



# DOCTORAL PROGRAM IN MATHEMATICAL MODELS AND METHODS IN ENGINEERING

Chair:  
**Prof. Roberto Lucchetti**

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 out 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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# REDUCED-ORDER MODELS FOR PATIENT-SPECIFIC HAEMODYNAMICS OF CORONARY ARTERY BYPASS GRAFTS

**Francesco Ballarin** - Supervisors: **Prof. Alfio Quarteroni, Dr. Roberto Scrofani**

Co-advisors: **Dr. Elena Faggiano, Dr. Andrea Manzoni, Prof. Gianluigi Rozza**

*Coronary artery bypass grafting (CABG)* is a surgical procedure in which one or more grafts are used to create new paths to restore blood flow to the myocardium when severe *coronary artery disease (CAD)* occurs. In this case, one or several major coronary arteries are occluded; this condition undermines the perfusion of oxygen-rich blood to the heart. Due to this critical issue, although several alternative treatments exist, CABG is still one of the largest components of surgical practice worldwide. However, current clinical experience suggests that, after some years, the implanted vessel themselves tend to occlude, leading to the failure of the surgery and the need of reintervention.

Investigating global and local features of the blood flow, in particular near the anastomoses, is of considerable clinical interest. In fact, some fluid dynamics indicators, such as wall shear stresses and oscillatory shear index, are strictly related to the development of intimal thickening and can be efficiently and accurately estimated by means of numerical simulations. In this thesis CFD methods are developed, focusing on complex geometries obtained from *clinical data*, with a special attention to *computational reduction techniques*, allowing

*individualized (patient-specific) simulations*.

The first part of the thesis contains a review of the available clinical data and a discussion of the proposed medical imaging pipeline. Patient-specific data have been acquired for fourteen patients, who have undergone a coronary artery bypass surgery. The current dataset features a broad variability of both disease (for example, different two- or three-vessels disease) and surgical intervention (for example, different combination of single or sequential grafts, Y-grafts or free grafts, radial artery or saphenous vein grafts). For each patient clinical collaborators at Ospedale Luigi Sacco in Milan acquire angiographical data in a pre-surgical phase and CT scan data in post-surgical phase. A clinical imaging pipeline is introduced and discussed in detail in this part. Figure 1 shows the reconstruction of a case in the current dataset.

The second part of the thesis deals with the computational reduction framework. In recent decades vast research interest has been devoted to *model order reduction techniques* for problems held by partial differential equations in a broad variety of contexts. The main motivation behind the use of *reduced-order models (ROM)* is that clinical interest lies not only

in the simulation on a patient-specific configuration, but also in addressing the variation of the flow conditions and of the geometry for a detailed analysis of several scenarios, aiming at a possible improvement of the design of the surgical operation. Unfortunately, relying on full-order discretization methods (such as finite element, finite volume, etc.) for each new scenario is usually too expensive from a computational point of view. ROMs, instead, allow to obtain an accurate description of the physical behavior of the system at greatly reduced computational costs.

In particular, POD-Galerkin methods are considered in this thesis. A finite element (FE) discretization is employed in a construction stage (offline), to be performed once, possibly on high performance computing (HPC) facilities. Afterwards, few relevant basis functions are computed from a set of snapshots of the full-order model, and the PDE is projected on the reduced basis space, that is, on the space spanned by these basis functions. Therefore, the number of degrees of freedom of the evaluation stage (online) is drastically reduced, enabling fast computations, which can be performed several times (e.g. for different physical and geometrical scenarios), possibly on a laptop.

The third part of the thesis deals with possible shape parametrization techniques for patient-specific configurations of coronary artery bypass grafts, in order to perform local geometrical variations of relevant interest in the clinical practice. Volume-based parametrizations are first introduced, together with a screening procedure for the selection of the geometrical design parameters. Furthermore, a new idea of shape parametrization is combined to the volume-based approach, namely the *centerlines-based shape parametrization*. This technique is based on the assumption that coronary arteries and bypass grafts can be represented as a network of tubular geometries. In this framework, we manage to obtain an intuitive description of the whole network, accounting for few parameters related to the variation of relevant design variables, such as stenoses severity and anastomosis features.

The fourth part of the thesis presents several results of the proposed framework on patient-specific CABG configurations. We examine variation of inlet flow rates (grafts and coronary arteries) among physical parameters; this is representative for example of different stress or rest conditions of the patient.

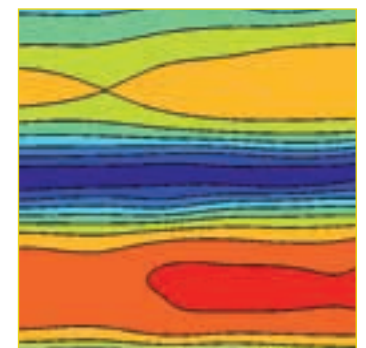
Moreover, both disease-related (stenosis severity) and surgery-related (anastomosis features) geometrical parameters are considered. As a first scenario, we show that inlet flow rates have a significant impact on the magnitude of wall shear stress (WSS, see also Figure 2) and the extension of the region of high oscillatory shear index (OSI). As a second scenario, we consider both variation of inlet flow rates and stenosis severity. The relation between stenosis severity and pressure drop or maximum WSS in the stenosis is explored, and local WSS patterns near the anastomosis are analyzed. As a third scenario, the variation of both stenosis and end-to-side anastomoses is considered. Possible relations between anastomosis type (related to the grafting angle, see also Figure 3) and locations where intimal thickening may occur are highlighted and discussed.



