcus Meyer, Hermann G. Matthies

Model Reduction Applied to the Aeroelastic Response of Wind Turbines

Topic: 10.2

To gain a high degree of accuracy in dynamic aeroelastic simulations, it is desirable to keep detailed models of the interacting subsystems during computation. But in repeated long-term simulations model reduction is essential to improve computing efficiency. We describe a projection-based model reduction of the nonlinear systems of equations. After comparing different choices of bases we will describe the application of dual-weighted-residual method to select proper basis vectors and nonlinear/postprocessed Galerkin method to increase the accuracy of the simulation.

3.11 Miscellaneous

Farid Ablayev, Aida Gainutdinova

On Computational Power of Quantum Branching Programs

Topic: 11.0

Quantum computations became intesively growing research area in the last decade. We would like to refer to a famous Shor result [1]. The model of classical Branching programs is well known in Practical and Theoretical Computer science [2]. In the talk we introduce a model of a Quantum Branching Program (QBP) and study its computational power. We define several natural restrictions of a general QBP model, such as a read-once and a read-k-times QBP, noting that *obliviousness* is inherent in a quantum nature of such programs.

In particular we show that any Boolean function can be computed deterministically (*exactly*) by a read-once QBP in width $O(2^n)$, contrary to the analogous situation for quantum finite automata. Further we display certain symmetric Boolean function which is computable by a read-once QBP with $O(\log n)$ width, which requires a width $\Omega(n)$ on any deterministic read-once BP and (classical) randomized read-once BP with permanent transitions in each levels.

We present a general lower bound for the width of read-once QBPs, showing that the upper bound for the considered symmetric function is almost tight.

1. P. Shor, Polynomial-time algorithms for prime factorization and discrete logarithms on a quantum computer, *SIAM J. on Computing*, 26(5), (1997), 1484-1509.
2. I. Wegener, Branching Programs and Binary Decision Diagrams - Theory and Applications, the SIAM Monograph in Discrete Mathematics and Its Applications, (2000).

I.V. Boikov

The Optimal with Respect to Accuracy and Complexity Algorithms of Solution of Weakly Singular Integral Equations

Topic: 11.0

Discussed optimal with respect to accuracy and complexity algorithms of solution of many-dimensional weakly singular integral equations

$$Kx \equiv x - Tx \equiv x(t) - \int_G h(t,\tau)x(\tau)d\tau = f(t), t, \tau \in G, \quad (1)$$

where $G \in R^l$ is the open bounded domain. There G is the square $G = \{t = (t_1, \ldots, t_l) \in R^l : -1 < t_i < 1, i = 1, 2, \ldots, l\}, t = (t_1, \ldots, t_l), \tau = (\tau_1, \ldots, \tau_l)$.

Let $\alpha = (\alpha_1, \ldots, \alpha_l), \beta = (\beta_1, \ldots, \beta_l)$ be mult-indexes with $\alpha_i, \beta_i \geq 0, \mid \alpha \mid = \alpha_1 + \cdots + \alpha_l$,
$D_x^\alpha = (\partial/\partial x_1)^{\alpha_1} \cdot \ldots \cdot (\partial/\partial x_l)^{\alpha_l}, D_{x+y}^\beta = (\partial/\partial x_1 + \partial/\partial y_1)^{\beta_1} \cdot \ldots \cdot (\partial/\partial x_l + \partial/\partial y_l)^{\beta_l}$.

The kernal $h(t,\tau)$ on the set $(D \times D) \setminus t = \tau$ has continuous derivatives $D_t^\alpha D_\tau^\beta h(t,\tau)$ $(\mid \alpha \mid + \mid \beta \mid) \leq m)$ to the order m $(m \geq 1)$ and exists a real number v that for the function $H(t,\tau) = \mid D_t^\alpha D_{t+\tau}^\beta h(t,\tau) \mid$
$(\mid \alpha \mid + \mid \beta \mid \leq m)$ the inequality

$$H(t,\tau) \leq C \begin{cases} 1 + \mid t-\tau \mid^{-v-|\alpha|}, & v + \mid \alpha \mid \neq 0, \\ 1 + \mid \log \mid t-\tau \mid\mid, & v + \mid \alpha \mid = 0. \end{cases}$$

occur.

The mechanical quadrature method for equation (1) was constructed. It was proved it optimality.

Alla Boikova

Approximation Methods of Calculation of Hypersingular Integrals and Their Applications to Transformer of Potential Fields.

Topic: 11.0

This paper is devoted to one interpolation method and its applications to calculation of integral transformers. In basis of this method is put the approximation of functions by interpolated polynomials, fundamental functions of which are characteristic functions of integral operators.

Let us consider the set of orthonormal polynomials $P_n(x)$ with some weight $p(x)$ of degree n. Denote by $\mu_k(k = 0, 1, 2, \ldots, n)$ the nodes of polynomial $P_{n+1}(x)$.

The polynomial

$$L_n f = \sum_{k=0}^{n} \frac{1}{\gamma_k} \sum_{i=0}^{n} P_i(\mu_k) P_i(\mu) f(\mu_k), \qquad \gamma_k = \sum_{l=0}^{n} P_l^2(\mu_k)$$

is interpolated polynomial of degree n interpolating function $f(\mu)$ on nodes $\mu_k(k = 0, 1, \ldots, n)$ of polynomial $P_{n+1}(\mu)$.

These polynomials and their applications to calculation of singular and hypersingular integrals were investigated in [1]. Their application to solution of singular integral equations and hypersingular integral equations was investigated in [2].

