Chair:
**Prof. Roberto Lucchetti**

# DOCTORAL PROGRAM IN MATHEMATICAL MODELS AND METHODS IN ENGINEERING

Equations are everywhere! Between the atmosphere and the wing of a spaceship, in the blood flowing in an artery, on the demarcation line between ice and water at the poles, in the motion of the tides, in the charge density of a semiconductor, in the compression algorithms of a signal sending images from outer space. Such equations represent real problems. The Mathematical Engineer can see and understand the nature of these equations, and can develop models in order to understand their relevant qualities and solve real problems.
This PhD program aims at training young researchers by providing them with a strong mathematical background and with ability to apply their knowledge to the solution of real-world problems that arise in various areas of science, technology, industry, finance, management, whenever advanced methods are required in analysis, design, planning, decision and control activities. PhD students carry our their research both in the development of new mathematical methods and in the implementation and improvement of advanced techniques in connection with specific contexts and applications.
The Faculty of the PhD program is responsible for the organization of the training and research activities of the PhD students. Decisions of the Faculty comply with the requirements and standards of the Doctoral School of the Politecnico di Milano. A Chairman is elected within the Faculty, for representative and coordination activities. Admission of students to the PhD program is decided after examination of the candidates. Students applying to our program must provide their CV, along with reference and motivation letters. After admission, each student is assigned a tutor. The tutor is a member of the Faculty who assists the student in the early stages of his career, especially in the choice of the courses and in identifying a thesis advisor.
The overall activity of the PhD students can be quantified in 180 credits. The PhD program has a duration of three years. Activity can be classified into:
introductory courses (no minimum number of credits required); main courses (at least 30 credits); specialized research training, including seminars, tutoring activity, participation to workshops/conferences, and scientific publications (at least 30 credits); development of a doctoral thesis (at least 90 credits).
At the end of each academic year, the PhD students report to the Faculty about their activity. The students report about attendance of courses and exams (and the corresponding grades), participation in various scientific activities (seminars, conferences, summer schools etc.), planning and intermediate results on their research project and preparation of the PhD thesis, and any other relevant activity. At the annual meeting the students also receive a grade by the Faculty. A negative grade may entail repetition of the current year of doctoral study (with suspension of the grant, if any) or exclusion from the PhD program, depending on the Faculty's decision. Mobility of PhD students to other institutions is strongly encouraged and financial support is provided to this purpose.
Among others, let us mention some typical types of professional skills and possible occupations of the graduated Doctors: analytic and numerical treatment of differential models for physical and industrial problems, quantitative methods in finance and risk management, operations research and optimisation, statistical modelling and data analysis. Placement of graduated Doctors is expected in the following positions: research and development divisions of businesses, businesses involved in innovative design activities, financial institutions such as banks or insurance companies, public or private research centres, public and/or governmental agencies for social, economical, scientific study, planning or evaluation, Universities.
Since the PhD program in Mathematical Models and Methods in Engineering (formerly, Mathematical Engineering) has been active since the year 2001, we expect that a larger number of institutions and businesses will soon become more and more aware of the professional skills and expertise of graduated doctors.

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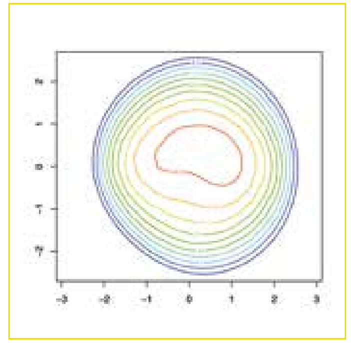
# BLOOD FLOW VELOCITY FIELD ESTIMATION VIA SPATIAL REGRESSION WITH PDE PENALIZATION

**Laura Azzimonti -** Supervisors: **Prof. Piercesare Secchi, Dott.ssa Laura Maria Sangalli**

In this work we propose a novel non-parametric smoothing technique for surface estimation on spatial domains with complex boundary conditions when a prior knowledge on the phenomenon under study is available. The prior knowledge included in the model derives from physics, physiology or geometry governing equations in the form of partial differential equations (PDEs) that the surface has to fulfill as well as the conditions at the boundary of the domain. The driving application concerns the study of the blood-flow velocity field on a cross-section of a carotid artery, using data provided by Echo-Color Doppler (ECD) acquisitions. This study is carried out within the project *MAthematichs for CARotid ENdarterectomy @ MOX* that aims at developing numerical and statistical tools for the study of the pathogenesis of atherosclerotic plaques in human carotids. Insights on the presence and the histological properties of the plaques based on information on the morphology of the blood vessel and the haemodynamics are of particular interest. Interactions between the fluid dynamics and atherosclerotic plaques have already been highlighted via patient-specific numerical simulations of the blood flow. Carotid ECD is a medical imaging procedure that uses reflected ultrasound waves to create detailed images of the carotid arteries and to measure the velocity of blood cells in some locations within these arteries. This technique does not require the use of contrast media or ionizing radiation and has relatively low costs. Even if ECD data are less rich of information than, for example, Phase Contrast Magnetic Resonance Imaging data, studying them is particularly interesting since they are frequently used by clinicians because of the short acquisition time and the non-invasivity of the technique. The estimation of the blood-velocity field on a cross-section of the carotid artery provides richer information for diagnostic purposes than the original ECD observations; it allows, in fact, to study the shape of the velocity profile and some of its relevant features, such as the eccentricity and the asymmetry of the blood flow or the reversion of the fluxes. For this reason, the development of new non-parametric techniques for the estimation of the blood-flow velocity field is very important. The estimated blood velocity fields will also be used to provide patient-specific and physiological inflow conditions for hemodynamics simulations. Moreover, the computation of the variance of the surface estimator will be used to investigate how the misspecification of inflow conditions affects the fluid dynamics numerical simulations. The blood velocity, projected in the longitudinal direction, is measured on 7 beams on the cross-section of the common carotid artery located 2 cm before the bifurcation. The ECD signal represents the histogram of the measured velocities, evolving in time, and it is summarized at each time with the mean velocity on the beam. We are interested, in the first place, in estimating the blood velocity field for a fixed time, in particular we consider the time corresponding to the systolic peak, but we also extend this framework to deal with the time dependence. The beams are located in a cross-shaped pattern that plays an important role in the smoothing estimate; in order to obtain physiological results, it is necessary to include in the model the prior knowledge on the fluid dynamics that govern the phenomenon under study. Thanks to classical fluid dynamics models, we expect the longitudinal velocity field to be similar in shape to a parabolic profile, with isolines resembling circles; however we don't want to impose a parametric model since the exact blood velocity field is influenced by the geometry of the artery and by the non-stationarity of the blood flow. We have also important information on the velocity near the boundary of the domain. The blood velocity has in fact to be equal to zero near the boundary due to the friction of the blood cells with the wall; these are the so-called no-slip boundary conditions.
Classical methods for surface estimation as thin-plate splines, tensor product splines, kernel smoothing, wavelet-based smoothing and kriging, do not include naturally information on the shape of the domain and on the value of the surface at the boundary. More complex smoothing methods, as for example spatial spline regression models and soap-film smoothing, can deal with the shape of the domain and the boundary conditions. Although being able to deal with the shape of the domain and general boundary conditions, these methods do not provide physiological estimates of the velocity field since the penalization of a measure of the local curvature oversmooths the surface in the regions where there are few observations.
On the other hand, the available prior knowledge on this phenomenon could be exploited to derive physiological estimates. We thus propose an extension of spatial spline regression models in order to include in the model the prior information on the shape of the surface in terms of PDEs that govern the phenomenon. More specifically we introduce a penalizing term that involves the misfit of a linear second order PDE that models to some extent the phenomenon under study. The surface estimator, which is proved to exist and to be unique, is then discretized by means of the mixed Finite Element method. The discrete surface estimator is linear in the observations and the classical inferential tools are derived. The comparison of the proposed method with the competitors in some simulation studies shows that the inclusion of the prior knowledge on the shape of the surface improves significantly the estimate of the surface, in particular when there some parts of the domain with few observations.
The proposed method is also generalized to take into account the fact that data in the ECD application are areal, in particular representing the mean value of the surface on a subdomain. Thanks to this generalization the blood velocity field on the carotid cross-section has been estimated.
The proposed method has good asymptotic properties, it's possible to prove that both the infinite dimensional estimator and the discrete one are consistent and converge almost surely to the true underlying surface when the number of observations increases and the parameter of the penalty term vanishes. Moreover, the mixed Finite Element method applied to this problem has an optimal convergence rate.

1. Echo-color Doppler image corresponding to the central point of the carotid cross-section located 2 cm before the carotid bifurcation.



2. Estimated velocity field on the carotid cross-section during the systolic phase.

# STATISTICAL MODELS AND METHODS FOR COMPLEX CLINICAL DATA

**Stefano Baraldo** - Supervisors: **Prof. Anna Maria Paganoni**

This work presents two distinct applications of statistical modeling and estimation in problems related to health care: the first part is dedicated to the statistical modeling of hospital admission data and their use for predictive purposes in the analysis of home telemonitoring for heart failure. The second part presents various statistical methods for the estimation of diffusion parameters in Magnetic Resonance Imaging (MRI) data, taking into account the distributional properties of the observed signals.

## Counting process modeling for heart failure data

Heart failure is a degenerative disease known as one of the most frequent causes of hospitalization among the eldest in the population.
Since the frequency of crises undergone by patients increases along time, more and more health care resources in terms of money, structures and personnel are needed. The necessity of a cost-effective solution for the care of this and other chronic pathologies has led to the experimentation of telemedicine as a possibly convenient strategy. The basic idea of telemonitoring is to keep the patient at home and to instruct her/him about the use of monitoring instruments, which send registered information (ECG, heart frequency, etc.) to the health institution via internet. The physician in charge evaluates received data to manage the home care program, for example by modifying drug doses and scheduling visits.
The telemonitoring outcome, i.e. the regular conclusion of the planned period or the early interruption by adverse events, should be related to the patients' clinical history to get better insight into the effectiveness and applicability of this strategy. To his aim, in this study we consider Hospital Dimission Forms extracted from the Italian Public Health Database (PHD), which gathers information about hospitalization periods. The use of information about hospitalizations to study telemonitoring outcome is an innovative approach, since no standard methodology exists to exploit this kind of data. Moreover, data conveyed by administrative databases are used for clinical investigation for the first time in Italy and in the field of telemonitoring.
Since heart failure is a pathology that alternates phases of stability to sudden worsenings of the patient's condition, a natural modeling approach, yet new in the field of telemonitoring, is to consider each patient's hospitalizations as points of a stochastic counting process. The model we consider is a Cox-type one, which allows to take into account many aspects that influence hospitalization risk and to compute the realized trajectories of underlying hazard process; these longitudinal data reduce complex characteristics of the patient's clinical history to a single curve that represents each patient's instantaneous risk of hospitalization. Hazard processes are then studied in the light of functional data analysis techniques to identify their main features, and used to construct a generalized linear model with functional covariates for predicting telemonitoring outcome.
Two sources of data are involved in the different phases of the analysis. First, hospital admission historical data from the PHD are used to estimate the parameters of a counting process and to construct patient-specific hazard functions, longitudinal data that reflect the evolution of rehospitalization risk before the application of the treatment.
The second phase is motivated by our main objective of predicting the outcome of the telemonitoring period; in this part of the analysis the data collected in the clinical survey are enriched with information gained from the previous clinical history of the patient, represented by the longitudinal data estimated in the first phase.

