BOOK OF ABSTRACTS

Mathematical Modelling Workshop
- MaMoW14 -

L'Aquila, 2014

Mathematics is much more than a language for dealing with the physical world. It is a source of models and abstractions which will enable us to obtain amazing new insights into the way in which nature operates. Indeed, the beauty and elegance of the physical laws themselves are only apparent when expressed in the appropriate mathematical framework.

—Melvin Schwartz

Contents

MaMoW14

Who are we?

The 1^{st} Mathematical Modelling Workshop was born from the wish to celebrate the initial 5 generations of the MathMods program, reinforce connections and present current work among all the master students and Alumni from the Erasmus Mundus Association (EMA) interested in Mathematical Modelling. The workshop also plays a role of a forum purposed for the exchange of ideas and discussions on topics related to mathematical modelling in engineering. Young researchers both from academia and private sectors are invited to participate, exchange their scientific knowledge and share information about different research groups, job opportunities and other relevant topics.

The Workshop consists of two parts. In the first two days, 14^{th} and 15^{th} of July, the Alumni meeting takes place: students from different EMA courses gathers to discuss their common experiences in round tables sessions, scientific camp and talks. This part of the Workshop is intended to foster collaborations in a friendly and creative environment. From 16^{th} to 18^{th} of July, the Mathematical Modelling Workshop with mini-lectures, talks contributions and poster session is held with a focus on the many aspects of mathematical modelling, numerics and applications. Speakers from Applied Mathematics and related areas, as well as Pure Mathematics, are welcome! Finally, on the last day, 19^{th} of July, a social trip to some beautiful nearby villages (like Santo Stefano di Sessanio and Rocca Calascio) is organised.

Thank you!

The Organization Committee would like to thank everyone involved in this workshop. First and foremost, we thank the students and their faculty advisers for their submissions to this workshop – without their research projects this conference wouldn't exist!

We also thank the rest of our team, members of the Scientific Committee, who reviewed student submissions and provided valuable feedback ensuring our firm belief in MaMoW14 scientific value. We would also like to extend our special thanks to the keynote speakers, and members of the round table discussions, for taking the time out of their busy schedules to participate in this event.

We are grateful to our sponsors, University of L'Aquila and University of Hamburg, joint together via EM MathMods programme, for their continued commitment and generous contributions that helped make this conference a reality. MaMoW14 would not have been possible without the great efforts made by the local arrangements who work tirelessly to ensure everything is running smoothly, and for this we extend a heartfelt thank you to Prof. Dr. Bruno Rubino from University of L'Aquila, as well as Prof. Dr. Ingenuin Gasser from University of Hamburg.

Finally, we take this opportunity to thank University of L'Aquila for hosting this conference and providing the needed resources.

We hope you will enjoy the workshop,
The Organization Committee

The Organization Committee

Alumni students - currently at the University of Hamburg

- Diana Gil
- Francesco Ludovici
- Arash Massoudi
- Petar Sapun

MathMods student representatives and EMA members

- Olena Burkovska
- Dinka Smajlagić

MathMods

- Danilo Larivera

The Scientific Committee

- Marco Di Francesco, University of Bath
- Chiara Simeoni, University of Nice-Sophia Antipolis
- Winnifried Wollner, University of Hamburg

Supporters

- University of L'Aquila
- University of Hamburg

MaMoW14 Schedule

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<tr><th colspan="2">Time</th><th colspan="2">Alumni meeting</th><th colspan="4">Mathematical Modeling workshop</th></tr>
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<tr><td>10:15</td><td>10:45</td><td rowspan="8">Registration</td><td rowspan="5">Scientific Camps (T-SC)</td><td>W-J3</td><td>F-J2</td></tr>
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<tr><td>14:15</td><td>14:45</td><td>Introduction</td><td rowspan="4">Round Table (T-R2)</td><td rowspan="3">Poster Session</td><td rowspan="3">T-ML</td><td rowspan="3">Alumni Assembly</td></tr>
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<tr><td></td><td></td><td></td><td></td><td>Social event</td><td>Workshop dinner</td><td>Social event</td></tr>
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MathMods Meeting:

- M-R1 Round Table Discussions: "The new perspective of Erasmus Mundus within Erasmus+ program"
- T-SC Participants can submit a topic on a real life aspects/problems to be discussed and analyzed.
- T-R2 Round Table Discussions: “Life after MathMods: PhD or a job in the industry?”