In this paper these interpolation polynomials are applied for calculation of transformers of potential fields.

These transformers are discribed expressions as

$$\int_{-\infty}^{\infty} \frac{f(\tau)}{\tau - t} d\tau,$$

$$\int_{-\infty}^{\infty} \frac{f(\tau)}{(\tau - t)^2} d\tau.$$

There are given the estimation of error of offered approximate methods of potential fields transformes.

References

1. A. Boikova, Methods for the approximate calculation of the Hadamard integral and solution of integral equations with Hadamard integrals. In the book Integral methods in science and engineering, Volume 2, (editors C. Constanda, J. Saranen, S. Seikkala) 1997. P. 59-63.

2. A. Boikova, An order one approximate method of solution of differential and integral equations In the book Integral methods in science and engineering, (editors B. Bertram, C. Constanda and A. Struthers) 1999. P. 73-79.

Ana Carpio

Wavefront Depinning Transitions in Discrete-Reaction Diffusion Systems

Topic: 11.0

Spatially discrete systems describe physical reality in many fields: propagation of nerve impulses along myelinated fibers, motion of dislocations in crystals...

A distinctive feature of discrete systems is wavefront pinning: below a certain critical value of a control parameter, fronts fail to propagate. We present a theory of wavefront depinning in one-dimensional discrete systems yielding critical parameter values, speed and shape of wavefronts. Propagating wavefronts lose continuity at the critical parameter value and become stationary.

Michael Dymkov

Feedback Control for Repetitive 2D Processes

Topic: 11.0

This paper introduces a general model of discrete and continuous-discrete 2D repetitive processes of both system theoretic and applications interest. The main efforts are concentrated on the developments of mature of optimization theory for relevant subclasses of these models. The obtained results yield a theoretical background for the design problem of optimal controllers for relevant basis processes. Some areas for short to medium term further research are also briefly discussed.

Boris Khoromskij, Wolfgang Hackbusch, Markus Melenk

Efficient Approximation to the Poincaré-Steklov Operators on Complicated Geometries

Topic: 11.0

We consider iterative methods of the linear-logarithmic complexity for efficient FE approximation to the Poincaré-Steklov operators associated with 2D elliptic equations on Lipschitz domains. The method is based on the *hp*-version of FEM using special geometric mesh by refinement towards the boundary [2].

The fast iterative solution process includes the construction of efficient, spectrally close (additive Schwarz type) preconditioner.

Preconditioning to the Schur-complement matrix on the boundary (mixed or Neumann boundary conditions) is based on the diagonal scaling or on the $\mathcal{H}$-matrix approximation on graded meshes [1]. In the case of constant coefficients, we also discuss the *h*-version of the refined interface method [3].

Finally, we present numerical results.

[1] W. Hackbusch and B.N. Khoromskij. *$\mathcal{H}$-Matrix Approximation on Graded Meshes.* The Mathematics of Finite Elements and Applications X, MAFELAP 1999, J.R. Whiteman (ed), Elsevier, Amsterdam, Chapter 19, 307-316, 2000.

[2] B.N. Khoromskij and J.M. Melenk. *Generalized Boundary Element Methods.* Preprint MPI Leipzig, 2001.

[3] B.N. Khoromskij. *On the fast computations with the inverse to harmonic potential operators via*

domain decomposition, J. Numer. Lin. Alg. with Applications, v. 3(2), 91-111 (1996).

Anastasia Kolodko, Karl Sabelfeld

Stochastic Lagrangian Method for Solving Spatially Inhomogeneous Smoluchowski Equation.

Topic: 11.0

The problem of numerical construction of solutions to spatially inhomogeneous Smoluchowski equation is treated by stochastic approach.

A stochastic variant of Lagrangian trajectories technique is suggested, based on solving the homogeneous equations along Lagrangian trajectories, governed by stochastic differential equations. The method provides an effective numerical algorithm. We analyse the relations between the Lagrangian and the Eulerian solutions.

Aziz Madrane, A. Madrane, P. Arminjon, A. Stcyr

High Resolution Non-Oscillatory Staggered Lax-Friedrichs Type Scheme for 3-D Flows on Unstructured Grids

Topic: 11.0

We present a 3D finite volume generalization of the 1-dimensional Lax-Friedrichs and Nessyahu-Tadmor schemes for hyperbolic equations on unstructured tetrahedral grids. The non-oscillatory central difference scheme of Nessyahu and Tadmor, in which the resolution of the Riemann problem at the cell interfaces is by-passed thanks to the use of the staggered Lax-Friedrichs scheme, is extended here to a two-step, three-dimensional non-oscillatory centered scheme in finite volume formulation. Piecewise linear cell interpolants using Venkatakrishnan's limiter combined with diverse techniques to estimate the gradients lead to a non-oscillatory spatial resolution of order 2. Numerical results for a linear advection problem with continuous initial conditions in 3D show the accuracy and stability of the method. We also include results for the 3D Euler system.

Markus Melenk, Barbara Wohlmuth

A Fully Adaptive Algorithm for hp-Finite Element Methods

Topic: 11.0

In the hp-version of the finite element method (hp-FEM), convergence can be achieved either through mesh refinement or by increasing the approximation order. In the hp-version of the finite element method (hp-FEM), convergence can be achieved either through mesh refinement or by increasing the approximation order. We present an hp-adaptive algorithm where the decision whether to perform h-refinement or p-enrichment is based on the local convergence history. The algorithm is based on local residual-based error indicators. Reliability of the error estimator is proved; the efficiency constant of the error estimator is O(p). p-enrichment is based on the local convergence history. The algorithm is based on local residual-based error indicators. Reliability of the error estimator is proved; the efficiency constant of the error estimator is O(p).