1. three-dimensional reconstruction of patient-specific CABG. Bypass grafts are represented in green colors. Coronary arteries are represented in red, pink, orange and yellow. Caption



2. plot of the wall shear stress near a Y-graft anastomosis.



3. maximum wall shear stress at the arterial bed as a function of time and anastomosis angle.

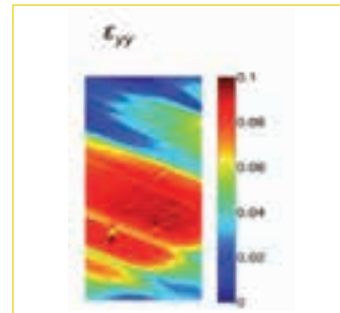
# INTERMITTENCY IN REVERSIBLE MARTENSITIC TRANSFORMATIONS

**Noemi Barrera** - Advisors: **Prof. Paolo Biscari**, Politecnico di Milano, and **Prof. Xavier Balandraud**, Université Blaise Pascal, Clermont-Ferrand

Martensitic Transformations (MT) are phase transitions among different solid states with different crystalline structures. These transitions are at the basis of the behavior of a class of smart materials, called Shape Memory Alloys (SMA). They are metallic alloys which combine the ability to store the memory of a given configuration and recover it after thermal or mechanical deformations (Shape Memory Effect) with the ability to deform to strain levels that are typical of rubbers and not of metals (Pseudo-Elasticity). The applications of these materials are many and in several fields, like aerospace, aeronautics, biomedical, nuclear and industrial in general. Thus, the knowledge of martensitic transformations becomes the key for the comprehension of the behavior of SMAs. The goal of this work is to go one step farther in the characterization of martensitic transformations. In order to do so, we analyze SMAs from different points of view. On one hand, we use a modeling approach by treating SMAs as macroscopic continua. In particular, we focus on the appearance of fatigue and permanent effects after cyclical transformations. Actually, many applications of shape memory alloys like actuators or coronary stents, require a cyclical behavior which remains stable for quite

long times. On the other hand, we address an experimental analysis of the phenomenon. The motivations in the choice of the experiment and of the method to be used for the data treatment are several: we wish for a significant amount of data and for a good quality in terms of resolution; moreover, we aim at a simple test with external conditions as simple as possible. By consequence, we choose a tensile uni-axial and uni-directional test in which the specimen is free to rotate without strong boundary conditions. The device also allows for slow loading rates. This puts the transformation in quasistatic conditions, avoiding inertial effects. Finally, we combine this experimental setting with a fullfield measurement method for the treatment of data, called *grid method*. This technique provides two-dimensional maps of the strain during all the martensitic transformation, with an excellent strain resolution. The amount of collected data and the resolution in the resulting information is such to perform a wide analysis on the transformation. Fig.1 shows an example of two-dimensional map obtained for the linear vertical strain component during the experiment. Different colors in the map indicate different solid phases in the specimen,

with a maximum strain in the vertical direction around 9%, according to the pseudo-elastic effect.

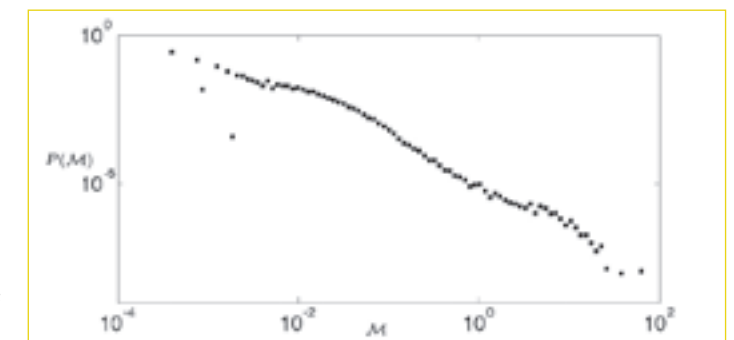


1. Linear vertical strain around the middle of the transformation.

A first step in the analysis consists in studying the overall behavior of the material. We thus find typical results of martensitic transformations when interpreted as a continuous phenomenon. But the focus of our analysis is above all on the presence of intermittency in the transformation. We consider a phenomenon as intermittent when it takes place in a non-periodic or non-predictable way. In particular, the kind of intermittency in which we are interested is the one that is present for many different scales in the same phenomenon. This feature is called *self-similarity*. A self-similar phenomenon is such that it is similar to itself but on various scales. For example,