The application of the proposed methodology could have an impact on the planning of this care strategy and provide support to the decision of allocating a patient to telemonitoring or to usual care.

## Likelihood methods in Diffusion Magnetic Resonance Imaging

Diffusion MRI is as an important tool in clinical research, as it allows to characterize some properties of biological tissues. When tumor areas are analyzed using this technique, it can be observed that the diffusion tensor, estimated from the MR magnitude signal, has reduced values in lesions with respect to surrounding tissues, allowing to identify pathological areas. When the region of interest can be considered as isotropic, the *Apparent Diffusion Coefficient* (ADC) is sufficient to characterize the diffusion properties of the tissue, and it is usually estimated as the exponential decay rate of the signal with respect to the *b-value*, the MR acquisition parameter. The assumption of isotropy is common and reasonable in various cases, like breast and prostate cancer. In many practical situations it may not be possible to collect more than few measures at different b-values, thus limiting the accuracy of the estimation. A reduction in the total number of measures necessary to achieve a desired accuracy would be convenient in term of costs, and would allow to keep the patient involved in the MR procedure for a shorter amount of time. In this work, different frequentist and Bayesian approaches for the estimation of the ADC are compared, underlining their statistical properties and computational issues, and an effective design of experiment for data acquisition is proposed. The criterion adopted, based on the Fisher Information Matrix, allows to choose a sequence of b-values for image acquisition that increases the accuracy of the estimated diffusion fields.
Another issue related to the analysis of diffusion MRI data is to account correctly for the non-gaussianity of the intensity signal. In particular, various estimation methods for the *Diffusion Tensor Imaging* (DTI) model have been extended to the Rician framework, which arises from natural modeling assumptions. The Rician model is effective in accounting for the signal skewness at low *Signal-to-Noise Ratios* (SNRs), but the assumptions for its validity are violated in presence of multi-coil scanners. If the signals received by the N coils are combined by sum of squares, the intensity signal follows a noncentral chi distribution. Moreover, different parallel acquisition and signal combination methods can modify the nature of this signal, often resulting in a noncentral chi variable with reduced degrees of freedom.
We present a methodology for maximum likelihood estimation of noncentral chi-distributed signals, applied in particular to the DTI model for brain imaging. We also propose a method for discriminating background from signal voxels basing on the noise distribution.
The noncentral chi estimation is compared to Gaussian and Rician estimation on a simulated phantom, and the performances of the estimators are presented analyzing real brain MRI data.

1. Estimated Apparent Diffusion Coefficient field on a brain slice

# MIMETIC FINITE DIFFERENCE METHODS FOR NONLINEAR AND CONTROL PROBLEMS

**Nadia Bigoni -** Supervisors: **Dr. Paola Francesca Antonietti, Dr. Marco Verani**

In this thesis we address the question of whether the Mimetic Finite Difference (MFD) method can be used to efficiently solve nonlinear and control problems. The MFD method is a very recent technique that has become a very popular numerical approach to successfully solve a wide range of problems. This is undoubtedly connected to its great flexibility in dealing with very general polygonal meshes and its capability of preserving the fundamental properties of the underlying physical and mathematical models.

The first part of this thesis is devoted to introduce and discuss the (primal and mixed) MFD method applied to elliptic problems. The main features of the method are recalled and several numerical examples assess its robustness and efficacy.

In the second part, we present the mimetic approximation of an elliptic control problem. We introduce the discrete formulation of the problem and we prove that it is well-posed. Next, we derive *a-priori* error estimates in suitable discrete norms and perform several numerical examples that confirm our theoretical analysis.

In the third part of the thesis, we study the application of the MFD method to solve a nonlinear elliptic problem of monotone type. After having introduced a proper mimetic discretization of the nonlinear term, we prove that the discrete problem admits a unique solution and an *a-priori* error estimate in suitable discrete norms is derived. We then apply the Kačanov method to solve numerically via linearization the nonlinear discrete problem. We show the efficacy of the algorithm through several numerical tests and we highlight that our *a-priori* error analysis is respected.

We next focus our attention on one of the most important manufacturing process employed in industry: *the extrusion process*. In this process a solid material is heated beyond the melting point to be enough malleable. Then, it is forced by one or more screws through a special die to produce a continuous manufactured item. The main problem linked to extrusion is the well-known *die-swell* phenomenon which is given by the increasing of the cross section of the material when it leaves the die. The numerical simulation of the extrusion process requires the solution of a *free-boundary* problem governed by (possibly) *non-newtonian* fluids. More precisely, the main aspect of a free-boundary problem is that the domain is not known a priori. This means that the problem, apart from the usual unknown quantities (e.g., velocity, pressure), contains additional geometrical unknowns.
In the fourth part of the thesis, we discuss the two main building blocks that will allow us to perform, in the next future, the mimetic numerical simulation of the extrusion process: the approximation of nonlinear Stokes problems and of free-boundary problems (recasted as shape optimization problems).

We start by addressing the approximation of nonlinear Stokes equations. To handle the nonlinear diffusion term, we resort to the ideas introduced in third part of the thesis. Moreover, in this context, the nonlinear problem is iteratively solved by means of the Uzawa's method and we show the performance of our algorithm with several numerical examples. More precisely, two different *non-newtonian* fluids have been considered: the first one governed by the *Carreau law* and the second by the *Cross model*.
Next, we give an overall description of the performance of the MFD method for solving shape optimization problems. To this aim, we explore the robustness of the MFD method for the approximation of some paradigmatic examples: the first two are shape optimization problems governed by an elliptic equation and a Stokes equation, respectively and the third one is related to the solution of an elliptic free-boundary problem. Our numerical examples show that the MFD method represents a very promising technology to solve this kind of problems and to handle the progressive deformation of the computational domain without resorting to any re-meshing strategy. This is a very new approach in the numerical solution of shape optimization problems. For the sake of completeness, adaptive strategies based on heuristic error indicators are also considered to validate the effectiveness of the numerical scheme.

Finally, in the last part of the thesis, we present a new technique called Virtual Element Method (VEM). The collocation of Virtual elements in the framework of numerical methods for partial differential equations can be seen in a twofold way: on the one hand, they can be seen as one of the many variants of Finite Element Methods for general polygonal and polyhedral elements. On the other hand, they are deeply related to the Mimetic Finite Differences, since many of their computational aspects are closely connected. In the thesis, we review the main feature of the method applied to an elliptic problem and we discuss its numerical performance through some numerical examples taken from the literature.

# ANALYSIS AND APPROXIMATION OF MOMENT EQUATIONS FOR PDES WITH STOCHASTIC DATA

**Francesca Bonizzoni** - Supervisor: **Prof. Fabio Nobile**

Mathematical models are helpful instruments for qualitative and quantitative investigation in many different disciplines. They provide an interpretation and predict the behavior of phenomena arising in natural science, biology, engineering, economy and finance. Numerical analysis develops and study algorithms for numerically solving problems coming from mathematical modeling. In many applications, the parameters of the model are not precisely known. This may be due to several factors: measurement errors, incomplete information or intrinsic variability. Recently, many efforts have been done in trying to treat and include this uncertainty in the model.
A very convenient framework is offered by the probability theory. In particular, starting from a suitable partial differential equation (PDE) model, the uncertain input data are described as random variables or random fields with known probability laws. This kind of mathematical models are known as *stochastic PDE* (SPDE).
The solution of an SPDE is itself stochastic: it is a function of space and time as well as of the random realizations.
The goal of the *Uncertainty Quantification* is to infer on the solution, that is to understand how the uncertainty in the input data of the model reflects onto the solution. The quantities of interest may be either the statistics of the solution, like mean and variance, or statistics of functionals of the solution.
Given complete statistical information on the input data, the aim of the present thesis is to derive suitable equations for the statistical moments of the stochastic solution of the SPDE. The technique we use is known as *"moment equations"*.
We take into account PDEs with randomness arising both in the loading term and in the coefficient.
For what concerns the first family, elliptic PDEs have already been studied in literature.
Our original contribution regards stochastic saddle-point problems. More in details, we study the stochastic counterpart of the mixed formulation of the Hodge Laplacian, a second order differential operator coming from the exterior calculus framework. The Hodge Laplacian unifies different problems important in applications, such as the Darcy problem, modeling the fluid flow in porous media, and the magnetostatic/electrostatic problems. In this setting, a stochastic loading term may represent an uncertain sink or source (Darcy problem) or an uncertain current (magnetostatic/electrostatic problem). Using the inf-sup operator for the deterministic Hodge Laplacian, we prove the well-posedness of the stochastic Hodge Laplacian.
The m-th moment problem is obtained tensorizing the stochastic Hodge Laplacian m times and then taking the expected value. For this reason, the forcing term of the m-th moment problem is the m-th statistical moment of the forcing term of the stochastic Hodge Laplacian and the differential operator is the Hodge Laplace operator tensorized with itself m times. This means that the m-th moment equation is itself a saddle-point problem, composed of m nested saddle-point problems. Hence, to prove its well-posedness, we need a tensorial inf-sup condition. We notice that the tensor product of an inf-sup operator is not straightforwardly an inf-sup operator. The first contribution of this work is the derivation of an inf-sup operator for the m-th moment problem. The natural finite element discretization for the m-th moment equation is obtained as full tensor product (FTP) of a finite element subspace for the deterministic Hodge Laplacian. Since the number of degrees of freedom grows exponentially in m (*curse of dimensionality*), this approach can not be pursed for m moderately large. To overcome this problem, we consider sparse tensor product (STP) finite element discretization techniques and prove stability and well-posedness of such discretization.
We then focus on the boundary value problem modeling the single phase flow (Darcy law) in a two or three dimensional heterogeneous porous medium. Following the geophysical literature, we describes the permeability as a stationary lognormal random field, that is the exponential of a stationary Gaussian random field Y. Under the assumption of small standard deviation of Y, we performs a *"perturbation analysis"*, which consists in expanding the solution of the SPDE in Taylor series with respect to Y.
As first task we investigate the approximation properties of the k-th order Taylor polynomial. We predict the divergence of the Taylor series and the existence of an optimal order k (depending on the standard deviation of Y) such that adding new terms to the k-th order Taylor polynomial will deteriorate the accuracy instead of improving it. These theoretical results are confirmed by numerical tests executed in a one dimensional physical domain.
We then use the perturbation technique to infer on the statistics of the solution. The idea is to approximate the statistical moments of the solution with the statistical moments of its k-th order Taylor polynomial, which we call k-th order approximation. Note that, if Y is a random variable or vector, the Taylor polynomial can be explicitly computed, whereas, in the infinite dimensional case (Y random field), the Taylor approximation can not be directly computed. However approximated equations for its moments can be derived.
We concentrate our attention mainly in the mean equation. The k-th order mean problem, that is the problem solved by the k-th order approximation of the mean, is recursive and requires the computation of k-points correlations. We state the well-posedness of the mean problem and regularity results for the correlation functions involved in the recursion. The high dimensionality of the problem represents an obstacle. We propose to store the correlations and make computations in a low-rank format: the Tensor-Train (TT) format. One tensor in TT format is expressed as a linear combination of three dimensional arrays, called cores of the TT decomposition. The algorithm which computes the TT decomposition of a given tensor is based on the recursive application of the singular value decomposition (SVD). The advantage is that the storage complexity of a tensor in TT format is no more exponential in the dimension. We develop a Matlab code in TT format to compute the k-th order approximation of the mean, and we compare our results to that obtained using the collocation or the Monte Carlo methods, in the case where the collocation can not be applied.

