E. Applications

5.1 Chemistry

Organizer : Iannis G. Kevrekidis

Key note lecture

New Chemistry and Mathematics

Alexander Mikhailov
Fritz-Haber-Institut der MPG, Berlin
email: mikhailov@fhi-berlin.mpg.de

Chemistry has changed and mathematics plays now an important role in this discipline. Chemical systems provide paradigmatic examples of nonlinear pattern formation described by reaction-diffusion models. Recent experimental developments in heterogeneous catalysis and biochemistry show that in some important cases one must go beyond this class of models. Chemical reactions in soft matter are coupled to structural phase transitions in such condensed systems and physical interactions between reacting particles should therefore be incorporated into a model. Enzymes and other proteins of a living cell form a network of molecular machines whose collective dynamics can show coherence and mutual synchronization, similar to the behaviour found in large populations of coupled nonlinear oscillators.

Invited lectures

Parity breaking bifurcations in reaction-diffusion systems with nonlocal coupling

Markus Bär
Max-Planck-Institut für Physik komplexer Systeme
Nöthnitzer Str. 38, 01187 Dresden, Germany
email: baer@mpipks-dresden.mpg.de

We study two component activator-inhibitor reaction-diffusion models with nonlocal coupling. It can be viewed either as a simple model of a pattern forming chemical reaction subject to a feedback with an intrinsic length scale (range of the nonlocal coupling) or as a limit case for a model describing the interaction of a single activator species with two inhibitor species, one with slow and the other with fast reaction dynamics. The nonlocal coupling introduces the possibility of an oscillatory instability with finite wavenumber (wave bifurcation) in addition to the well known stationary bifurcation with finite wavenumber (Turing bifurcation) and an oscillatory instability with zero wavenumber. The linear stability analysis is performed and gives analytic criteria for the occurence of wave bifurcation as well as various codimension-2 bifurcations, out of which we focus on the simultaneous wave and Turing bifurcation.

Amplitude equations of Ginzburg-Landau type are derived for the codimension-2 Turing-wave point and enable us to predict the nonlinear behavior with respect to the appearance of traveling or standing waves and the competition of waves and Turing patterns. Under conditions of bistability of these structures, we observe a new type of pattern, cellular drifting states that represent a finite width inclusion of waves in a Turing pattern background that travels in the direction opposite to the constituting waves. This structures are unstable in the amplitude equations and appear only in a finite distance to the onset of pattern formation. The drifting states have been studied in detail by extensive numerical studies. Their structure is similar to phenomena occuring in experimental and theoretical studies of parity breaking instabilities in stationary cellular patterns. We compare our results to alternative approaches based on symmetry considerations. Further away from the wave or Turing bifurcation, the models exhibit bistable behavior including the parity breaking front bifurcations studied in pure reaction-diffusion systems. Thus, we have studied the transition from this regime of large amplitude localized coherent structures (pulses, fronts) to a regime closer to onset where periodic patterns described by amplitude equations appear. In the intermediate regime, complex traveling patterns and patches of periodic stationary patterns are observed.

Nano-scale Pattern Formation in Electrodissolution

Hsueh-Chia Chang
Department of Chemical Engineering, University of Notre Dame, Notre Dame, IN 46556 USA
email: `Hsueh-Chia.Chang.2@nd.edu`

We investigate the pattern formation dynamics of two important electrodissolution processes-electropolishing and anodization. Electropolishing is a century-old technology that exploits the stability of free-surface dissolution dynamics to smooth metal surfaces. An applied voltage is used to preferentially dissolve microscopic bumps on the metal surface in an electropolishing electrolyte. In contradiction to this old wisdom, our group discovered 5 years ago that electropolishing is actually unstable at submicron scales. More interestingly, using Atomic Force Micrography, this new instability is found to produce very regular hexagonal and stripe patterns beneath the hydrodynamic boundary layer. In the past three years, we have deciphered the electrochemical origin of this new free-surface instability and have derived a simple evolution equation for its dyanamics. Numerical simulation of the equation and bifurcation analyses of the resulting amplitude equations provide the windows of applied voltage and electrolyte concentrations when both regular patterns appear. They are in good quantitative agreement with our measured experimental data. We can potentially use these results to generate nanoscale self-assembly very cheaply.

Anodization is another electrodissolution process that involves the break down of a metal oxide layer under an applied voltage. It is the fundamental mechanism behind pitting corrosion of protective aluminum oxide layers–a major problem in pollution. We have formulated this free-surface problem into a fingering process. The eletric potential satifies the Laplace equation within a thin strip around the growing finger and nonlinear curvature-dependent boundary conditions at the strip boundary due to field-assisted dissolution and double-layer cuvature effects. Using matched asymptotics and numerical conformal mapping techniques, we obtained the critical voltage for the onset of fingering and the finger dimensions as functions of the electrolyte chemistry. The results are favorably compared to our experimental data. They allow us to determine when corrosion of a metal oxide layer occurs and the size of the resulting pits. We can also generate hexagonally arranged pits that, if properly shrunk in dimension, can be used to house quantum dots.

Mathematical issues in modeling chemically reacting systems

Iannis G. Kevrekidis
Department of Chemical Engineering and PACM, Princeton University

Raymond E. Goldstein
Department of Physics, University of Arizona

The research area of spatiotemporal dynamics in systems involving chemical mechanisms and their mathematical models (e.g. reaction-diffusion PDEs) is characterized by a fruitful interplay between mathematics and experimentation. The development of spatially and temporally resolved observation and analysis techniques, beyond model validation, provide constant motivation for exploring certain types of PDEs and their solutions. The purpose of this chapter is to chart this interaction, provide a summary of recent cases of cross-fertilization between chemistry and mathematics, and discuss future directions for this research area.

We start by discussing certain classical reaction-diffusion and reaction engineering paradigms (the chemistry involved in the BZ and related reactions as well as the chemistry of catalytic surface reactions like CO oxidation; the CSTR and the tubular reactor as well as reverse flow reactors). Certain elements of numerical techniques for the computer-assisted study of such models are also briefly reviewed.

We then proceed to discuss a number of current issues including

- pattern formation on inhomogeneous and anisotropic media (PDEs with spatially varying coefficients and issues of homogenization, both analytical and numerical);
- pattern formation in spatiotemporally forced systems (PDEs with spatiotemporally varying coefficients and their use in elucidating chemical and biochemical mechanisms);
- issues of local versus longer-range (up to global) interactions and their effect on reaction dynamics;
- complex geometry issues;
- dissipativity and its implications in low-dimensionality of the dynamics;
- the extraction of features (like fronts and pulses) and the derivation of asymptotic dynamic equations for their evolution;
- kinetically based models of reacting media and their dynamics;

- molecular level modeling of reaction dynamics and its real time observation;

We conclude by a discussion of current technological developments (ranging from the technology of microreactor fabrication to wavelet based “real-time” homogenization techniques and to issues of computational chemistry) which, we believe, will affect the way chemically reacting systems are modelled and analyzed in the near future.

Long-Time Dynamics of Dissipative PDEs with Applications to Reaction-Diffusion Systems

Edriss S. Titi
University of California - Irvine
email: `etiti@math.uci.edu`

In this talk we will discuss the long-time behavior of dissipative evolution PDEs, with emphasize on models of fluid flows and reaction-difussion systems. In particular, we will survey the results concerning determining degrees of freedom in such systems, such as determining modes and nodes, global attractors and invariant inertial manifolds. Later we will introduce a novel numerical method for integrating dissipative PDEs - the post-processing Galerkin method. We will present numerical experiments that will demonstrate the superiority, in computational efficiency, of this method in comparison to the standard Galerkin and nonlinear Galerkin methods. Finally, we will present a numerical criterion for designing a linear feed-back controller for stabilizing unstable steady states of parabolic dissipative equations including reaction-difussion systems.

Contributed talks

Existence and mass conservation for the coagulation-fragmentation equation

P.B. Dubovski
Institute of Numerical Mathematics, Russian Academy of Sciences
email: `dubovski@inm.ras.ru`

We prove existence theorem and reveal the cases when the coagulation-fragmentation equation possesses the mass conservation property. From physical point of view the mass conservation is usually treated as the absence of gel point.

References

[1] Dubovski P.B. and Stewart I.W., ”Existence, uniqueness and mass conservation for the coagulation-fragmentation equation,” *Math. Meth. Appl. Sci.*, **19**: 571–591 (1996).

The mathemetical model for the combined oxydational treatment of water with phosphorus-organical pesticidic contaminants

Ilya Gorenko
email: timur@akcecc.net

The scheme of free-radical reactions in water surroundings was proposed for a decomposition of organical contaminants under the combined treatment of ozone, UV and H_2O_2. A system of quadratic ordinary differential equations was built, which describes this system kinetics, an investigation of dynamics and characteristic of its peculiar points was installed. On basis of experimental data the problem of identification was stated and solved, also the problem of system optimal control was stated:

$$\frac{dc_i}{dt} = A_i c + c^T B_i c + U_i, \quad i = \overline{1,n}$$

$$J(U) = \sum_{l=1}^{k} \alpha_l c_l^2(T) \to \min U$$

$$\int_0^T U_2(t)dt = a, \quad \int_0^T U_3(t)dt = b,$$

$$c(0) = c_0.$$

- $c = (c_1, c_2, \ldots, c_n)^T$ -vector of substance's concentrations in water surrounding
- $A_i = (a_1 i, a_2 i, \ldots, a_n i)$ -coefficients vector for the linear part of kinetics differntial equation with number i
- B_i -the matrice of quadratic form, which describes the non-linear part of kinetics differential equation with number i
- $U = (0, U_2, U_3, 0, \ldots, 0)$-the control vector (we can only control concentrations of ozone and H_2O_2)
- $k, (k < n)$ -quantity of pollutants in water surrounding
- T -the final time point of oxydatinal process
- a -quantity of ozone
- b -quantity of H_2O_2
- c_0 - vector of starting conditions

The solving of optimal control problem was conducted by means of Hamilton-Pontryagin's method.

Kinetic scheme reduction in first order differential equation models

Sybille Handrock-Meyer
Technical University Chemnitz
email: Sybille.Handrock@mathematik.tu-chemnitz.de

Modelling reaction kinetics in a homogeneous medium usually leads to stiff systems of ordinary differential equations the dimension of which can be large. A well-known approach to reduce the dimension of such systems is the quasi-steady state assumption (QSSA): the derivative of fast variables is assumed to be zero. This procedure requires some knowledge of the underlying chemistry, moreover the corresponding differential system must be explicitely given. In this paper we shall describe and justify a procedure for a local reduction of the dimension of state space which does not require chemical insight as well as an explicit knowlegde of the system in a singularly perturbed form. The mathematical justification is based on the theory of invariant manifolds.

Continuation of Waves in Reaction-Diffusion-Convection Systems via Heteroclinic and Homoclinic Orbits

Milan Kubíček
Prague Institute of Chemical Technology
email: kubicek@vscht.cz

Numerical methods for tracking of homoclinic and heteroclinic orbits provide a powerful tool in analysing bifurcation problems of practical importance, such as a sudden appearance (or extinction) of large amplitude oscillations in stirred tank reactors or occurrence of travelling waves in tubular reactors. Typically, such methods are formulated as a special boundary value problem.

We formulate efficient methods for numerical tracking and continuation of homoclinic/heteroclinic orbits with a nonoscillatory approach to the steady state(s) in systems of ordinary differential equations. The method allows for studying waves in spatially one-dimensional systems upon the moving frame coordinate transformation. In the case of homoclinic orbits, the method provides velocity-parameter curves for solitary pulse waves. Tracking of heteroclinic orbits can be used for finding one-parameter families of front waves. A computer implementation of the methods included in a continuation program CONT is applied to two problems: the first one deals with pulse and front waves in a reaction-diffusion system and the second one focuses on shock waves in adsorption columns.

Posters

Bifurcations to mixed mode oscillations in chemical systems

Alexandra Milik
Technische Universität Wien
email: amilik@umbriel.tuwien.ac.at

Mixed mode oscillations consist of alternating large and small amplitude oscillations and are a common phenomenon in oscillatory chemical systems. To study this phenomenon I analyze an extended version of the Boissonade de Kepper model which is a three dimensional Van der Pol Duffing like oscillator and shares some qualitative properties with models derived by first principles from chemical mechanisms. The model is analyzed by means of geometric singular perturbation theory and an adapted version of Melnikov's method, which allows to derive approximating formulas for some of the codimension one and two bifurcation curves.

5.2 Chemotaxis, Cross-Diffusion and Blow-Up

Organizer : Angela Stevens

Invited lectures

On a reaction–diffusion system modelling chemotaxis

Herbert Gajewski
WIAS Berlin
email: gajewski@wias-berlin.de
Klaus Zacharias
WIAS Berlin
email: zacharias@wias-berlin.de

Chemotaxis as the oriented migration of organisms under the influence of chemical substances can be modelled by partial differential equations of reaction–diffusion type of the form

$$\frac{\partial U}{\partial t} = \Delta U - \chi \nabla \cdot (U \nabla V), \quad \frac{\partial V}{\partial t} = \alpha \Delta V - \beta V + \delta U.$$

Here U denotes the population density, V the density of the chemotactic agent. The system is considered for positive initial values U_0, V_0 under homogeneous Neumann conditions on $\mathbb{R}_+ \times \Omega$ where $\Omega \subset \mathbb{R}^2$ is a piecewise smooth domain; α, β, δ, χ are positive constants. The system has the Lyapunov function

$$F(U,V) = \int_\Omega \left\{ \frac{\chi}{2\delta} \left(\alpha |\nabla V|^2 + \beta V^2 \right) + U(\log U - \chi V) \right\} dx$$

i.e. this functional decays along solutions as time increases. If

$$\frac{\delta \chi \|U_0\|_{L_1}}{4 \alpha \Theta} < 1 \,,$$

where Θ is the smallest interior angle formed by the boundary curves of Ω, then the Lyapunov function remains bounded from below for all times. Under this smallness condition for the initial values there is a (possibly nontrivial) asymptotic state $(U^\star, V^\star)$. For large initial values the system can show blow–up.

References

[1] H. Gajewski, K. Zacharias. Global Behaviour of a Reaction–Diffusion System Modelling Chemotaxis. *Math. Nachrichten*, **195**: 77–114, (1998).

Hyperbolic Models For Chemotaxis

Thomas Hillen
Universität Tübingen
email: thomas.hillen@uni-tuebingen.de

Parabolic models for chemotaxis (e.g. Keller-Segel type models) are well known and widely studied in the literature. They describe experiments well but are under discussion for several reasons. First they allow for infinite speed of propagation; secondly the relevant parameters (motility and chemotactic sensitivity) are not directly related to the individual movement of the investigated species.

In this talk I will present hyperbolic models and transport equations for chemotaxis. The general transport model (Alt's equation [1]) is based on the individual movement of the particles, and the way they respond to external stimuli. I will present results on local and global existence of solutions of hyperbolic chemotaxis models in one dimension ([2], [3]). In the case of global existence, the asymptotic behavior of solutions is described by parabolic models (*parabolic limit*). Finally, some numerical simulations show interesting behavior like pattern formation and finite time blow up (see [2]) and the formation of shocks (see [3]).

The results on the 1-D model are joint work with Angela Stevens (Leipzig) and Christian Rohde (Freiburg).

References

[1] W. Alt. Biased random walk model for chemotaxis and related diffusion approximation. *J. Math. Biol.*, **9**:147-177, (1980).
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Behavior of Solutions to a System Related to Chemotaxis

Takasi Senba
Miyazaki University, Japan
email: t0f302u@cc.miyazaki-u.ac.jp

We will talk about blow-up of solutions of the following system related to chemotaxis

$$
\text{(KS)} \qquad \begin{cases} u_t = \nabla \cdot (\nabla u - \chi u \nabla v), & x \in \Omega,\ t > 0, \\ \tau v_t = \Delta v - \gamma v + \alpha u, & x \in \Omega,\ t > 0, \\ \dfrac{\partial u}{\partial n} = \dfrac{\partial v}{\partial n} = 0, & x \in \partial\Omega,\ t > 0, \\ u(\cdot, 0) = u_0, v(\cdot, 0) = v_0, & x \in \Omega. \end{cases}
$$

Here Ω is a bounded domain in $\mathbf{R}^2$ with smooth boundary $\partial\Omega$, χ, γ, α and τ are positive constants, and u_0 and v_0 are non-negative smooth functions on Ω.