this happens for earthquakes, from the biggest ones to the small movements of the earth crust, for fractals, lung inflation, economical dynamics and many phenomena in different fields and at different scales. Self-similarity can be very useful. On one hand, within the same phenomenon it enables us to focus on the overall behavior, instead of considering small and precise details that become negligible at bigger scales. On the other hand, it allows some comparisons among phenomena that are apparently very different but whose statistical behavior is the same. Among all the phenomena which have been found to display intermittency and self-similarity there are also martensitic transformations in shape memory alloys (together with many other materials like superconductors, ferromagnets or porous media). This feature is particularly interesting because martensitic transitions are usually described as continuous phenomena while in practice, when looking at the details, the transition is not continuous but obtained as a sum of several events of different dimensions. From a mathematical point of view, this kind of phenomena are characterized by the so-called *power-law distributions* of events, that is  $P(X) = X^{-\alpha}$ . These laws can be found in

many fields: Gutenberg-Richter law for earthquakes, Zipf's law in Social Sciences and Pareto's law in Economics. In our case, we identify the different events that contribute to the transformation and we analyse their features, like the size or the magnitude, that is a measure of the energy related to each event. The novelty of the result is above all in the two-dimensionality of the information, since until now only one-dimensional measures have been analyzed in the study of intermittency of SMAs. Figure 2 shows the log-log plot of the probability distribution function of the magnitude of the different events during the transformation. The use of the log-log plot is the common practice when dealing with power laws, since the slope of the straight line on which the points are distributed corresponds to the exponent



2. Log-log plot of the probability distribution function of the transformation events magnitude.

that characterizes the law. We can notice that the magnitude spans for almost six decades and shows a distribution that can be fitted with a power law. Its exponent can be estimated in the range [1.5,1.8], in agreement with previous experimental results. In conclusion, the main result of this thesis is provided by the combination of a suitable experimental device with a high-resolution full-field measurement technique: it allowed us to analyze various aspects (also some poorly investigated ones) of intermittency in a martensitic transformation.

## ADVANCED TECHNIQUES FOR THE GENERATION AND ADAPTATION OF COMPLEX SURFACE MESHES

**Franco Dassi** - Supervisor: **Prof. Simona Perotto** - Tutor: **Prof. Luca Formaggia**

In this thesis we develop new tools for optimizing computational grids in view of the approximation of partial differential equations on surfaces as well as of different applications: from the statistical analysis of large data sets, to the mesh generation of CAD models, to the analysis of geological seismic data in basins of interest. More precisely, we focus on surface meshes composed by triangular elements and we consider both isotropic and anisotropic grids. Independently of the field of interest, we pursue the goal of identifying the “best mesh”, i.e., the mesh that provides the best approximation. As expected, this does not represent a straightforward task. In the literature the same concept of “best mesh” often represents an open issue, since strictly related to the application we are dealing with. As a consequence, according to the framework under investigation, we have developed ad hoc mesh adaptation and/or mesh generation methods to properly fit the specific demands. Different original contributions are provided in this thesis: a new a priori and a posteriori error analysis for the generation of anisotropic surface adapted meshes; a new mesh simplification strategy to reduce the computational cost

associated with the statistical analysis of huge amounts of data; a new anisotropic mesh generation method to approximate the geometry of a CAD model based on the embedding of the starting grid into a higher dimensional space; specific surface mesh operations to manage the complex geometries characterizing geological domains.



## OBJECT ORIENTED GEOSTATISTICS

**Alessandra Menafoglio** - Advisor: **Prof. Piercesare Secchi**

In recent years, the increasing availability of complex and high-dimensional data has motivated a fast and extensive growth of Object Oriented Data Analysis. In OODA the focus is on the statistical unit as the *atom* of the analysis, which is interpreted as a point in a finite-or infinite-dimensional space. For instance, a multivariate datum of dimension  $p$  is typically embedded into the Euclidean space  $\mathbb{R}^p$ , where standard multivariate techniques are available. A  $B$ -part composition – i.e., a  $B$ -dimensional constrained vector, describing the proportions (or percent amounts) of a whole according to a given partition of the domain – can be analyzed via the embedding into the  $(B-1)$ -dimensional simplex endowed with the Aitchison geometry. Even infinite-dimensional data can be dealt with within the framework of OODA, if embedded into a suitable functional space (e.g., the space  $L_2$  of square-integrable functions). As such, OODA unifies within the same framework the classical settings of real and multivariate analysis, with those at the frontier of statistics such as Compositional Data Analysis (CoDa) or Functional Data Analysis (FDA). The aim of this work is to introduce and explore Object Oriented Geostatistics