# ON SOME MULTI-PHASE PROBLEMS IN CONTINUUM MECHANICS

**Stefano Bosia** - Supervisors: **Prof. Maurizio Grasselli, Prof. Andrei Constantinescu**

This research project deals with some modelling problems arising in continuum mechanics in connection with multi-phase systems. Three main issues have been investigated:
diffuse interface models in phase separation of binary mixtures (e.g., coarsening of alloys or bistable polymeric fluids);
the operation of electronic devices (in particular p-n junctions) under mechanical deformations.
lifetime predictions in polycrystalline metals under periodic loading.

## The flow of binary fluid mixtures

A typical phase separation model used to describe the flow of a binary mixture is the well-known model H. This results from the coupling of the convective Cahn-Hilliard equation with the Navier-Stokes system through the so-called Korteweg force.
Our research focused on the study of the asymptotic properties of some variants of this system of PDEs within the general framework of the theory of infinite dimensional dynamical systems.
Both the Navier-Stokes and the Cahn-Hilliard systems of equations pose challenging open problems for contemporary mathematical analysis. In particular, we still lack a complete understanding of the well-posedness of the Navier-Stokes system in 3D. In this long standing quest, only existence of weak (variational) solutions is known as well as the uniqueness of strong solutions within the larger class of weak solutions.
Concerning the Cahn-Hilliard equations, several problems have drawn the attention of researchers in the last years. Among these, dealing with the thermodynamically relevant logarithmic singular potential is probably one of the most interesting ones. Indeed, a rigorous derivation of the Cahn-Hilliard model within statistical physics leads to a double-well potential describing the evolution of the composition of the mixture. For physical relevance, this potential is defined only on a bounded interval of real numbers, being continuous there, but having infinite slope at its endpoints.
In our work, three different generalisations of the model H were considered: non-newtonian shear-thickening fluids, chemically reacting fluids and nonlocal interactions between the different constituents of the mixture.
The nonlinear Ladyzhenskaya model for viscosity was used to represent shear-thickening fluids. Under this constitutive assumption, existence of solutions was proved on bounded domains in 3D. In this case, a singular, logarithmic type, double-well potential was assumed to model phase separation in the Cahn-Hilliard equation. Since uniqueness of solutions is still unknown for this system, its long-term beahaviour was studied using the theory of trajectory attractors. Resulting from the work of Chepyzhov and Vishik. This theory overcomes uniqueness issues by considering a suitable extended phase space, which is made up by whole trajectories (i.e. solutions) departing from time 0 and extending up to infinity.
Chemically reacting fluids can be modelled by considering a reaction (or Oono) term in the Cahn-Hilliard equation. In contrast with the usual results known for the Cahn-Hilliard equation or for the model H, this choice implies that the average composition of the mixture can evolve over time. We focus on 2D bounded domains and on regular (polynomial) double-well potentials. After investigating the well-posedness of this system and after proving that it admits an exponential attractor, a robustness analysis is conducted. The result is the existence of a family of exponential attractors, which continuously depends on the kinetic constant of the chemical reaction.
Finally we consider a nonlocal model for the interactions between the different components of the mixture. These non-local interactions are represented through convolution with a singular kernel instead of the usual Laplace term.
Considering the Cahn-Hilliard equation alone with a singular (possibly of logarithmic type) double-well potential, we prove existence and uniqueness of solutions for this system. Moreover, we are also able to characterise its long-term dynamics by proving that it admits a global attractor. This study is challenging because no obvious equivalent differential problem can be associated to the energetic formulation considered here. More precisely, due to the incomplete regularity theory for the non-local diffusion operator, the natural boundary conditions for this system are unknown. A partial answer to this regularity problem is also given: in the case of regular solutions and under weak assumptions on the interaction kernel the usual homogeneous Neumann boundary conditions are recovered.

## Strain in semiconductors

The second topic considered is the coupling between mechanical and electronic properties in semiconductors. This study is relevant for flexible electronic devices and applications, going from plastic substrate solar cells to wearable electronics. The description of the electronic devices we consider is based on the drift-diffusion model for electrons and holes. The first part of the study is devoted to the identification of those mechanisms responsible for the relevant strain effects in semiconductors. In particular, two of these seem critical in view of the photovoltaic applications: mobility effects and changes in the generation/recombination terms due to shifts in the equilibrium concentration of carriers.
The next step of our study is the derivation of a macroscopic continuum model for strained semiconductors. This goal can be reached by writing an energetic formulation of the drift-diffusion model. This can naturally be extended to an electro-mechanical model for the continuum. Constraints on the mobilities imposed by thermodynamical consistency of the model are also obtained.
The effect of strain on the characteristic curve of a p-n junction (or solar cell under no light) is the final result of our investigation. This problem can be studied with approximate solutions depending either only on physical assumptions or involving formal and rigorous mathematical asymptotic expansions. The preliminary results obtained are currently awaiting experimental confirmation. However, the necessary data should be available soon from an experimental campaign being conducted presently at the partner university of this cotutelle PhD (Ecole Polytechnique).

## High cycle fatigue

The final part of the thesis presents an application of the theory of dynamical systems to the prediction of the lifetime for polycrystalline metals subjected to high cycle fatigue regimes.
The material is modelled as an elastic matrix surrounding an elastoplastic inclusion. This inclusion is representative of those few grains that suffer the largest shear stresses due to their alignment and therefore undergo plastic deformations.
A new model involving a non-linear hardening rule for the inclusion is proposed. Despite of the additional theoretical complexity, explicit analytical estimates on the lifetime of the material are deduced. This is possible by studying the resulting system of ODEs within the theory of dynamical systems and bifurcations. These results are then compared with the existing literature achieving similar prediction reliability.

# FINITE VOLUME METHODS AND DISCONTINUOUS GALERKIN METHODS FOR THE NUMERICAL MODELING OF MULTIPHASE GAS-PARTICLE FLOWS

**Susanna Carcano -** Supervisors: **Luca Bonaventura, Augusto Neri**

The thesis is devoted to the numerical modeling of multiphase gas-particle flows. This work has been originally motivated by the need of developing numerical tools for the simulation of explosive volcanic eruptions. Due to the complexity of volcanic phenomena, that does not allow to reproduce them at the laboratory scale, mathematical and numerical models are achieving an essential role.

Several theoretical and numerical challenges arise in the field of the simulation of explosive volcanic eruptions. The mathematical description of the real multiphase fluid is not trivial, due to the presence of a wide spectrum of solid components and a large number of chemical gaseous components that interact with each other. Concerning the numerical modeling of explosive volcanic eruptions, the main difficulties are related to the multiscale nature of the phenomena and to the wide variety of flow regimes involved. Further difficulties are related to the rigorous model verification and validation. In conclusion, the accurate and efficient simulation of realistic eruptive scenarios still represents a challenge for computational fluid dynamics.

After a discussion on different approaches to the mathematical modeling of multiphase gas-particle flows, a model based on the Eulerian-Eulerian approach is presented for a mixture of a gaseous phase and N classes of solid particles, able to handle the widest range of physical phenomena. The mathematical model consists in a set of balance equations representing the mass, momentum and energy conservation. Appropriate closure equations are introduced, based on literature review. The dimensional analysis of the multiphase equations is carried out for significant test problems, both on the volcanic scale and the laboratory scale. In complex flow regimes, such as those encountered in natural volcanic phenomena, dimensional analysis is an effective tool to interpret numerical simulations and to reduce the physical and computational complexity of the model. The relative importance of different physical phenomena that take place in the volcanic jet and in the pyroclastic density current are assessed. In the volcanic jet problem, we show that the ejected multiphase mixture can be well approximated as inviscid. Gravitational effects and dissipation due to viscous and drag forces are negligible. Compressibility effects are important and a transonic regime can be expected. Moreover, the hypothesis of equilibrium between different phases is not valid and a fully multiphase mathematical model is needed to investigate the non-equilibrium dynamics between different phases. After the volcanic column collapse, in the pyroclastic current gravitational effects become dominant. When reproducing a multiphase jet on the laboratory scale, particle dynamics is strongly decoupled from gas dynamics. Moreover, viscous dissipation and the work done by the drag force may play a key role in the thermodynamics of the mixture. As a consequence, the thermodynamics processes that influence the jet dynamics on the laboratory scale may differ from those characterizing the volcanic jet dynamics.

Two distinct numerical approximations of the multiphase flow equations are presented and validated, based on the finite volume and the discontinuous Galerkin approach. The proposed finite volume scheme achieves second order accuracy in space and time and it is validated against experimental and numerical results in both supersonic and subsonic regimes. The underexpanded jet problem on the laboratory and volcanic scale, the particle-laden gravity current and the collapsing jet problem are taken as benchmark tests. Supersonic and subsonic regimes are well described by the finite volume scheme. The multidimensional second order spatial discretization is essential to accurately capture the shock wave pattern observed in underexpanded jets and to reduce numerical diffusion. Validation against experiments and comparison against numerical results is satisfactory.

The alternative p-adaptive discontinuous Galerkin approach allows to achieve higher accuracy, while keeping a small computational stencil and a relatively limited computational cost thanks to a p-adaptivity approach. In the present work, the discontinuous Galerkin scheme is applied to solve multiphase gas-particle equations that accounts for drag and heat exchange coupling between different phases. Appropriate flux limiting and slope limiting techniques are applied to the proposed discontinuous Galerkin approximation of the multiphase flow equations. The discontinuous Galerkin approach is tested on several benchmark problems in the one-dimensional case. In particular, monophase and multiphase shock tube test cases are considered in order to assess the accuracy, the limiting techniques properties and the computational efficiency obtained thanks to the p-adaptive approach. We show that slope limiting and flux limiting techniques are essential in multiphase shock tube problems to guarantee the positivity of physical quantities and the stability of the numerical solution. The p-adaptive approach is able to reduce the computational cost up to 50% by keeping a good accuracy on the numerical solution.

In the last part of the work, the finite volume numerical model is applied to study the effect of gas-particle non-equilibrium on underexpanded volcanic jets by assuming monodisperse, bidisperse and polydisperse mixtures. By means of a scaling analysis based on particle Stokes numbers *St*, i.e., the ratio between the particle relaxation time and the Mach disk formation time of the underexpanded jet, we classify solid particulate into two categories, namely *fine* and *coarse* particles. Fine particles are tightly coupled with the gas phase and do not modify the structure of the shock wave pattern in the jet. On the contrary, coarser particles are decoupled from the gas phase and strongly influence the jet decompression structure, including the intensity, shape and position of the Mach disk. On the basis of the results of the time scale analysis, an hybrid pseudogas-multiphase model is proposed, in which fine particles and the gas phase are modeled together as a pseudogas with average thermodynamics properties, whereas coarse particles are grouped together into a representative class of solid particles with average properties. Depending on the mass ratio between fine ($St \ll 1$) and coarse ($St \gg 1$) particles, the jet flow pattern can dramatically change, leading to the obliteration of the Mach disk structure. Numerical results confirm the validity of the hybrid approach for the simulation of monodisperse, bidisperse and polydisperse underexpanded jets and highlight the key effect of the total grain size distribution on the underexpanded jet and on the overall stability properties of the eruptive column.