There exists a unique solution (u, v) to (KS) defined on a maximal interval of existence $[0, T_{max})$, which is smooth in $x \in \overline{\Omega}$ and $0 < t < T_{max}$. If $u_0 \gneqq 0$ in Ω, the solution satisfies that $u(x,t) > 0$, $v(x,t) > 0$ for $(x,t) \in \Omega \times (0, T_{max})$(see [6]). If $T_{max} < \infty$, we can observe that $\lim_{t \nearrow T_{max}} \|u(\cdot,t)\|_{L^\infty(\Omega)} = \infty$, which we mean that the solution blows up in finite time.

We refer to the system (KS) as Keller-Segel model. Keller-Segel model is a classical model to describe the initiation of chemotactic aggregation of cellular slime molds. On the system (KS), the existence of the solutions has been studied by [1,2,6] and the blow-up of the solutions has been studied by [3].

Particularly, Herrero and Velázquez [3] constructed a radially symmetric solution with u which forms a delta function singularity in a finite time. Such a phenomenon is referred to as the chemotactic collapse.

We will talk about some results concerning the chemotactic collapse.

References

[1] P. Biler. Local and global solvability of some parabolic systems modeling chemotaxis. *Adv. Math. Sci. Appl.*, **8**:715–743, (1998).

[2] H. Gajewski and K. Zacharias. Global behaviour of a reaction-diffusion system modelling chemotaxis. *Math. Nachr.*, **195**:77–114, (1998).

[3] M. A. Herrero and J. J. L. Velázquez. A blow-up mechanism for a chemotaxis model. *Ann. Scuola Norm. Sup. Pisa IV*, **24**(4):633–683, (1997).

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Systems of Reaction Diffusion Equations Modelling Chemotaxis and Angiogenesis

B.D. Sleeman

Department of Applied Mathematics, University of Leeds, Leeds, LS2 9JT, UK

email: `bds@amstra.leeds.ac.uk`

In this paper we present a class of reaction diffusion equations based on the theory of reinforced random walks which are being developed to model problems of chemotaxis and tumour angiogenesis.

Results concerning local existence are presented together with a qualitative analysis of global existence and blow-up. We also present a class of exact similarity solutions.

Contributed talks

Numerical Blow-Up Time Convergence for Discretizations of Reaction-Diffusion Equations

Luis M. Abia
Dpto. de Matemática Aplicada y Computación, Facultad de Ciencias, Universidad de Valladolid, Valladolid, Spain
email: `abia@mac.cie.uva.es`

Juan C. López-Marcos
Dpto. de Matemática Aplicada y Computación, Facultad de Ciencias, Universidad de Valladolid, Valladolid, Spain
email: `lopezmar@mac.cie.uva.es`

Julia Martínez
Dpto. de Economía Aplicada (Matemáticas), Facultad de Ciencias Económicas y Empresariales, Universidad de Valladolid, Valladolid, Spain
email: `julia@esgueva.eco.uva.es`

Convergence of the numerical blow-up times of finite-difference discretizations on a uniform mesh of a $1D$ reaction-diffusion model is analyzed and special attention is devoted to symmetric solutions. Also nonsymmetric solutions are considered when the reaction term $f(u)$ is such that $f(0) = 0$. Sufficient conditions for blow-up in such discretizations are established and upper bounds of the blow-up time, which depend on the maximum norm of the initial conditions are provided. These results, although considering a simple situation of blow-up, extend similar ones by Chen [1] and contribute to a better understanding on how to approximate the blow-up time of solutions of reaction-diffusion equations [2].

References

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Some blowup results for the Keller-Segel model

Dirk Horstmann
Mathematisches Institut der Universität zu Köln
email: `dhorst@mi.uni-koeln.de`

In this talk we consider the so-called Keller-Segel model

$$\left.\begin{array}{rcll} a_t(x,t) & = & \nabla\cdot(\nabla a(x,t) - \chi a(x,t)\nabla c(x,t)), & x\in\Omega\subset\mathrm{IR}^2, \quad t>0 \\ c_t(x,t) & = & k_c\Delta c(x,t) - \gamma c(x,t) + \alpha a(x,t), & x\in\Omega, \quad t>0 \\ \partial a/\partial n & = & \partial c/\partial n \ = \ 0, & x\in\partial\Omega, \quad t>0 \\ a(0,x) & = & a_0(x), & x\in\Omega \\ c(0,x) & = & c_0(x), & x\in\Omega \end{array}\right\} \quad (1)$$

which has been introduced in [1] and [2]. We prove the existence of radialsymmetric initial data for which the solution of (1) blows up in finite or infinite time. For the proof we assume that Ω is a disk, $\gamma = 0$ and

$$\alpha\chi \int_\Omega a_0(x)dx > 8\pi k_c,$$

where $(\alpha\chi \int_\Omega a_0(x)dx)/k_c$ is not equal to a multiple of 8π.

In a second result we show that if the solution blows up in the nonsymmetric case, the blowup must happen at the boundary of Ω, provided that $\Omega \subset \mathbb{R}^2$ is a smooth domain and

$$8\pi k_c > \alpha\chi \int_\Omega a_0(x)dx > 4\pi k_c.$$

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Long-wave unstable thin film equations — blow-up and steady-states

M. C. Pugh
University of Pennsylvania
email: mpugh@math.upenn.edu
R. S. Laugesen
University of Illinois at Urbana-Champaign
email: laugesen@math.uiuc.edu
A. L. Bertozzi
Duke University
email: bertozzi@math.duke.edu

We consider long-wave unstable parabolic PDEs of the type

$$h_t = -(h^n h_{xxx})_x - B(h^m h_x)_x$$

where $B > 0$, and n and m are positive exponents. Such equations arise in modelling the flow of thin liquid films, driven motion in a Hele-Shaw cell, the aggregation of aphids, and models of Type-II superconductors.

Bertozzi and I conjectured that if $m < n + 2$ then solutions remain L^∞ bounded for all time, if $m \geq n + 2$ and $m \leq n/2$ the solutions can grow at most exponentially in time, and if both $m > n + 2$ and $m > n/2$ then there is initial data whose solution has L^∞ norm becoming infinite in finite time. We prove the subcritical case $m < n + 2$ and discuss a specific critical and super-critical case $n = 1$, $m \geq n + 2 = 3$.

Laugesen and I have classified a large class of nontrivial steady states of PDEs of the above type. Here, we present the steady states, analytical and numerical results on the linear and nonlinear stability of these steady states, and numerical simulations of the initial value problem.

References

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[2] "Properties of Steady States for Thin Film Equations" with R. S. Laugesen, to appear in EJAM.
[3] "Long-wave instabilities and saturation in thin film equations" with A. L. Bertozzi, CPAM 51(1998)625-661.

5.3 Industrial Applications

Organizer : Andreas Schuppert

Key note lecture

Dynamic Systems in Electronics Industry

Albert B. Gilg
Corporate Technology Dept., Siemens AG, ZT PP 2, D-81730 Munich, Germany
email: `Albert.Gilg@mchp.siemens.de`

Globalization in industrial competition speeds up an increase in systems complexity at reduced innovation cycle times. Systems modeling gained a key role in keeping pace in this race. Increasing system complexity therefore enforces to keep track with scaling-up problems of model evaluation algorithms. Furthermore it is still not possible to fully cover industrial systems analysis and design at abstraction levels describing systems dynamics by discrete modeling paradigms. This leads to a key challenge to deal with continuous models, typically modeled by sets of differential equations, tightly coupled within a discrete model environment, e.g. control structures. Another source of problems originates of top-down design methodologies, trying to design a system by small modifications of already existing designs or by combination from available modules and components. This enforces a component or block-based modeling concept leading to problems in dynamic systems analysis not yet satisfactorily solved. We discuss these core problems in a number of different electronic systems application fields of our company, e.g. microelectronics design, industrial plant design, automotive electronics and railway traffic applications.

Invited lectures

An Efficient Reduced SQP Strategy for Large-Scale Dynamic Process Optimization

Daniel Leineweber
Bayer AG, Leverkusen
email: `Daniel.Leineweber.DL@Bayer-AG.De`

Efficient and robust techniques for the optimization of dynamic chemical processes are presented. In particular, we address the solution of large, multistage optimal control and design optimization problems for processes which can be described by differential-algebraic equation (DAE) models of index one. A new simultaneous solution strategy – based on multiple shooting and partially reduced sequential quadratic programming (PRSQP) – has been developed to fully exploit the structure of large sparse DAE process models. Unlike other simultaneous strategies based on collocation, direct use is made of existing advanced, fully adaptive DAE solvers. Since the integrations on different multiple shooting intervals are completely decoupled, the approach lends itself well to parallel computation.

A practical implementation is provided within the modular optimal control package MUSCOD-II (Leineweber, 1999). The advanced BDF code DAESOL (Bauer *et al.*, 1997) is used for the efficient calculation of the required directional sensitivities. As a typical application, we discuss the optimization of a batch distillation process. This example involves a sparse nonlinear DAE model with several hundred states, leading to a nonlinear programming (NLP) problem with several thousand variables. It is shown that such problems can still be efficiently solved on a standard workstation using the simultaneous strategy presented. Hence optimization strategies of this type are expected to find widespread practical use in the near future.

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Mathematics in industry—the balance between science and economy?

Andreas Schuppert
Bayer AG
email: `ANDREAS.SCHUPPERT.AS@bayer-ag.de`

Although mathematical methods have a significant impact on industrial practice, the acceptance of mathematical science in industry is comparably poor. This is on the one side due to a lack in mathematical education of engineers and economists, on the other side there seems to be a gap between the structure of mathematical research and research and development structures in industry.

In this presentation on the example of mathematical applications in process industry it will be shown how the develpopment of mathematical methods and industrial R&D structures can be brought together.

The scope of the presentation is

- to clarify how R&D projects are structured in industry,
- to show how benefits of mathematical development can be estimated even in an economic sense

- to stimulate the discussion how to improve dynamical systems applications.

Contributed talks

Two-dimensional modelling of pollutant transport in a shallow basin

Moulay Mustapha Charafi
CRREE, LPEE, Groupe sédimentologie, Km7, routed'Eljadida, Casablanca, Morocco
email: `mcharafi@hotmail.com`

Abdelaziz Sadok
CRREE, LPEE, Group of sedimentology

Abdelaziz Kamal
CRREE, LPEE, Group of sedimentology, Morocco

Shallow basins are often used for treatment processes such a sedimentation, waste stabilisation, etc. In this paper, a two dimensional numerical model was developed to simulate the sediment and pollutant transport in a shallow basin. The developed model consists of two modules: Hydrodynamic module and sediment/pollutant transport module. A numerical hydrodynamic module based on the St-Venant equations, is resolved by a MacCormack numerical scheme and is used to simulate the circulation pattern in the basin. The obtained flow circulation is used as input to the sediment/pollutant transport module to simulate the transport and dispersion of a pollutant emitted into the basin. To calibrate the numerical model, the distorted scale model of the Windermere Basin (JIAN WU and TSANIS, 1994) was used. In this physical model, the flow visualisation and pollutant transport experiments provide a good calibration. The simulated results were found to be in good agreement with the experimental measurements and the JIAN WU results. With the aid of the validated model, the influence of the construction of dikes on the residence time distributions in the basin were examined.

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On the non-isothermal formation of polymeric fibers

Thomas Hagen
Department of Mathematics, The University of Wales, Aberystwyth, SY23 3BZ,UK
email: `toh@aber.ac.uk`
Michael Renardy
Department of Mathematics, Virginia Tech, Blacksburg, VA 24061-0123, USA
email: `renardym@math.vt.edu`

The focus of this presentation is the nonlinear hyperbolic system governing the one-dimensional formation of viscous or viscoelastic polymeric fibers under non-isothermal flow conditions ("melt-spinning"). Two issues will be discussed in detail (cf. references):

1. We will address the fundamental question of well-posedness of the system in the viscous and viscoelastic regime. The viscoelastic flow will be described through appropriate quasi-linear fluid models in differential form. The problem of well-posedness will be tackled through suitable energy methods.

2. We will furnish a rigorous proof that the stability of the steady-state solution for the linearized equations in the exemplary viscous regime is determined by the eigenvalues of the associated semigroup generator. Since the underlying equations are hyperbolic, this result has to precede any numerical resolution of the spectrum of the semigroup generator.

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Equality of two variable means: reduction to differential equations

László Losonczi
Department of Mathematics and Computer Sc., Kuwait University
email: `losonczi@math-1.sci.kuniv.edu.kw`

Let Φ be a strictly monotonic continuous function and F be a positive function on an interval I. Then for any $\mathbf{x} = (x_1, \ldots, x_n) \in I^n$ the quantity

$$M_{\Phi\, F}(\mathbf{x}) = \Phi^{-1}\left(\frac{\sum\limits_{i=1}^{n} \Phi(x_i)F(x_i)}{\sum\limits_{i=1}^{n} F(x_i)}\right)$$

lies between the maximum and minimum of the x_i's. It is called *quasiarithmetic mean weighted by the weightfunction F*. The equality problem for two such means:

$$M_{\Phi\, F}(\mathbf{x}) = M_{\Psi\, G}(\mathbf{x}) \quad (\mathbf{x} \in \mathbf{I^n})$$

was solved by Bajraktarević [1] if $n \geq 3$ is *fixed* and the functions are twice differentiable. Aczél and Daróczy [2] solved the same functional equation, assuming that $n\,(\geq 2)$ is *arbitrary* and the functions are continuous.

The aim of this paper is to solve the $n = 2$ *variable equality problem*, assuming, that the functions involved are *six times differentiable.*

We can easily rewrite this problem in the form

$$E(x,y) := \frac{\varphi(x)f(x)+\varphi(y)f(y)}{f(x)+f(y)} - \varphi\left(\frac{g(x)x+g(y)y}{g(x)+g(y)}\right) = 0 \quad (x,y \in J)$$

where $J = \{\Psi(x) \,:\, x \in I\}, g = G \circ \Psi^{-1}, f = F \circ \Psi^{-1}, \varphi = \Phi \circ \Psi^{-1}$. First we obtain a system of differential equations from $E_{xx}(x,x) = 0, E_{xxyy}(x,x) = 0, E_{xxxyyy}(x,x) = 0$ (here the subscripts denote partial derivatives, the first, third and fifth order derivatives of E do not give independent equations).

These derivatives were calculated by the software package MapleV. Eliminating from our system the functions g, f we end up with the equation

$$4U'''U^2 - 18UU'U'' + 15(U')^3 = 0$$

where $U(x) = 4\frac{\varphi'''(x)}{\varphi'(x)} - 6\left(\frac{\varphi''(x)}{\varphi'(x)}\right)^2$. Finding U is relatively simple. To determine φ we have to solve, among others, four Riccati equations. Then we can find g, f. The functions so obtained are also solutions of the functional equation, provided that we make suitable restrictions on their domains. The functional equation has 33 families of solutions and 32 of them are new, compared to the case $n \geq 3$.

References

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Non-Newtonian Fluids

Šárka Matušů -Nečasová

Mathematical Institute of Academy od Sciences,Žitná 25,11567 Prague 1,Czech Republic,

email: `matus@math.cas.cz, matusu@ math.utl.ist.pt`

The investigation of the motion of viscoelastic fluids has been largely studied by many authors but the rigorous mathematical analysis of compressible viscoelastic fluids has been only recently considered.There exists a proof of the existence of the slightly compressible fluids of the steady motion given by Talhouk [6] and the existence of classical solution of the steady motion of compressible viscoelastic fluids of White-Metzner type in a bounded domain was showed by Sy [5].

The aim of this lecture is to show the existence of classical solution of the steady motion of viscoelastic compressible fluids of Oldroyd type in an exterior domain. Further, the existence and asymptotic behaviour of steady motion of Maxwell compressible fluids will be shown as well as the existence of weak solution of the unsteady motion of Oldroyd type. This is a joint work with A.Sequeira, J.H. Videman, see [1–4].

References

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5.4 Mechanics

Organizers : Jerrold E. Marsden, Jürgen Scheurle

Key note lecture

Dynamical Systems, the Three Body Problem, and Space Mission Design.

Jerrold E. Marsden
Caltech
email: marsden@cds.caltech.edu

Wang-Sang Koon
Caltech
email: koon@cds.caltech.edu

Martin Lo
Jet Propulsion Laboratory
email: mwl@trantor.Jpl.Nasa.Gov

Shane Ross
Caltech
email: shane@cds.caltech.edu

This talk concerns the application of dynamical systems techniques to the problem of heteroclinic connections and resonance transitions in the planar circular restricted three-body problem. These related phenomena have been of concern for some time in topics such as the capture of comets and asteroids and with the design of trajectories for space missions such as the *Genesis Discovery Mission.*

The main new technical result reported on in this talk is the numerical proof of the existence of a heteroclinic connection between pairs of periodic orbits, one around the libration point L_1 and the other around L_2, with the two periodic orbits having the same energy. This result is applied to the resonance transition problem and to the explicit numerical construction of interesting orbits with prescribed itineraries.