(OOGeoStat) as a new branch of OODA addressing the problem of geostatistically characterizing sets of spatially dependent object data. The extension of geostatistical techniques, and particularly Kriging, to the OODA setting arises as a natural answer to the need of treating disparate types of spatially distributed complex data. The unifying idea of this work is to consider the available data as object data, and accordingly interpret a georeferenced dataset as a partial observation of a random field valued in an appropriate space (finite-or infinite-dimensional). The relevance of this new viewpoint to geostatistics is twofold: (i) it allows to treat a broad class of georeferenced complex data which are nowadays commonly available in industrial and environmental studies (e.g., temperature profiles, data on soil composition, etc.), and (ii) it provides new insights in well-established multivariate methods, such as Cokriging. We approach OOGeoStat progressively, by proposing original methodologies to treat increasingly complex scenarios. We first focus on OOGeoStat for data embedded into a separable Hilbert space. This case appears of particular interest for applications, as the Hilbert-space embedding allows to deal with most types

of data which are commonly available in environmental and industrial statistics (e.g., multivariate, compositional or functional data). As a first key element of innovation, we establish a novel and coherent theoretical framework for the geostatistical analysis of data in any Hilbert space, not just  $L_2$ . We define novel global notion of spatial dependence based on the concepts of norm and inner product in a Hilbert space, and consistently develop an original Universal Kriging methodology for random fields valued in any separable Hilbert space. From an application viewpoint, this is particularly relevant, as it significantly broadens the applicability of the theory on geostatistics for functional data currently available. For instance, in our setting, both point-wise and differential properties characterizing functional data can be explicitly incorporated in the stochastic model, e.g., by embedding the data into an appropriate Sobolev space. This new approach to geostatistics constitutes the rich soil upon which all the subsequent developments of this work are grounded. Amongst these, a particular emphasis is given to constrained object data, in the form of Functional Compositions (FCs). The latter are functions constrained to be non-negative and to integrate

to a constant and are the infinite-dimensional counterparts of compositional data. The statistical analysis of FCs was pioneered in 2006 by Egozcue *et al.*, who established a Hilbert space structure for FCs based on the log-ratio approach, upon which the Aitchison geometry is grounded. We rely on this theory and on our first developments to address a key issue in earth sciences, that is the geostatistical characterization of soil particle-size curves (PSCs). These data describe the distribution of grains sizes within a given soil sample and are relevant to applications related to groundwater hydrology, soil science, geophysics, petroleum engineering and geochemistry, with emphasis on applications oriented towards modeling physical and chemical processes occurring in heterogeneous earth systems. As a key element of innovation, we here propose to analyze particle-size distributions through their densities, interpreted as object data within the Hilbert space of FCs, endowed with the generalized Aitchison geometry. A relevant advantage of our approach lies in the possibility of obtaining predictions of the entire particle-size curve at unsampled locations, as opposed to classical or compositional Kriging which only allow for finite-dimensional predictions, based on a set of selected features (or synthetic indices) of the curve. As such, our developments allow for a complete assessment of the information content embedded into PSCs, which is critical to the proper modeling of several physical and chemical processes occurring in

heterogeneous earth systems, which are affected by the local composition of the host soil/rock matrix. In a number of situations, the Hilbert-space embedding cannot be employed. This is the case, for instance, when the covariation between phenomena is the focus of the analysis. This kind of information is usually available in the form of manifold data, such as covariance matrices or operators. Even though the analysis of data belonging to Riemannian manifolds is relevant (e.g., in shape analysis, diffusion tensor imaging or the analysis of covariance structures), the nonlinear geometry of Riemannian manifolds often prevents a proper account for the spatial dependence which may exist among data when these are georeferenced. Another instance of non-Hilbert data is the case of environmental variables associated to continuous profiles: a natural embedding for this kind of object data is the space  $C$  of continuous functions, which is a separable Banach space with the uniform norm, but cannot be equipped with a complete metric induced by an inner product (i.e., it cannot be a Hilbert space). In  $C$  however, the point-wise evaluation of a function is meaningful, unlike the case of the space  $L_2$  which is typically employed in FDA. Even in these cases, the abstract viewpoint of our approach offers a new perspective to address these issues. These ideas are explored in the last part of this work, which seeks to go further beyond Hilbert spaces, in the challenging directions of object data in Riemannian manifold

and in Banach spaces. We recognize important differences in the complexity of these object data, which reflect on the strategies we employ for their statistical analysis. To face the problem of the non-linearity in a Riemannian manifold, we employ a projection strategy relying upon the observation that, if the dispersion of the data on the manifold is not too large, these can be projected on a suitably chosen tangent space, where additive models and linear predictors can be used. Instead, in the absence of an inner product, we consider an extension of the Kriging methodology to the Banach-space embedding, grounded on the theory of Gaussian processes in function spaces. The latter developments are proved to be fully consistent with the methodology proposed in the first part, and are part of an ongoing research project aiming to unify within the same theoretical framework multivariate, space-time and functional geostatistics.