The developed methodology and techniques are general and can be extended to the many different multiphase gas-particle flows that can be encountered in geophysical and industrial applications.

# FEM FOR PDES WITH UNFITTED INTERFACES: APPLICATION TO FLOW THROUGH HETEROGENEOUS MEDIA AND MICROCIRCULATION

**Laura Cattaneo -** Supervisors: **Prof. Paolo Zunino, Prof. Davide Ambrosi**

Mathematical models and numerical methods have emerged as fundamental tools in the investigation of life sciences. In the real world many problems, that we want to describe through mathematical models, are characterized by field quantities that change rapidly over length scales that are small with respect to the observed domain.
These kind of problems arise from different fields, such as geosciences, nanotechnologies, bioengineering and systems biology.
For example, in plate tectonics and basin evolution, mantles, plates and sedimentary layers can be modeled as heterogeneous viscous fluids, featuring non standard frictional interactions at their interfaces.
Again, many geophysical applications, such as groundwater flows or two-phase flows for oil migration, are characterized by the presence of strong heterogeneities of the model parameters and the permeability of the considered medium (the ground, or, at a larger scale, a geological basin) may easily span several orders of magnitude.
In many bioengineering studies, in order to handle the heterogeneous coupling between blood flow and plasma filtration, we need to develop numerical models capable to deal with extremely variable parameters, such as the blood viscosity and Darcy's permeability of the arterial walls and the external tissue.
The heterogeneities that characterize these systems are described also by the geometry of the systems themselves. Indeed the different layers of a basin are separated by fractures or interfaces and, in a similar way, the vessel walls separate the blood system from the external tissue.
Therefore, in order to predict in a proper way the model results, it is needed to well describe both the physical and the geometrical properties of the system.
At the same time, the geometrical description could be too difficult, so it is very important to find a correct trade off between the accurate description of the included structures and the reduction of the geometrical complexity of the system.
On one hand it is fundamental to use real geometries for the computational modeling, since they allow for an accurate description of the non-smooth behavior of the system. In this direction, for example, the enormous development of clinical imaging such as magnetic resonance or computed tomography opens a new way toward a detailed patient-specific description of the actual geometry.
On the other hand it could be computational too expensive to describe in details the embedded structures because at the level of the numerical solver, we may have to use refined meshes or graded meshes.
For all these reasons, it is fundamental to study and develop reduced numerical models able to simplify the geometrical complexity without loss of information.

The aim of this thesis is to develop mathematical and numerical models of partial differential equations with unfitted interfaces.
On one hand we will study multidomain problems with homogeneous dimensionality, i.e. problems characterized by two means of the same dimension separated with one another through an interface.
On the other hand, we will focus on multidomain problems with heterogeneous dimensionality, that is the case where a one dimensional structure is completely embedded into a three dimensional structure.
In both situations, the different parts of the system feature different physical properties and, depending on the problem, the solution involves discontinuities or singularities.
The common strategy to solve both kinds of problems plans to develop numerical models characterized by the use of computational meshes that do not fit the geometry of the embedded structures. The discretization of the external domain and the discretization of the internal structure are therefore completely independent.

The thesis is divided in two parts, each of which is focused on the study of a different model problem.

The first part of this thesis is focused on multidomain problems with homogeneous dimensionality. We study contrast problems, which is the case where different means of the same dimensions are separated by an interface. In particular we analyze elliptic equations and saddle point problems.
To solve these kind of problems we apply the eXtended Finite Element Method, (XFEM), that is based on the local enrichment of the approximation space of the classical FEM, such that the non-smooth solution properties are accounted for correctly, independently of the mesh.

The second part of the thesis is focused on multidomain problems with heterogeneous dimensionality. We develop a multiscale method to study blood flow and transport phenomena in living tissues, applying a special coupling between a micro-circulation network surrounded by a permeable medium.
We use the Immersed Boundary (IB) method to couple the one-dimensional with the three-dimensional flow through the network and the interstitial volume, respectively. The main idea consists in replacing the immersed actual three dimensional network with an equivalent concentrated source term. In this way we facilitate the analysis of complex capillary bed configurations and we end up with an heterogeneous system characterized by one dimensional channels embedded into a porous medium.
The resulting numerical method is characterized by the fact that the partitions into elements of the one dimensional network and the three dimensional tissue are completely independent.

# PROBABILISTIC REPRESENTATION OF SOME CLASSES OF NONLINEAR PDES AND CONNECTIONS WITH STOCHASTIC OPTIMAL CONTROL AND STOCHASTIC ANALYSIS

**Andrea Cosso** - Supervisors: **Prof. Marco Fuhrman**

The present Ph.D. dissertation studies three different topics related to stochastic optimal control and stochastic analysis, pivoting on the theme of probabilistic representation formulae for viscosity solutions to nonlinear partial differential equations.
After a general introduction, in the second chapter of the thesis we study double-obstacle quasi-variational inequalities, which are Hamilton-Jacobi-Bellman-Isaacs equations arising in two-player zero-sum stochastic differential games involving impulse controls.
We first establish the dynamic programming principle for both the lower value function and the upper value function of the stochastic differential game. This allows us to prove that they satisfy, in the viscosity sense, the corresponding dynamic programming equation. We also provide a comparison theorem for the Hamilton-Jacobi-Bellman-Isaacs equation, from which it follows that the two value functions coincide and that the stochastic differential game admits a value.
The third and fourth chapters of the dissertation deal with probabilistic representation formulae for viscosity solutions to path-dependent PDEs, in finite and infinite dimensions. More precisely, in the third chapter we focus on the finite dimensional case, and we adopt the definition of viscosity solutions for path-dependent PDEs recently introduced by Ekren, Touzi, and Zhang. We prove that non-Markovian forward-backward stochastic differential equations provide functional nonlinear Feynman-Kac formulae for viscosity solutions to semilinear path-dependent PDEs. This extends the result presented in Ekren, Keller, Touzi, and Zhang to the case with a possibly degenerate diffusion coefficient in the forward dynamics. The fourth chapter, on the other hand, is devoted to generalize the theory of viscosity solutions for path-dependent PDEs to the infinite dimensional case, providing also, as in the third chapter, a functional nonlinear Feynman-Kac representation formula for these equations.
Finally, in the last chapter of the thesis we introduce a class of reflected backward stochastic differential equations with nonpositive jumps and upper barrier. We prove that there exists a unique minimal solution through a double penalization approach, under regularity assumptions on the barrier. In a suitable Markovian framework, we show that the minimal solution to our class of BSDEs provides a nonlinear Feynman-Kac formula to fully nonlinear variational inequalities of Hamilton-Jacobi-Bellman-Isaacs type arising in general zero-sum stochastic differential controller-and-stopper games, where control can affect both drift and diffusion term, and the diffusion coefficient can be degenerate. We also obtain a dual game formula for our BSDE minimal solution in terms of a family of equivalent probability measures and discount factors, which gives rise to an original representation for the value function of zero-sum stochastic differential controller-and-stopper games.

# ASYMPTOTIC ANALYSIS OF EVOLUTION EQUATIONS WITH NONCLASSICAL HEAT CONDUCTION

**Filippo Dell'Oro -** Supervisors: **Prof. Vittorino Pata**

The main aim of the doctoral thesis is a rigorous and detailed mathematical analysis of well-posedness and asymptotic behavior of several linear and nonlinear dissipative partial differential equations with nonclassical heat conduction, that is, thermal evolutions where the temperature may travel with finite speed propagation. This area of nonclassical diffusion is nowadays very topical, since there is an increasing evidence, also supported by physical experiments, that thermal motion is indeed a wave-type mechanism. Accordingly, several theories have been proposed through the years as candidates to describe the phenomenon. In the present thesis, we principally consider the approaches of Maxwell-Cattaneo, Gurtin-Pipkin, Coleman-Gurtin and Green and Naghdi.

Linear and nonlinear infinite-dimensional dynamical systems play a crucial role in the modern study of several physical phenomena where some kind of evolution is taken into account. In particular, many dynamics are characterized by the presence of some dissipation mechanisms (e.g. friction or viscosity) which produce a loss of energy in the system. Roughly speaking, from the mathematical viewpoint, dissipation is represented by the existence of a set in the phase space called "absorbing set". Nevertheless, in order to have a better understanding of the asymptotic behavior of the system as time goes to infinity, some additional "good" geometrical and topological properties (e.g. compactness or finite fractal/Hausdorff dimension) are necessary. This leads to the modern concept of "attractor" that is, the minimal compact set which attracts uniformly all the bounded sets of the phase space. In the linear case, the results contained in the thesis mainly focus on the stability properties of the associated strongly continuous semigroups, analyzing the uniform and non-uniform decay to zero of the solutions. At the same time, in the nonlinear situations, we dwell on existence and regularity of finite fractal-dimensional global and exponential attractors, as well as existence of absorbing sets reflecting the dissipative character of the system. In this way, we are able to provide a complete description of the asymptotic dynamics as time goes to infinity by means of suitable "small" regions of the phase space.

Specifically, we first consider strongly damped nonlinear wave equations in a three dimensional bounded smooth domain. These equations serve as a model in the description of type III thermal evolution within the theory of Green and Naghdi, but other physical interpretations are possible, for example viscoelasticity of Kelvin-Voigt type. In particular, the two nonlinearities are allowed to be nonmonotone and to exhibit a critical polynomial growth. The main focus is the longterm analysis of the related solution semigroup, which is shown to possess global and exponential attractors of optimal regularity in the natural weak energy space. In particular, to prove the existence of absorbing sets, the standard techniques based on the use of the Gronwall lemma do not work, and it is necessary to exploit novel Gronwall-type lemmas with parameters. Moreover, in order to show the existence of the attractor, several challenging partial regularization estimates have to be performed. Then, we analyze two evolution systems ruling the dynamics of type III thermoelastic extensible beams or Berger plates. In the linear case, we provide a description of the stability properties in dependence of the coupling parameter, while in the nonlinear situation we show existence of the regular global attractor, along with a geometric characterization. In this latter case, the presence of a memory component in the system (in the form of a time-convolution against a suitable memory kernel) produces a lack of compactness in the phase space, and thus a careful and more challenging analysis is need. Moreover, we study the asymptotic behavior of a nonlinear type III Caginalp phase-field system in presence of two nonlinearities both of critical polynomial growth, proving existence and regularity of the global attractors for the associated dynamical system, and generalizing several previously known results. Finally, we discuss the decay properties of a linear Timoshenko system with Gurtin-Pipkin thermal law. A necessary and sufficient condition for exponential stability is established in terms of the structural parameters of the equations. In particular, by means of suitable singular limits procedures, we generalize previously known results on the Fourier-Timoshenko beam model. In addition, for a particular choice of the memory kernel, we recover and subsume some known results on the Maxwell-Cattaneo-Timoshenko thermoelastic system. It is also worth noting that our approach is based on the construction of explicit energy-type functionals. As a consequence, the argument can be exported to the nonlinear case, allowing for example to prove existence of absorbing sets and regular global and exponential attractors. Moreover, the procedure can be likely used in the study of singular limits in nonlinear Timoshenko systems and related perturbation problems.