The point of view developed is that the invariant manifold structures associated to L_1 and L_2 as well as the aforementioned heteroclinic connection are fundamental tools that can aid in understanding dynamical channels throughout the solar system as well as transport between the "interior" and "exterior" Hill's regions and other resonant phenomena.

Using these tools, a new technique for constructing missions, such as a petit grand tour of the moons of Jupiter will be given. Other issues such as the use of variational integration algorithms and optimal control techniques for low thrust missions will also be discussed.

Invited lectures

Quasi-Periodic Motions of the Perturbed Euler Top

Heinz Hanßmann
Institut für Reine und Angewandte Mathematik der RWTH Aachen
email: `Heinz@iram.rwth-aachen.de`

Let the (rotational) motion of a rigid body, fixed at one point, be perturbed by a weak external force field. A normal form approach yields an integrable approximation, and the 2-torus action induced by the unperturbed system allows to reduce to one degree of freedom. This reduced system describes the (approximate) motion of the angular momentum in space. In the same way that the domains of rotational and librational motions of the angular momentum are separated by stable and unstable manifolds of hyperbolic equilibria and shrink down to elliptic equilibria, the invariant 3-tori of the integrable approximation are organised by the invariant 2-tori. This extends to the Cantor families of persistent invariant tori of the original perturbed system.

The Hamiltonian structure of the dynamics of ideal liquid bridges

Hans-Peter Kruse
Zentrum Mathematik, TU München
email: `kruse@mathematik.tu-muenchen.de`

A *liquid bridge* is a fluid drop that is trapped between two plates. The state of the bridge is determined by the position of the free boundary Σ of the drop and its velocity field v. In [2] and [5] a Hamiltonian formulation was introduced for the dynamics of an ideal inviscid liquid bridge moving under the influence of surface tension and adhesion forces. In this model the contact lines of Σ with the two plates are allowed to move freely along the plates. The Hamiltonian formulation has been used in [3] to study the stability of rigidly rotating liquid bridges with cylindrical shape and bifurcations from the family of rotating liquid cylinders which occur upon variation of the angular velocity of the bridge or its angular momentum, respectively. In [1] a model is introduced to describe axisymmetric potential flow of ideal inviscid liquid bridges with *fixed* contact lines. In this talk we present a Hamiltonian formulation of the equations of motion of an ideal inviscid liquid bridge with fixed contact lines that moves under the influence of surface tension acting on its free boundary Σ. We do not assume that the velocity field of the fluid comes from a potential or that the velocity field is axisymmetric. The configuration space of the liquid bridge in the Lagrangian description has the structure of an infinite-dimensional Hilbert manifold (compare [4]). Using the methods of [3] and [6] we study the stability of rigidly rotating liquid bridges with respect to perturbations that fix the contact lines of the bridge and bifurcations from the family of rigidly rotating liquid cylinders.

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Singular relative normal modes for nonlinear Hamiltonian systems

Juan-Pablo Ortega
Département de Mathématiques, École Polytechnique Fédérale de Lausanne. CH 1015 Lausanne. Switzerland.
email: `Juan-Pablo.Ortega@epfl.ch`

An estimate on the number of relative periodic orbits around a relative equilibrium in a Hamiltonian system with continuous symmetry is given. This estimate depends in general on the topology of the singular reduced spaces, except for a few particular cases that are also analyzed.

Symmetric Hamiltonian Systems

Tudor S. Ratiu
Ecole Polytechnique Fédérale de Lausanne
email: `Tudor.Ratiu@epfl.ch`

Singular reduction tools to study the dynamics induced by a G–invariant Hamiltonian are introduced. Several local and global approaches to the reduction problem are presented and compared. The so–called *reconstruction equations* are discussed in order to provide a local picture of the equations that govern G–Hamiltonian dynamics.

References

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Relative Equilibria of Molecules

Mark Roberts
University of Warwick
email: mark@maths.warwick.ac.uk

This talk will describe joint work with Igor Kozin (Warwick) and Jonathan Tennyson (UCL) on the role that relative equilibria can play in the prediction and interpretation of molecular spectra. The presentation will concentrate on the example of the molecular ion H_3^+. The global relative equilibrium bifurcation diagram for this example will be described and 'harmonic' quantization and induced representation theory applied to predict how the energies and symmetries of the lowest lying quantum states change as angular momentum increases. A brief description of the possible spectral manifestations of Hamiltonian Hopf bifurcations of relative equilibria will also be given.

References

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Examples of Relative Equilibria

Jürgen Scheurle
University of Technology Munich
email: scheurle@mathematik.tu-muenchen.de

Analyzing the dynamics of a mechanical system usually starts with computing equilibria or, in other words, steady state solutions and studying their stability properties. If a system has symmetries in the sense that there exists a group of transformations in phase space under which the equations of motion are covariant, then the class of most basic solutions extends to so-called relative equilibria. The talk focuses on recent existence, stability and bifurcation results for relative equilibria of examples for both, dissipative and conservative mechanical systems.

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Contributed talks

On the influence of the kinetic energy on the stability of equilibria of natural Lagrangian systems

Maria Letizia Bertotti
Università degli Studi di Palermo - ITALY
email: `bertotti@dipmat.math.unipa.it`

Sergey V. Bolotin
Moscow State University - RUSSIA
email: `bolotin@mech.math.msu.su`

We consider natural Lagrangian systems (T, Π) on $\mathbb{R}^2$ described by the equation $\frac{d}{dt}\frac{\partial T}{\partial \dot{q}} - \frac{\partial T}{\partial q} = -\frac{\partial \Pi}{\partial q}$, where $T(q, \dot{q})$ is for all $q \in \mathbb{R}^2$ a positive definite quadratic form in $\dot{q}$ and $\Pi(q)$ has a critical point at 0. We are concerned with the question, whether the kinetic energy can influence the stability properties of the equilibrium 0. We show that there exist a C^∞ potential energy Π and two C^∞ kinetic energies T and $\widetilde{T}$ such that the equilibrium $q(t) \equiv 0$ is stable for the system (T, Π) and unstable for the system $(\widetilde{T}, \Pi)$. We conclude that for C^∞ natural systems the kinetic energy can influence the stability. In the analytic category this isn't true.

References

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On the stability of relative equilibria of tethered satellite systems

Martin Krupa
Technische Universität Wien
email: `krupa@umbriel.tuwien.ac.at`

Martin Schagerl
Technische Universität Wien
email: `martin.schagerl@tuwien.ac.at`

Alois Steindl
Technische Universität Wien
email: `alois.steindl@tuwien.ac.at`

Hans Troger
Technische Universität Wien
email: `hans.troger@tuwien.ac.at`

We consider the stability problem of the orbital motion of a system of two satellites joined by a flexible continuous elastic tether, which can have a length up to 100 km. The system moves under the action of the gravitational field of a perfectly spherical Earth

[1]. This stability problem is quite complicated, because an infinite dimensional system, described by a set of coupled nonlinear ordinary and partial differential equations, must be analysed. Analytical solutions may be expected only in special cases.

One special case is given by a circular orbit of the system's center of mass. Due to the $O(3)$-symmetry there exist relative equilibria, which correspond to equilibria in properly rotating frames. These states are of great practical interest. Their stability will be investigated by means of the reduced energy momentum method [2] since by symmetry, besides energy, also the angular momentum is conserved.

We will distinguish between two different types of relative equilibria, existing for the considered system. One are the so-called trivial relative equilibria, for example, the practically most important state where the tether is in its radial configuration. The nontrivial (wavy) tether configurations require active control of the motion of at least one of the satellites. By means of the application of the reduced energy momentum method we show that the trivial radial relative equilibrium state is stable provided the tether is not too long. For the nontrivial relative equilibria we formulate a bifurcation problem, where we vary the position of one of the satellites relative to the other and check the stability of the resulting configuration of the tether, which is supposed to be longer than the straight distance between the two satellites.

Numerical methods have to be applied, first, in the calculation of the relative equilibria by Finite Differences and, further, in the evaluation of the stability condition following from the reduced energy momentum method. This is done by formulating an eigenvalue problem.

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Evolution of rotations of a rigid body under the action of perturbed moment

Dmytro Leshchenko
Odessa State Academy of Civil Engineering
email: `zernov@usm.tm.odessa.ua`

The authors investigated perturbed rotational motions of a rigid body, similar to regular precession in the Lagrange case, under the action of the moment that is slowly changed in time. The average system of equations of motion is obtained in the first approximation. Examples are considered. The qualitative features of the motion are noted. Perturbed rotational motions of a rigid body, similar to regular precession in the Lagrange case, when the restoring moment depends on the rotation angle are investigated. The averaged system of equations of motion is obtained and investigated in the first and second approximations. Specific mechanical models of the perturbations are considered.

Nonlinear stability of periodic and relative periodic orbits in Hamiltonian systems

Juan-Pablo Ortega
Département de Mathématiques, École Polytechnique Fédérale de Lausanne. CH 1015 Lausanne. Switzerland.
email: Juan-Pablo.Ortega@epfl.ch

The classical Dirichlet criterion on the stability of equilibria in Hamiltonian systems is generalized to handle the orbital stability of periodic orbits. The result obtained is adapted to the study of the stability of relative periodic orbits in Hamiltonian systems with symmetry.

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Posters

An Explicit Smale Horseshoe for Generic Quadratic Maps

Diego Vaz Bevilaqua
Instituto de Física, Universidade Federal do Rio de Janeiro
email: dvaz@if.ufrj.br

Mário Basílio de Matos
Instituto de Física, Universidade Federal do Rio de Janeiro
email: mario@if.ufrj.br

The aim of this work is to present some new results regarding the distribution of homoclinic and periodic points in generic quadratic mappings. We show that it is possible to obtain asymptotic formula for the coordinates of such points. The main feature of these formula is that they depend only on the eigenvalue of the fixed point and give the coordinates in terms of integers.

5.5 Models in Biology, Medicine and Physiology

Organizer : Philip Maini

Key note lecture

From microscopic models of individuals to continuum chemotaxis equations

Hans G. Othmer

Department of Mathematics, University of Utah
email: `othmer@math.utah.edu`

A characteristic feature of living systems is that they sense the environment in which they reside and respond to it. The directed motile response of organisms to chemical cues is called *chemotaxis*. Frequently this individual response is manifested by the collective movement of a population up a gradient of concentration of some *chemoattractant*. Smaller organisms such as bacteria frequently rely on some form of *kinesis*, which involves modulation of either the speed or the duration of movement in response to environmental conditions. Both taxes and kineses are often described by macroscopic chemotaxis equations of the form

$$\frac{\partial \rho}{\partial \tau} = \nabla \cdot (D \nabla \rho - \rho \chi(c) \nabla c), \tag{1}$$

where ρ is the density of 'particles' and c is the attractant density, even though the stochastic processes that describe movement at the single-organism level may be quite different. Chemotaxis equations have been derived from a variety of standpoints, and we will discuss several of these. In particular, we show how these can be obtained either from reinforced random walks on a lattice [1], or from a transport equation that describes the velocity jump stochastic process [2].

The simplest version of the mathematical model describing the velocity jump process leads to the equation

$$\frac{\partial}{\partial t} p(x,v,t) + v \cdot \nabla p(x,v,t) = -\lambda p(x,v,t) + \lambda \int_V T(v,v') p(x,v',t) dv', \tag{2}$$

where $p(x,v,t)$ denotes the density of particles at spatial position $x \in \Omega \subset \mathbb{R}^n$, moving with velocity $v \in V \subset \mathbb{R}^n$ at time $t \geq 0$. We first show how to derive a diffusion equation in the diffusion limit of (2), using only a generalized Perron-Frobenius property of the integral operator. In the diffusion limit the diffusion matrix D is not diagonal in general, and we discuss necessary and sufficient conditions under which D reduces to a scalar times the identity. We also show that to derive chemotaxis equations such as (1) we must require suitable conditions on the strength of the bias due to the external field, we give an estimate for the accuracy of the limit equation, and we show how to obtain higher order approximations.

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Invited lectures

Bifurcation analysis of an orientational aggregation model

Edith Geigant

Theoretical Biology, University Bonn, Germany
email: `edith.geigant@uni-bonn.de`

We consider the following integro-differential equation for the development of a function f on the circle $S^1 = \mathbb{R}/\mathbb{Z}$ over time.

$$\dot{f}(\theta) = -\int_{S^1} W[f](\theta,\psi) f(\theta)\, d\psi + \int_{S^1} W[f](\psi,\theta) f(\psi)\, d\psi \tag{1}$$

Here W is a functional mapping functions on S^1 to functions on $S^1 \times S^1$. We choose the following form for W.

$$W[f](\theta,\psi) = \int_{S^1} h(\phi-\theta)\, G_\sigma(\psi-\theta-v(\phi-\theta))\, f(\phi)\, d\phi\,, \tag{2}$$

where G_σ is a periodic Gaussian of deviation σ, $v : S^1 \longrightarrow S^1$ is an odd function, and $h : S^1 \longrightarrow \mathbb{R}_{\geq 0}$ is an even function of total mass $\int_{S^1} h = 1$.

Equations (1, 2) describe orientational aggregation of particles (e.g., acting filaments) by a jump process, where a particle located at an angle θ interacting with another particle located at an angle ϕ changes its orientation instantly to an angle ψ. This new angle is chosen relative to the locations of the interaction partners; its preferred value is given by v, and the accuracy of the movement is measured by σ. The rate (or probability) of interaction depends on the relative angle $\phi - \theta$; it is given by h.

We study the bifurcation behaviour of the model (1, 2) in some detail. In particular, we show that when there is a generic bifurcation from the homogeneous distribution (i.e., exactly one of the eigenmodes changes stability), there is an analytic branch of stationary solutions emanating from the bifurcation point whose power series expansion can be computed explicitly. Moreover we show that our model can exhibit a wide variety of types of dynamical behaviour, for example travelling waves, periodic solutions not of travelling wave type, and solutions combining characteristics of both.

Modelling the cellular response to multiple guidance cues

Kevin Painter
Department of Mathematics, University of Utah
email: `painter@maths.ox.ac.uk`

The chemotactic response of a cell population to a single chemical species has been characterized experimentally for many cell types and has been extensively studied from a theoretical standpoint. However, cells frequently have multiple receptor types and can detect and respond chemotactically to more than one chemical. How these signals are integrated within the cell is not known, and a macroscopic phenomenological approach is therefore often adopted. In this talk, I present chemotactic models based on partial differential (chemotaxis) equations for cell movement in response to multiple chemotactic cues. The derivation generalizes the approach of Othmer and Stevens, [1], who have recently developed a modeling framework for studying different chemotactic responses to a single chemical species. The importance of such a generalization is illustrated by the effect of multiple chemical cues on the chemotactic sensitivity and the spatial pattern of cell densities in several examples. The model can be shown to generate the complex patterns observed on the skin of certain animal species, and used to model a variety of biological phenomena, including patterning in bacteria populations and axonal guidance during development of the nervous system.

References

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Contributed talks

Bifurcations of traveling wave solutions in population models with taxis

Faina Berezovskaya
Center of Forest Ecology R.A.S.
email: `faina@cepl.rssi.ru`

Georgy Karev
Center of Forest Ecology R.A.S.
email: `Gkarev@hotmail.com`

We study the conceptual polynomial model of population with auto-taxis:

$$P_t = F(P) + (P_r/Fi_1(P)/Fi_2(S)S_r)_r, \qquad (A)$$
$$S_t = T_1(P)T_2(S)$$

where P, S are correspondingly density of population and substance produced by population, functions $F(P)$ and $T(P,S) = T_1(P)T_2(S)$ describe the kinetics of population and its substance, constant $D > 0$ is a diffusion coefficient and function $F(P,S) = /Fi_1(P)/Fi_2(S)$ is cross-diffusion coefficient. Under condition of $/Fi_2(S)T_2(S) = const$ (see Othmer, 1997) we describe all principal wave solutions $P(r,t) = P(r+ct) = p(x)$ and corresponding wave regimes of the model arising with non-linear autotaxis for linear, quadratic and cubic local kinetic function $F(P)$. We describe also rearrangements of such regimes with change of parameters of function F and the velocity c of wave propagation.

Investigation of the model (A) is based on transition to corresponding wave ODE system and systematic using of bifurcation diagrams of normal forms ODE to which wave systems are reduced by linear transformations.

Some possible applications of obtained results to study of dynamics of ameba populations, forest insect outbreaks, etc. are discussed.