# WEIGHTED FUNCTIONAL INEQUALITIES AND NONLINEAR DIFFUSIONS OF POROUS MEDIUM TYPE

**Matteo Muratori** - Supervisors: **Gabriele Grillo, Bruno Nazaret**

This thesis deals with a class of nonlinear diffusion equations whose prototype is  $u_t = \Delta(|u|^{m-1}u)$ , known as porous medium equation (PME) for  $m > 1$  and as fast diffusion equation (FDE) for  $m < 1$ . One may see it as a particular nonlinear version of the heat equation whose diffusion coefficient is a power of the solution itself. Such coefficient becomes degenerate or singular at  $u=0$  depending on whether one considers the PME or the FDE, respectively. Evolution equations of porous medium type have a long history, both as concerns the applications which motivate their consideration and from the mathematical point of view. Here we are concerned with a number of (weighted) variants and extensions of the PME or the FDE, for which we address several fundamental issues such as existence and uniqueness of solutions and their asymptotic behaviour. Our analysis aims at linking as far as possible the properties of the solutions with functional inequalities associated with the underlying functional spaces. Below we outline the main topics investigated in the thesis, which is divided into four chapters. In chapter 1 we deal with

the weighted PME, namely  $\rho_\mu(x)u_t = \operatorname{div}[\rho_\mu(x)\nabla(|u|^{m-1}u)]$ , where  $\rho_\nu$  and  $\rho_\mu$  are suitable positive functions (weights). The weight  $\rho_\nu$  corresponds to an inhomogeneous mass distribution, whereas  $\rho_\mu$  corresponds to an inhomogeneous diffusion coefficient. It is natural to introduce the measure  $d\nu := \rho_\nu(x)dx$ , whose associated Lebesgue spaces we denote as  $L^p(\nu)$  for  $p \geq 1$ . Our first concern consists in considering  $L^q(\nu) - L^p(\nu)$  smoothing and decay properties of solutions, where  $u(t) \in L^p(\nu)$  as a consequence of  $u_0 \in L^q(\nu)$ . It is a classical problem in linear semigroup theory, which has widely been studied in the nonlinear setting as well. Here we prove full equivalence between suitable versions of such smoothing and decay estimates and appropriate Poincaré-, Sobolev- or Gagliardo-Nirenberg-type inequalities. These estimates may not be satisfied up to  $p = \infty$  unless Sobolev- or Gagliardo-Nirenberg-type inequalities hold true (i.e. a Poincaré-type inequality is not enough). The details of the stated equivalence depend on the particular problem at hand: we consider Euclidean domains with both homogeneous Dirichlet and homogeneous Neumann

boundary conditions. In the same chapter we also consider an inhomogeneous filtration equation in the Euclidean space  $R^d$ , namely a weighted PME where  $\rho_\mu \equiv 1$  and  $|u|^{m-1}u$  is replaced by a more general function  $G(u)$ . It is known that nonuniqueness phenomena can occur even for bounded data and solutions. Uniqueness can then be restored by adding a suitable nonhomogeneous condition at infinity. Here we prove existence and uniqueness results, under suitable assumptions on  $\rho_\nu(x)$  and  $G(u)$  and provided certain pointwise conditions at infinity are prescribed. Chapter 2 is devoted to the study of nonnegative solutions to the fractional porous medium equation (FPME)  $u_t = -(-\Delta)^s(u^m)$ , where  $m > 1$  and for  $s \in (0,1)$  we denote as  $(-\Delta)^s$  the fractional Laplacian operator on  $R^d$ . The investigation of such a class of equations has been started recently by J. L. Vázquez et al.; in particular, well-posedness of the evolution is proved for general  $L^1$  data. Existence and uniqueness of Barenblatt-type solutions, namely solutions having a Dirac delta as initial datum, have been proved again by Vázquez. Motivated by these results, we have tackled the problem of (existence and) uniqueness of weak solutions to the FPME with initial datum

a general positive finite Radon measure. This is performed by adapting a clever argument first introduced by M. Pierre a long ago, whose applicability is however far from obvious in the present context. In fact our method, based on Riesz potential techniques, also works in the case of the weighted FPME (WFPME)  $\rho(x)u_t = -(-\Delta)^s(u^m)$ , provided some power-type conditions on  $\rho(x)$  are required both at the origin, where it can be singular, and at infinity. Being able to prove existence and uniqueness of Barenblatt-type solutions in the weighted case as well, we can study the asymptotic behaviour of general solutions to the WFPME in terms of Barenblatt-type solutions, at least when  $\rho$  decays slowly at infinity. The convergence result exploits scaling properties of the Barenblatt-type solution associated with a singular-power density even if the equation at hand involves a regular density. The asymptotics of solutions to the WFPME with rapidly decaying densities is quite different. In fact we prove that the latter is determined by a separable solution which involves the solution of a suitable fractional sublinear elliptic equation. This requires techniques completely different from the ones we use in the slowly decaying case. In chapter 3 we address the problem of finding the functions that optimize a family of Caffarelli-Kohn-Nirenberg (CKN) inequalities, which can be obtained by interpolation from Hardy's inequality and from the Sobolev inequality: they depend on the weight  $|x|^{-\gamma}$  ( $\gamma \in (0,2)$ ) and on  $p \in (1, (d-\gamma)/(d-2))$ . Finding optimal functions for CKN