Mathematical Modeling Workshop:

- W-J1 Olga Chernomor - Modelling of Evolutionary Relationships: problems and challenges in Phylogenetics and its Applications
- W-J2 Krystyna Isakova – Mechanics of tamponade fluids in the vitreous chamber of the eye
- W-J3 Andjela Davidovic - Role and modelling of some heterogeneities for cardiac electrophysiology
- W-J4 Petar Sapun - Numerical results of the Berestycki’s fast line diffusion model
- W-S1 Monika Twarogowska – A well-balanced numerical scheme for a one-dimensioanl quasilinear hyperbolic model of chemotaxis
- T-S1 Federica di Michele – Bohmenian type boundary conditions for quantum hydrodynamics
- T-J1 Agnieszka L. Kozub - Electronic structure of Co impurities in Cu hosts
- T-J2 Diana Gil - Kinetic-Induced Moment Systems for Conservation Laws
- T-J3 Francesco Ludovici - Optimal control of parabolic PDE with Constraints on the Gradient of the State
- T-ML Fabio Antonelli – Stochastic Differential Equations and Finance
- F-J1 Muhammad Junaid Kamboh - Error estimation and implementation of new physics modes in PolyDE
- F-J2 Arash Massoudi - Five Things You Should Know About Control of PDE Systems
- F-ML Winnifried Wollner – Adaptive finite elements and a posteriori error estimations

Abstracts

1 Talks

1.1 Mini Lectures

Fabio Antonelli
Stochastic Differential Equations and Finance
University of L'Aquila

Winnifried Wollner
Adaptive finite elements and a posteriori error estimations
University of Hamburg

1.2 Senior Talks

1.2.1 Federica Di Michele

Bohmenian type boundary conditions for quantum hydrodynamics
University of L'Aquila

The quantum hydrodynamical model(QHD) coupled with the Poisson equation is able to describe the quantum effect appearing at nanoscale in many modern semiconductor devices. It can be obtained adding the Böhm potential to the classical hydrodynamical equations (HD) or directly from the Shröedinger equation. Here we derive (heuristically) a physically reasonable set boundary conditions (BCs) for QHD-Poisson system. We just consider unipolar case, thus the hole concentration is neglected. These new BCs have two interesting explanations from the physical viewpoint.

Firstly, if we consider the Böhm term as a correction for the pressure functional, it implies the conservation of the generalized enthalpy at the interface between metal-semiconductor. Alternatively, assuming that the Böhm term works together with the electrical potential, the BCs.

The existence and the uniqueness of a regular solution for the QHD-Poisson system is then discussed using these new BCs. The model is tested numerically on a case study device and the linear stability of the solution is discussed in a special case. The same consideration can be used to derive interface conditions between QHD and HD in the contest of the hybrid models

1.2.2 Monika Twarogowska

A well-balanced numerical scheme for a one-dimensioanl quasilinear hyperbolic model of chemotaxis

IAC-CNR Rome

We consider a quasilinear hyperbolic/parabolic system, motivated by the chemotaxis dynamics of endothelial cells during the vasculogenesis. It describes the time evolution of the density $\rho(x,t)$ of cells, their velocity $u(x,t)$ and the concentration $\phi(x,t)$ of a chemoattractant. In one space dimension the system writes as

$$\begin{cases} \rho_t + (\rho u)_x = 0, \\ (\rho u)_t + \Big(\rho u^2 + P(\rho)\Big)_x = -\alpha(x)\rho u + \chi \rho \phi_x, \\ \phi_t = D\phi_{xx} + a\rho - b\phi. \end{cases} \tag{1.1}$$

for $t > 0$, and $x \in [0, L]$ in a bounded interval endowed with a no-flux boundary condition. The function $P(\rho)$ is given by the pressure law for isentropic gases that is $P(\rho) = \kappa\rho^\gamma$, $\gamma > 1$.

This model was developed to describe formation of capillary-like networks from randomly seeded cells. Emerging such structured patterns corresponds to the formation of non constant stationary solutions. In fact, system (1.1) is meant to stabilize on a class of asymptotic regimes with $\rho u = 0$ and, for certain values of the parameters, with density distribution containing regions where ρ is strictly positive and regions where it vanishes. We provide a detailed description in the case $\gamma = 2$ of the non constant stationary solutions composed of vacuum and only one interval where $\rho > 0$.