Reinhard Nabben

Algebraic Theory of Domain Decomposition Methods

Topic: 11.0

Domain decomposition methods are widely used for solving partial differential equations. The principal advantages include enhancement of parallelism and a localized treatment. But these advantages can also be used to solve other problems.

Strongly connected with domain decomposition methods are the multiplicative and additive Schwarz-type methods for solving linear systems. Here we present an algebraic theory which gives a number of new convergence results. The algebraic analysis presented complements the analysis usually done on these methods using Sobolov spaces. The effect on convergence of algorithmic parameters such as the number of subdomains, the amount of overlap, the result of inexact local solves and of coarse grid corrections (global coarse solves) is analyzed in an algebraic setting. Moreover we give convergence results for the so-called 'restricted' Schwarz methods. These methods are widely used in practice and are the default preconditioner in the PETSc software package.

Daniela Nikolova-Popova, Eugene Plotkin

Matrix Equations in Linear Groups

Topic: 11.0

It is a well known fact that a finite group is nilpotent iff it satisfies an Engel law of some length. The subject of our recent research has been to establish a similar characterization for finite soluble groups. It is sufficient to check the problem on two-generated subgroups. For this purpose a sequence of two-variable commutator formulae are investigated (Conjecture of B.I. Plotkin).

The solubility is checked by examining a counter-example of least possible order, i.e. to show that in minimal simple groups there are no such identities. Thus, we solve equations in matrix groups, especially for the generic case G = PSL(2,p).

There is a strong evidence that Plotkin's conjecture is true. We give some results by computer calculations using GAP and formulate some conjectures.

The solution of such equations is connected with some well-known problems in finite matrix groups, as for example the Ore conjecture.

Similar result was obtained for finitely dimensional Lie algebras by E.B. Plotkin and B. Kunyavski

Antje Noack, Ch. Grossmann, R. Vanselow

Numerical Effects Caused by Reduced Regularity in the Boundary Control of Parabolic Systems

Topic: 11.0

Parabolic problems with piecewise constant boundary controls arising e.g. in discretized optimal control problems governed by evolution equations naturally lead to solutions with reduced regularity. We study piecewise constant Dirichlet controls which result in dramatically refined grids if step size procedures are applied. In the spatial 1D case a prestructuring of the state into the explicitly given response to the discontinuity and a solution of a more regular parabolic problem can be used to improve the discretization technique.

George Osipenko

Calculation of Structural Characteristics of Dynamical Systems

Topic: 11.0

The evolution of complex dynamic systems is determined by structure of locally maximal invariant sets and their characteristics, such as Lyapunov exponents, the Morse Spectrum, the Conley Index, the topological entropy and dimension. Methods of applied symbolic dynamics, which gives an opportunity to obtain and information about the qualitative behavior of a system without any preliminary information about the system, are considered. These methods are based on the synthesis of theoretical results and computer-oriented algorithms for the qualitative studying of dynamic systems. A dynamical system is associated with a directive graph called the symbolic image, which is an approximation of this system. Valuable information about the system may come from analysis of the symbolic image. In particular, the mentioned characteristics can be found.

Abedallah Rababah

Transformation of Chebyshev-Bernstein Polynomial Basis

Topic: 11.0

The Bernstein polynomials have been studied extensively, and there is a fair amount of literature on these bases. They possess important properties like partition of unity, having a recursion formula, besides their importance for the development of Bézier curves and surfaces in Computer Aided Geometric Design.

On the other hand the fact that they are not orthogonal turns out to their disadvantage in the use in the least-squares approximation, and thus the calculations performed in obtaining the least-squares approximation polynomial of degree n do not reduce the calculations to obtain the least-squares approximation polynomial of degree $n+1$.

The Chebyshev polynomials of first kind $T_n(u)$ are orthogonal on [0,1] with respect to the weight function $w(u) = \frac{1}{\sqrt{4u-4u^2}}$. In this paper we derive the matrix of transformation of Chebyshev polynomials of first kind into Bernstein polynomials and vice versa. We study also the stability of these linear maps and show that the Chebyshev-Bernstein basis conversion is remarkably well-conditioned, allowing one to combine the superior least-squares performance of Chebyshev series with the geometrical insight of the Bernstein form. We also compare it to other basis transformations such as Bernstein-Hermite, power-Hermite, and Bernstein-Legendre basis transformations.

Victor Shutyaev

Control Operators and Iterative Algorithms in Variational Data Assimilation

Topic: 11.0

The data assimilation problems are formulated as optimal control problems for the models governed by quasilinear evolution equation with the aim to identify the initial data and/or the right-hand-side functions of the original equation. The properties of the control operators are studied. The solvability of linear and nonlinear data assimilation problems in specific functional spaces is proved. The iterative algorithms for solving the data assimilation problems are formulated and justified, the convergence rate estimates are derived. Numerical examples for applications are presented.