# HPC SIMULATION OF SEDIMENTARY BASIN

**Nur Fadel** - Supervisors: **Prof. Luca Formaggia**

The upper part of the Earth crust is modelled as superimposed regions of homogeneous rock with constant physical properties. On geological time frames, rocks can be considered fluids with very high viscosity and their evolution can be described by the Stokes equations. To solve the problem in a reasonable time it is important to develop a parallel implementation. In this work, the solution of the Stokes problem is coupled with a suitable algorithm to track the interfaces between rock layers. The parallel implementation of this solver presents some challenges: we need to find suitable parallel preconditioner for the Stokes problem and to devise an efficient strategy for the set of hyperbolic equations governing the interface tracking. Simulations have been performed on several HPC architectures to test and optimize the proposed solutions. Details on performance and scalability are given.

# STATISTICAL PROPERTIES OF URN MODELS IN RESPONSE-ADAPTIVE DESIGNS

**Andrea Ghiglietti** - Supervisors: **Prof. Anna Maria Paganoni**

The thesis is focused on mathematical and statistical aspects of urn models used as randomized devices in the field of design of experiments. In particular, we consider the context of clinical trials, where the experimentation involves human subjects. In this framework, a central role is played by the randomization, which is now an essential feature of the scientific method. These procedures randomly assign the subjects that sequentially enter the trial to the treatments under study.
The benefit of randomization has been deeply studied in many areas of research, especially in the clinical trial context. The strategy adopted to randomly allocate units to treatments generates different types of experimental designs.
In the thesis, we focus on response-adaptive procedures, in which the allocations depend also on the responses given by the subjects previously assigned. This feature enables to create designs that change the probability of assignment of the subjects according to the treatments performances.
This factor is very important, especially in clinical experimentation, where the ethical aspect is significant more than in other scientific fields. For this reason, the theory of clinical trials has been always characterized by a trade-off between the individual ethics of the subjects involved in the experiment and the collective ethics of the entire community. The first aims at maximizing the individual probability to receive the best treatment, while the second aims at maximizing the power of the procedure that determines the best treatment.

A large class of response-adaptive randomized designs is based on urn models, since they represent classical tools to guarantee a randomized device. Urn procedures can be characterized by different strategies of reinforcement and in this thesis we consider urn models with random non-negative reinforcements concerning only the extracted colour. These designs have been called Play the Winner or Randomly Reinforced Urn (RRU) designs, and they are randomized devices able to asymptotically allocate subjects to the optimal treatment. These procedures had a good success, since their asymptotic behaviour maximizes the individual ethics. Nevertheless, these designs are unsatisfactory for the collective ethics, since their statistical properties present some problems.
At first, because there are many results for designs whose asymptotic allocation is a value within the interval (0,1), that cannot be applied to RRU models since their asymptotic allocation is exactly either 0 or 1. Moreover, these models generate groups with very different sample sizes. Then, the inferential procedures based on these designs are usually characterized by a very low power in comparing treatments effects.
For these reasons, we have modified the reinforcement scheme of the urn to construct a design that asymptotically targets an allocation proportion is a value within (0,1).
The term target indicates the limit of the urn proportion process.
We will denote this urn model as the Modified Randomly Reinforced Urn (MRRU) design.

At first, we introduce the MRRU model and we prove strong convergence of the urn proportion to the target allocation in (0,1).
Further first-order asymptotic properties of the urn model have been investigated.
The study of the asymptotic behaviour has been particularly challenging since the modified urn process does not present the sub/supermartingality properties presented by the RRU.

Then, we adopt the MRRU model to improve the statistical performance of different tests for comparing the mean effect of two treatments. We show that a response adaptive design as the MRRU for implementing the random allocation procedure enables to get good properties from both ethical and statistical points of view. In particular, we achieve both the goals of increasing the power of the test and of assigning fewer subjects to the inferior treatment.
Simulation studies on the statistical performances of this procedure have been conducted. We applied this procedure to a real case study and the results of the analysis have been reported.

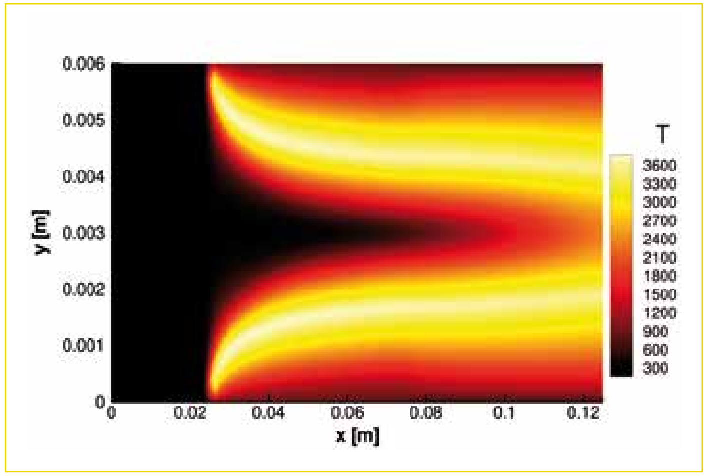
Moreover, we investigate the second-order asymptotic properties of the MRRU model. In particular, we compute the rate of convergence of the urn process and we study its asymptotic probability distribution. Then, we compare theoretically and empirically the inferential performances of the MRRU model with the ones provided by the RRU model, whose asymptotic allocation is 0-1.

Finally, we construct a randomly reinforced urn model able to target an asymptotic allocation within (0,1), which is a function of unknown parameters modelling the responses distribution.
First-order asymptotic results under different conditions have been investigated.
In particular, we prove the couple convergence (almost sure and in probability) of the urn proportion to the desired allocation function of the unknown parameters.

# NUMERICAL MODELING AND SIMULATIONS OF COMBUSTION PROCESSES IN HYBRID ROCKET ENGINES

**Alessandro Mazzetti -** Supervisors: **Paolo F. Barbante**

Nowadays, two are the most intriguing mid-long term challenges for space propulsion technology research and development. The first one is to achieve reliable, safe, flexible, low-cost and possibly mass access to space. The second one is to realize hypersonic aircrafts for goods and passenger transports which are able to cross intercontinental distances in a limited number of hours. Hybrid rockets might be the answer. They conjugate throttleability, precision and safety of liquid-fuelled rockets with design simplicity and low cost of solid-fuelled rockets. However a major drawback in hybrid rocket engines is the low regression rate of traditional fuels. This leads to inadequate performance levels in terms of thrust and specific impulse, forfeiting the reach for aforementioned achievements. Research effort to overcome low burning fuel speed is addressed towards testing of high energetic additives (micro- and nano- sized metals, metallic hydrides) and innovative paraffin-based fuel formulations. The latter rely on entrainment effect to increase performance: returning heat from the flame zone creates a molten layer on top of the fuel grain; injected oxidizer makes unstable this thin film and fuel spray is generated; these fuel droplets are then burned. Physical phenomena involved are very complex and difficult to model: the flow inside the rocket engine is turbulent, multi-species, multiphase and chemically reacting. Therefore main research is still fully experimental. The development of an accurate and reliable numerical tool could be a relevant contribution to research in this field. In fact this kind of tool can be used to analyze combustion processes in hybrid rockets, in order to get a better understanding of the problem physics. A reliable numerical model capable of predicting performance parameters and behavior of hybrid rockets is of major importance for the design of the next generation of hybrid rocket engines. Such tool can be used as support and guidance for fuel formulation investigation and for engine performance estimation.
In fact, nowadays, numerical simulations of combustion processes in hybrid rockets are only considered as a qualitative tool used to describe fluid-dynamic field inside the rocket. A research effort could be of major importance in order to change this trend, by obtaining results which are quantitatively accurate.
This work faces this open research problem addressing the issues related to the simulation of such complex and interdependent problems as the ones present in the problem physics.
The governing equations of the addressed problem are discussed, with particular attention to the accuracy of the closure models and of the boundary conditions. In fact, as the state of the art review reveals, several simplifications are generally applied in order to reduce problem modeling complexity.
This work applies a more rigorous approach in the modeling of energy equation and in the modeling of closure terms. This requires the identification of adequate models for turbulence and chemical reactions. Moreover thermodynamic and transport properties of both the single reacting species and the gas mixture are to be modeled.
Two different chemical models are evaluated in order to verify their coherence with problem physics. In addition, in order to address the limits of quasi-laminar chemistry versus a fully turbulent chemistry approach, both approaches for the chemistry source term are implemented and verified.
In order to focus the work on the combustion modeling description, a modular object-oriented scientific computing environment is used: this is COOLFluID code, developed at von Karman Institute for Fluid Dynamics.
Results are presented under an increasing problem complexity philosophy: at first non-reacting testcases are performed in both laminar and turbulent fashion, in order to obtain the base validation of the code.
The first reacting testcases are analyzed with a simplified boundary condition for the fuel inlet, with constant velocity of injected gaseous fuel based on experimental data, and at constant pressure.
An accurate boundary condition considering the energy balance at the fuel inlet region is then described and implemented.




1. Temperature field for 2D double fuel slab simulation of hybrid rocket engine combustion chamber. In bright colors, the diffusion flames corresponding to two fuel slabs at the wall. The scale is stretched in y direction in order to achieve better visibility.

This is mandatory in order to obtain an estimation of both local and average fuel regression rate, the most important parameter for the comparison of hybrid rocket engines performance.
An additional analysis is performed in order to assess the influence of both oxidizer mass flux and pressure increase on the combustion flowfield and on the regression rate. The effect of pressure on regression rate is yet an open research question in hybrid rocket science, with controversial interpretation.
This work addresses the problem through the analysis of simulation results.
Therefore this simulation results obtained are innovative and important because their apply some original ideas, such as: accurate treatment of energy equation, accurate energy balance at fuel wall and multi-time PaSR approach for a fully turbulent simulation of chemical reactions.
In conclusion, this research work is an important step towards the understanding of the combustion phenomena in hybrid rocket engines and the further development of this technology, because it offers a new starting-point tool for quantitative analyses and simulations of hybrid rockets.

# ADJOINT-BASED PARAMETER ESTIMATION IN HUMAN VASCULAR ONE DIMENSIONAL MODELS.

**Alessandro Melani -** Supervisors: **Prof. Luca Formaggia, Prof. Fabio Nobile**

Vascular network models are used to describe the propagation of pulse waves in the cardiovascular system. However they depend on several parameters that are difficult (if not impossible) to measure *in vivo* with sufficient confidence. Yet, their knowledge could provide useful information to physicians on the state of the vessels. It is therefore crucial to develop suitable techniques that allow to estimate these parameters adequately, starting from available measurements.

In this thesis, we focus on the estimation of the compliance of arterial walls in vascular networks. We represent the network as the combination of one-dimensional non linear models (one for each vessel) coupled through suitable interface conditions and boundary conditions. These are reduced models (and consequently less computationally expensive than three dimensional models ) but nevertheless they are able to capture the main characteristics of the physical phenomena, like the propagation of pressure waves. The compliance of the vessel appears in the model as a parameter and, in general, it varies from one vessel to another and may even vary within a single vessel, for instance, because of the presence of a stenosis.