Hyperbolic part of system (1.1) belongs to a class of balance laws which can stabilize onto non-constant solutions characterized by an accurate balance between the transport and the sources. Moreover they can contain parameters which variation can influence significantly the behavior of solutions. Correct numerical approximations have to reproduce on the computational grids the aforementioned behaviors. Usually this is obtained by using sophisticated numerical fluxes consistent not only with the convection terms but also with other parts of the equation. We present some examples in which fractional-steps methods are unable to deal with such particular problems. Then we propose a numerical scheme for the chemotaxis system (1.1) that couples a well-balanced strategy to capture the non constant equilibria for $\gamma > 1$ with an adapted flux solver in order to treat vacuum. Moreover, we describe the asymptotic preserving property of this scheme with the parabolic model in the high friction and long time limit.

1.3 Junior Talks

1.3.1 Olga Chernomor

Modelling of Evolutionary Relationships: problems and challenges in Phylogenetics and its applications
Center for Integrative Bioinformatics Vienna (CIBIV)

Abstract:

Evolutionary process refers to the changes in inherited characteristics of species, which are observed in successive generations of biological populations. Acting on different levels of biological organization ranging from species to genes and proteins, evolution is responsible for the diversity of life on Earth.

One of the main goals of evolutionary theory is the reconstruction of the so-called Tree of Life, the representation of the evolutionary relationships between species. With the advances of sequencing technologies the study of such relationships has moved from the usual analysis of morphological data to the analysis of genetic information.

Phylogenetics aims to reconstruct evolutionary tree of group of species based on their genes. One of the main approaches to tackle this problem is the famous maximum likelihood method [1]. Given gene sequences arranged in the multiple sequence alignment and evolutionary model, one searches through the tree space for the maximum likelihood tree. Evaluation of all the possible trees is only feasible for the small number of species. This poses an optimization problem of finding the maximum likelihood tree in reasonable amount of time.

Under the maximum likelihood inference, assuming that each gene evolves under its own substitution model, the tree search might suffer from the missing sequence information. It might happen that several trees have exactly the same maximum likelihood [2]. They are said to belong to the same phylogenetic terrace. During the search it simply means that one needs to do many unnecessary recomputations. We propose a phylogenetic terrace aware (PTA) data structure to efficiently deal with such cases [3]. The main idea is to map a parent tree onto the gene subtrees. Whenever the parent tree is changed using mappings we can quickly identify whether we need to recompute the likelihood or not.

One of the applications of Phylogenetics is found in Conservation Biology, where one is interested in selecting a subset of species under certain measure of species diversity and additional constraints. The selected subset of species is used for further conservation actions. Phylogenetic Diversity (PD) was introduced by Faith [4] and has become quite popular in conservation planning. We will discuss the optimization problem of Viable taxon selection under Split Diversity (SD), which is a generalization of PD [5]. Here, the aim is to select a subset of species that maximizes SD subject to predatorprey constraints. Though the problem is NP hard, it can be modelled in terms of the well-known Integer Programming and solved optimally within seconds [6].

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2. Sanderson, M.J., McMahon, M.M., and Steel, M. (2011) Ter-

races in phylogenetic tree space. Science, 333, 448-450.
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6. Chernomor, O., Minh, B.Q., Forest, F., Klaere, S., Ingram, T., Henzinger, M, and von Haeseler, A. (2014) Split Diversity in Constrained Conservation Prioritization using Integer Programming, submitted.

1.3.2 Andjela Davidović

Role and modelling of some heterogeneities for cardiac electrophysiology
INRIA, University of Bordeaux, IMB, LYRIC, France

Abstract:

Introduction: The most used model in the elctrophysiology of the heart, known as the bidomain model, is the system of degenerate parabolic PDEs coupled with the non-linear ODE. Even though these equations provide quite accurate results, they are based on the fact that active cardiomyocytes are present everywhere in the heart, while it is known that non-small regions exist where fibroblasts and other non-excitable cells or additional extracellular media take place. These regions, which play an important role in diseased hearts, are often taken into account through ad-hoc rough tuning of the tissue conductivities. In this work, we introduce a rigorous way to derive these conductivities from a microscopic description of the heterogeneities in the tissue.

Method: We assume a periodic alternation of the healthy tissue (bidomain model) and the fibrotic tissue (diffusive part). In order to reduce the computational cost, we derive a homogenized model at the macroscopic scale, following a two-scale convergence method. There are two problems rising here. First one has to deal with the degeneracy of parabolic equations and second one comes from the non-linearity of the ionic model of the cardiac cells. In order to study the model and illustrate its relevance, we computed numerical simulations of both the microscopic and homogenized models based on a non-physical linear model, and then on the Mitchell-Schaeffer ionic model.

