Mathematisches Forschungsinstitut Oberwolfach

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Reactive Flow and Transport Through Complex Systems

Organised by
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Oktober 30th – November 5th, 2005

ABSTRACT. The meeting focused on mathematical aspects of reactive flow, diffusion and transport through complex systems. The research interest of the participants varied from physical modeling using PDEs, mathematical modeling using upscaling and homogenization, numerical analysis of PDEs describing reactive transport, PDEs from fluid mechanics, computational methods for random media and computational multiscale methods.

Introduction by the Organisers

The workshop *Reactive Flow and Transport Through Complex Systems*, organized by Cornelius J. van Duijn (Eindhoven), Andro Mikelić (Lyon) and Christoph Schwab (Zürich) was held October 30th–November 5th, 2005.

This meeting was attended by over 46 participants with broad geographic representation from all continents.

The theme of the conference,

modeling, analysis and numerical simulation of diffusion and transport processes in complex systems,

is a response to the need for more accurate, quantitative prediction in a growing number of scientific disciplines, particularly those related to biological applications. Here, simple mathematical models have been found, in particular due to the vastly increased available experimental data from these systems, to offer only inadequate and incomplete understanding of the observed phenomena.

This resulted in increased requirements for quantitative, verified predictions from sophisticated mathematical as well as computational models. The continuous development of complex mathematical and computational models and their

verification and validation against available experimental data is a continuous source of challenges for applied and computational mathematicians.

The complexity of the systems arises from several sources: highly irregular geometries of membranes and interfaces (as, e.g. in bone marrow, cell membranes, root systems of plants, membrane structures in human organs), physical or chemical properties of the systems (e.g., models for spread of pollution in underground medium which has uncertain material properties, where chemical reactions take place between constituents, and where strong transport effects on a macroscopic scale coexist with diffusion phenomena at the grain interfaces).

Quantitative mathematical and computational models of such phenomena are not only essential for a deeper understanding of these systems but, at least equally importantly, are a keystone in the development of new technologies which increasingly mimic and adapt biological phenomena for industrial purposes (e.g., root-reactor technology for the efficient production of organic compounds, bioinspired catalysts for waste processing, to name but a few).

Accordingly, the rather wide scope of the topic of the conference and the blend of researchers working in several areas of applied mathematics was a necessary condition to review modelling approaches across a number of application areas as well as across several mathematical disciplines.

Accordingly, during the meeting, talks were presented on homogenization, analysis and computation of multiscale problems, models of porous media, biological flow problems, to name but a few.

In addition to the regular presentations, there were three evening sessions organized "on the spot" based on the discussions which started in the first half of the meeting. These were in each case opened by a presentation from a person invited by the organizers, and were devoted to the topics:

(1) Mathematical Models in Biology – Results and challenges in the mathematical modelling of biological systems, (animated by W. Jäger, Uni and IWR Heidelberg),
(2) Density driven flows – analytical and computational results and challenges (animated by C. van Duijn, Einhoven and F. Otto, Bonn),
(3) Numerical Models of PDEs with stochastic coefficients (animated by H. Matthies, TU Braunschweig and by C. Schwab, ETH)

The presentations of the experts present at the meeting comprised, naturally, a much wider scope of topics:

- – Flow, transport and reactions in micro-reactors and micro-channels
- – Effective laws for processes on surfaces
- – Effective laws for transports and reactions in membranes
- – Polymer flow through porous media
- – Homogenization of processes in networks (neural networks, vessels .....)
- – Overall elastic properties of fiber structures and textiles
- – Flow through deformable structures with evolving process depending geometry
- – Growth of crystals, biological structures like dendrites or vessels.

- – Flow and transport in bifurcating vessels with rigid and flexible walls
- – Effects of walls
- – Wall laws and interface laws

These talks touched on advanced mathematical methods from dynamical systems, especially infinite dimensional ones arising with spatially heterogeneous problems (PDEs), asymptotic analysis, homogenization and averaging methods, numerical multiscale methods, methods from stochastic analysis and statistics.

Apart from advancing *disciplinary* mathematical methods in these areas, in the present meeting also qualitatively new mathematical developments emerged: for example, mathematical and computational modelling of PDEs with stochastic data which are spatially inhomogeneous and do *not* satisfy stationarity or ergodic hypotheses.

In processing experimental data (which becomes increasingly available at lower cost and, e.g. through modern scanning techniques, also at high volume and spatial and temporal resolution) new techniques of image and data processing have to be developed, and the mathematical models of complex systems have to allow for incorporation of statistical data extracted from these experiments.