The method that we developed can be placed in the wider class of data assimilation that consists in combining in an optimal way the mathematical information provided by the models and the physical information given by the observations, generally sparse and noisy. Data assimilation had a huge development in the last two decades in the field of cardiovascular simulations.

One of the major novelties of our methods stay in the fact that it is the first attempt to estimate a parameter in one dimensional network models by a variational data assimilation approach. Firstly, we define a cost functional that takes into account the difference between the observations and the output of the 1D-FSI model and consequently we introduced the Lagrangian functional that we minimized by solving the coupled system of first order conditions (the so-called Karush-Kuhn-Tucker conditions), namely *state problem*, that describes blood flow in the vessels and that depends on parameters; *adjoint problem*, that gives us the sensitivity of state model to the variation of parameters and that depends on both state problem solution and parameters; *optimality condition*, that permits us to understand when we reach the minimum and that depends on both state and adjoint problem solutions. In this process, a particular attention is devoted to the treatment of adjoint boundary conditions and adjoint coupling conditions. Therefore we build up an iterative optimization framework in which we first solve the state and adjoint equation and, then, we update the parameter by computing the optimality condition and applying finite dimensional optimization methods, until a certain tolerance is reached. The optimization problem is solved by using line search methods (in particular we implement steepest descent method, Barzilai-Borwein method and Newton method) and a scaling strategy to be sure that the updated parameter is admissible.

We implemented this framework in *LifeV*, a C++ finite elements library. In particular, we are able to manage and estimate different distributions of the compliance parameter inside each vessel or part of vessel.

We test the method and our implementation on different networks and we studied the influence of noise and of sparse observations, by using simulated observations. We note that Barzilai-Borwein method permits to obtain a good accuracy in the estimation with a low computational cost.

Finally, we apply the developed method to a patient specific case employing real medical data, which is another of the main contributions of our work. In particular, we study and pre-process real observations and then we estimate the elastic properties of carotid that underwent thromboendoarteroctomy with patch insertion. We employ two type of observations:
eco color doppler, from which we obtain velocity profile to enforce inflow boundary condition;
4D magnetic resonance imaging, from which we extract the evolution of section area in 17 locations of the carotid bifurcation in 25 time instants.
The results of the application of our method seem to highlight a difference in the compliance parameter in the region of the patch with respect to the rest of the vessels.

# MATHEMATICAL AND NUMERICAL MODELING IN GEODYNAMIC APPLICATIONS

**Mattia Penati -** Supervisor: **Prof. Edie Miglio**

Plate tectonics is a theory that describes the evolution of Earth's lithosphere. The lithosphere is broken up in a set of regions called plates moving on the fluid-like asthenosphere; due to this motions earthquakes, volcanic activity and orogeny occur along plates boundaries. The relative motions of plates determine the type and the surface phenomena occurring along boundaries; three different types of boundaries exist: transform, divergent and convergent.
Oceanic rift processes are due to divergent plates which are moving away from each other and the asthenospheric mantle rises up creating new oceanic crust. These regions are particularly interesting for studying interaction between lithosphere and asthenosphere. During the last years the amount of available data on mid-ocean ridge increases providing evidences on the fact that symmetry of mid-ocean ridge is less common than originally believed; in particular asymmetries have been observed in the seafloor depth and in the subsidence rate of the ridge flanks.  Recent studies have shown that the rift zone and the plates are moving with respect to the underlying asthenospheric mantle, this process has been considered as one of the possible explanation of such asymmetries.
The aim of this thesis is the development of advanced mathematical and numerical models for the simulation of geodynamic processes, in particular the migration of the mid-ocean ridges and the induced asymmetries. Both heuristic explanations and mathematical models have been proposed in order to show the relationship between the migration processes and ridge asymmetries. In this work a rigorous dimensional analysis is performed in order to define the proper mathematical models; some simplifications based only on scale analysis (using direct measurements) are introduced. Moreover novel numerical techniques are proposed for the solution of the viscous and elastic problems arising in the numerical simulation of geodynamic processes; in particular we deal with:

- preconditioning techniques of Darcy and Stokes problem with highly variable coefficients;
- arbitrarily high order geometric integrators for the nonlinear elastic problem.

We have investigated the mathematical and numerical modeling for geodynamic applications, with a focus on the mid-ocean ridges. A rigorous dimensional analysis has been performed in order to obtain an appropriated mathematical model for the simulation of mid-ocean ridge migration process. From our point of view this a key point in order to define a proper mathematical model and to our knowledge it has never been carried out in details. Moreover this analysis has shown that some heuristic assumptions considered in previous works are not totally justified. Another outcome of this analysis is the definition of a proper model which can be applied for studying of large portions of lithosphere, this gives us a new tool to define proper boundary conditions for the problem at hand. Numerical results shown that these boundary conditions are less invasive than the ones adopted by other authors; this fact allowed us to perform the same numerical simulations carried out by other authors using smaller domains without boundary effects and reducing the computational cost. The reduction of the computational cost is of great importance especially in view of three dimensional simulations. From the geological point of view this model predicts a small asymmetry of the lithospheric depth between the two flanks of the ridge; such difference has been obtained taking into account only the migration process, we expect to get more details including one or more of the following extensions:

- introduction of the density variation and the buoyancy force term;
- an improvement of the rheology model for the lithosphere and asthenosphere, for example taking into account the presence of the Low Viscosity Zone;
- tracking the rocks mineralogical composition, the water content and the melting rate in order to give a more detailed image of the rift.

The main difficulty we have encountered is the preconditioning of the problems arising from the geodynamic applications since they usually involve highly variable coefficients. This difficulty has been solved introducing a novel mixed formulation for the Stokes problem and using an effective preconditioning technique which has been proposed by Arnold. In this thesis a new application and a detailed analysis of this preconditioning technique is proposed. The results show the effectiveness and robustness of this preconditioner. Future works in this context will include:

- the application of the mixed formulation of Stokes problem and the proposed preconditioning techniques for the solution of unsteady problems;
- using a mixed-hybrid discretization technique to reduce the number of the unknowns and obtaining a more efficient solver.

The last part of this work is a preliminary study of the application of Galerkin variational integrators to the nonlinear elastic problem or more generally to the continuum mechanics. The analysis of the Galerkin variational integrators has been recast in a more natural framework: some results which have been proved by other authors can be seen as a special case of the proposed general theory. These kind of numerical integrators are well suited for the mechanical system and for long time simulations.

# MULTISCALE HOMOGENIZATION AND ITS APPLICATION TO TUMOR BIOLOGY: FLUID AND DRUG TRANSPORT PHENOMENA AND PORO MECHANICS OF GROWING MATERIALS

**Raimondo Penta** - Supervisor: **Prof. Davide Ambrosi**

Aim of the present thesis is the development of novel mathematical models to describe the fluid and drug transport processes in malignant biological tissues, as well as their mechanical properties and growth. The work falls within the framework of classical methods of mathematical physics, in particular multiscale *homogenization* , applied to the behavior of biological systems pointed out by recent experiments.

The tumor microvasculature represents an *ad hoc* supply network, which is sprout out via the so called angiogenesis process, in order for the malignant mass to obtain nutrients for growth.
The angiogenic blood vessels are characterized by functional and structural abnormalities and heterogeneities and they are in general highly permeable, leaking and tortuous, such that the blood circulation through these vessels can be impaired and hard to predict.

In this scenario, several complex and coupled physical phenomena take place, including blood and drug circulation in the angiogenic capillary network, fluid and drug transport, as well as chemical reactions in the interstitial space and blood leakage through the vessels membrane, which enables the coupling between the two compartments. A complete description of the physics in the tumor system represents a challenging issue from a mathematical modelling and computing viewpoint.
We thus exploit the sharp length scale separation between the characteristic tumor length (the *macroscale*) and the intercapillary distance (*the microscale*), such that, via asymptotic homogenization, we are able to decouple spatial variations and obtain a robust macroscale theoretical framework.

The resulting model takes into account both the relevant physical phenomena occuring in the system and reduces mathematical complexity; a major aim for this work is, in perspective, to achieve a practical tool which can help the setup of effective anti-cancer therapies. The role of the microvascular geometrical complexity is encoded in the model coefficients, which are computed via numerical simulations of classical differential problem on a single representative *cell*.

Tumor growth and its mechanical properties are important issues to tackle. The multiscale analysis of poroelastic growing materials (where, in this case, the micro and macro spatial scales are identified with the pore radius and medium length, respectively) we carried out represents a theoretical starting point to improve our physical insight about the interplay between material growth and elastic strains and it can be applied to the tumor mass, which has been shown to be behave as a poroelastic material.

The thesis is organized as follows:

In the first chapter, a system of differential equations for coupled fluid and drug transport in vascularized (*malignant*) tissues is derived by a multiscale expansion.
We start from mass and momentum balance equations, stated in the physical domain, geometrically characterized by the intercapillary distance (*the microscale*).
The Kedem-Katchalsky equations are used to account for blood and drug exchange across the capillary walls.
The multiscale technique (*homogenization*) is used to formulate continuum equations describing the coupling of fluid and drug transport on the tumor length scale (*the macroscale*), under the assumption of local periodicity; macroscale variations of the microstructure account for spatial heterogeneities of the angiogenic capillary network.
A double porous medium model for the fluid dynamics in the tumor is obtained, where the drug dynamics is represented by a double advection-diffusion-reaction model.
The homogenized equations are straightforward to approximate, as the role of the vascular geometry is recovered at an average level by solving standard cell differential problems.
Fluid and drug fluxes now read as effective mass sources in the macroscale model, which upscale the interplay between blood and drug dynamics on the tissue scale. We aim to provide a theoretical setting to support the design of effective anti-cancer therapies.

In the second chapter, the role of the microvascular network geometry on transport phenomena in solid tumors and its interplay with leakage through the vessels is qualitatively and quantitatively discussed. Our starting point is multiscale homogenization, which can be applied assuming a sharp length scale separation between the characteristic vessels and tumor tissue spatial scales, referred to as the *microscale* and the *macroscale*, respectively. The coupling between interstitial and capillary compartment is described by a double Darcy model on the macroscale, whereas the geometric information on the microvascular structure is encoded in the effective hydraulic conductivities, which are numerically computed solving classical differential problems on the microscale representative *cell*. Then, microscale information is injected into the macroscopic model, which is analytically solved in a prototypical geometry and compared with previous experimentally validated, phenomenological models. In this way, we are able to capture the role of the standard blood flow determinants in the tumor, such as the tumor radius, tissue hydraulic conductivity and vessels permeability, as well as the influence of the vascular *tortuosity* on fluid convection. The results quantitatively confirm that transport of blood (and, as a consequence, of any advected anti-cancer drug) can be dramatically impaired by increasing geometrical complexity of the microvasculature. Hence, our quantitative analysis supports the argument that geometric regularization of the capillary network improve blood transport and drug delivery in the tumor mass.