means finding those functions which attain the best constant in the inequality. Such problem was solved by M. Del Pino and J. Dolbeault in the non-weighted case  $\gamma = 0$ . In particular, they show that the optimal functions coincide with  $b_0(x) := (1+|x|^2)^{-1/(p-1)}$ , up to a multiplication by a constant and a scaling. Our aim is to generalize this result to CKN, namely to prove that their optimal functions are of the type of  $b_\gamma(x) := (1+|x|^{2-\gamma})^{-1/(p-1)}$ . Establishing that  $b_\gamma$  optimizes CKN among radial functions is easy. Hence, our analysis amounts to proving that the optimal functions are radial, which is not trivial even if the weight  $|x|^{-\gamma}$  is radial (in general symmetry breaking phenomena can occur). By means of a perturbation argument involving concentration-compactness techniques, we show that the result is true provided  $\gamma > 0$  is small. This has interesting consequences for the asymptotics of nonnegative solutions to the power-weighted Euclidean FDE  $|x|^{-\gamma}u_t = \Delta(u^m)$  in the range  $(2d-\gamma-2)/[2(d-\gamma)] < m < 1$ . In fact, the optimality of  $b_\gamma$  for CKN is equivalent to the validity of a sharp free energy-Fisher information inequality, which is in turn equivalent to a sharp exponential decay estimate for the free energy functional. The latter is a measure of the distance between a general solution and  $b_\gamma$ , after a standard time-space scaling. Finally, in chapter 4 we study the FDE on hyperbolic space  $H^N(N \geq 2)$ . As it happens for the fast diffusion equation on bounded Euclidean domains with homogeneous Dirichlet boundary conditions, solutions

become identically zero in a finite time  $T > 0$ . The asymptotics of nonnegative radial solutions (i.e. solutions depending on the spatial component only through the geodesic distance  $r$  from a given pole) turns out to be, in the range  $m \in ((N-2)/(N+2), 1)$ , driven by a separable solution with the same extinction time  $T$ , which involves the unique positive energy solution  $V$  to an elliptic Emden-Fowler equation. Convergence to the separable solution is proved in a strong sense, namely in the uniform norm of the relative error and at the level of all derivatives. We point out that, at least in the special case of spherically symmetric Riemannian manifolds known as model manifolds, we basically fall in the class of equations described by a two-weight FDE. In fact, in this framework, the radial component of the Riemannian Laplacian can be written in the form  $\rho^{-1}(r)\partial_r(\rho(r)\partial_r)$  in geodesic polar coordinates. Here we perform a detailed analysis on hyperbolic space only, as the topologically simplest example of noncompact, negatively curved model manifold. We believe however that our results can be extended at least to more general model manifolds with strictly negative curvature.

# NUMERICAL APPROXIMATION OF THE ELECTRICAL ACTIVITY IN THE LEFT VENTRICLE WITH THE INCLUSION OF THE PURKINJE FIBERS

**Simone Palamara** - Supervisors: **Prof. Alfio Quarteroni, Dr. Christian Vergara**

Cardiovascular diseases are the leading cause of death in the world. This highlights the vital role of the cardiovascular system, that allows blood to circulate, supplying oxygen and nutrients to tissues and removing wastes from them. Due to its importance, scientists during the last century have developed bio-mathematical models of the cardiovascular system, exploiting the increase in the computational power in combination with new technologies for both the acquisition of clinical data and the design of new experiments. These efforts are crucial to gain better insight on the mechanisms regulating cardiovascular system activity and to provide the clinicians with a powerful instrument for diagnosis and therapeutic design. In this thesis we concentrate on the study of the heart electrical activity, that is fundamental since it is the spreading of the electrical signal that triggers the heart contraction. The purpose of this work is the numerical modelization of the electrical activity in the left ventricle with the inclusion of Purkinje fibers. Because of its role, a dysfunction of the normal electrical propagation causes a disorganized and irregular contraction of the whole heart, that in the worst case

can lead to sudden death. Therefore, in the last years, detailed and sophisticated electrophysiological models of the heart have been developed with the aim of revealing and describing the causes and the major mechanisms arising in different pathologies. In particular, we can identify two main classes of models: (i) *cardiac tissue and cell models* that describe the structure of the cardiac tissue and all the cellular mechanisms involved in the generation and propagation of the electrical signal; and (ii) *cardiac anatomical models*, that describe instead all the anatomical structures that regulate and influence the spreading of the electrical signal. Both these classes of models are fundamental to obtain accurate, reliable and realistic description of the electrical activity in the heart. To the first class of models belongs for example the so called *bidomain model*, that is the most accurate model for describing the spreading of the signal through the cardiac tissue, capable of representing different phenomena, from normal propagation to tachycardia and defibrillation. Coupled to the bidomain model, detailed models of the heart cells have been developed, describing the dynamics that lead to the generation of the electrical signal at the cell level.