Homoclinic bifurcation in a Hodgkin-Huxley Model of Thermally Sensitive Neurons

Ulrike Feudel
Institut of Physics, University of Potsdam, Germany
email: `ulrike.feudel@agnld.uni-potsdam.de`

Alexander Neiman
Center for Neurodynamics, University of Missouri at St. Louis
email: `neiman@neurodyn.umsl.edu`
Xing Pei
Center for Neurodynamics, University of Missouri at St. Louis
email: `xpei@newton.umsl.edu`
Winfried Wojtenek
Center for Neurodynamics, University of Missouri at St. Louis
email: `wojtenek@umsl.edu`
Frank Moss
Center for Neurodynamics, University of Missouri at St. Louis
email: `mossf@umslvma.umsl.edu`

Bursting and irregular spiking activity of neurons is often observed in electrophysiological experiments. Recently, several studies give strong arguments that this irregular behavior can be explained in terms of low-dimensional dynamics. To investigate the spiking activity of thermally sensitive neurons we study global bifurcation phenomena, in particular homoclinic bifurcations, in a modified Hodgkin-Huxley model. This model has been proposed by Braun et al. [1] and mimics the action potential observed in electroreceptors from dogfish [1], catfish [2], from facial cold receptors [3] and hypothalamic neurons of the rat [4]. Using the temperature as the control parameter, a large region of chaotic behavior is identified. In a certain temperature region we obtain a sudden increase in the Poincaré return time. We provide numerical evidence that this increase can be explained as a result of a homoclinic bifurcation related to a fixed point of saddle-focus type in the four-dimensional state space. The transition is accompanied by intermittent behavior which obeys the universal scaling law for the average "laminar phase" with the distance from the homoclinic bifurcation. Furthermore, we discuss the influence of noise on the homoclinic bifurcation in the modified Hodgkin-Huxley model to compare our results with observations from electrophysiological experiments, which are always contaminated by noise. In such experiments, the only measurable quantity are interspike intervals which can be regarded as a direct measurement of the Poincaré return time. We present experimental results of interspike interval measurements taken from the crayfish caudal photoreceptor, which qualitatively demonstrate the same bifurcation structure.

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General models of size-dependent population dynamics with nonlinear growth rate

Nobuyuki Kato
Shimane University
email: `nkato@math.shimane-u.ac.jp`

We shall investigate the size structured population models having the birth and aging functions of general type with the growth rate depending on the individual's size and total population. The models are described as the following initial boundary value problem with nonlocal boundary condition:

$$\begin{cases} u_t + (V(x, P(t))u)_x = G(u(\cdot, t))(x), \quad x \in [0, l), \ 0 \le t \le T, \\ V(0, P(t))u(0, t) = C(t) + F(u(\cdot, t)), \quad 0 \le t \le T, \\ u(x, 0) = u_0(x), \quad x \in [0, l), \\ P(t) = \int_0^l u(x, t)dx, \quad 0 \le t \le T, \end{cases}$$

where the unknown function $u(x, t)$ stands for the density of the population of size x at time t and $l \in (0, \infty]$ is the maximum size, and so $P(t)$ is the total population at time t. The mappings F and G correspond to the birth and aging functions respectively. The function $V(x, P(t))$ represents the growth rate depending on the size x and the total population $P(t)$ at each time. The function C describes the inflow of zero-size individuals from an external source.

Our aim is to generalize the results of A. Calsina and J. Saldaña [1], where they treated the birth and aging functions of the Gurtin-MacCamy type:

$$\begin{aligned} F(u(\cdot, t)) &= \int_0^l \beta(x, P(t))u(x, t)dx, \\ G(u(\cdot, t))(x) &= -m(x, P(t))u(x, t). \end{aligned}$$

This assumption is essential in their arguments. We deal with the birth and aging functions of general type as treated in [2] by G. Webb in the age dependent case (which is equivalent to the case $V \equiv 1$) and we show the existence of the solution.

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Modeling of heterogeneous populations

Georgy Karev

Center of Forest Ecology and Productivity of Russian Academy Sciences

email: gkarev@hotmail.com , karev@cepl.rssi.ru, Georgy.Karev@epc.u-sud.fr

Individual-based models of dynamics of heterogeneous population with distributed values of parameter and initial conditions of variables are suggested. The resulting model represents the system of ODE (note that under standard approaches the dynamics of heterogeneous population is described usually by partial differential equations). The formulae for calculation of current average values and dispersions of phase variables and parameters with the help of auxiliaries variables satisfying to a system of equations in variations are obtained. Two main examples are considered: 1) the phenomenon of formation of patterns (known as gap, locus, cenon) in tree populations from initial heterogeneous subpopulation of trees; 2) the models of number dynamics of population with distributed values of a reproduction factor and/or environment parameters. The interesting new effect was founded even for simple population model by Alle' type. Namely, even small non-zero dispersion of environment parameter can result to probably short-lived, but having large amplitude number outbreaks. The research was supported by grants RFFI N 98-04-48502 and 99-04-00234.

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Nonlinear mathematical model of pulsed-therapy of heterogeneous tumors

Abdelkader Lakmeche
University of Sidi Bel Abbes
email: `Lakmeche@yahoo.fr`

The impulsive models arise, generally, in the description of phenomena in the applied sciences subjected to abrupt external changes, where the time of the change can be neglegted, and can be considered as a jump in the simulation of the phenomena under study.

More specifically, we consider the following heterogeneous tumor model

$$\dot{x} = r_1(x,y)\,x \tag{1}$$

$$\dot{y} = r_2(x,y)\,y \tag{2}$$

$$x\left(t_n^+\right) = \eta_n\left(D, x\left(t_n\right), y\left(t_n\right)\right) \tag{3}$$

$$y\left(t_n^+\right) = \theta_n\left(D, x\left(t_n\right), y\left(t_n\right)\right) \tag{4}$$

where D is the drug dose administered, x and y are, respectively, the biomass of sensitive cells and drug resistant cells. The values $r_1(x,y)$, $r_2(x,y)$ are, respectively, the growth rates of sensitive and drug resistant cells. The values $\eta_n\left(D, x\left(t_n\right), y\left(t_n\right)\right)$ and $\theta_n\left(D, x\left(t_n\right), y\left(t_n\right)\right)$ are, respectively, the biomass of sensitive and resistant cells which survive after the nth drug dose D administered at the moment t_n, the sequence (t_i) is strictly increasing.

Travelling wave solutions for reaction diffusion equations

Luisa Malaguti
Department of Mathematics - University of Modena and Reggio Emilia (Italy)
email: `malaguti@unimo.it`

As it is well-known, the following general reaction diffusion equation

$$\frac{\partial u}{\partial t} + \frac{\partial h(u)}{\partial x} = \frac{\partial}{\partial x}\left[d(u)\frac{\partial u}{\partial x}\right] + g(u) \tag{1}$$

frequently occurs in many biological and chemical models (see i.e. [2] and [3]). It takes into account both a non-linear convection effect introduced by the term $\frac{\partial h(u)}{\partial x}$ and a density dependent diffusion given by the function $d(u)$.

In [1] we provide results on the existence of *travelling wave solutions*, that is solutions $u(t,x)$ of equation (1) such that $u(t,x) = u(z)$ with $z = x + ct$. The constant c stands for the *speed* of the wave. To be physically realistic $u(z)$ has to be bounded for all z and non-negative. Therefore, the existence of bounded travelling fronts for equation (1) essentially reduces to the study of the following boundary value problem on the real line

$$\begin{cases} ((d(u)u')' - ((c + h'(u))\, u' + g(u) = 0 & \left(' = \frac{d}{dz}\right) \\ \\ u(-\infty) = 0, \quad u(+\infty) = 1 \end{cases} \tag{2}$$

where we stress that also the real constant c is an unknown of the model.

Using lower and upper solutions techniques, we get an existence and uniqueness result of monotone solutions of (2) for any speed $c \geq c^*$, and provide an estimate for the threshold value c^* .

Main Result *Assume that h', g, d are continuous in [0,1], with* $\min d(u) > 0$*. Then, if $D^+(dg)(0) < +\infty$, there exists a constant c^* with*

$$2\sqrt{D_+(dg)(0)} - h'(0) \leq c^* \leq 2\sqrt{\sup_{u\in]0,1]} \frac{d(u)g(u)}{u}} - \min_{u\in[0,1]} h'(u)$$

such that (2) admits monotone solutions if and only if $c \geq c^*$. Moreover, the solution is unique (up to a translaction of the origin).

Whereas, if $D_+(dg)(0) = +\infty$, problem (2) does not admit monotone solutions for any speed c.

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The Basic Reproduction Number for STD's and Linear Chains

Johannes Müller

Biomathematics, University of Tübingen

email: `johannes.mueller@uni-tuebingen.de`

In models for infectious diseases, the basic reproduction number is the crucial parameter which determines the stability of the uninfected situation, i.e. the possibility of an outbreak. In simple situations it depends in a monotone way on the infectivity. Non-monotone behavior may occur in diseases where infectivity depends on time since infection and where transmission depends on social structure [1]. A typical application is the HIV infection where transmission rates depend on existing pair bonds and infectivity changes drastically over time.

A class of epidemic models with pair formation and infectivity depending on time since infection is defined within the framework of hyperbolic PDE's. The reproduction number is derived and leads to a non-autonomous cyclic linear reaction chain

$$x_1 \rightarrow x_2 \leftrightarrow x_3 \leftrightarrow \cdots \leftrightarrow x_n \leftrightarrow x_1$$

where additionally there is an outflow from each state with a rate $\mu(t)$. Note that no transition is possible from state two to state one. Let furthermore $\alpha_1(t)$ be the transition rate from state one to state two. If we choose as initial values $x_1(0) = 1$ and $x_i(0) = 0$ for $i = 1, .., n$, the reproduction number can be represented as the number of transitions from state one to state two,

$$R_0 = \int_0^\infty \alpha_1(\tau) x_1(\tau)\, d\tau.$$

The monotonicity of R_0 with respect to the infectivity function is equivalent to the the monotonicity of $\int_0^\infty \alpha_1(\tau)x_1(\tau)\, d\tau$ with respect to an increase of the transition rates from the states i to states $i+1$, and a decrease of the transition rates from the states $i+1$ to states i.

The crucial idea of the proof of this monotonicity theorem is to reformulate the solution of the ODE as an integral of sequences, which mimic a stochastic random walk. We do not directly use the stochastic process but a construction that has similar properties, such that it is possible to apply methods from the theory of stochastic particle systems [2].

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Model reduction by extended quasi-steady-state approximation

Klaus R. Schneider
WIAS Berlin
email: `schneider@wias-berlin.de`

Thomas Wilhelm
Institut für Gewässerökologie und Binnenfischerei
email: `wilhelm@igb-berlin.de`

The quasi-steady-state assumption (QSSA) can be justified mathematically by the existence of an exponentially attracting integral manifold for the corresponding system of singularly perturbed differential equations. We extend the QSSA with respect to the class of differential systems as well as with respect to the order of approximation. Especially, we extend it to the class of singular singularly perturbed systems where the associated system has a first integral. That means, we may introduce slow pool variables by means of a (nonlinear) coordinate transformation. As an application we prove that the trimolecular autocatalator can be approximated by a fast bimolecular reaction system. Finally we describe a class of singularly perturbed systems for which the first order QSSA can easily be obtained.

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Periodicity versus chaos in population dynamics

Hans Thunberg
Dep. of Mathematics, KTH, Stockholm
email: `hasset@math.kth.se`

Using recent results on the asymptotics of families of one-dimensional mappings we investigate two standard models in population dynamics, namely the Ricker family

$$R_{\lambda,\beta}(x) = \lambda x e^{-\beta x} \qquad \lambda > 1, \quad \beta > 0$$

and the Hassell family

$$H_{\lambda,\beta}(x) = \frac{\lambda x}{(1+x)^{\beta}}, \qquad \lambda > 1, \quad \beta > 1.$$

These models seek to describe certain single-species population dynamics, where λ is the intrinsic reproduction rate, and β controls the damping for large populations due to the environmental effects. Lately the work by Gyllenberg, Hanski and Lindström shows that models such as these also can be derived from more complicated models with structured competition processes.

Our focus is on generic behavior seen for many parameters and many initial conditions. There is an almost dichotomy between maps with stable cycles and strongly chaotic maps. Strongly chaotic maps here means maps with global, exponential sensitivity to initial conditions and an invariant probability measure, with integrable density, describing the asymptotics of almost all initial conditions.

The following generic results are applicable to the families above: (i) Each map has a unique metric attractor; (ii) Maps with stable cycles are dense in parameter space; (iii) Strongly chaotic maps appears with positive frequency in parameter space; (iv) Asymptotic dynamics is almost independent of initial conditions, and can in most cases be described by an invariant probability measure; (v) Various (in)stability properties of these asymptotic distributions.

Posters

Parameter estimation and model selection in ODEs: the lipid metabolism

Thorsten G. Müller
Freiburger Zentrum für Datenanalyse und Modellbildung
email: `muellert@fdm.uni-freiburg.de`

Karl Winkler
Freiburger Universitätsklinik
email: winkler@ukl.uni-freiburg.de

Jens Timmer
Freiburger Zentrum für Datenanalyse und Modellbildung
email: jeti@fdm.uni-freiburg.de

Modelling biological non-linear dynamical systems is often done using ordinary differential equations (ODE). To analyze these systems and the underlying mechanisms with help of data it is crucial to evaluate different modelling approaches and to estimate parameters of the models. To get numerically stable estimates of the parameters we apply the so-called multiple-shooting method [1], [2]. To identify the model which fits the data best we apply likelihood-ratio-tests which have to be adjusted to the occuring non-standard conditions. This concept is exemplified with a data set from human lipoprotein metabolism where different compartment models are compared.

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5.6 Molecular Modelling

Organizer : Folkmar Bornemann

Key note lecture

Conformational Dynamics: How to Compute Almost Invariant Structures in the Complicated Motion of Molecular Ensembles

Christof Schütte
Konrad-Zuse-Zentrum, Takustr. 7, D-14195 Berlin, Germany
email: schuette@zib.de

The function of many important biomolecules comes from their dynamic properties and their ability to switch between different *conformations*. In a conformation, the large scale geometric structure of the molecule is understood to be conserved, whereas on smaller scales the system may well rotate, oscillate or fluctuate. In [2], it has been demonstrated that conformations can be understood as almost invariant sets of the Hamiltonian system governing the molecular dynamics. Moreover, it has been proposed to follow Dellnitz and Junge [1] in computing these almost invariant sets via certain eigenvectors of the Frobenius Perron operator of the system. We will shortly review this approach in its application to molecular dynamics and discuss its potential drawbacks in this particular case. Analysis of these drawbacks will lead us to the insight that the Frobenius-Perron operator must be replaced by some specific Markov operator T that correctly describes the statistical fluctuations within the molecular ensemble [3]. This reformulation leads to nonlinear state space Markov chains that replace the deterministic Hamiltonian systems of the original approach. The conformations are identified using eigenvectors of T corresponding to the eigenvalue cluster near the maximal eigenvalue 1. Following [4], we illustrate and justify this approach by discussing statistical and spectral properties of T and the associated Markov chain. In order to approximate the desired eigenvectors of T, we discretize the corresponding eigenvalue problem by means of a specific Galerkin procedure. This results in a stochastic discretization matrix T_N [5] for which, even for large molecules, the eigenvectors can be computed efficiently. Finally, it is demonstrated how this leads to approximate conformational subsets. Our approach allows for the first time to identify dynamical conformations of molecular ensembles including their stability life spans and the rate of transitions between them.

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Invited lectures

Molecular Propagation through Crossings and Avoided Crossings of Electron Energy Levels

George A. Hagedorn

Virginia Polytechnic Institute and State University

email: `hagedorn@math.vt.edu`

Most information about molecular propagation is obtained from the time–dependent Born–Oppenheimer approximation. This approximation fails to apply if two electron energy levels cross or approach close to one another for some configuration of the nuclei. In this talk we describe the time–dependent Born–Oppenheimer approximation and discuss what happens when a molecular system propagates through a generic level crossing or avoided crossing.

Adiabatic Evolution of Systems with Infinitely many Eigenvalue Crossings

Alain Joye
Institut Fourier, Grenoble
email: `alain.joye@ujf-grenoble.fr`

Monti Francois
LPUB Dijon

Guérin Stéphane
LPUB Dijon

Jauslin Hans
LPUB Dijon

We formulate an adiabatic theorem adapted to models that present an instantaneous eigenvalue experiencing an infinite number of crossings with the rest of the spectrum. We give an upper bound on the leading correction terms with respect to the adiabatic limit. The result requires only differentiability of the considered spectral projector, and some geometric hypothesis on the local behaviour of the eigenvalues at the crossings.