In the third chapter, a new mathematical model is developed for the macroscopic behaviour of a porous, linear elastic solid, saturated with a slowly-flowing incompressible, viscous fluid, with surface accretion of the solid phase.
The derivation uses a formal two-scale asymptotic expansion to exploit the well-separated length scales of the material: the pores are small compared to the macroscale, with a spatially-periodic microstructure.
Surface accretion occurs at the interface between the solid and fluid phases, resulting in growth of the solid phase through mass exchange from the fluid at a prescribed rate (and *vice versa*).
The averaging derives a new poroelastic model, which reduces to the classical result of Burridge and Keller in the limit of no growth. The new model is of relevance to a large range of applications including packed snow, tissue growth, biofilms and subsurface rocks or soils.

# MECHANICS OF THE HEART: CONSTITUTIVE ISSUES AND NUMERICAL EXPERIMENTS

**Simone Pezzuto -** Supervisor: **Prof. Davide Ambrosi**

The functional role of the heart in a living system is to pump the blood throughout the body, so that oxygen and nutrients can be distributed to all the tissues and metabolic waste product can be collected for disposal. This basic physiological job is performed in an extremely sophisticated way, the effectiveness of the mechanical activity as well as its regulation are performed according to rules that exploit the laws of mechanics in service of the needs of the organism.

The thesis deals with the mathematical modeling and numerical simulation of the cardiac activity. We are interested in understanding and reproduce numerically how the heart is able to produce work and regulate its functions. There are at least two motivations behind this work: the first one, is to contribute to advance the human understanding of its functionality by the support of mathematics, shedding some light on the reason why its architecture and physiology make its performance so effective and stable.
The second motivation, in a long--term vision, is the ambition that a computer--aided medicine, if properly calibrated, can provide the clinicians a support to improve their diagnosis and prognosis.

In this work the emphasis is on two keywords: calibration and stability. A good mathematical model, must be able to reproduce, to a certain extent, some of the peculiarities of the system it has been thought for. In the case of the heart, examples of striking features are the ability to adapt the propulsive force depending on the load, or to torque in order to accommodate the ejection of blood from the ventricle. On the other hand, the introduced complexity possibly with the specific purpose of capturing aspects of the underlying physiology, must not compromise the stability of the model. Secondly, after fixing the properties of the model and its numerical implementation, there is the need to calibrate all the involved parameters.

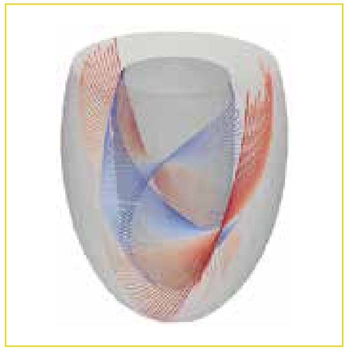
The first chapter concerns the passive ventricular mechanics, where the chamber is supposed to be an elastic body, without residual stress, that deforms under the action of a pressure difference. The ventricle, which is approximately ellipsoid shaped, has a thick wall composed of, among other things, specifically oriented muscle fibers organized into laminar sheets. This is an essential mechanical characteristic of the myocardium because it determines the ability of the ventricle to twist and swell correctly during the filling phase.

We analyze in detail an hyperelastic model proposed by Holzapfel and Ogden in 2009, to describe the mechanics of the passive myocardium. The model is gaining an increasing popularity because of its simple invariant--based formulation and the small set of material parameters invoked, at least when compared to other models in the literature. It has also already been exploited in patient--specific simulations.

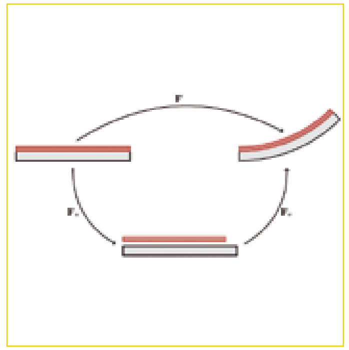
We discuss the sensitivity of the numerical results on the microstructure (which is always known with a large uncertainty) on the basis of various geometries and configurations. We study the influence of different boundary conditions on the solution and the prescriptions to obtain mathematically well--posed problem. While the authors of the model suggest to deactivate the fibres--specific elastic energy contribution when fibers undergo a compressive regime, here we show which problems can occur if this modification is neglected.

In the second and last chapter, we study the contractility of the heart, as a muscle, its ability to spend energy at the microscale to produce work at the macroscale. This interaction between biochemistry and mechanics is usually represented, at the macroscale, by an active stress to be added to the linear momentum balance.
The constitutive equation of the passive contribution is usually addressed by standard stress--strain tests without electric excitation; conversely the active term can be barely decoupled from the passive contribution at a tissue scale and therefore its constitutive form is usually provided on the basis of the observed cell--scale behavior.

A less popular biomechanical approach is to introduce just one stress term, while splitting the gradient of deformation into two factors: a passive one and an active one. In this case, standard stress--strain tests are expected to provide the form of the passive (inert) strain--energy function; the determination of the active strain as a function of the activation fields (concentration of ionic species) has to be prescribed on the basis of cell type experiments. From a thermodynamic point of view, the key assumption here is that the distortion induced by the active term does not store recoverable energy, so that the strain--energy has to be evaluated with respect to such distortion.



1. Fibres distribution on a idealized left ventricle



2. Active strain approach for muscular thin films.

Both the “active stress” and the “active strain” approaches should satisfy due mathematical properties, namely frame indifference and rank--one ellipticity of the total stress. From this point of view, the active strain approach simply inherits these properties from the strain--energy. The rank--one ellipticity of an active stress needs instead to be verified case by case, in particular in the compressive regime.
In the first part of the chapter we discuss examples of active stress and active strain laws in terms of precise mathematical and physiological properties.

Constitutive laws deduced from the cell--level dynamics should reproduce the observed physiological behavior of the specific living tissue at the macroscale, when both active and passive forces contribute. Archetypical requirement in cardiac dynamics is to reproduce the correct pressure--volume relationship and torsion. Intuitively, the heart has to be able to generate the necessary pressure to open the aortic valve and let the blood flow throughout the body. As in the previous chapter, we perform several sensitivity analysis of the model by means of numerical simulations, and we show that the microstructure plays an even more prominent role than the case of a purely passive inflation of the ventricle, since non--physiological orientations of the fibers are not appropriate to produce the expected pressure.

# BLIND SOURCE SEPARATION METHODS FOR HIGH-DIMENSIONAL, MASSIVE, AND COMPLEX DATA

**Paolo Zanini -** Supervisors: **Prof. Piercesare Secchi, Dr. Simone Vantini**

The aim of this manuscript is to analyze Blind Source Separation problems for high-dimensional, massive, and complex data, and to propose new methods to face these statistical problems. Blind Source Separation problem consists of retrieving a set of unobserved source signals from a set of observed mixed signals, according to some a priori hypotheses on the sources and/or on the mixing process. Specifically we rely on the following model; let X in $R^p$ be a random vector and assume the existence of a vector S in $R^K$ representing K latent random sources and such that X = A(S), where A: $R^K$ à $R^p$ is an unknown mapping from $R^K$ to $R^p$ called mixing process. In this manuscript we consider two simplified assumptions related to this model. In particular we assume K ≤ p and A is a linear process. Then the previous model reads X = AS, where A is an unknown p x K matrix of real numbers called mixing matrix. Therefore the columns of A constitute a basis of a K-dimensional subspace of $R^p$; for this reason A is also called basis matrix. If the rows of the n x p matrix X collect n observed realizations $x_1,\dots,x_n$ in $R^p$ of the random vector X while the rows of the n x K matrix S represent the corresponding unobserved realizations of the latent random vector S, our model becomes X = $SA^T$. A BSS problem consists in estimating A and S, given X.

BSS problems are widespread in a lot of different fields. They became popular for those areas focused on temporal signals, like speech and audio signals, telecommunication systems and medical signal processing (e.g., electroencephalograms signals). Nowadays BSS methods are also frequently applied to more complex data, such as texts, images and tensors. Image processing, in particular, provides very different applications for BSS techniques. A typical example is the functional Magnetic Resonance Imaging (fMRI), a functional neuroimaging procedure that measures brain activity and provides brain images that can be processed through BSS methods. Another possible application is the analysis of geo-referred images gathered by GIS systems. All these applications share a common feature; the complexity of the available data is sharply increasing, due to the big improvements in the technology. Then, new statistical methods need to deal with high-dimensional, massive, and complex data, that often contain redundant information and hence make it difficult to extrapolate the relevant features. The crucial purpose is to find a space of small dimension where data can be easily analyzed without losing their significative features.

Many approaches are commonly used to solve a BSS problem. The most common is Principal Component Analysis (PCA). PCA is a powerful method to find optimal subspaces where to represent data, but it presents some drawbacks. In particular, PCA yields an orthonormal basis (i.e., the columns of A are orthogonal vectors); in many circumstances orthogonality is a desirable property but in some it introduces an artificial constraint not related to the phenomenological characteristics of the analyzed problem. For this reason basis elements provided by PCA might not represent physical features of the phenomenon under study. Indeed PCA is a model free method and this lack of assumptions might lead to solution that cannot be interpretable. The idea, instead, is to take into account some assumptions on the model. These assumptions can be made on the source matrix S and/or on the basis matrix A. Among the methods that make assumptions on the sources the most popular is Independent Component Analysis (ICA), which surmises the stochastic independence between the sources. Other approaches, instead, look for a sparse basis matrix, since some of the relevant features may involve a great number of the primitive variables describing the data set while others may be restricted only to a few. Hence a multi-resolution analysis is desirable. Among the others we cite Wavelets and Treelets. In a third group of BSS methods can be considered those methods which aim to find interpretable solution imposing some constraints on S and/or A in the estimate procedure. These constraints typically come from some a priori knowledge on the source matrix and the basis matrix. Among these methods we cite the Nonnegative Matrix Factorization (NMF), which solves the BSS problem imposing the nonnegativity constraint on both the elements of S and A.

In this manuscript we present new methods and interesting applications for BSS problems, particularly suited for high-dimensional, massive, and complex dataset. Specifically in the first part of the manuscript we present Hierarchical Independent Component Analysis (HICA), a new method which simultaneously introduces sparsity and multi-resolution on the basis matrix A to obtain meaningful basis elements and sources. We apply HICA to an Electroencephalography (EEG) dataset, comparing the results provided by HICA with those obtained through other popular methods. In the second part we present spatial colored Independent Component Analysis (scICA), a new method that extends ICA by exploiting the dependence structure within the sources, precisely when sources are generated by a spatial stochastic process. We apply scICA to a geo-referenced dataset describing the mobile-phone traffic in the area of Milan, Italy. We compare scICA with other popular methods, also considering the HICA method. In the third part part we analyze the resolution of the Nonnegative Matrix Factorization through an Alternating Least Square algorithm. In particular we focus on two issues. The first one is related on how to face the problem when different kind of constraints have to be imposed. The second regards the Alternating Least Square algorithm for functional data and, in particular, how to deal with the problem of misalignment of functional data. We show an application to the analysis of the gas chromatograms of chemical mixtures. Finally we also present the help of the package fastHICA we developed to implement HICA method in the statistical software R.