Results: Interestingly, we recover a bidomain type model, but with modified conductivities, that depend on the volume fraction of the diffusive inclusions but also on their geometries. The numerical results confirm the convergence of the microscopic model to the homogenized equations in the linear case. We are currently working on the numerical simulations for the non-linear case, where we expect to observe the in uence of the diffusive inclusions on the propagation of action potentials.

Conclusion: With the final non-linear model, we shall provide cheap modeling tools to account for tissue heterogeneities at intermediate scales, as can be observed, e.g., in the fibrotic tissue.

References:

1. Allaire, Homogenisation and two scale convergence, SIAM J. MATH. ANAL. Vol. 23, No. 6, pp. 1482-1518, November 1992.

1.3.3 Diana Gil

Kinetic-Induced Moment Systems for Conservation Laws
University of Hamburg, Mathematics Faculty

Abstract:

Based on the relation between kinetic theory and non-linear hyperbolic equations, we derive a kinetic-induced moment system for the spatially one-dimensional Burgers' Equation [1] and Shallow Water Equations [2]. The derivation is based on an artificial Boltzmann-like transport equation with a BGK-relaxation [3]

$$\partial_t f(t,x,\xi) + \xi \partial_x f(t,x,\xi) = \frac{1}{\epsilon}[f_0(Q,\xi) - f(t,x,\xi)], \quad 0 < \epsilon \ll 1$$

and its corresponding moments,

$$W_k = \int_{\mathbb{R}} \xi^k f(t,x,\xi) d\xi, \quad with\ k \in \mathbb{Z}_{\geq 0}$$

The resulting infinite system is a coupled system of balance laws, which depends on the relaxation parameter ϵ coming from the kinetic equation. Using Chapman-Enskog-like asymptotic expansion techniques [4], it will be shown that at each order of ϵ, a scale-induced closure is possible, which results in a finite number of moment equations.

Of particular interest is the above mentioned coupled system obtained from a third order closure, which in the formal limit $\epsilon \to 0$, yields the original system of equations with an additional variable that acts as a monitoring function of particular ow structure (like shocks and rarefaction waves) and their potential applications in the description of small-scale geophysical

ows. This new unknown can be used on the one hand into the construction of adaptive numerical methods, and on the other hand as a basis to derive novel parametrizations for subgrid closures.

The first results of the research are contained in G. Diana and J. Struckmeier [2], which involves the coupled system derivation for the one-dimensional Shallow Water Equation. Currently a following paper is in preparation G. Diana, H. Struchtrup and J. Struckmeier [1], containing the earliest results on the construction of adaptive discretization techniques using a novel refinement parameter given by the kinetic-induced moment system.

Conclusion: With the final non-linear model, we shall provide cheap modeling tools to account for tissue heterogeneities at intermediate scales, as can be observed, e.g., in the fibrotic tissue.

References:

1. G. Diana, H. Struchtrup and J. Struckmeier: A Kinetic-Induced Moment System for Burgers Equation, 2014 (in preparation).
2. G. Diana and J. Struckmeier: Kinetic-Induced Moment Systems for the Saint-Venant Equations, TASK QUARTERLY, 2013, Vol. 17 No. 1-2, pp. 6390.
3. B. Perthame, Kinetic Formulation of Conservation Laws, OXFORD University Press, NY, 2002.
4. H. Struchtrup, Macroscopic Transport Equations for Rare ed Gas Flows, Springer-Verlag, Berlin, 2005.

1.3.4 Krystyna Isakova

Mechanics of tamponade uids in the vitreous chamber of the eye

University of Genova

Abstract:

Retinal detachment (RD) occurs when the sensory layer of the retina detaches from the retinal pigment epithelium. This is a serious condition that might lead to permanent loss of sight and needs immediate treatment. A commonly adopted surgical technique to tread RD is vitrectomy: the vitreous body is removed from the vitreous chamber and a tamponade uid, typically a silicon oil, is inserted. The amount of uid inserted in the eye depends on the patient condition. Tamponade uids are immiscible with water and their role is to push back the retinal in contact with the pigment epithelium. Owing to their hydrophobic properties tamponade uids coexist in the vitreous chamber with a certain amount of aqueous humour which is the uid produced in the anterior segment of the eye.