Enhanced Quantum–Classical Molecular Dynamics: Models and Numerical Integrators

Peter Nettesheim
Konrad–Zuse–Zentrum Berlin, Berlin, Germany
email: `nettesheim@zib.de`

Christof Schütte
Konrad–Zuse–Zentrum Berlin, Berlin, Germany
email: `schuette@zib.de`

In recent years, *mixed quantum–classical models* have attracted much interest as approximation to a full quantum dynamical description in molecular dynamics. The attention is based on the hope to overcome the obstacles of the widely used Born-Oppenheimer approximation. In this particular model, the dynamics of light particles (i.e., electrons) is *adiabatically* coupled to the classical dynamics of heavier nuclei. It has been assumed that the so–called QCMD model, which consists of a *singularly perturbed* Schrödinger equation nonlinearly coupled to Newtonian equations, might describe the — in many applications crucial — *nonadiabatic effects* as well. The approximation properties of QCMD were thoroughly analyzed [1,2]. It could be shown that QCMD is a valid approximation under certain assumptions and in mildly nonadiabatic scenarios only. A novel and much more promising approach for nonadiabatic systems leads to the Quantum–Classical–Liouville equation [3] implying some kind of QCMD surface–hopping [4].
But not only the modelling should gain attention. To efficiently obtain a reliable numerical solution of the model equations the development of numerical integrators for the case of a singularly-perturbed PDE coupled to a Hamiltonian ODE is required. Due to the great variation of application problems, there are many different ways to discretize the system: using structure conserving [5], long–time–step [6] and averaging methods [7,8].
The first part of the talk is dedicated to an overview of the approximation properties of

some quantum–classical models. In the second part of the talk numerical algorithms to solve the derived model equations will be considered.

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Contributed talks

Electronic structure calculations via reduced density matrices and semidefinite programming

Bastiaan J. Braams
Courant Institute, NYU
email: `braams@courant.nyu.edu`

Joint work with Shidong Jiang, Madhu Nayakkankuppam, Michael L. Overton and Jerome K. Percus (Courant Institute) and François Oustry (INRIA-Grenoble). The ground state variational problem for a many-electron system may be formulated in terms of the one-body and two-body reduced density matrices instead of the complete wavefunction [1-2]. A central issue is the "representability problem" of characterizing (through convex inequalities) the class of functions that can arise as density matrix of a many-electron system. The calculation of ground-state properties then reduces to a linear optimization problem subject to the representability constraints, of which the simplest ones are a finite set of linear equalities and bounds on eigenvalues, as in semidefinite programming. Significant work on this application was done in the 1970s [3], but interest has waned since, partly because of the unsettled status of the representability problem and partly because of the computational cost of solving the associated optimization problem. Recent advances in the application of interior-point and related methods to semidefinite programs [4] have encouraged us to revisit the reduced density matrix approach to electronic structure calculations. Our research follows two tracks. On one hand we are using analytical and numerical approaches to develop new representability conditions. Our new conditions extend fundamentally the known "diagonal" conditions developed in the 1970s [5], which correspond to the well-studied problem of characterizing the Cut Polytope [6]. While a complete solution of this problem appears intractable, we hope that our approach will bring the status of the complete representability problem to the same level as has been achieved for the diagonal problem. On the other hand, we are exploring numerically the strength of the known representability conditions by calculations on model systems, in which we compare the ground state energy found by the optimization approach with the ground state energy found using full configuration interaction.

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5.7 Patterns

Organizer : Paul C. Fife

Key note lecture

The Viscous Nonlinear Dynamics of Twist and Writhe

Raymond E. Goldstein
Department of Physics, University of Arizona, Tucson, AZ 85721
email: `gold@physics.arizona.edu`

Motivated by diverse phenomena in cellular biophysics, including DNA transcription and replication, and bacterial flagellar motion, I describe recent work on four aspects of the overdamped nonlinear dynamics of a an elastic filament in the low Reynolds number regime. (i) A geometrically exact and gauge-invariant intrinsic formulation, utilizing the "natural" frame of space curves, that yields coupled nonlinear PDES for the time evolution of the complex curvature and twist density, and thereby describes the dynamic interplay of twist and writhe. (ii) A class of problems in the dynamics of forced elastic filaments (and related experimental work) that reveals the basic principles of elastohydrodynamics, and in the case of rotational forcing, the competition between twist injection, twist diffusion, and writhing instabilities. (iii) A mechanistic explanation for "chirality inversions" observed in helical bacterial flagella in external flow fields. (iv) Preliminary experiments with optical trapping techniques on the elasticity of supercoiled bacterial fibers that reveal for the first time the bending modulus of a bacterial cell.

Invited lectures

Modelling Bioconvection at Low and High Volume Fractions of Swimming Bacteria

John O. Kessler
Department of Physics, University of Arizona, Tucson, AZ 85721
email: kessler@physics.arizona.edu

Modelling the dynamics of suspensions containing swimming micro-organisms requires equations governing (1)conservation of organisms, (2)conservation of advected and diffusing passive scalars which may be emitted or consumed, and which may affect the probability density functions for the organisms' swimmng velocity, (3)conservation of mass, and (4)conservation of momentum, the Navier-Stokes equations. Conservation of mass conventionally leads to divU=0, where U is the fluid velocity. When organisms can swim relative to U, and when their volume fraction becomes large, e.g 0.1, this equation must be augmented. The variability of fluid density, due to swimming, must also be accounted for in the D(momentum)/Dt term of the Navier Stokes equations. The experimental motivation for this research, observations of "microturbulence" in concentrated bacterial suspensions, will be described.

Spatio-Temporal Phase Patterns in Forced Oscillatory Systems

Ehud Meron
Institute for Desert Research and the Physics Department, Ben-Gurion University, Sede Boqer Campus, 84990, Israel
email: ehud@bgumail.bgu.ac.il

Periodic forcing of an oscillatory system produces frequency locking bands within which the system frequency is rationally related to the forcing frequency. We study extended oscillatory systems that respond to uniform periodic forcing at one quarter of the forcing frequency (the 4:1 resonance). These systems possess four coexisting stable states, corresponding to uniform oscillations with successive phase shifts of $\pi/2$.

Using an amplitude equation approach near a Hopf bifurcation to uniform oscillations, we study front solutions connecting different phase states. These solutions divide into two groups: π-fronts separating states with a phase shift of π and $\pi/2$-fronts separating states with a phase shift of $\pi/2$. We find a new type of front instability where a stationary π-front "decomposes" into a pair of traveling $\pi/2$-fronts as the forcing strength is decreased. The instability is degenerate for an amplitude equation with cubic nonlinearities. At the instability point a continuous family of pair solutions exists, consisting of $\pi/2$-fronts separated by distances ranging from zero to infinity. Quintic nonlinearities lift the degeneracy at the instability point but do not change the gross effects of the instability. We conjecture the existence of similar instabilities in higher $2n$:1 resonances ($n = 3, 4, ..$) where stationary π-fronts decompose into n traveling π/n-fronts.

The instabilities designate transitions from stationary two-phase patterns to traveling $2n$-phase patterns. As an example, we demonstrate with a numerical solution the collapse of a four-phase spiral wave into a stationary two-phase pattern as the forcing strength within the 4:1 resonance is increased. Comparisons of theoretical results with experimental data obtained by Lin and Swinney on the periodically forced Belousov-Zhabotinsky reaction are discussed.

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Complex Pulse Dynamics in Nonlinear Dissipative Systems

Yasumasa Nishiura
Hokkaido University
email: `nishiura@aurora.es.hokudai.ac.jp`

Pulse dynamics is one of the typical patterns in dissipative systems, which conveys information from one place to another. Like a propagating pulse in nerve axon, such waves in general annihilate upon collision and it has been regarded as a characteristic distinction from solitons in nonlinear dispersive systems. A different class of pulse waves, however, has been found for several reaction diffusion systems including the Gray-Scott model: bouncing pulse waves upon collision or self-replicating patterns. In this talk firstly we discuss a *skeleton structure of self-replicating patterns* from global bifurcational point of view. It turns out that the *aftereffect* of hierarchy structure of saddle-node bifurcation is responsible for self-replicating process. Also pulse interaction approach is quite useful to understand the manner of splitting asymptotically. Secondly we discuss about the *self-destruction* phenomena arising in the Gray-Scott model, which appears typically after the self-replicating process, namely the whole domain is filled by the localized islands through self-replication, then several groups of islands disappear followed by the invading process from the surroundings with replication, and this process repeats over and over again in a chaotic way. The saddle-node structure of the Turing branch of the highest mode as well as the instability of the critical point is crucial to understand this complex dynamics.

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Localized waves: worms in electroconvection

Hermann Riecke
Northwestern University
email: `h-riecke@nwu.edu`

A wide range of physical systems undergoes bifurcations to spatial and temporal patterns when they are driven sufficiently strongly. Of great recent interest have been systems in which the appearing patterns do not extend over the whole system but become localized in only a small part of it, although the system is translationally invariant. In contrast to fronts that connect two stable states these localized patterns are not topologically stable, and their stability depends on the dynamics of the system.

Usually, localized structures arise in systems that exhibit a bistability between the feature-less state and the spatially extended pattern. Recently, however, localized waves ('worms') have been observed in experiments on electroconvection of nematic liquid crystals in the absence of a bistability between the basic state and the spatially extended pattern [1]. We show that this can be understood if the waves are coupled to a slowly decaying large-scale field [2]. We discuss a Ginzburg-Landau-type model for this coupling that captures various aspects of the experimental observations, e.g. the shape and stability of the worms.

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Spinodal Decomposition for the Cahn-Hilliard Model

Thomas Wanner
Department of Mathematics and Statistics
University of Maryland, Baltimore County
Baltimore, MD 21250, USA
email: wanner@math.umbc.edu

Some forty years ago J.W. Cahn and J.E. Hilliard introduced the fourth-order parabolic partial differential equation

$$\begin{aligned} u_t &= -\Delta(\varepsilon^2 \Delta u + f(u)) \quad \text{in} \quad \Omega\,, \\ & \frac{\partial u}{\partial \nu} = \frac{\partial \Delta u}{\partial \nu} = 0 \quad \text{on} \quad \partial\Omega \end{aligned}$$

as a model for several physical phenomena occurring in binary alloys. One particularly intriguing phenomenon is spinodal decomposition: If a homogeneous high-temperature mixture of two metallic components is rapidly quenched to a certain lower temperature, then a sudden phase separation sets in. The mixture quickly becomes inhomogeneous and forms a complicated, fine-grained structure, more or less alternating between the two alloy components.

In this talk I present recent mathematical progress in explaining spinodal decomposition for the Cahn-Hilliard equation. This includes both a description of the main characteristics of the generated patterns, as well as an explanation of the surprising mechanism underlying the phase separation. I will also address the case of multi-component alloys, which is modeled by a system of Cahn-Hilliard equations.

These results were obtained in collaboration with Stanislaus Maier-Paape, Evelyn Sander, and Barbara Stoth.

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Contributed talks

Spinodal decomposition for the stochastic Cahn-Hilliard equation

Dirk Blömker
University of Augsburg
email: `Dirk.Bloemker@Math.Uni-Augsburg.DE`

The talk addresses the spinodal decomposition for the stochastic Cahn-Hilliard equation

$$u_t = -\epsilon^2 \Delta^2 u + \Delta(u^3 - u) + \xi$$

in a domain Ω with Neumann and no flux boundary conditions. $\Omega \subset \mathbb{R}^d$, $d = 1, 2, 3$ is a domain with sufficiently smooth boundary and ξ a Gaussian white noise process. Based on the work of Maier-Paape and Wanner [1,2] for the Cahn-Hilliard equation, it is shown, that with high probability solutions of the linearized equation starting at $u = 0$ will leave a neighborhood of 0 along a strongly unstable manifold, provided ϵ small enough. This will give solutions with a characteristic wavelength, as discussed in [1]. This linear result is then extended to the nonlinear stochastic equation near the origin.

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Bifurcation for reaction-diffusion systems with nonstandard boundary conditions

Jan Eisner
Mathematical Institute of Academy of Sciences,
Žitná 25, 115 67 Prague 1, Czech Republic
email: `eisner@math.cas.cz`

Let us consider a reaction-diffusion system of activator-inhibitor type

$$\begin{aligned} u_t &= \sigma_1(s)u_{xx} + f(u,v) \\ v_t &= \sigma_2(s)v_{xx} + g(u,v) \end{aligned} \quad \text{on } (0,+\infty)\times(0,1) \tag{1}$$

with boundary conditions

$$u(0)=\overline{u},\ v(0)=\overline{v}, \quad u_x(1)\in -m_1(u(x_1)), v_x(1)\in -m_2(v(x_2)) \tag{2}$$

where $\sigma : \mathbb{R} \to \mathbb{R}^2_+$ is a smooth curve, $s \in \mathbb{R}$ is a bifurcation parameter, $\overline{u}, \overline{v}$ are real numbers, $f, g : \mathbb{R}^2 \to \mathbb{R}$ are real differentiable functions such that $f(\overline{u},\overline{v}) = g(\overline{u},\overline{v}) = 0$ (i.e. $[\overline{u},\overline{v}]$ is a steady state of (1), (2)), $x_1, x_2 \in (0,1]$ and $m_1, m_2 : \mathbb{R} \to 2^{\mathbb{R}}$ are multivalued functions of a certain type.

The multivalued conditions in (2) with certain m_1 and m_2 describe for example semipermeable membranes on the part of the boundary with sensors in x_1 and x_2, respectively. Particularly, the sensors can be the interior of the domain and therefore at different points than the sources.

There exists a bifurcation point $s_I \in \mathbb{R}$ of (1), (2) at which stationary spatially nonconstant solutions (spatial patterns) bifurcate from the branch of trivial solution $[\overline{u},\overline{v}]$. Moreover, s_I lies in the region of stability of $[\overline{u},\overline{v}]$ as a solution to a corresponding stationary problem to (1) with classical boundary conditions

$$u(0)=\overline{u},\ v(0)=\overline{v}, \quad u_x(1)=v_x(1)=0, \tag{3}$$

particularly in the region, where bifurcation for (1) with (3) is excluded.

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Lagrangian turbulence and the dynamo effect in Magnetohydrodynamics

Fred Feudel
Institute of Physics, University of Potsdam, Germany
email: `fred.feudel@agnld.uni-potsdam.de`

Sten Rüdiger
Institute of Physics, University of Potsdam, Germany
email: `sten@agnld.uni-potsdam.de`

Annette Witt
Institute of Physics, University of Potsdam, Germany
email: `annette.witt@agnld.uni-potsdam.de`

The generation and maintenance of magnetic fields by the motion of electrically conducting fluids are the subject of dynamo theory. It is a prevalent assumption that this phenomenon can be modeled by the magnetohydrodynamic (MHD) equations which consist of the coupled system of Navier-Stokes equations (NSE) and induction equation.

The general idea is that the mechanical energy pumped into the fluid by heating or other mechanisms is transferred into the induction equation producing the dynamo. We report on bifurcations of the MHD equations which are driven by an external forcing of the Roberts type [1,2]. It drives a flow which serves as a model for the convection in the outer core of the Earth [3] and is realized in an ongoing laboratory experiment aimed at demonstrating a dynamo effect. The symmetry group of the problem is determined and we study in detail the first symmetry breaking transition from the nonmagnetic state. The appearance of the magnetic field is spacially correlated with the location of stagnation points. We observed that the magnetic field is stongly amplified in the neighborhood of the fixed points of the velocity field which have an one-dimensional stable and a two-dimensional unstable manifold. The Lagrangian chaos of passive tracers in this region gives numerical evidence that intersections of stable and unstable manifolds of fixed points of different type are responsible for the creation of the dynamo in this model.

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Asymptotic profiles of nonlinear diffusion problems

Jorge García-Melián
Departamento de Análisis Matemático, Universidad de La Laguna, Spain
garmel@ull.es

José Sabina de Lis
Departamento de Análisis Matemático, Universidad de La Laguna, Spain
email: josabina@ull.es

We are describing the existence, uniqueness and profile structure as $\lambda \to +\infty$ of positive solutions to the logistic type problems,

$$\begin{array}{rcll} -\Delta_p u &=& \lambda u^{p-1} - u^q - f(u) & x \in \Omega \\ u &=& 0 & x \in \partial\Omega, \end{array}$$

$\Omega \subset \mathbb{R}^n$ a smooth and bounded domain, Δ_p the p-Laplacian, $q+1 > p > 2$ while f is C^1 and both satisfies $f = o(u^{p-1})$, $f = o(u^q)$ respectively as $u \to 0$, $u \to +\infty$. The case Ω radially symmetric will studied in detail while spacial emphasis will be put in the arising, on general domains Ω, of dead cores, i.e. sets $\mathcal{O}_\lambda := \{x : u(x) = \bar{u}(\lambda)\}$ where u is a positive solution and $\bar{u}(\lambda)$ satisfies $\lambda u^{p-1} - u^q - f(u)$ (see [1],[2]).