Instead, cardiac anatomical models concentrate their efforts in including the major structures involved in the electrical propagation, based on anatomical knowledge or driven by clinical data. For example, the reconstruction of the three-dimensional geometry of the heart through medical images, the inclusion of the muscular fibers and the modelization of the cardiac conduction system, that regulates the propagation of the electrical signal through the heart. The choice of which structure to be included depends on the level of accuracy required and on the clinical problem that is addressed. In this thesis, we focus on modelling the electrical activity in the left ventricle, using clinical data on the activation times and medical images provided by the Division of Cardiology, Ospedale S. Maria del Carmine, Rovereto, Trento, Italy and by the operative unit of Radiology of Borgo-Pergine, Ospedale di Borgo Valsugana, Trento, Italy. Clinicians are interested in the electrical activity of the left ventricle, since this cardiac chamber pumps blood in the whole body (except for the lungs) and therefore electrical pathologies affecting the left ventricle can be life-threatening, such as the ventricular tachycardia or ventricular defibrillation. The electrical

activity in the left ventricle is regulated by the peripheral part of the cardiac conduction system, the *Purkinje fibers*. These fibers regulate the propagation of the electrical signal in normal conditions, but they also play a role during abnormal electrical propagations. In the latter situation, the inclusion of the Purkinje fibers is essential also to design new therapies or to optimize existing ones. The present work can be regarded in this framework, since it concerns with the study of electrical activation of the left ventricle with the inclusion of the Purkinje fibers, with the final aim of addressing cases of clinical interest, related to healthy and pathological propagations. In particular, the principal goals of this work are: the study of different strategies for solving the coupled problem given by the interaction between the Purkinje fibers and the ventricular myocardium, arising at the endpoints of the fibers, the Purkinje-Muscle junctions (PMJ). The electrophysiology models considered are the monodomain and eikonal equations. After a brief introduction, the thesis is organized as follows. In Chapter 2 we introduce the biological notions about the heart physiology, focusing on the role of the Purkinje fibers in the ventricular activation, on the

studied pathologies (myocardial infarction, Wolff Parkinson White syndrome and left bundle branch block) and therapies (cardiac resynchronization therapy and ablation therapy). In Chapter 3 we present the clinical data, consisting in medical images of the left ventricle and in endocardial measures of the activation times acquired by means of the Navx system. At the best of the author's knowledge, these data have been used for computational purposes only in one paper, for the definition of a space-dependent muscular conduction velocity. In Chapter 4 we study the mathematical models of the electrical activity, focusing on the monodomain and eikonal problems. We study different strategies for modelling the coupled problem given by the interaction between the Purkinje fibers, represented as a one-dimensional network, and the myocardium. Finally, we propose some numerical tests to compare the different strategies and we present a preliminary result on the inclusion of the Purkinje network in an electro-mechanical simulation. This is, at the best of author's knowledge, the first attempt to include the Purkinje fibers in the electro-mechanical simulations. In Chapter 5 we detail the major and original achievement of this thesis,

consisting in a methodology for the generation of a patient-specific Purkinje network, driven by available clinical measures of the activation times acquired on the endocardium of the left ventricle. At the best of the author's knowledge, this is the first time that clinical data are used to generate a patient-specific Purkinje network. Finally, in Chapter 6 we present several numerical results of what discussed in the previous chapters, both in an ideal geometry with synthetic data and in real geometries with clinical measures of healthy and pathological propagations. Moreover, we consider an application to the cardiac resynchronization therapy (CRT), with an optimization study to identify the best timings and locations of the stimuli produced by the CRT-device. The numerical simulations have been performed both in ideal geometries and in a real geometry with a patient-specific Purkinje network.



## THE ROLE OF MECHANICS IN MORPHOGENESIS: THEORY AND NUMERICS

**Viola Pettinati** - Advisor: **Davide Ambrosi**

Morphogenesis is the ensemble of biological processes that lead to the emergence of an organism shape. The orchestrated cellular process of differentiation and duplication yields organs that have a precise shape and size. An important role in this phase is held by molecules that were first hypothesized by Alan Turing. In his seminal work, he described how the concentration of chemical substances in a tissue evolves in time because of reaction and diffusion processes. The density patterns, dictated by instability, can be conjectured to drive the system shaping. Even if he did not precisely identify such molecules, Turing called them morphogens to convey the idea of shape generation.

A fundamental contribution to the theory of morphogens is due to Lewis Wolpert, who proposed the "French flag model". The central element of this model is the spatial distribution of the concentration of specific substances in the tissue: it is detected by the cells which, according to specific thresholds, trigger the transcription of distinct sets of genes. According to this theory, there is a direct correlation between the input (the concentration level) and the output (the response of the tissue): each threshold corresponds to the border of an expression territory. Many

efforts have been made to understand how morphogens influence growth, and Turing's idea was extended: not only morphogens are responsible of pattern formation, they also specify mutual cell position and then influence organism growth. Examples of morphogens are the Decapentaplegic (DPP), Hedgehog, and Wingless. The theoretical argument that the concentration of a morphogen can drive growth is fascinating and successful in some cases, but such an appealing explanation is to be corroborated by other physical mechanisms. An alternative approach to explain how the size in the tissue growth is controlled by a limited proliferation is based on mechanobiology. In the study of the responsible mechanisms for the tissue size determination, the most popular model organisms is the *Drosophila Melanogaster*, also known as fruit fly. We concentrate our attention on the *Drosophila* wing imaginal disc, the structure of the larva from which the adult insect wing originates. Mechanical stress is known to play a role in tissue development, sometimes in conjunction or superposition with chemical signaling. In particular, evaluation of the stress in the wing imaginal disc by photoelasticity has been the subject of recent experimental