It is of clinical interest to have an estimate of the retinal coverage provided by a tamponade uid depending on the volume injected. We have established a mathematical model that determines the percentage of coverage by predicting the shape of the interface between aqueous humour and substitute, given the vitreous chamber shape and uid properties. In addition to that we provided an estimate of the wall shear stress on the retina in presence of tamponade uids during eye rotations. This grows with the viscosity of substitute and tends to a constant value for very viscous uids. However, it decreases dramatically when a layer of aqueous is present inhibiting direct contact be-

tween the vitreous substitute and the retina.

Silicon oils cannot be left for too long in the vitreous chamber since they tend to produce an emulsion of oil droplets in the aqueous. Several clinical studies have tried to investigate the conditions leading to the formation of an emulsion, but the problem remains essentially not understood. Many authors, however, believe that shear stresses at the oil- aqueous interface generated during eye rotations might be responsible for the generation of an emulsion (e.g. [1, 2]).

Owing to the lack of understanding of this instability process we consider a higly idealised problem as a starting point to understand the mechanisms leading to instabilty. We perform a linear stability analysis of aquoeus-silicone oil interface using the normal mode approach and assumig quasi-steady ow condition of the base ow. The results show that instability is possible in a range of parameters that can be encountered during eye movemets.

References:

1. de Silva, D.J„ Lim, K. S. and Schulenburg, W.E., "An experimental study on the effect of encircling band procedure on silicone oil emulsfication", Br.J. Ophtalmol., 89, 1348-1350 (2005).
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cation", Retina, 32(10), 2039- 2044(2012).

1.3.5 Muhammad Junaid Kamboh

Error estimation and implementation of new physics modes in PolyDE
Technical University of Hamburg

Abstract:

PolyDE is an FEM (finite element method) based simulation software being developed at the Institute for Microsystems Technology, Hamburg University of Technology under the supervision of Prof. Dr. -Ing Manfred Kasper and contributions from his doctoral students. The software is fully adaptive i.e. allows for h-, p- and hp-adaptation and is capable of solving steady state scalar and multiphysics problems in 2D and 3D . The language chosen for the implementation is FORTRAN . A generalized mathematical approach has been taken so that underlying PDE (partial differential equation) and system of PDEs ensure suficient flexibility to suitably solve problems from various physical areas. To this end, several physics modes are available for use. However, main emphasize is on the functionality to simulate MEMS devices. PolyDE can employ element shape functions up to polynomial order of 20 which is its unique feature and inspiration for the name PolyDE. Some external libraries and program parts are also used in the implementation code. Various results pertaining to adaptation and shape functions by the contributors have been published in journals and conferences. Recently, new physics modes in 2D have been implemented, namely , Stoke's flow in micro-channel and mixing process in t-shaped microdevice . The obtained results are compared with commercial software "COMSOL Multiphysics" and as yet are not ready to be published. However, progress and dificulties will be the point of discussion. Further course of work

is to implement new physics modes, improving the adaptation process and possibly incorporate a novel error estimator.

References:

1. Kasper, M. 2000 Mikrosystementwurf: Entwurf Und Simulation Von Mikrosystemen, Springer.
2. Zienkiewicz, Olek C., Taylor, Robert L. and Nithiarasu, P. 2005 The finite element method for uid dynamics, Elsevier.
3. Verfurth. R.. 1996 A review of a posteriori error estimation and adaptive mesh- refinement techniques, Wiley-Teubner.

1.3.6 A. L. Kozub

Electronic structure of Co impurities in Cu hosts
Gdansk University of Technology

Abstract:

I will present the theoretical procedure to investigate magnetic transition metal impurities located in non-magnetic transition-metal hosts. The impurities are described in terms of the multi-orbital Anderson model (AIM) [1] that takes into account the complete 3d shell of the impurity atom, the repulsive Coulomb interaction at the impurity site, and the hybridization between the impurity orbitals and the conduction-electron states in the host lattice. The AIM is parametrized to match the LDA [2] electronic structure and solved using the Lanczos method [3]. To demonstrate the method, I will present unpublished results of cobalt impurities located in the bulk and on the surface of copper. I emphasis on systematic description of the many-body ground state and excitation spectra. The effect of spin-orbit interaction and the lowered symmetry due to the surface on the formation of the magnetic and nonmagnetic ground states is analyzed. The results are compared to those obtained using the continuoustime quantum Monte Carlo (CT-QMC) method [4].