We are also dealing with a second kind of spatially dependent diffusion problems, namely,

$$\begin{array}{rcll} -\Delta_p u &=& \lambda u^{p-1} - a(x)(u^q + f(u)) & x \in \Omega \\ u &=& 0 & x \in \partial\Omega, \end{array} \tag{1}$$

where $a = a(x) \in C^1(\overline{\Omega})$, $a(x) \geq 0$ but the relevant fact is $D := \text{supp } a \subset \Omega$. We are considering the issues of existence and uniqueness of positive solutions and showing that such solutions ceases to exist when $\lambda > \lambda_1(\Omega \backslash D)$. In fact, we are showing that positive solutions blow-up for λ close $\lambda_1(\Omega \backslash D)$ and we will provide a detailed account on the profile of such solutions when $\lambda \to \lambda_1(\Omega \backslash D)$ (see [3] for earlier results).

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Convective Cahn-Hilliard models for kinetically controlled crystal growth

Alexander Golovin
Department of Chemical Engineering, Technion, Haifa 32000, Israel
email: `cersgsg@techunix.technion.ac.il`

Steven Davis
Department of Engineering Sciences and Applied Mathematics, Northwestern University, Evanston, Illinois 60208-3100
email: `sdavis@nwu.edu`

Alexander Nepomnyashchy
Department of Mathematics, Technion, Haifa 32000, Israel
email: `nepom@leeor.math.technion.ac.il`

Michael Zaks
Department of Nonlinear Dynamics, Institute of Physics, Potsdam University, D-14415, Potsdam, Germany
email: `zaks@agnld.uni-potsdam.de`

We consider solidification into a hypercooled melt in which kinetic undercooling and anisotropic surface energy are present. We allow the anisotropy to be strong enough that equilibrium configurations would contain facets.

In one-dimensional case, the formation of facets is governed by the convective Cahn-Hilliard equation

$$u_t + Duu_x + (u_{xx} + u - u^3)_{xx} = 0,$$

where $u(x, t)$ is proportional to the slope of the interface. Depending on the parameter D, the derived equation describes the coarsening of facets (kinks), development of a steady spatially-periodic surface relief and appearance of a non-periodic attractor (roughening). The bifurcations and stability of spatially-periodic solutions, as well as the rate of coarsening, are studied.

In two-dimensional case, several generalizations of the convective Cahn-Hilliard equation have been derived for different orientations of growing surfaces. The numerical simulation reveals the formation of hill-and-valley structures in the form of coarsening square, triangular and rhombic pyramids and grooves.

Spatial patterns for reaction-diffusion systems with nonstandard boundary conditions

Milan Kučera
Mathematical Institute, Academy of Sciences,
Žitná 25, 115 67 Prague 1, Czech Republic
email: `kucera@math.cas.cz`

Reaction diffusion systems of the activator-inhibitor type

$$u_t = d_1 \Delta u + f(u,v),\ v_t = d_2 \Delta v + g(u,v)$$

will be considered under the assumptions guaranteing the loss of stability of the spatially homogeneous stationary solution (diffusion driven instability) in case of classical boundary conditions. The existence and location of a bifurcation of stationary spatially nonhomogeneous solutions (spatial patterns) will be discussed for the case when classical boundary conditions are replaced by nonstandard nonlinear boundary conditions or supplemented by some additional restrictions in the interior of the domain. The class of conditions under consideration includes a description of unilateral membranes or some regulation on the boundary or in the interior of the domain (e.g. a thermostat type regulation). The simplest example are boundary conditions

$$\frac{\partial u}{\partial n} \in m_1(u),\ \frac{\partial v}{\partial n} \in m_2(v)$$

where m_1, m_2 are multivalued functions of a certain type. The method used can be applied to the case when $f,\ g$ contain jumping nonlinearities. The results can be formulated in the abstract form for general inclusions of the type

$$x - T(\mu)x - G(\mu, x) \in -M(x)$$

where for any μ, $T(\mu)$ is a linear completely continuous operator, G is a small compact perturbation, M is a multivalued mapping of a certain type in a Hilbert space, μ is a bifurcation parameter. The main common feature of the problems under consideration is that they cannot be linearized and therefore the classical approaches to bifurcation and stability cannot be used.

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Existence of bounded trajectories via upper and lower solutions

Cristina Marcelli
Department of Mathematics - University of Perugia (Italy)
email: marcelli@unipg.it

The talk deals with the boundary value problem on the whole line

$$(P) \qquad \begin{cases} u'' - f(u,u') + g(u) = 0 \\ u(-\infty) = 0 \quad u(+\infty) = 1 \end{cases}$$

where $g : R \to R$ denotes a continuous non-negative function having support $]0,1[$, and $f : R^2 \to R$ is a continuous function. In [2] we propose a new approach in order to treat (P), based on a combination of lower and upper-solutions methods and phase-plane techniques, by means of which we achieve both an existence and non-existence result:

Main theorem. *Assume that* $f(u,0) = 0$ *for any* $u \in [0,1]$ *. Then, if*

$$\frac{f(u,u')}{u'} \geq 2\sqrt{\sup_{u\in]0,1]} \frac{g(u)}{u}} \qquad \text{for every } u \in [0,1], u' > 0 \tag{1}$$

problem (P) admits monotone solutions. Moreover, if the function $\frac{f(u,u')}{u'}$ *is non-decreasing with respect to* u'*, then the solution is unique (up to translation of the origin). Whereas, if*

$$\limsup_{(u,u')\to(0,0)} \frac{f(u,u')}{u'} < 2\sqrt{D_+ g(0)} \tag{2}$$

then problem (P) does not admit monotone solutions.

As an application of previous result we are able to discuss the existence of travelling wave solutions for a reaction diffusion equation of the general type (see [3])

$$\frac{\partial u}{\partial t} + \frac{\partial h(u)}{\partial x} = \frac{\partial}{\partial x}[d(u)\frac{\partial u}{\partial x}] + g(u)$$

which appears in several biological and chemical models (see i.e. [1] and [4]).

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Asymptotics, existence and stability of solutions with internal layers of "fast" and slow elliptic systems

Nikolai Nefedov
Lomonosov Moscow State University
email: nefedov@mt384.phys.msu.su

Elliptic problems, including systems with "fast" and slow equations are considered. We demonstrate our approach for the system

$$\varepsilon^2 \triangle u = g(u, v, x, \varepsilon), \ \triangle v = f(u, v, x, \varepsilon), \ x \in D \tag{1}$$

with prescribed boundary conditions on ∂D.

We give some sufficient conditions of existence of solutions with internal layers. The proof is based on asymptotic method of differential inequalities. Some relevant problems for integro-differential equations are also disscussed.

More detailed consideration of some of the presented problems in scalar case can be found in the papers [1-2].

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Multibump patterns near a co-dimension 2 point

Vivi Rottschäfer
Boston University
email: vivik@bu.edu

The behaviour of marginally unstable small solutions in a reaction-diffusion model problem is studied near a co-dimension 2 point. At this co-dimension 2 point the 'classical' Ginzburg-Landau equation approximation breaks down. In numerical simulations on the reaction-diffusion system asymptotically stable multibump patterns are observed. By applying normal form theory, these multibump patterns are found theoretically.

Stabilizing unstable periodic orbits in reaction diffusion systems by global time-delayed feedback control

Scott M. Zoldi
Los Alamos National Laboratory, Los Alamos, NM,USA
email: zoldi@cnls.lanl.gov

Giorgio Franceschini
Institut für Theoretische Physik, Technische Universität Berlin
email: franceschini@physik.tu-berlin.de

Sumit Bose
Institut für Theoretische Physik, Technische Universität Berlin
email: bose@physik.tu-berlin.de

Eckehard Schöll
Institut für Theoretische Physik, Technische Universität Berlin
email: `schoell@physik.tu-berlin.de`

The success of chaos control in high-dimensional spatially extended dynamical systems is examined by applying the extended time-delay autosynchronisation control method. The control technique is applied to a globally coupled reaction-diffusion system which describes charge transport in a bistable semiconductor. In our system, the control signal,

$$\epsilon(t) = K \left((1-R) \sum_{m=1}^{\infty} R^{m-1} y(t-m\tau) - y(t) \right) \qquad 0 \leq R < 1. \tag{1}$$

utilizes a control variable $y(t)$ given by the spatial average $y = \langle a \rangle$ of the field $a(x,t)$. We note that with increasing R orbits of higher period and orbits with larger Lyapunov exponents should be stabilized [1]. Using a damped Newton algorithm [2], we explicitly compute the unstable periodic orbits (UPOs) associated with the spatiotemporal chaotic reaction-diffusion system. A variety of spatiotemporal UPOs of period-one, period-two, or period-four can be stabilized if the product of the period τ and the largest Lyapunov exponent λ is less than 1.9. Even though we can compute spatiotemporal UPOs to within a high precision, we can not stabilize the computed long-period UPOs or UPOs with large Lyapunov exponents if $\lambda\tau > 1.9$. This result is in contrast with the approximate theoretical limit of control for low-dimensional temporal chaos [1] where stabilization is possible for $\lambda\tau \leq 2(1+R)/(1-R)$ using the extended time-delay autosynchronisation method.

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Patterns in an electrically driven conducting fluid layer

Norbert Seehafer
Institute of Physics, University of Potsdam, Germany
email: `seehafer@agnld.uni-potsdam.de`

Jörg Schumacher
Department of Physics, University of Marburg, Germany
email: `Joerg.Schumacher@physik.uni-marburg.de`

A numerical stability and bifurcation analysis is presented for an incompressible, viscous and electrically conducting fluid sheet, bounded by stress-free parallel planes and driven by an external electric field tangential to the boundaries. For the case of a uniform electrical conductivity it is found that the quiescent basic state, in which the current density is uniform and the magnetic field profile across the sheet linear, remains stable, no matter how strong the driving electric field. Instability is possible, however, for appropriately varying conductivity. We have studied in detail the Harris equilibrium, where the conductivity varies across the sheet in such a way that the current is largely concentrated in a layer centered about the midplane of the sheet and the magnetic field has a hyperbolic-tangent profile. A Squire's theorem could be proven stating that two-dimensional perturbations become unstable first. By varying several parameters of the equilibrium, stability boundaries were determined. The unstable perturbations are tearing modes, characterized by current filaments, magnetic islands associated with them and a fluid motion in convection-like rolls. Restricting the problem to two spatial dimensions, the nonlinear evolution of the tearing modes was followed up to time-asymptotic steady states. These are linearly stable with respect to two-dimensional perturbations, but prove to be sensitive to three-dimensional ones even close to the primary bifurcation point. Again stability boundaries were determind by varying the system parameters. The unstably perturbed states were followed up in their three-dimensional nonlinear evolution.

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Some Properties of Transcendental Integrable Dynamical Systems

Maxim V. Shamolin

Institute of Mechanics, Lomonosov Moscow State University

email: `shamolin@inmech.msu.su`

It is well-known that the concept of integrability has the various aspects due to in what functions an integration is made (analytical, smooth, meromorphic etc.) [1,2]. In the given activity the problem of integrability of systems of ordinary differential equations in the class of transcendental functions, i.e. functions, after which prolongation in complex area they have essentially singular points is discussed [2]. Concept of integrability of the class of transcendental functions arises for the reason of availability of this system asymptotic (attracting or repelling) limited sets, i.e. sets that have the neighborhood which consist of diversities of dimensionality above 1.

In this paper, we touch upon some qualitative questions of the theory of ordinary differential equations important for study of dynamical systems. The lots of them are arising in dynamics of a rigid body interacting with a medium. We shall review such problems as 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.

We are also dealing with the existence and uniqueness of trajectories of dynamical systems on a plane which have infinitely remote points as α- and ω-limit sets. So, on

Riemann or Poincare spheres, limit sets of such trajectories is the north pole. These are key trajectories by definition because an infinitely remote point is always singular [3-5].

Recall that in a phase space a trajectory is Poisson stable if in a finite time it returns to any sufficiently small neighborhood of its point.

Sufficient conditions for the existence of Poisson stable trajectories will be formulated in this work.

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5.8 Semiconductors

Organizer : Herbert Gajewski

Key note lecture

Wigner Transforms,Homogenisation and Dispersive Problems

Peter Markowich
Universitaet Wien
email: Peter.Markowich@univie.ac.at

It is well known by now that Wigner transforms are the appropriate tool to carry out the semiclassical limit of the Schroedinger equation. The weak limit of the Wigner transform of the wave function (the so called Wigner measure) then satisfies the Liouville phase space equation and limits of physical observables can be calculated by essentially computing moments of the Wigner measure. This limit procedure is not at all influenced by the possible occurance of caustics. In the talk we shall generalize the methodology of Wigner transforms to various applied p.d.e. problems. We consider zero pressure and compressible isentropic quantumhydrodynamics, the incompressible Euler limit from the nonlinear Schroedinger equation and mean field Schroedinger-Poisson coupling.

Also we show how the Wigner transform approach can be used to carry out homogenisation limits of quadratic functions (functionals) of solutions of linear and weakly nonlinear antiselfadjoint (pseudodifferential) initial value problems. As typical examples we discuss electrons in crystal lattices, the Maxwell equations in a periodic medium and the classical limit of the Dirac equation (to the relativistic Vlasov equation). Finally, we present a Wigner-function based method to derive dispersion and Morawetz-type estimates for wave-like equations.

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Invited lectures

Moment equations for carrier transport in semiconductors

Angelo Marcello Anile
Dipartimento di Matematica, Universitá di Catania, Italy
email: `anile@dipmat.unict.it`

Nikos Nikiforakis
D.A.M.T.P Cambridge University
email: `N.Nikiforakis@damtp.cam.ac.uk`

Rosa Maria Pidatella
Dipartimento di Matematica, Universitá di Catania, Italy
email: `rosa@dipmat.unict.it`

Hydrodynamical models are currently used in order to describe carrier transport in submicron semiconductor devices. Hydrodynamical models are obtained as moment equations of the kinetic Boltzmann transport equation, with appropriate closure assumptions. Lately a class of hydrodynamical models has been introduced with the closure based on the maximum entropy ansatz (in the formulation of Extended Thermodynamics) by Anile, Romano and Russo. Mathematically the models consist of a hyperbolic system of conservation laws with sources, endowed with convex entropy and coupled to the Poisson equation.

The simulation of a realistic device, like the $n^+ - n - n^+$ diode, introduces strong gradients in the density at the junctions and therefore requires, for an accurate solution, high order methods suitable for hyperbolic systems of conservation laws. In this article we report on the numerical solution of these models by using a high accuracy, high-order, centred TVD schemes namely the FLIC (Flux LImiter Centred) method introduced by Toro. The homogeneous part of the system was solved using the FLIC scheme, while various conventional methods were employed for the solution of the forcing terms in the framework of a splitting strategy. One of the important advantages of using the FLIC scheme is that this method can be implemented with ease for non stationary problems in several dimensions and arbitrary geometries. Various classes of models have been investigated (according to the various approximations which can be made when applying the maximum entropy approach) and the results have been compared with those of Monte Carlo simulations.

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About some mathematical questions concerning the embedding of Schrödinger–Poisson systems into the drift–diffusion model of semiconductor devices

Hans–Christoph Kaiser

Weierstrass Institute for Applied Analysis and Stochastics, Berlin

email: `kaiser@wias-berlin.de`

Joachim Rehberg

Weierstrass Institute for Applied Analysis and Stochastics, Berlin

email: `rehberg@wias-berlin.de`

Nanostructures — quantum wells, quantum wires and quantum dots — become ever more important for the performance of semiconductor devices. While Van Roosbroeck's equations provide a good landscape view on an electronic device, Schrödinger–Poisson systems portrait the individual features of a nanostructure within the device. This leads to the embedding of Schrödinger–Poisson systems, often including an effective Kohn–Sham operator, into phenomenological models for semiconductor devices. For connecting the different models boundary conditions for both Van Roosbroeck's equations and the Schrödinger–Poisson systems obviously play an important role. This leads to the question about the regularity of basic quantities as density and current on the interface between regions governed by different models.

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The dynamics of some quantum open systems with short-range nonlinearities

Francis Nier
CPT, Luminy Case 907, F-13288 Marseille Cedex 9, France
email: `nier@cpt.univ-mrs.fr`

We consider the simplest model of quantum open systems, which is the case of one-body statistical physics with inflow boundary conditions at infinity. We develop a functional framework for some nonlinear dynamics, where the nonlinearities are (very) short-range perturbations of a given Hamiltonian. In this framework, one can prove the global in time existence and uniqueness of a solution for the time dependent problem and the existence of steady states of which the form can be specified. This approach relies on some tools of quantum scattering theory, namely on Mourre theory and Sigal-Soffer propagation estimates. This problem arises from the modelling of semiconductors and the proposed functional framework especially applies to the models described in [1][2][3] and [4].