Nijole Simeliene

Optimization Strategies for Optimization Procedures

Topic: 11.0

New theory of circle patterns (or packing) is now well developed. We present a new approach concerned with a theory of discrete multistage optimization. Mathematical model is investigated in which control variables are described by a sequence of nonnegative variables $u^i_{1,k}$. The process under consideration, including the most popular models, can be nested within the following dynamics:

$$\frac{u^{i+1}_{1,k} - u^i_{1,k}}{\frac{R^i}{R^{i+1}} + 1} = k^i.$$

Finally the stochastic properties of systems defined this way will be investigated.

Marko Vrdoljak

Optimal Design for the Principal Eigenvalue of Stationary Diffusion Problems

Topic: 11.0

The optimal design problem for the first (principal) eigenvalue associated to the stationary diffusion equation with symmetric matrix of coefficients (or the elasticity system) was considered by many authors. In the case of nonsymmetric coefficients, that is addressed here, applied techniques are of little use. We describe the behaviour of the principal eigenvalue in the homogenisation process, leading to relaxation. The Harnack inequality and the Krein-Rutman theorem are crucial for the proof.

Yousef Zahaykah, M. Lukáčová-Medvidová, G. Warnecke

On Evolution Galerkin Methods for the Multi-Dimensional Wave Equation System
Topic: 11.0

The subject of the paper is the development of evolution Galerkin schemes for the multidimensional wave equation system. The aim is to construct a method which takes into account better the infinitely many directions of propagation of waves. To do this the initial function is evolved using the characteristic cone and then projected onto a finite element space. We apply this technique to two and to three dimensional wave equation system with continuous and discontinuous initial data using periodical and radial boundary conditions respectively. We study numerically the stability of these two dimensional evolution Galerkin schemes. Numerical examples are given to compare between the new method and other existing methods.

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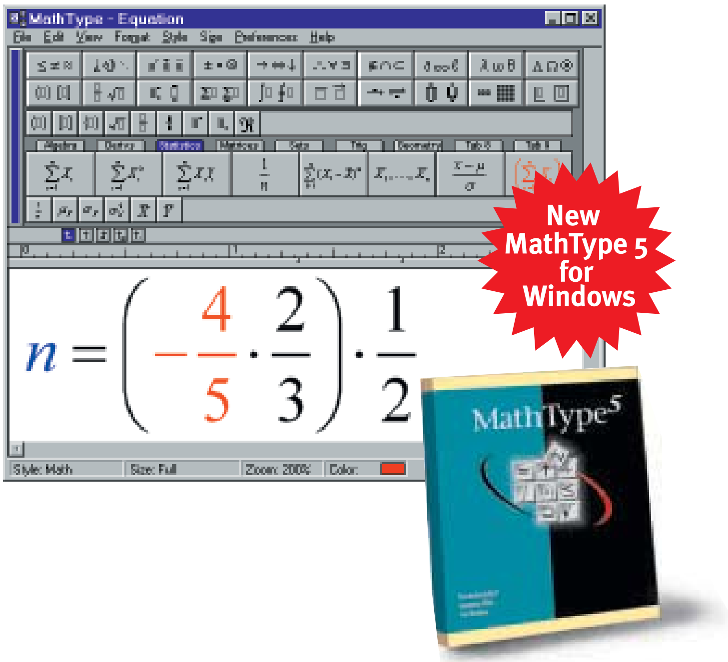

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4 Abstracts of Poster Session

4.1 Medicine

Philipp G. Batchelor, Derek L.G. Hill, Dave Atkinson

Reconstruction of Tensor and Vector Data from Diffusion Tensor MRI.

Topic: 1.1

Diffusion Tensor MRI provides images which are interpreted as samples of a quadratic form in different directions. Skare et al, JMR 147,340-352(2000) ran a downhill simplex minimisation of the condition of the associated system. They found a minimum of 1.32 for every number N of directions they tried (N=6,10,20,30,40). We investigate this further, we show that the limit of the condition number when N goes to infinity (uniform directions) is 1.5811.

Stefan Henn, Kristian Witsch

An Inverse Problem In Digital Image Matching With Application To Human Brains

Topic: 1.1

We consider an inverse problem for digital image matching with application to medical imaging. This yields a nonlinear ill conditioned inverse problem. A Tikhonov regularization method is considered to rule out discontinuous and irregular solutions. An important problem is a proper choice of the regularization parameter. For the practical choice of the parameter we use iterative regularization methods based on nonlinear multigrid techniques.To obtain a suitable initial guess, we use an approach similar to the full multigrid approach.

Marius Lysaker, Arvid Lundervold, Xue-Cheng Tai, Michael Bock, Lothar Schad

Noise Removal with Tissue Boundary Preservation

Topic: 1.1

A partial differential equation of 4th order is used to remove noise from MR images. We are trying to get a new image that has the same noise level but with a smallest norm for the second order derivatives. This minimization problem is solved by a Lagrangian technique in connection with finite difference approximation. The algorithm smooths out noise in homogenous tissue region and in the same time preserve boundary tissue.

Emiliana Ursianu

Mathematical Modelling of Epidemic Spreading

Topic: 1.6

The inference about parameters are made in ANOVA model with errors generated by a first order autoregressive process when the data are collected sequentially in time. The existing autocorrelation in process made impracticable the classical Shewhart X-bar control chart. The efficiency of the fixed (FSI) versus variable (VSI) sampling intervals is investigated employing their lengths ratio and some recommendation on the advantages of VSI. An example of epidemic spreading is given.