This has repercussions for the mathematical research *and* implies that novel algorithms are needed to generate computational grids adapted to voxel data.

In the last five years mathematicians from analysis, stochastics and numerics started cooperation in this interdisciplinary field of research.

New journals specifically devoted to these issues such as the SIAM Journal of Multiscale Analysis and Simulation, have been successfully launched.

The previous meeting in Oberwolfach " Multiple Scale Systems - Modeling, Analysis and Numerics " from July 27 to August 2, 2003, gathered 42 scientists, among them approximately 15 junior scientists, from these areas.

Since multiscale tools are crucial in many of the above themes, in the previous meeting mainly diffusion problems were treated. Reactive flow and transport, which were central themes in the present meeting, emerged only recently as key issues.

The meeting was, exactly because of its wide scope, successful particularly in cross fertilizing different areas of applied mathematics and also raised a huge number of questions and challenges to participants documenting that the applications of mathematics to biological, social and other "complex systems" which has been emerging in the past years, is in the process of gaining momentum and, more importantly, stimulates development of new techniques and approaches in applied and computational mathematics at an increasing rate.

List of all talks

- Monday, October 31, 2005:
    - 9h15–10h: Andrea BRAIDES: A Model for a Weak Membrane with Defects
    - 10h-10h45: Gregory A. CHECHKIN: Prandtl boundary layer equations in the presence of rough boundaries
    - 11h30–12h30: Eduard MARUŠIĆ-PALOKA: Rigorous Justification of Compressible Reynolds Equation for Gas Lubrication
    - 16h-16h45: Maria NEUSS-RADU : Homogenization of thin porous layers and applications to ion transport through channels of biological membranes
    - 16h45–17h30: Angela STEVENS: Propagation speed in inhomogeneous media
    - 17h45–18h30: Barbara NIETHAMMER: A statistical mechanics approach for effective theories of domain coarsening
- Tuesday, November 1, 2005
    - 9h00–9h45: Hermann G. MATTHIES: Computational Approaches for Stochastic Models in Flow Through Stochastic Porous Media
    - 9h45-10h30: Assyr ABDULLE: Fully Discrete Heterogeneous Multiscale Methods and Application to Transport Problems in Microarrays
    - 11h–11h45 Radu A. TODOR: Sparse Perturbation Algorithms for Elliptic Problems with Stochastic Data
    - 15h30–16h15: Guy BOUCHITTÉ: Some asymptotic problems on optimal transportation.
    - 16h15-17h: Michel LENZINGER: Viscous fluid flow in bifurcating channels and pipes
    - 17h15–18h René de BORST: Stability and Dispersion in Damaging Multiphase Media
- Wednesday, November 2, 2005
    - 9h00–9h45: Michel KERN: Reactive Flow and Transport Through Complex Systems
    - 9h45-10h30: Vincent GIOVANGIGLI: Gaseous flows with multicomponent transport and complex chemistry
    - 11h–11h45 Sorin I. POP: Dissolution and Precipitation in Porous Media
    - 11h45 – 12h30: Giovanna GUIDOBONI: Uniqueness of weak solutions for a fluid-structure interaction problem

- Thursday, November 3, 2005
    - 9h00–9h45: Björn ENQUIST: The Heterogeneous Multiscale Method for Flow in Complex Systems
    - 9h45-10h30: Peter KNABNER: Efficient Accurate Simulation of General Reaction Multispecies Transport Processes in Porous Media by Reduction and Selective Decoupling
    - 10h45–11h30 Raúl TEMPONE: Spectral Collocation for Partial Differential Equations with Random Coefficients
    - 11h30-12h15: Leonid BERLYAND: Two analytical models of random composites: polydispersity and correlations
    - 15h15–16h: Jérome JAFFRÉ: Riemann solvers for flows through rocks changing type
    - 16h00–16h45: Ben SCHWEIZER: Averaging of unsaturated flow in stochastic porous media
    - 16h45-17h30: Rudolf HILFER: Can homogenization solve the upscaling problem for 2 phase flow equations in porous media?
    - 17h45–18h30 Alain BOURGEAT: Some Problems in upscaling source terms in a waste disposal
- Friday, November 4, 2005:
    - 9h00–9h45: Jérome POUSIN : Order 2 in time schemes for discontinuous reactive terms operator splitting for reaction diffusion with a singular reaction term.
    - 9h45-10h30: Peter BASTIAN: ADG method for flow in complex domains
    - 10h45–11h30 Eric BONNETIER: Can one detect a misplaced inclusion in a periodic composite by boundary measurements ?