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Contributed talks

Mathematical analysis of electrostatics BVP for dielectrics in powerful electrical fields

Igor Brigadnov
North-Western Polytechnical Institute, St. Petersburg, Russia
email: `brigadnov@ip.nwpi.ru`

It is well known that in powerful electrical fields the behaviour of real dielectrics is essentially non-linear and it is not possible to use the linear model in many cases. For dielecrics with non-linear vector-function of saturation $D = D(x, E)$, the appropriate

BVP is formulated as the variational problem for the scalar electrical potential u such that $E = -\nabla u$. For dielectrics with ideal saturation, where $|D| \leq \lambda < +\infty$, the existence of the limited electrostatic load (such external charges with no solution of BVP) and discontinuous electrical potentials with breaks of the first type has been proved by the author recently [1]. From the physical point of view these effects are treated as the electrical puncture of dielectric.

For estimation of the electrical durability of the dielectrical body $\Omega \in R^3$ the following variational problem must be solved [1]

$$t_* = \inf \left\{ \int_\Omega |\nabla u(x)| \lambda(x)\, dx : \ u \in V, \ L(u) = 1 \right\}, \tag{1}$$

$$L(u) = \int_\Omega \rho u\, dx + \int_{\Gamma^2} \sigma u\, d\gamma, \qquad \lambda(x) = \liminf_{|E| \to \infty} \frac{\Phi(x, E)}{|E|},$$

$$\Phi(x, E) = E_i \int_0^1 D_i(x, tE)\, dt,$$

where $V = \{u \in W^{1,1}(\Omega) : \ u(x) = U(x), \ x \in \Gamma^1\}$ is the set of admissible electrical potentials, U is the given potential on a portion Γ^1 of the boundary $\partial\Omega$, ρ and σ are the external bulk and surface charges, respectively; $\Gamma^2 = \partial\Omega \setminus \Gamma^1$, $a_2 \geq a_1 > 0$ and $a_0 \in R$ are the constants. The limited electrostatic load is $(\rho_*, \sigma_*) = t_*(\rho, \sigma)$. If $t_* < 1$, then the appropriate electrostatics BVP has no solution.

From the mathematical point of view the variational problem (1) is non-correct and, therefore, needs regularization. We use the partial regularization which is based on the special discontinuous finite-element approximation (FEA) [2]. After this discontinuous FEA the problem (1) is transformed into the non-linear system of algebraic equations which is badly determined. Therefore, for the numerical solution the decomposition method of adaptive block relaxation is used [3,4]. The main idea of this method consists of iterative improvement of zones with "proportional" fields by special decomposition of variables, and separate calculation on these variables.

The numerical results show that, for finding the main parameter t_* of a limited electrostatic load, the proposed technique has the qualitative advantage over the standard continuous finite-element approimations.

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The Small Debye Lenght Limit in the Drift-Diffusion Model for Semiconductors

Ingenuin Gasser
Institut für Angewandte Mathematik, Universität Hamburg
email: gasser@math.uni-hamburg.de

We are going to study some aspects of the so called Drift Diffusion Model for semiconductors, which is well known from semiconductor physics. The equations for the electron and hole densities n^λ and p^λ, respectively, and for the electric field E^λ read

$$\begin{aligned} n_t^\lambda &= \mu_n(\Delta n^\lambda + \operatorname{div}(n^\lambda E^\lambda)) \\ p_t^\lambda &= \mu_p(\Delta p^\lambda - \operatorname{div}(p^\lambda E^\lambda)) \\ -\lambda^2 \operatorname{div} E^\lambda &= n^\lambda - p^\lambda - C \\ n^\lambda(t=0,x) = n_0^\lambda(x), &\qquad p^\lambda(t=0,x) = p_0^\lambda(x) \end{aligned}$$

with $x \in \mathbf{R^d}$, $t \geq 0$. The quantities μ_n, μ_p denote the electron and hole mobilities and $C = C(x)$ is the dopingprofile. A complete existence theory for this model was given in [1]. The problem we are going to focus on is the vanishing Debye length limit $\lambda \to 0$ (the superscript λ denotes the $\lambda-$dependence).

On the initial time layer scale $s = \frac{t}{\lambda^2}$ the formal limit equations for the limits n, p and F of n^λ, p^λ and $\lambda^2 E^\lambda$, respectively, are given by

$$\begin{aligned} n_s &= \mu_n \operatorname{div}(nF) \\ p_s &= \mu_p \operatorname{div}(pF) \\ -\operatorname{div} F &= n - p - C \\ p(t=0,x) = n_0(x), &\qquad n(t=0,x) = p_0(x), \end{aligned}$$

where n_0 and p_0 are the limits of n_0^λ and p_0^λ as $\lambda \to 0$. We give a rigorous prove of this fact and discuss the limit $s \to \infty$ in the limiting layer equations.

On the original (slow) time scale t the limit $\lambda \to 0$ is completely different. Formally, for $\mu_n = \mu_p = 1$ and $C = 0$ we obtain quasineutrality $n - p = 0$ and as limit the heat equation for the limit w of $w^\lambda = n^\lambda + p^\lambda$

$$\begin{aligned} w_t &= \Delta w \\ w(0,x) &= n_0(x) + p_0(x). \end{aligned}$$

We show this rigorously using an entropy estimate. The cases for differing μ_n and μ_p and nonvanishing C are studied in [2].

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Rigorous derivation of a hierarchie of macroscopic models for semiconductors and plasmas

Ansgar Jüngel
Fachbereich Mathematik, Technische Universität Berlin
email: `jungel@math.tu-berlin.de`

Under special physical conditions, certain parameters in the quasi-hydrodynamic equations for semiconductors and plasmas are small compared to reference values. Neglecting the corresponding terms, one gets simplified equations which are numerically easier to solve and which contain the important physical informations. The study of the asymptotic limits and their mathematical verification is of great importance to understand the validity of the various models.

In this talk we analyze three asymptotic limits: relaxation-time limit, zero-electron-mass limit, and zero-space-charge limit in the hydrodynamic (Euler-Poisson) model and the drift-diffusion equations. In particular, we prove the following:

(i) *Zero-electron-mass limit.* When the kinetic energy of the electrons is small compared to the kinetic energy of the positively charged ions (in plasmas) or holes (in semiconductors), the continuity equation for the electrons can be reduced asymptotically to a nonlinear relation between the electro-static potential and the electron density, such that the Poisson equation becomes nonlinear. This model is known by physicists for 'weakly ionized plasmas'. The limit is studied both in the hydrodynamic and the drift-diffusion equations [1,3].

(ii) *Relaxation-time limit.* In the relaxation-time limit, the hydrodynamic model reduces to the drift-diffusion model. This limit is performed for both weakly ionized and not weakly ionized plasmas in the adiabatic (or isentropic) case [2,4].

(iii) *Zero-space-charge limit.* For small scaled Debye lengths, the electron and ion densities are comparable. We study this limit rigorously for the drift-diffusion equations [5]. In the case of plasmas, this limit is also called quasi-neutral limit.

The proofs of the above results are all based on a priori estimates given by the entropy functional and appropriate compactness methods (compensated compactness, compactness-by-convexity). The entropy estimates are useful not only for the hyperbolic Euler equations, but also for the parabolic drift-diffusion models. Therefore, the entropy method proves to be a very powerful tool also for parabolic systems.

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Asymptotics of bound states and resonances for laterally coupled waveguides

Igor Yu. Popov
Leningrad Institute of Fine Mechanics and Optics, Sablinskaya, 14, St.-Petersburg, 197101, Russia
email: popov@mail.ifmo.ru

Sergei V. Frolov
Leningrad Institute of Fine Mechanics and Optics

A problem of quantum waveguides with Dirichlet boundary condition which are coupled laterally through small apertures of width $2a$ is considered. Asymptotics in a of an eigenvalue close to the threshold is obtained. The result is in good correlation with variational estimates of Exner and Vugalter and with the corresponding results for zero-width slit model based on the theory of self-adjoint extensions of symmetric operators (Popov). The cases of two different and two identical waveguides are studied. The asymptotics of the eigenvalue for waveguides coupled through finite number of windows is obtained. It is shown that a measure of "common width of apertures" is a sum of two-dimensional harmonic capacities of the windows. Asymptotics of real and imaginary part of resonances (quasi-bound states) close to $N-$th threshold ($N > 1$) is found. The background for the construction is the method of matching of asymptotic expansions of solutions of boundary problems.

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Simulation of current filamentation in an extended drift-diffusion model

Georg Schwarz
Institut für Theoretische Physik, Technische Universität Berlin
email: schwarz@physik.tu-berlin.de

Eckehard Schöll
Institut für Theoretische Physik, Technische Universität Berlin
email: schoell@physik.tu-berlin.de

Reiner Nürnberg
Weierstraß-Institut für Angewandte Analysis und Stochastik Berlin
email: `nuernberg@wias-berlin.de`

Herbert Gajewski
Weierstraß-Institut für Angewandte Analysis und Stochastik Berlin
email: `gajewski@wias-berlin.de`

We simulate the nonlinear spatio-temporal dynamics of current filaments in doped semiconductors in the regime of low temperature impurity breakdown. Charge transport is modeled by a drift-diffusion approach combined with local generation-recombination (GR) kinetics describing the autocatalytic impurity impact ionization which sets in above a certain threshold field. This is shown to result in an S-shaped current density-field relation. The parameters of our model have been determined by a Monte Carlo simulation of the microscopic scattering processes. The transport equations are solved self-consistently with Poisson's equation on two-dimensional spatial domains using a finite element discretization in space and a backward Euler scheme in time. Because of the very different timescales, and the steep spatial gradients between the current density inside and outside the filaments, which differ by several orders of magnitude, our problem poses high challenges to the numerics.

We consider different sample geometries, where we employ Dirichlet boundary conditions at the contacts and Neumann boundary conditions elsewhere. For a rectangular spatial domain with two small circular contacts we find that the nascence of current filaments upon application of a dc bias is induced by two impact ionization fronts originating from both cathode and anode. After their coalescence they form a pre-filament between the two contacts which subsequently grows into a fully developed filament. The action of an external perpendicular magnetic field leads to an asymmetrically broadened or bent filament due to the Lorentz force. For radially symmetric samples with two concentric circular contacts ("Corbino disks") we find spontaneous symmetry breaking which results in a break-up of the initial radial impact ionization front into several streamers. These develop into a number of radial pre-filaments. Due to the global coupling via the external load resistance competition between the pre-filaments occurs, with only a limited number of them surviving as stable filaments depending upon the bias conditions ("winner takes all dynamics"). Our results are in good agreement with experimental investigations of current filamentation in thin n-doped GaAs films at low temperatures for different contact geometries [1].

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5.9 Steady Water Waves

Organizer : Gérard Iooss

Key note lecture

Phenomena beyond all orders and bifurcation of reversible homoclinic connections

Eric Lombardi
I.N.L.N, UMR 6618 CNRS-UNSA, Nice, France
email: `lombardi@inln.cnrs.fr`

We have developed a general method to obtain an exponentially small equivalent of oscillatory integral when it involves solutions of *nonlinear differential equations.* The method is based on a very precise description of the holomorphic continuation of the solutions of the perturbed equation and in particular of their behavior near the complex singularities of the solutions of the unperturbed system. The method that we use to build step by step the holomorphic continuation of the solutions is a rigorous version for this problem of the formal theory of Matching Asymptotic Expansions (M.A.E.). In particular, the construction of the holomorphic continuation of the solutions near the singularities is based on the study of an "inner system" which is well known in the theory of M.A.E. and which appears to be the relevant part of the equation near the singularities.

This method enables us to study the problem of the persistence of homoclinic connections to 0 for the one parameter families $V(.,\mu)$ of reversible vector fields which admit at the origin a $0^2 i\omega$ resonance, i.e. vector fields for which the origin is a fixed point and for which 0 is a double non semi simple eigenvalues and $\pm i\omega$ are simple eigenvalues of the differential at the origin $DV_u(0,0)$. This problem cannot be solved by a direct Melnikov approach since the Melnikov function is given by an oscillatory integral and is exponentially small. Our "Exponential tools" enable us to prove [2] that generically, vector fields admitting at 0 a $0^2 i\omega$ resonance at the origin do not admit any homoclinic connection to 0, whereas we proved in [1] that they always admit homoclinic connections to exponentially small periodic orbits. One example of such a vector field in infinite dimensions occurs when describing the irrotational flow of an inviscid fluid layer under the influence of gravity and small surface tension (Bond number $b < 1/3$) for a Froude number F close to 1. In this context a homoclinic connection to 0 would be called a solitary wave.

We have also developed a general method to obtain an exponentially small equivalent of bi-oscillatory integrals. In this case, the interaction between the two frequencies, makes the study more intricate and a partial complexification of time is necessary. This last method enables to study the $(i\omega_0)^2 i\omega_1$ resonance, i.e. one parameter families $V(\cdot,\mu)$ of reversible vector fields for which $\pm i\omega_0$ are a double non semi simple eigenvalues and $\pm i\omega_1$ are simple eigenvalues of the differential at the origin $DV_u(0,0)$. Such a resonance occurs for water waves when studying several layers problems and for chains of coupled nonlinear oscillators.

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Invited lectures

Symplecticity and criticality: extending criticality to finite-amplitude vortical steady waves

Tom Bridges
University of Surrey
email: mas1tb@mcs.surrey.ac.uk

At the cornerstone of the theory and practice of open channel hydraulics is the concept of criticality of uniform flows. In the setting of uniform flows, criticality can be defined in a number of different – but equivalent – ways, but the most fundamental definition is generally given in terms of an energy-momentum argument. Considering the fundamental nature of criticality, it is remarkable that it has never been generalized as far as we are aware to finite-amplitude states or any steady state wave other than a uniform flow. On the other hand it is not at all obvious how this might be accomplished. In this talk we show that the classical definition can be interpreted in terms of a symplectic variational principle, and that this definition easily generalises. The theory is then applied to steady water waves with constant vorticity. Much like in the uniform flow case, we show that criticality for finite-amplitude steady water waves is related to the bifurcation of solitary waves, although in this case the solitary waves are biasymptotic to periodic travelling waves of finite amplitude.

Multiplicity of algebraically decaying solitary waves

Boris Buffoni
Department of Mathematics, Swiss Federal Institute of Technology–Lausanne
email: Boris.Buffoni@epfl.ch

Philippe Bolle
Département de mathématiques, Université d'Avignon
email: Philippe.Bolle@univ-avignon.fr

It is known that, for appropriate values of the parameters (densities, gravity, surface tension, depths of the layers, propagation speed), two solitary waves decaying algebraically exist at the interface between two finite layers of perfect fluids [1]. The mathematical model consists of a system of partial differential equations with a free boundary. It can be reduced by the centre-manifold theorem to a four-dimensional Hamiltonian system with a centre equilibrium that has two non semi-simple and imaginary eigenvalues. Homoclinic orbits, which correspond to solitary waves, are then obtained by normal form theory and a careful persistence analysis.

Our main result states that there are not only two solitary waves, but in fact infinitely many that decay algebraically. More precisely, either there is a circle of solitary waves or we can establish the existence of so-called "multibump" solutions, in the spirit of [2] where saddle-focus equilibria are considered.

The dynamics near the centre can only be fully understood by taking into account the third and fourth order terms of the Taylor expansion of the Hamiltonian at the equilibrium. In general it is not true that the set of points in the phase space that converge to a centre is a manifold. Thanks to the fact that some coefficient of the normal form at the centre is negative, we can nevertheless establish the existence of two-dimensional stable and unstable manifolds made of orbits converging polynomially to the equilibrium. Moreover the Calculus of Variations allows us to obtain other orbits near the equilibrium that are reminiscent of those provided by the lambda-lemma in hyperbolic dynamical systems.

Then we show that the existence of a homoclinic orbit that is the topological intersection of the stable and unstable manifolds implies the existence of infinitely many "multibump" homoclinic solutions and the topological entropy of the system is positive. In addition, for interfacial waves, if the intersection is not topologically transverse, we can deduce that the stable and unstable manifolds coincide and consist of a circle of homoclinic orbit.