4.2 Biotechnology

Billie Sandak, A. Brandt

Fast Multiscale Electrostatics of Long Range Charge and Dipolar Interactions

Topic: 2.0

We present a multiscale algorithm for solving the N-body problem of the fast summation of long range interactions. Namely, the rapid evaluation of the electrostatic potential and energy induced in homogeneous and heterogeneous *point-charge* and *dipolar* systems. We have achieved this using *linear* complexity of $O(N)$. This means that although we are summing $O(N^2)$ Coulombic interactions, the execution time grows only linearly with the number N of particles. This approach is beneficial to large-scale problems such as molecular statics and dynamics, equilibrium statistics (Monte-Carlo simulations), molecular docking, and bioinformatics. It is also advantageous for calculation of moving particles.

Billie Sandak, R. Nussinov, H.J. Wolfson

Biomolecular Structural Recognition and Docking Allowing Conformational Flexibility

Topic: 2.0

A key problem in rational drug design and in biomolecular structural recognition is the generation of binding modes between molecules, also known as *molecular docking*. Here we present our generic docking method which allows it flexible hinge induced motions to exist either in the receptor (e.g., enzyme) or ligand (e.g., drug). Our method is capable of handling molecules of diverse sizes (e.g., from 20 to 3000 atoms), obtaining *fast* running times. By gearing our method to database screening it may also facilitate in lead discovery. The generality of our approach can also be used in the search for hinge-bent motifs aiding in protein folding.

Francisco Torrens

Fractal Dimension of Transdermal-Delivery Drug Models

Topic: 2.2

The fractal dimension D is calculated for a series of phenyl alcohols as models for transdermal-delivery drugs. TOPO is used for the calculation of the solvent-accessible surface AS. D is calculated from the dependence of AS on the solvent molecular radius. The results agree with reference calculations (Kantola et al.). The linear correlations between D, Q and log_P point to the ability to predict and tailor drug properties.

4.3 Materials Science

Liliana Emilia Bejan

Phenomenological Fracture Using Invariants of the Eigenvectors of Woven Composite
Topic: 3.0
The Kelvin formulation of the linear Hooke's law allow construction of the eigentensor for the anisotropic symmetries.The eigentensors are significant because they identify preferred modes of deformation associated with particular anisotropic elastic symmetries.The invariants of eigentensors was used in the reformulation of failure criteria of woven composite materials.

Pavel Bondarev

An Approach to the Porous Piezocomposites Simulation by the Homogenization and FEM
Topic: 3.1
Last years the porous piezocomposites have begun to receive broad appeal in biomedicine, acoustic and NDT applications. Because of high heterogeneity of concerned composites it is impossible to simulate the effective properties of such materials directly as analytically as numerically, especially for 3D case. The Homogenization and FEM are used for the problem. The Homogenization method connects the averaged macroparameters of the representative composite volume with coordinate distributions of microparameters that are calculated by FEM.

Vladyslav Danishevs'kyy, Dieter Weichert, Igor Andrianov

Asymptotic Evaluation of Effective Elastic Moduli of Periodical Composite Materials
Topic: 3.1
We propose a new asymptotic procedure for effective elastic moduli of periodical composite materials. We start with asymptotic expansions by ratios of elastic constants. Then we use homogenization method. Cell problems are solved by consequent application of self-consistent scheme, perturbation technique and two-point Pade approximants. As illustrative examples we consider fibre-reinforced composites. Approximate analytical formulas for effective moduli are derived. In some cases our procedure allows establishing direct analogy between effective elastic and transport properties.

Leela Rakesh, Stanley Hirschi, Sonia Ramirez

Rheological Modeling of Conductive Polymeric Material
Topic: 3.1
Electrorheological (ER) fluids undergo a rapid reversible transition resulting in development of a yield stress and increased viscosity by the application of electrical fields. The project involves modeling the rheology of such conductive (thermal and electrical) materials. These materials tend to be highly filled and require specific flow characteristics for success in the marketplace. Present pap would be an attempt in the theoretical impact of filler size, shape, treatment and loading on the rheology of silicone based systems.

Alexander Alshin, M.O. Korpusov, Yu.D. Pletner, A.G. Sveshnikov

Sobolev Equations as Mathematical Models of Processes in Mediums with a non-Isotropic Dispersion
Topic: 3.1
The main aim of our investigation is the problem of reduction of vectorial mathematical models for a wide set of physical processes in ferromagnetics and antiferromagnetics, plasma in magnetic field etc. to initial-boundary value problems for sufficiently uniform scalar high order PDE of composite type. By means of theory of dynamical potentials the classical unique solvability of constructed scalar models was proved.

The asymptotic behavior at large time for explicit solutions of some initial-boundary value problems were considered. The method for proving the unique solvability of the problem with moving boundaries based on the parametric prolongation of solution was constructed.

4.4 Environmental Science

Peter Kirkegaard, Leif Kristensen

A Nonlinear Integral Equation for Two-Particle Dispersion
Topic: 4.0
A model is described for neutrally buoyant particles suspended in a fluid in which the turbulence is stationary and isotropic. By using Gaussian statistics we show how this model can predict the 2-particle variance $\mathrm{d}^2(t)$ at any time t by solving a symmetric 2D nonlinear integral equation system

$$\psi(\theta',\theta'') = f(\theta') + f(\theta'') - \int_0^{\theta'} \mathrm{d}\vartheta' \int_0^{\theta''} \mathrm{d}\vartheta'' \rho_{\mathrm{L2}}(\vartheta',\vartheta'')$$

$$\rho_{\mathrm{L2}}(\theta',\theta'') = f''(\theta''-\theta') + \frac{3}{2}\alpha_1 \times$$

$$\int_0^\infty \frac{\exp(-\mu|\theta''-\theta'|s)}{s^2}\Big\{\exp(-\psi(\theta',\theta'')s^3)\cos(\Delta_\circ s^{\frac{3}{2}}) -$$

$$\exp(-f(\theta''-\theta')s^3)\Big\}\mathrm{d}s$$

for ψ with $(\theta',\theta'') \in [0,\infty)\times[0,\infty)$. Asymptotic properties of the model are studied and numerical procedures outlined.