References:

1. A. Georges and G. Kotliar, Hubbard model in infinite dimensions, Phys. Rev. B 45, 6479 (1992).
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4. B. Surer, M. Troyer, P. Werner, T. O. Wehling, A. M. Läuchli, A. Wilhelm, and A. I. Lichtenstein. Multiorbital Kondo physics of Co in Cu hosts, Phys. Rev. B, 85, 085114 (2012).

1.3.7 Francesco Ludovici

Optimal control of parabolic PDE with Constraints on the Gradient of the State

University of Hamburg

Abstract:

Optimal control problems with state constraints arise in glass and steel production during heating/cooling processes, [5]. In these processes the temperature plays the role of the state variable and to preserve the product quality the internal thermal stress should be avoided leading naturally to the consideration of gradient state constraints.

In this talk we will consider a simplified model. Namely, we are concerned with the distributed optimal control problem

$$\textit{Minimize} \quad \frac{1}{2}\int_I \int_\Omega (u(x,t) - u_d(x,t))^2 dx\, dt + \frac{\alpha}{2}\int_I q(t)^2 dt,$$

where u_d is a prescribed temperature profile and the state $u(x,t)$ and the control $q(t)$ are coupled by a linear PDE.

In addition, we consider the integral gradient state constraint

$$\int_\Omega |\nabla u(x,t)|^2 \omega(x) dx \le b, \quad \forall t \in [0,T],$$

where $\omega(x)$ is a weighting function reflecting constraints on stress averages. The time discretization is based on the discontinuous Galerkin time stepping scheme while for the space discretization we use classical conforming finite elements. The control variable is discretized implicitly by the optimality conditions using the variational approach.

We focus on the diffculties behind the study of problems with gradient state constraints and on the derivation of an a priori error estimates. This is performed analysing separately the error introduced by the time and space discretization, [2].

In a second step, we extend our approach to a more realistic case where a semilinear parabolic PDE is considered. We highlight the main differences and criticalities with respect to the linear case. The second part is a joint work with Ira Neitzel (TUM).

References:

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4. D. Meidner, R. Rannacher, and B. Vexler, A priori error estimates for finite element discretizations of parabolic optimization problems with pointwise state constraints in time, SIAM J. Control Optim., 49 (2011), pp.1961-1997.
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1.3.8 Arash Massoudi

Five Things You Should Know About Control of PDE Systems

University of Hamburg

Abstract:

In this talk, I present the newest trends in the control and observation of partial differential equations (PDEs) from a system theory point of view. To this end, I start with a motivating example to show how one can use the already developed tools of dynamical systems to control PDE models. Subsequently, we will see how this connection allows us to tackle the field of linear quadratic optimal control problem for PDEs.

Afterwards, I will present the main challenges concerning the numerical approximation of partial differential equations in the context of optimal control problem. We will learn where it is preferable to first optimize the system and then discretize it, as opposed to the classical approach of first discretizing the system and then optimizing it. To this end, we focus on two fundamental examples which are motivated by practical applications. These examples are

1. Convection-Diffusion equation in a bounded 2-dimensional domain with boundary control and observation.
2. The transport equation in one dimension with boundary observation and pointwise control

Finally, I close the talk by presenting our recent works concerning the control of PDE models and the main open problems in this field. We will see how this fascinating area of research

has joined many expertise in the field of applied mathematics.

References:

1. Olof J. Staffans. Well-posed linear systems. Cambridge University Press, Cambridge, 2005.
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3. Martin Weiss and George Weiss. Optimal control of stable weakly regular linear systems. Math. Control Signals Systems, 10(4):287330, 1997.
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1.3.9 Petar Sapun

Numerical results of the Berestycki's fast line diffusion model

University of Hamburg

Abstract:

The goal of the talk is to present numerical simulations a differential model describing the spread of disease trough population in the urban environment. For this purpose, it is assumed that the physical domain can be separated in to two subdomains called road (street), with strong, direction dependent diffusion acting on it, and field, with not oriented weak diffusion. The underlying mathematical model has been proposed by Henry et al. Berestycki [1] [2] and it consists of a system of parabolic differential equations each acting on the specific part of the domain (the road is modelled in 1D and field is modelled in 2D) coupled by reaction terms given as an exchange between populations. The discretization is based on finite difference schemes [3] set on Cartesian grids. Numerical experiments have shown the expected (long-time) behaviour of the model and this results will be presented. Finally, possible comparisons with a global reaction-diffusion model with anisotropic diffusion tensor [4] are also discussed.