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Interfacial waves in the presence of a free surface

Frédéric Dias
Institut Non-Linéaire de Nice
email: `dias@inln.cnrs.fr`

In a two-fluid system where the lower fluid is bounded below by a rigid bottom and the upper fluid is bounded above by a free surface, two kinds of solitary waves can propagate along the interface and the free surface: classical solitary waves characterized by a solitary pulse or generalized solitary waves with in addition nondecaying oscillations in their tails. The origin of these nonlocal solitary waves can be easily understood from a physical point of view. The dispersion relation for the above system shows that short waves can propagate at the same speed as a solitary wave. The interaction between the solitary wave and the short waves creates a nonlocal solitary wave. In this talk, the interfacial-wave problem is reduced to a system of ordinary differential equations by using a classical perturbation method. The classical as well as the generalized solitary waves which are solutions of this system of model equations are constructed.

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Two- and three-dimensional steady gravity-capillary water waves via Hamiltonian spatial dynamics

Mark Groves
Loughborough University, UK
email: `M.D.Groves@lboro.ac.uk`

The hydrodynamic problem concerning the irrotational flow of a perfect fluid of constant density in a domain bounded above by a free surface and below by a rigid bottom is known as the water-wave problem. Here we examine the gravity-capillary steady water-wave problem, in which the fluid is acted upon by the forces of gravity and surface tension and all waves are uniformly translating with constant speed. The problem depends upon two dimensionless combinations α and β of the various physical quantities. We consider the two-dimensional version of the problem, in which x is the horizontal direction of uniform translation and y points vertically upward, together with a three-dimensional version in which the waves have an additional periodic dependence upon the horizontal direction z perpendicular to x.

Starting from a variational principle, we show that the two- and three-dimensional steady water-wave problems can be formulated as infinite-dimensional Hamiltonian systems in which x plays the role of the time-like variable. A centre-manifold reduction technique is then used to show that the problem is locally equivalent to an ordinary differential equation whose solution set can be analysed. In the two-dimensional problem we look for the existence of solitary waves, that is solutions to the system which decay to zero at large values of $|x|$. We identify two regions (I and II) of (β, α)-parameter space in which the system has infinitely many solitary waves. In region I these waves are multi-troughed waves of depression with exponentially decaying outskirts; in region II they are modulated waves.

In the three-dimensional problem we identify regions of (β, α)-parameter space in which there are generalised solitary waves, that is waves which decay to a spatially periodic motion at large $|x|$. In particular, we find a family of three-dimensional disturbances which decay to two-dimensional periodic waves at large $|x|$.

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Three-dimensional capillary-gravity waves

Mariana Haragus-Courcelle
Mathematisches Institut A, Universität Stuttgart, Germany
email: `haragus@mathematik.uni-stuttgart.de`

We study analytically the existence of three-dimensional (3D) surface waves, i.e. waves for which the associated free-surface displacement varies in two horizontal directions, the third direction being the vertical direction, as solutions of the full Euler equations. The waves are assumed to travel at a constant speed on the free surface of an inviscid fluid layer of finite depth under the influence of gravity and surface tension. We consider small-amplitude waves bifurcating from the state of rest that are periodic in one of the two horizontal directions.

The method which we apply is based on ideas from the theory of dynamical systems. The water-wave problem is formulated as a dynamical system in which the evolutionary variable is the variable in the unbounded horizontal direction. The bounded solutions are orbits in an infinite-dimensional phase-space consisting of functions living on the bounded cross-section of the domain. Restricting to solutions of small amplitude the corresponding orbits live on a finite-dimensional - center - manifold and are described by a finite-dimensional system of ODEs. The normal form of this system can be obtained. The reversibility and the $O(2)$-symmetry of the system play an important role in the analysis.

Two types of 3D waves are considered: waves which are periodic in the direction transverse to propagation that we call periodically modulated traveling waves, and waves which are periodic in the direction of propagation that we call periodic traveling waves. We have two different formulations of the system depending on which of the two types of waves above we are looking for. In both cases, an infinite sequence of bifurcations of increasing complexity as the surface tension tends to zero is found. In the case of periodically modulated traveling waves, the simplest bifurcation, for the lowest periodic mode, leads to a reduced system of dimension ten, and in the case of periodic traveling waves, to a reduced system of dimension four. Various types of 3D symmetric or asymmetric waves are obtained. Similar waves have been found for a model equation for three-dimensional water-waves in [2] and [3]. For the Euler equations, several types of reversible periodically modulated traveling waves have been constructed in [1] by using a Hamiltonian formulation of the system.

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Gravity and Capillary-gravity traveling waves for superposed fluid layers, one being deep

Gérard Iooss
Institut Universitaire de France, INLN, UMR CNRS-UNSA 6618,
1361 route des Lucioles, F-06560 Valbonne
email: `iooss@inln.cnrs.fr`

The mathematical study of 2D traveling waves in the potential flow of two superposed layers of perfect fluid, with free surface and interfaces (with or without surface tensions) and with the bottom layer of infinite depth, is formulated as a *ill-posed reversible evolution problem*, in a suitable function space, where the horizontal coordinate plays the role of a "time". We give the structure of the spectrum of the linearized operator L_μ near equilibrium (μ denotes the set of parameters). This spectrum consists in a set of isolated eigenvalues of finite multiplicities, a small number of which lie near or on the imaginary axis, and of the *entire real axis* which constitutes the *essential spectrum* where there is no eigenvalue, except 0 in some cases.

A *normal form analysis in infinite dimensional space* is performed. We split the space into i) an invariant subspace belonging to the continuous spectrum (which crosses the imaginary axis) and to eigenvalues far from the imaginary axis and ii) a complementary invariant subspace belonging to eigenvalues near or on the imaginary axis, including 0, if this one is an eigenvalue. This splitting and normal form analysis are made possible thanks to the explicit knowledge of the resolvent of the linear operator L_μn near 0, and to good estimates of the resolvent on the imaginary axis.

Concerning periodic waves, we give a general constructive proof of bifurcating solutions, adapting the Lyapunov-Schmidt method to the present (reversible) case where 0 (which is "resonant") belongs to the continuous spectrum. In particular we give the results for the generic case and for the 1:1 resonance case.

For the 1:1 resonance case, (with an additional 0 eigenvalue embedded in the continuous spectrum in some cases), in the case of the two reversible homoclinic orbits for the reduced normal form, we can show that they do persist for the full system. They correspond to *traveling solitary waves*, with oscillations *algebraically damped* at infinity (the non exponential damping being due to the continuous spectrum).

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Existence and Non-existence of Solitary Waves in Water

Shu-Ming Sun

Virginia Polytechnic Institute and State University

email: `sun@math.vt.edu`

This talk concerns permanent capillary-gravity waves on the free surface of a two-dimensional incompressible inviscid fluid of finite depth with small surface tension. Assume that the flow is irrotational and a single hump wave, called solitary wave, moving with a constant speed will be studied. The existence of solitary waves with small oscillations at infinity, called generalized solitary waves, is considered and the relationship between the amplitude and the phase shift of the oscillation is fully discussed. There are two approaches to obtain the generalized solitary waves, assuming the magnitude of the amplitude first or fixing the phase shift first. It will be shown that the generalized

solitary waves obtained from these two approaches are actually connected. By letting the amplitude be a function of the phase shift δ and the long-wave parameter ϵ, it is obtained that there exists a curve in δ-ϵ plane. When δ and ϵ are near this curve, the amplitude can become arbitrary large. Otherwise, the amplitude is exponentially small. For some surface tension close to 1/3, the amplitude never become zero for small ϵ, which gives the non-existence of truly solitary waves.

Contributed talks

The wave resistance problem for a surface-piercing body

Carlo Domenico Pagani
Politecnico di Milano, Italy
email: carpag@mate.polimi.it

Dario Pierotti
Politecnico di Milano, Italy

One considers a "slender" cylinder semisubmerged in a heavy incompressible and inviscid fluid and moving at uniform, supercritical speed in the direction orthogonal to its generators; the problem is to find the resulting steady two-dimensional flow.

By a hodograph transformation, the problem (originally set up in a domain with a free boundary) reduces to the determination of a function, holomorphic in a fixed domain, satisfying different conditions (one of which, the Bernoulli condition, is nonlinear) on different parts of the boundary; but two separating points between these parts, corresponding to the points of contact fluid-cylinder, are unknown and their determination is part of the problem. One proves the existence of a "smooth" solution for which the free boundary and the cylinder profile (which is assumed convex and reasonably smooth) form a single C^1–streamline; furthermore the free boundary is monotone increasing downstream, monotone decreasing upstream and lies under the level of calm water. This is not the only solution of the problem; for one proves that under additional assumptions, another solution exists, which is singular at the contact points fluid-cylinder; such points appear as stagnation points for the flow.

The linear approximation of the wave resistance problem (called Neumann-Kelvin problem) has been extensively studied (see, e.g. [1] and [2]). The analogous problem for a completely submerged body has been treated in [3] and [4].

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5.10 Unsteady Hydrodynamic Waves

Organizer : John F. Toland

Key note lecture

Boundary Integral Methods for Water Waves

J. Thomas Beale
Duke University
email: `beale@math.duke.edu`

We discuss numerical methods for time-dependent water waves and the analysis needed to prove the convergence of properly designed versions to the actual solution. Boundary integral methods have been widely used for water waves; they are based on singular integrals arising from potential theory. The water surface is tracked by points which move with the fluid velocity. The velocity is determined from an integral equation on the surface. (For a recent survey, see [2].) We will begin by reviewing the equations of water waves and their qualitative properties. We then present the boundary integral formulation and describe its use as a numerical method, with emphasis on the three-dimensional case. In [1] a version of the boundary integral method for doubly periodic water waves is proved to converge to the actual solution. We will discuss several issues related to the design and analysis of this method. A new approach is used for the computation of singular integrals, such as a single layer potential on a surface; the Green's function is regularized and an efficient local correction is computed for the trapezoidal sum. The numerical stability depends on choosing discretizations so that the errors are governed by equations with structure analogous to that of the full equations. For the stability estimates, mapping properties of the discrete integral operators are used which are found by treating the sums as discrete versions of pseudodifferential operators. The Dirichlet-to-Neumann operator on the surface is a fundamental part of the equations of motion; the wavelike character of the motion depends on the positivity of this operator. Similarly, the stability of the numerical method seems to depend on the positivity of the discrete version of this operator.

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Invited lectures

Nash-Moser Theory for Standing Water Waves

Pavel Plotnikov
Lavrentyev Institute of Hydrodynamics
email: Plotnikov@hydro.nsc.ru

John F. Toland
University of Bath
email: J.F.Toland@maths.bath.ac.uk

Unlike progressive (or steady) Stokes waves, standing waves are a truly time-dependent phenomenon in the sense that they can not be regarded as stationary relative to a moving reference frame and we believe that, until now, there has been no existence theory, even for the case of small amplitude waves.

Our purpose is to show how the Nash-Moser iteration method can be used to give a rigorous proof of the existence of certain small-amplitude standing water waves on an incompressible irrotational flow of finite depth over a horizontal bottom under gravity, when surface tension is neglected. The waves in question are solutions of the Euler equations, formulated in Lagrangian coordinates, for an ideal incompressible fluid which satisfy exactly the constant-pressure and kinematic boundary conditions on the free surface. But in addition, the solutions for which existence is established satisfy further constraints which are expressed in terms of the normal component of pressure gradient on the free surface. These constraints are designed to facilitate the mathematical development here, with particular regard to the method for obtaining a priori bounds necessary for the Nash-Moser method. They have no obvious analogue for it in the theory of Stokes waves.

Because the proof is long and quite technical it will be possible only to outline the main result and to sketch the method in the limited time available.

Justification of quasistationary approximation in the problem of evolution of a capillary drop

Vsevolod Solonnikov
V.A.Steklov Mathematical Institute, S.Petersburg Department
email: solonnik@pdmi.ras.ru

The problem of motion of a viscous capillary drop consists in the determination of a bounded domain $\Omega_t \subset R^3$, of the velocity vector field $\vec{v} = (v_1(x,t), v_2(x,t).v_3(x,t))$ and of the scalar pressure $p(x,t)$, $x \in \Omega_t$, satisfying the Navier-Stokes equations

$$\varepsilon(\vec{v}_t + (\vec{v}\cdot\nabla)\vec{v}) - \nabla^2\vec{v} + \nabla p = 0, \qquad \nabla\cdot\vec{v} = 0, \tag{1}$$

initial condition

$$\vec{v}(x,0) = \vec{v}_0(x) \tag{2}$$

in a given domain Ω_0 and the conditions at the free boundary $\Gamma_t = \partial\Omega_t$

$$\vec{v}\cdot\vec{n} = V_n, \qquad T(\vec{v},p)\vec{n} - H\vec{n} = 0. \tag{3}$$

Here ε is a positive parameter proportional to the Reynolds number, V_n is the velocity of evolution of Γ_t in the normal direction $\vec{n}$, T is the stress tensor and H is the doubled mean curvature of Γ_t. Quasistationary approximation consists in setting $\varepsilon = 0$ in (1) (which removes the time derivative $\vec{v}_t$ and the nonlinear term) and in the elimination of the initial condition (2) for $\vec{v}$ (but not for Ω_t). One can expect that the approximating solution is close to $(\vec{v}, p)$ in the case of small ε.

We prove that the problem (1)-(3) is uniquelly solvable on a certain finite time interval $(0, t_1)$ independent of ε and that the difference between the exact and the approximating solutions has the order of magnitude $O(\varepsilon)$ for $t > t_0 > 0$.

The proof is based on a new Schauder type estimate for the linearized problem (1)-(3).

Well-posedness in Sobolev spaces of the full water wave problem

Sijue Wu
Univ. of Maryland and Univ. of Iowa
email: `sijue@math.umd.edu`

We consider the motion of the interface separating an inviscid, incompressible, irrotational fluid from a region of zero density in the three dimensional space; we assume that the fluid region is below the region of vacuum and the fluid is under the influence of gravity and the surface tension is zero. Assume that the density of mass of the fluid is one, the gravitational field is $(0, 0, -1)$, and at time $t \geq 0$, the free interface is $\Sigma(t)$, and the fluid occupies the region $\Omega(t)$, the motion of the fluid is described by

$$\begin{aligned} v_t + v \cdot \nabla v &= -(0,0,1) - \nabla p \qquad on\ \Omega(t),\ t \geq 0, & (1)\\ div\, v &= 0 \qquad on\ \Omega(t),\ t \geq 0, & (2)\\ curl\, v &= 0, \qquad on\ \Omega(t),\ t \geq 0. & (3)\end{aligned}$$

where $v = (v_1, v_2, v_3)$ is the fluid velocity, p is the fluid pressure. Since we neglect the surface tension, the pressure is zero on the interface. So on the interface:

$$p = 0, \qquad on\ \Sigma(t) \tag{4}$$

$$(1, v) \text{ is tangent to the free surface } (t, \Sigma(t)). \tag{5}$$

The above model is a 3-dimensional water wave model. It is generally known that when surface tension is neglected, the motion of the interface between an inviscid fluid and vacuum under the influence of gravity can be subject to Taylor instability [1], [2]. In a previous work [3], we studied the 2-dimensional water wave model, we showed that for 2-D water wave, the sign condition relating to Taylor instability always holds for nonself-intersecting interface, that is, the motion of the interface is not subject to Taylor instability; we showed further that the 2-D full nonlinear water wave problem is wellposed in Sobolev spaces, locally in time, for any initially nonself-intersecting interface.

In this talk, I will show that the results we obtained for the 2-D water wave also hold for 3-D, that is, the motion of 3-D water wave is not subject to Taylor instability and the full 3-D water wave problem is uniquely solvable in Sobolev spaces for any nonself-intersecting initial interface. I will demonstrate that Clifford analysis is an effective tool for 3-D water wave problem.

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Contributed talks

Surface waves for an incompressible ideal fluid

Atusi Tani
Keio University
email: `tani@math.keio.ac.jp`

In this communication, we are concerned with a free boundary problem for the motion of an incompressible ideal fluid under the gravitational field in a two-dimensional domain of infinite extent and of finite depth. Our problem is to find the two-dimensional domain occupied by the fluid which is bounded below by the fixed bottom and above by the free surface together with the velocity vector field and the pressure of the fluid satisfying the system of Euler equations and the initial-boundary conditions. The Euler equations consist of the conservations of mass and momentum under the gravitational field in a downward direction. The purpose of this paper is to establish the temporary local solvability in a Sobolev space.

We also consider the same problem as above taking into account of the surface tension on the free surface. For this problem we prove the temporary local existence theorem irrespective of the direction of the gravitational field, and the convergence of this solution to the cprreponding one as the surface tension coefficient tends to zero if the gravitational field acts in a downward direction.

For the proof, we rely on the methods due to Nalimov and Yosihara for the water waves, and to Iguchi-Tanaka-Tani for the vortical water waves of infinite depth.