Kristian Witsch, Stefan Henn

Multigrid Methods For An Inverse Problem To Determine Atmospheric Motion Vectors

Topic: 4.2

Winds estimated from the tracking of clouds in satellite image sequences is an important data source for numerical weather prediction. We describe an algorithm for determining optical flow based on variational and partial differential equation (PDE) methods to calculate the wind direction and velocity. This yields a nonlinear ill-posed inverse problem, which is solved by a Landweber iteration. Multigrid methods are used to speed up the solution process.

Elena Alshina, N.N. Kalitkin, I.A. Sokolova

Effective Method for Estimating Pollutants Concentrations in Burning Flows

Topic: 4.3

Simulating of viscous chemical-reacting flows through channel with variable cross section and curved wall is important for many scientific and applied problems, partially for estimating concentrations of pollutants in the environment. Numerical investigations of 2D and 3D equations while taking into account tens different chemical species and hundred chemical kinetic reactions is very hard and labor-consuming computation problem. The system of a chemical kinetics is the stiff one and requires special methods for solution. New effective numerical method based on quasi-one-dimensional model of smooth channel and stiff method of lines is constructed by authors. Numerical results prove the efficiency of this approach.

Pavel Bortnikov

Model of Heavy Meal Migration in the System

Topic: 4.3

Dynamic of metal concentration (Zn, Pb, Cu, Cd) in surface water of tailings ponds is the subject of investigation. Computer simulations were carried out for three ponds located in the Kemerovo region (Russia) where tailings of sulfide ore are stored. Factors rendering the most influence on surface water quality were considered during simulations. They are: confluent, outflow, atmospheric precipitation, evaporation, convective and molecular diffuse of solutions, autodestraction, sedimentation.

4.5 Nanoscale Technology

Ramon Escobedo, Luis L. Bonilla, F. J. Higuera

Recycling and Motion of Axisymmetric Electric Field Domains in Bulk Semiconductors

Topic: 5.2

We have solved numerically the Kroemer drift-diffusion model for the Gunn effect in a circular (Corbino) disk with a circular cathode at its center and an outer circular anode at its boundary. Axisymmetric pulses of the electric field are periodically shed by the cathode when the dc voltage bias between contacts surpasses a certain onset. These waves decay as they advance towards the anode, which they may not reach. Meanwhile the current continuously increases and then abruptly decreases when a new wave is shed. The resulting periodic oscillation of the current has frequencies in the microwave range. Depending on the bias, more complex patterns with multiple shedding of pulses at the cathode are possible. The numerical results are interpreted by means of an asymptotic analysis based on the assumption of a small ratio of the pulse width to the disk radius. Our results explain existing experiments on two dimensional geometries.

4.7 Traffic

Luis Margalho, Carla Fidalgo, Maria do Céu Amorim Faulhaber

Pedestrian Crossings and Speed Control Systems

Topic: 7.0

Traffic intensity can be dangerous for pedestrians due to their exposure on public roads. Foot travelers include important characteristics such as reduced speed, vulnerability and dependence upon given environmental conditions surrounding them. For these reasons, they are considered to be the most susceptible users. Definitions of different kinds of pedestrian crossings, as well as criterion followed in some countries for the chosen of the typology of these same crossings will be presented. A comparative description of the operation of semaphorical systems will also be given. Finally, the effectiveness of one of these systems for the city of Coimbra, Portugal will be analysed. Key-words: Pedestrian Crossings, Semaphorical Systems.

Eliodor Constantinescu

Container Control in Liner Shipping

Topic: 7.1

This paper develops a mathematical model capable of dealing with container leasing, purchasing, stocking and allocation so as to yield the least cost solutions for both container capital investment decisions (size of container stock) and routine operating decisions (allocation of empty containers) under a variety of plausible patterns.

The models present the process of container control in a typical liner shipping company. Several special container loading problems such as selecting one container from several alternatives, weight balance and variable container length are addressed. The modifications to the general model needed for these situations are also provided. Numerical examples are illustrated to validate the models.

Sanja Marusic

Boundary Layers and Boundary Conditions for the LWR Model

Topic: 7.3

We study the boundary conditions of the BLN type for the standard LWR model for the traffic flow. In the context of traffic flow the BLN conditions have some natural interpretation. We introduce the BLN conditions using two approaches: the method of characteristics and the boundary layer theory for the vanishing viscosity method. We discuss the conditions on density and on the flow and their meaning in real-life situations.

Joanne Morgan

A Comparison of Macroscopic Models for Motorway Traffic

Topic: 7.3

Deterministic fluid based models are non linear differential equations with flux functions which may be nonconvex and require numerical solution. The schemes applied to these models need to be capable of capturing shocks and are often of conservative upwind type. Here, we discuss the Lighthill-Whitham-Richards model with different velocity functions, the Payne-Whitham model and the more recent Aw-Rascle model. The numerical results are compared to averaged data from a section of a UK motorway with no on/off ramps.