References:

1. H. Berestycki, J.-M. Roquejoffre, L. Rossi. The influence of a line with fast diffusion on Fisher-KPP propagation. J. Math. Biol. 66 (2013), 743-766.

2. H. Berestycki, J.-M. Roquejoffre, L. Rossi. Fisher-KPP propagation in the presence of a line: further effects. Nonlinearity 26 (2013) 2623-2640

3. LeVeque, Randall J. Finite Difference Methods for Differential Equations. University of Washington, 2005.
4. Weickert, Joachim. Anisotropic Diffusion in Image Processing. ECMI Series, Teubner-Verlag, Stuttgar, 1998.

2 Posters

1. **Finite Element approximation of semilinear elliptic optimal control problems with pointwise state constraints**
   - **Author**: Ahmed Ali
   - **Institution**: Department of Mathematics, University of Hamburg.
   - **Description**: We consider the finite element approximation of semilinear elliptic optimal control problems with distributed control and pointwise state constraints. In particular, we discretize the optimal control problem by means of linear finite elements and study the order of convergence.

2. **Parameter Identification for the viscous Shallow Water Equation**

   - **Author**: Marco Capo
   - **Institution**: Department of Mathematics, University of Hamburg.
   - **Description**: It is well known that the quality of the initial conditions plays an important role in the analysis of atmospheric dynamics and weather forecast. This is a direct consequence of the nonlinearity of all these geophysical processes which imposes an important sensitivity to the initial conditions. Parameter Identification has become a relevant topic in environmental sciences, since it combines effectively all the sources of information (e.g. Observations of the ocean) with models and numerical methods. In this project we present an application of this technique on the Shallow Water Equations. In order to do this we solve the associated optimization problem by the means of the Newton method over a Finite Element framework (Q1). The implementation of the optimization algorithms and the different time step methods (Backward Euler, Crank Nicolson and Fractional Theta method) are obtained from the C++ library DopeLib.

3. **Numerical boundary conditions in the FEM simulation of the Navier Stokes equations and their role in the adjoint equation**

    - **Author**: Gabriela Cirtala
    - **Institution**: Department of Mathematics, University of Hamburg.
    - **Description**: We consider the incompressible Navier-Stokes equations in a 2 or 3 dimensional domain. I take the boundary of the domain as consisting of a Dirichlet part (S0) and a natural outflow part (S1). Therefore, on S0 I impose the homogeneous Dirichlet condition, while on S1 I consider the directional do nothing boundary condition. Formulating it as a control problem and applying Lagrange calculus I obtained the optimality conditions. Further steps in this thesis include the implementation of the directional do nothing condition (DDN) and the implementation of the DDN for the adjoint equation in Matlab.

4. **Efficient methods for defect classification in non-destructive evaluation of materials**
    - **Author**: José Fernando Cuenca Jiménez
    - **Institution**: Department of Mathematics, University of Hamburg.
    - **Description**: Ultrasonic non-destructive evaluation of material involves many challenging problems. Nowadays, the behaviour of ultrasound in material is well known and many simulation and reconstruction methods are available from the literature. Nevertheless, the data given by the non-destructive testing method has to be analyzed in a fast and reliable way. In addition, the acquired data is also often very noisy, and has missing information (missing data), because only few measurements can be taken. In this poster, it is discussed how topology and methods from persistent homology can be a useful tool for clustering in a point cloud data (PCD), and could be seen as a reasonable alternative to other methods (DBSCAN, k-mean, etc) for detecting and classifying defects.

5. **Advanced motion planning algorithms for robots and manipulators**
   - **Author**: Irina Gulina
   - **Institution**: Brno University of Technology
   - **Description**: The research is concentrated on the motion planning problem and particularly the family of random sampling algorithms. One of the most time consuming parts of the RRTs-based algorithms is the search for the nearest neighbor node. This resent research contributes to the improvements of the runtime of the nearest neighbor function by using the spatial index.