# MICROSTRUCTURE EVOLUTION IN MARTENSITIC TRANSFORMATION AND CRYSTAL PLASTICITY

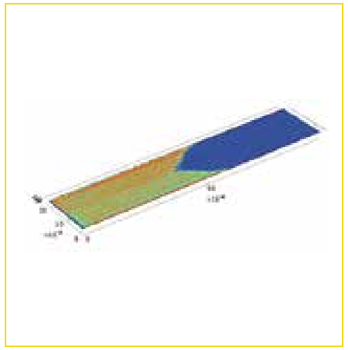
**Anna Zanzottera** - Supervisors: **Prof. Paolo Biscari, Dott. Marco Urbano**

This work arises from a fruitful collaboration with the R$\&$D group of the SAES GETTERS company (http://www.saesgetters.com). The problem under investigation is the mechanical behavior of shape memory alloys (SMAs), for the sake of a deeper insight in the functional fatigue process of SMAs when subjected to superelastic cycling. The main challenge is to find the link between the relevant mechanisms of reversible martensitic phase transformation (MT) and plastic deformation (PD), occurring at crystallographic level, and the macroscopic behavior of the material. SMAs enjoy very interesting thermo-mechanics properties for a variety of applications ranging from aerospace and robotics to biomedics. The key element at the origin of these properties is the martensitic transformation. It is characterized by an abrupt change of crystal structure that modifies the mechanical properties of the material, allowing for shape memory effect and pseudoelastic behavior. Shape memory effect is the ability of the material to recover, upon heating, the deformation suffered below a critical temperature. Pseudoelasticity is the ability to recover strains beyond their apparent elastic limit.

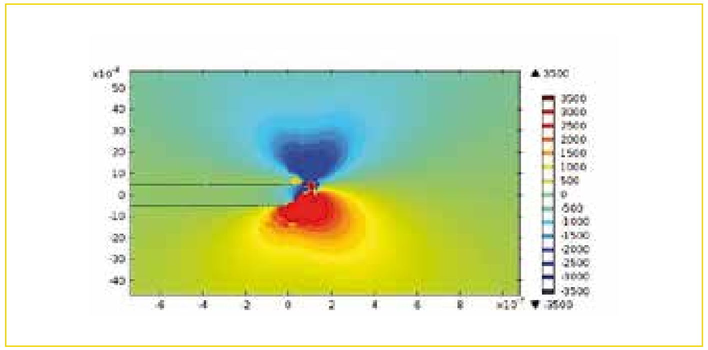
The reversibility of the phase transformation, i.e. the ability to go back and forth through the transformation many times without degradation of functional properties is crucial for applications. However, plastic phenomena very often occur during repeated cycles of transformation inducing a not complete recover of the shape and a significative deterioration of SMAs functional properties. It is generally believed that the degradation of functional properties is due to the creation and evolution of dislocations, possibly driven by the accumulation of stress at the transition layer between transformation phases. The undesirable degradation effects are exemplified by internal crack formation and growth, leading to failure in many applications. A deeper understanding of PD and MT as well as their interplay is an active topic of investigation both in terms of fundamental and applied research. In the literature the topic is tackled with a twofold perspective: a) reducing the causes of dislocation activity. It has been conjectured and experimentally confirmed that if peculiar geometric compatibility conditions between martensitic parent and product phases are satisfied (`good fitting of the phases'), the resistance to transformational fatigue is improved. This approach leads to the search of new materials where the alloys composition is tuned to satisfy the peculiar compatibility conditions; b) accepting the presence of dislocation activity during MT and derive reliable models to predict formation and evolution of plastic phenomena in MT.

We present a modeling framework to explore MT and PD in a single crystal. At the crystallographic level, MT is associated with a lattice symmetry breaking deformation. On the other hand plastic slip is associated with an arbitrary large shear deformation that locally preserves the lattice symmetry. Within the phase field approach and in the framework of finite elasticity, we implement and analyze a model for MT, and propose a new model for PD. The model for MT is characterized by a strain energy which, by construction, accounts for the finite number of symmetry breaking stretches associated with the phase transformation. On the other hand, the model for plastic deformation is set to deal with the infinite number of lattice invariant plastic slips. The latter are described by deformations whose gradient belongs to the infinite global symmetry group. In both models the elastic strain is coupled with a finite number of phase field variables which evolve according to a gradient flow type equation.





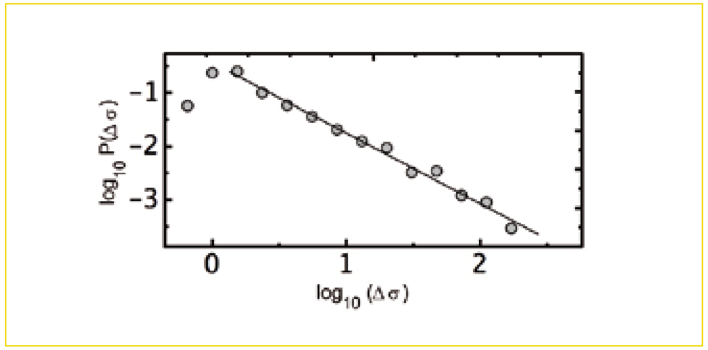
1. Microstructure evolution during mechanical induced MT.



2. Contour plots of a component of the stress tensor close to an edge dislocation.

In MT the phase field variables label the spatial arrangement of transformation phases, in PD they select the deformation path and an auxiliary plastic map identifies the plastic deformation at each position and time. The non compatible discontinuities of such map allow to track position and character of crystal dislocations.

We present numerical simulations for the proposed models in a number of experiments. Mechanically and thermally induced martensitic phase transformation are simulated and the arising microstructure is analyzed (see Figure 1). Hysteresis loops are compared to investigate the influence of orientation of the crystal and temperature. We discuss the importance of working in a geometrically nonlinear framework rather than a linear elastic one. Creation and evolution of dislocations are investigated via displacement controlled shear tests (see Figure 2). The effect of an initial defect density on the mechanical response is analyzed. We show the model is able to capture the intermittent character of the plastic dynamics, analyzing the statistical distribution of the associated fluctuations (see Figure 3).




3. Power law distribution for the amplitude of stress drops in a shear experiment.

As future perspective, it would be interesting to study the MT and PD in a coupled model by combining the formulations we have introduced. In fact, our phase field approach can be generalized in a natural way to take into account for both dislocations formation and martensitic phase transformation. The two phenomena can be modeled in a similar way: the only difference is that in the case of phase transformation (unlike in crystal plasticity) the possible equilibrium configurations are finitely many and characterized by symmetry breaking deformations.

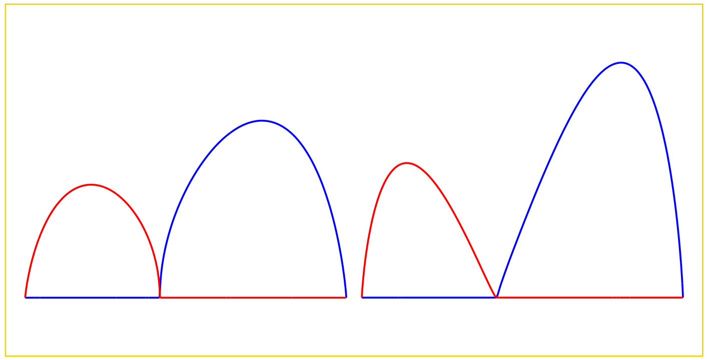
# ON MONOTONICITY FORMULAE, FRACTIONAL OPERATORS AND STRONG COMPETITION

**Alessandro Zilio** - Supervisors: **Gianmaria Verzini, Susanna Terracini**

The main focus of the thesis is on qualitative properties of solutions to system of elliptic semilinear equations which contain interaction-competition terms. The manuscript is divided in two parts, corresponding to the two main subjects of the thesis. In the first part we deal with uniform estimates in appropriate spaces for solutions to fractional elliptic system involving strong competition. In the second and last part, for a system of elliptic equations concerning the study of Bose-Einstein condensates, we shall prove existence of entire solutions which exhibit an exponential growth at infinity. The main theme, common to the two parts, is the use of monotonicity formulae of Alt-Caffarelli-Friedman and Almgren type in the study of solutions of elliptic systems.

Uniform Hölder bounds for strongly competing systems

The first part of the thesis is concerned with the common regularity shared by the solutions of fractional elliptic systems with a strong reciprocal competition mechanism. The competition term is represented by a function of the two interacting densities, and in general it satisfies different assumptions according to the modeling aspects of the problem under investigation: of the many possible choices, we have considered two types of competition which are most important in applied sciences, namely the variational competition (which appears, for instance, in the Gross-Pitaevskii equation for Bose-Einstein condensates), and symmetric one (of interest in mathematical biology, namely in the Lotka-Volterra model for population dynamics). Our main aim is the study of the behavior of the solutions to such systems as the strength of the competition (with respect to the diffusion and internal reaction features) diverges. The description of the limiting profiles is quite important from an applied point of view, since the limiting systems associated to these models appear in many contest, such as pattern formation and optimal partition problems. It should be mentioned that the limiting problem is in general hard to study, due to the sharp transitions imposed by the diverging competition term, thus an approach based on approximations, as the one proposed, is useful in this sense. But the importance of the description of the behavior of the solutions as the competition diverges is crucial also by itself. Moreover, this analysis helps to identify the correct conditions that the solutions of the limiting system have to satisfy. We should mention that the present problem, in the case of standard diffusion processes, has already been object of study by the scientific community: as of now, a quite precise picture of the phenomenon of segregation is now available. The aim is then to try and generalize such results to the fractional contest. As a result, in the first part of the thesis we show that uniformly



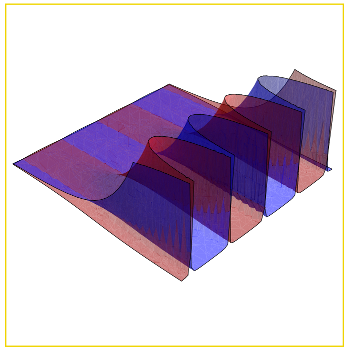
1. Solutions to the system of fractional elliptic equations. On the left, a solution in the case of variational competition, while on the right a solution in the case of symmetric competition. The difference in the regularity is evident.



bounded family of solutions to both the variational and the symmetric system are compact in suitable Hölder spaces, and that the limit configuration (obtained, that is to say, with infinitely strong competition) are segregated. The most interesting fact is that the optimal exponent of regularity does depend on the type of competition and that, in a great contrast with the standard diffusion case, the choice of the competition term affects deeply the geometry, the regularity and also the limiting condition enjoyed by the segregated states of the solutions.

Existence and qualitative properties of solutions to competing elliptic systems

As already mentioned, with respect to the fractional diffusion models introduced before, the standard diffusion case has been already object of a deep analysis by the scientific community. In particular, for the corresponding system it has been shown (both in the symmetric and in the variational contest) that uniform boundedness in the supremum norm of a family of solutions is sufficient to guarantee the optimal regularity of the limiting solutions as the competition diverges. This and related results have then been used in order to study existence and qualitative properties of the solutions, as well as to describe precisely how the segregation phenomenon occurs. In particular, it has been shown that, in the limit of strong competition, appropriate scaled versions of the segregating functions converge locally to entire solutions of a peculiar system of interacting elliptic equations and thus a complete characterization of the solutions of such system has become an important subject. The symmetric case was already studied in one of the pioneering papers on this subject. In the variational setting, only recently in the papers the authors were able to show in existence of algebraically growing solutions. Motivated by this result, in the second part of the thesis we show that the variational system admits also solutions which exhibit an exponential growth.



2. A particular of the solutions to the variational system exhibiting exponential growth.