4.8 Market and Finance

Mark Leidman, R. Pocs, Ye. Tsarkov

Stochastic Analysis of Marshall-Samuelson Market

Topic: 8.0

The paper deals with an adaptive single-component market, taking into account no linearity of demand, time delay in supply and permanent random perturbations of elasticity functions. Our approach is based on stochastic calculus and asymptotic methods of bifurcation theory. It allows not only to advance in price equilibrium stability analysis, but also to detect a price stochastic business cycle and to prove that time delay of supply exerts significant influence on market price dynamics.

Mehdi Ahmadinia, Vadim Shmyrev, Maxim Osadchii

Leasing Payments Optimization by Complementary Variables

Topic: 8.1

The specific class of optimization problems arising from modeling of leasing in view of taxation and budget constraints of parties to a contract is investigated. Initial problem of leasing payments optimization is reduced to linear programming problem with additional condition of complementarity of assigned pairs of variables characterizing lessor's profit and losses. It was shown that the problem admits solution by means of linear programming.

Maria Emília Bigotte De Almeida, Maria do Céu Barbosa

A Combinatorial Optimization Application in Statistical Disclosure Control of Microdata

Topic: 8.1

In this Information Age critical activities of society are fuelled by data. Users of statistical data rely especially upon government statistical agencies to collect reliable data and disseminate it in a timely and broadly useful way. As a standard practice statistical agencies do not release microdata but rather provide the public with various forms of aggregate totals (tabular data) from their surveys. As a result, only a fraction of the potential utility of the collected respondent data is made available to the public. Statistical Disclosure Control of microdata concerns the different methodologies of modification of the original microdata in ways that the confidentiality of the respondent data is not compromised. Microaggregation, one of these methods, consists in grouping records from the microdata according to some notion of similarity and creating a new set of microaggregates whose records are group averages of the original microdata. In this talk we formalize the microaggregation problem as a (new) combinatorial optimization problem, show that for some parameter values it is polynomial solvable and provide numerical experiments that show the effectiveness of some heuristics and optimization methods.

Marek Niezgoda

Applications of Normal Decomposition Systems

Topic: 8.1

Normal decomposition systems (NDS) play a unifying role in many problems of statistics, probability, matrix theory, Lie theory and optimization. The first idea comes from Lewis (1996, 2000) who employed NDS to study some problems of optimization and programming. In the paper the author gives a unified treatment of majorization inequalities for linear maps using NDS. Necessary and sufficient conditions are given for inequalities to hold. Some classical inequalities regarding eigenvalues and singular values of a matrix are deduced in this way.

Raúl Tempone, T. Bj

Monte Carlo Euler Approximation of HJM Term Structure Financial Models

Topic: 8.1

We present two Monte Carlo Euler methods for the HJM term structure model, based on Itó stochastic differential equations in infinite dimensional spaces, and prove error estimates. These error estimates can be used to identify different error contributions arising from time and maturity discretization as well as the statistical error due to finite sampling. Due to the structure of the HJM models considered here, our sharp error estimates require just a small extra computational work.

4.10 Engineering Design

Thomas Viklands, Per-Åke Wedin

Computing Rigid Body Movement by Global Minimization of a Penrose Regression Problem

Topic: 10.0

Consider the least squares problem (Penrose) $\min |f(M) - b|_2^2$ where $f(M)$ is a linear function and M is a 3×3 rotation matrix. This problem appears in many applications related to rigid body movement. Generally it has several local minima. We give an algorithm that computes a global minimum by using ellipses on the surface $f(M)$.

Juan Delgado-Romero, E. Hernandez-Morales, R. S. Gonzalez-Garza

Robustness Analysis of Systems: Other Application Conditions

Topic: 10.2

In this work we describe some application conditions to guarantee robust stability of electric and electronic circuits represented by a linear time invariant system with parametric uncertainty. An interval matrix is used to give the parametric uncertainty. The principal motivation of this work is given by the existence of dynamic systems with parametric uncertainty in their models. We know the stability of a continuous linear time invariant systems is given only by A matrix, if the system contains parametric uncertainty, then A can be an interval matrix. In this work we give practical conditions to guarantee the robust stability and some examples to show the application.

Toshiaki Itoh

Coherent Sheaf Condition for Conservative Algebraic Finite Difference Equations

Topic: 10.2

Integrable and conservative properties for finite difference equation are treated by algebraic geometrically. Here coherent sheaf condition for difference equation is introduced. By this condition we can judge conservative property of the difference equation algebraically, in spite of its solution function is analytic object.

Albert Seidl, Peter Richter

Mathematical Models for Locksmithing Problems

Topic: 10.3

A mechanical master key system realizes access control to a building. The system-function is coded by mechanical means using key-cuts and cylinder fillings. The objective of this paper is to clarify different aspects of the problem by offering alternative mathematical descriptions: (1) A relational model. (2) A description as an integer nonlinear programming problem for a simple case. (3) A problem-description using the notation of coding theory.

4.11 Miscellaneous

Florica Aldea

Some remarks of the surjectivity results of Kasahara

Topic: 11.0

In this paper we present a new formulation and proof of the surjectivity theorem of Kasahara. Also, some consequences of this theorem are given.

Natalia Chinchaladze

Vibration of Cusped Shells

Topic: 11.0

The main purpose of this paper is to study the IBVP for elastic cusped prismatic shell type bodies. In cusped edges all unknown quantities are defined as the corresponding limits. From this definition follows that on the cusped edges admissible are only 4 type boundary conditions. IBVP can be reduced to the integro-differential equation with symmetric kernel. The solution of this problem can be written as infinite series, whose convergence is proved.