6. **Surface-Enhanced Infrared Absorption (SEIRA) of Silicon Nitride onto Plasmonic Nanoantenna arrays**
   - **Author**: Mohammed Janneh
   - **Institution**: Department of Industrial, Information Engineering, and Economics - University of L'Aquila.
   - **Description**: Plasmonic nanoantennas operating in the mid-infrared region have attracted much attention as a powerful engineer sensing device. Plasmonic nanoantennas have the ability to receive, focus, and transmit incoming optical and infrared electromagnetic radiation by mean of surface plasmon. In this way it is possible to localize excitation of molecules onto metal surface, enabling these materials to detect and characterize ultrasensitive biological and chemical substances, as well as environment hazard monitoring. We report a plasmonic engineered gold nanoantenna arrays tailored with silicon nitride (Si_3N_4) to measure its optical absorbance as a function of it thickness in mid-infrared region. Initially, we introduced different configurations of Si_3N_4 medium onto the surface of the nanoantenna arrays geometry and, as well altered the dimensions of the nanoantenna geometry, to demonstrate the influence on the average sensitivity of the SEIRA gain for sensor applications. However, analytical results were supported by numerical simulations with finite element method.

7. **Thermal Fluid-Structure Interaction Method**
   - **Author**: Azahar Monge
   - **Institution**: Center for Mathematical Sciences, Lunds University.
   - **Description**: Thermal Fluid-Structure Interaction is observed in many industrial processes. For instance, the cooling process in a steel forging process. There, one considers the coupling of the Navier-Stokes equations as a model for the fluid and the heat equation as a model for the temperature distribution in steel. The semi-discrete coupled system is solved using stiffly stable SDIRK methods of higher order, where on each stage a fluid-structure-coupling problem is solved. For the resulting method it is shown by numerical experiments that a second order convergence rate is obtained. This property is further used to implement a simple time-step control, which saves considerable computational time and, at the same time, guarantees a specified maximum error of time integration.!

8. **Design optimization of the ship hulls**
   - **Author**: Orest Mykhaskiv
   - **Institution**: Department of Mathematics, University of Hamburg and Institute of Fluid Dynamics and Ship Theory, Technical University of Hamburg-Harburg (TUHH).
   - **Description**: The concepts of adjoint optimization are applied to the hydrodynamic design problems. The air and water drag cost function is to be minimized with incompressible turbulent Navier-Stokes equation for two-phase flow as constraints. The inhomogeneity of the fluid is resolved by Volume of Fluid (VOF) method coupling with Navier-Stokes equations. Continuous- and discrete-adjoint formulation for the system is derived. Gradient/Sensitivity function is obtained to find the optimal shape parameters. The corresponding numerical experiments are conducted to verify stated model. The numerical schemes are based on Finite Volume (FV) method and high-performance algorithms of TUHH in-house fluid dynamics software FreSCo.

9. **Phase envelope calculation for multicomponent mixtures with capillary pressure**
    - **Author**: Diego Sandoval
    - **Institution**: DTU-Kemi, Technical University of Denmark.
    - **Description**: A multicomponent mixture in confined spaces is typical in petroleum reservoirs. In particular for tight reservoirs and shales, the pore size can get down to tens of nanometers. Such systems are characterized by large area/volume ratios and high capillary forces. The influence of capillary pressures on the phase behavior of the mixture can become significant. There are several studies on the influence of capillary pressures on phase equilibrium in shale due to the recent interest in shale gas production. This work presents an algorithm for the construction of the phase envelope for multicomponent mixtures involving capillary pressure. A full Newton method was employed to solve the governing equations of the vapor-liquid equilibria coupled with the capillary pressure equation. Results are presented for systems with pore radius down to 10 nm. A change in the saturation pressures was observed in the whole phase envelope except in the critical point. The bubble point curve shows a negative displacement of the saturation pressure in the whole temperature interval. The dew point curve shows both, a positive and negative displacement of the saturation pressure in the upper dew point branch and the lower dew point branch, respectively.

10. **Metabolic Regulation by Leptin**
    - **Author**: Cansu Uluseker
    - **Institution**: Department of Industrial, Information Engineering, and Economics - University of L'Aquila.
    - **Description**: We develop a mathematical model of leptin dynamics, with parameters derived from published experimental data, to provide information on the leptin hormone, its role in food intake, body weight, their mechanism of action, and in acute appetite control. This model considers that leptin is measured in plasma and brain in wild type (WT) mice and leptin knockout (LepKo) mice which is also called ob/ob mice. The assessment of the relationship between leptin concentrations, food intake, and the energy expenditure are set as a function of leptin. The effects of body weight are examined by two separate systems – with and without control by an explicit set-point. This effect is investigated by changing dietary caloric content for weeks in mice. Collectively, the results presented in this thesis highlight the role of leptin on energy metabolism and differences between the "settling point" and "set-point" systems and changes in response to different energy caloric content. Strategies targeted at metabolic regulation by leptin and possibility of multiple steady states for body weight open up new venues for future research.