Natalia Chinchaladze

Some Contact Problems for Solid-Fluid Interaction

Topic: 11.0

We investigate transmission conditions between a three-dimensional fluid part and a solid part of prismatic cusped shell shell type, based on the classical bending theory of plates. Proposing angle between the outward normal to the plate and axis$(0x_3)$ sufficient small, and plate is thin, we can assume that:

- Fluid occupies the whole space but the middle plane(Ω) of the plate;
- Geometry of the solid along thickness is taken into account in the coefficients of the bending equation;
- Transmission conditions we can be transferred at appropriate points of Ω.

Emmanuel Degryse, Mottelet, Stephane

Shape Optimization of Sensors/Actuators for the Control of Feedback Systems

Topic: 11.0

In this work, we focus on the optimal design of piezoelectric sensors and actuators for the control of plates.

First, a new criterion for designing non-collocated sensors and actuators is derived and then reformulated as a shape optimization problem for which we will give some theoretical and numerical results. We will also compute low-order controllers for the resulting system: the closed-loop behavior show that our approach is very promising.

Vitalie Geru, Vladimir Zolotarevsky

Approximate Solution of Some Classes of Integral Equations on Vandermonde Nodes
Topic: 11.0
Interpolation of function on Vandermonde nodes are studied. The estimations for the approximate of complex variable functions by Lagrange interpolate polynomials on these nodes are obtained. The case when the nodes are situated on the unitary circle of complex plane is examined. These results are applied for theoretical justification of approximate methods for some classes of integral equations.

Frank Hülsemann

Hierarchical Hybrid Grids: A Grid Framework for High Performance Computation
Topic: 11.0
Grid based methods for PDEs such as finite elements lead to sparse linear algebraic systems, which often dominate the overall computational effort. A novel grid framework for iterative linear solvers is presented that combines the flexibility of unstructured grids with the high performance of structured ones. Experiments on a variety of computer architectures demonstrate the potential of the approach. The framework is very flexible and not limited to any particular type of PDE.

Carlos E. Mejia, Carlos D. Acosta

On Regularization by Discrete Mollification
Topic: 11.0
We present a definition of discrete mollification which works with a nonsymmetric kernel and two different procedures for the automatic selection of mollification parameters, with no knowledge of the amount of noise in the data required. The new version of discrete mollification satisfies standard consistency and stability estimates which are illustrated by numerical experiments. For the application of discrete mollification to differentiation, we improved some known stability estimates.

Kyoung-Sook Moon, Anders Szepessy, Raúl Tempone, Georgios E. Zouraris

Adaptive Algorithms for Deterministic and Stochastic Differential Equations
Topic: 11.0
An adaptive algorithm for approximation of ordinary differential equations including dividing and merging of time steps is proven to stop with the optimal number of steps up to a problem independent factor. Furthermore, the global error is proven to be asymptotically bounded by the specified error tolerance.

Similar results are proven for weak approximation of Itó stochastic differential equations.

Peter Petek

Periodic Points in Quaternionic Dynamics
Topic: 11.0
For a specific choice of the parameter in quaternionic quadratic family, there is an invariant circle, carrying periodic points. These are connected to periodic points in the complex plane by curves of a given periodic itinerary. Topologically, these curves can be circles or double spirals. It is interesting to observe the bifurcation that interchanges them.

Mirjana Stojanovic

Generalized Solutions to Semilinear Parabolic Equations with Non-Lipschitz Nonlinearity and Singular Initial Data
Topic: 11.0
We consider Cauchy problem for semilinear parabolic equation

$$\partial_t u - \delta u + g(u) = 0,\ t > 0,\ x \in \mathbf{R}^n,$$

$g(u) \in L^1_{loc}(\mathbf{R}^n)$ and does not satisfy Lipschitz condition and the initial data are strongly singular (e.g. $u(0,\cdot) = \mu \in \mathcal{M}^k(\mathbf{R}^n) \subset \mathcal{D}(\mathbf{R}^n)$, $k \in \mathbf{Z}_+$. We find special regularization to g (cut-off method of regularization) and another kind of regularization to initial data (convolution with delta sequences) to obtain existence and uniqueness results in Colombeau algebra of generalized functions. The same results holds for semilinear parabolic equation with conservative nonlinear term

$$\partial_t u - \delta u + \partial_x \vec{g}(u) = 0,\ t > 0,\ x \in \mathbf{R}^n,$$

$$u(0) = D^k\psi, ; \psi \in L^p(\mathbf{R}^n),\ 1 \le p \le \infty.$$

If $p = 1$, $\psi \in \mathcal{M}(\mathbf{R}^n)$ is the space of Radon measures.

Nenad Teofanov, Srboljub Simic

Approximate Solutions of Biharmonic Equation Using Wavelet Subspaces
Topic: 11.0
Variational method unifies many diverse branches of science, leading to new theoretical results and powerful methods of calculation. The inverse variational problem is to find an equivalent variational formulation of the previously formulated boundary-value problem for operator equations. In this presentation we show that a sequence of wavelet subspaces could be successfully used in order to find an approximate solution of a problem of an equilibrium of an elastic half-plane with a continuously distributed force on its boundary.

5 Authors

References to invited talks are bold, to mini symposia talks italic. If the author is the speaker the page number is underlined.