works. One of the aims of this thesis is to address whether a continuum mechanics model can reproduce a stress pattern qualitatively similar to the one reported and reconstructed by these experiments. The stress is a long range field, natural candidate for intercellular communication, and, as a matter of fact, cells are well known to modulate their motility and reproduction rate on the basis of their own tensional state. We formalize different conjectures about possible morphogenetic mechanisms in mathematical equations and analyze them in terms of physical admissibility. Our standpoint is that a physical field is an admissible mechanism of local transduction of global information if, under homogeneous growth, it depends in a specific way on the domain size and on its relative position in the organ only. By means of finite elasticity calculations under plane strain-plane stress assumption in a circular disc, we show that, prescribing an active contraction in a circular portion of the domain, possibly dictated by high concentration of morphogens, the force balance equation yields a stress distribution of the desired form: the stress locally provides the cells the information about the size of the tissue, and such a signal is compatible

with a homogeneous growth. Moreover, it is compressive, it grows at a given position fixed in space as the disc becomes larger. These results are qualitatively in agreement with recent experimental observation. Then, we corroborate and extend this idea to the case of a full three-dimensional domain with the support of numerical simulations. We have developed a finite element code to determine the stress distribution induced by an inhomogeneous active contraction in a 3D monolayer. Two geometrical settings are considered: a thin circular cylinder and the real shape of the wing imaginal disc. Both radial and biaxial symmetries in the morphogens' concentration can be set on the basis of possible line sources and then determine the active region. The flexibility of the numerical simulations allows us to enforce different symmetries when experimental reports obtained by different techniques are apparently in conflict. These simulations also validate numerically the assumptions that were at the basis of our analytical results. They confirm that the planar components of the stress strongly resemble the ones obtained in the 2D case, confirming that the planar axisymmetric approximation is able to catch the relevant features of the stress distribution. Moreover, the z-components of the computed stress is much smaller than the other components and do not significantly vary along the thickness, thus supporting our simplifying assumptions. Therefore, our analysis of the *Drosophila* development provides an effective mechanism

for the regulation of tissue size in growing organisms. It is known that mechanics plays an important role also in the emergence of organism shape. Coordination and integration of forces by long-range force transmission and mechanosensing of cells within tissues produce large-scale tissue shape changes. The limb has long been considered a paradigm of the organogenesis. Experimental studies on mouse and chick limb bud, the embryonic precursor of the limb, have provided extended knowledge of the underlying chemical processes involved in organogenesis. However, the gene effects on shape have still to be determined. There have been several attempts to quantify the spatiotemporal distribution of growth in the limb bud. The prominent hypothesis is called the proliferation gradient hypothesis. According to this mechanism, the elongation of the limb bud is achieved by distal cells being stimulated to divide faster than proximal cells, without invoking any kind of directional behavior: high distal rate of non-oriented proliferation are considered to be sufficient to drive tissue growth. Recent studies call into question this idea. They indicate that cell elongation and division have preferential directions, and therefore the oriented cell behaviors are important for driving tissue elongation. How much of the growth is due to phenomena like convergent extension, the process by which the tissue of an embryo is restructured to converge along one axis and extend along a perpendicular axis by cellular movement, and how much

is due to homogeneous and anisotropic growth has still to be understood, and calls for mechanical models. Moreover, evidence of anisotropy in the limb bud tissue have already been provided: the basal membrane, which surrounds the limb bud, can be classified as a transversal anisotropic material. In this thesis we propose a preliminary mixture model for vertebrate limb bud growth. In our model, the limb bud is described as a three phase mixture, made of the fluid and the solid components of the extracellular matrix, and of (fluid) cells. A water inflow triggered by the active transport of chemical species increases the ECM fluid phase, and mass transfer among different components induces their growth. This study represents a first step to connect the chemical signals and the mechanical response of the tissue in a context of mixture theory. We feel that this context is the most appropriate to describe a realistic limb bud, especially because, through the ECM fiber distribution, the tissue anisotropy can be taken into account.

# GLOBAL AND COMPONENT-WISE DISTRIBUTION-FREE INFERENCE FOR FUNCTIONAL DATA: METHODS AND APPLICATIONS

Alessia Pini - Supervisor: Prof. Simone Vantini

Functional Data Analysis, i.e., the statistical analysis of sets of curves, is a lively area of statistics. New possibilities introduced by recent technologies of recording high-resolution data representable as functions, leave statisticians with the problem of developing novel methodologies to analyze this type of data. In the thesis, the problem of inference on functional data is addressed, from both a methodological and an application point of view. Functional data are typically modeled as random elements of infinite dimensional separable Hilbert spaces, and one of the main issues is the impossibility of defining a probability density function for random functions. However, the problem of developing suitable inferential tools for functional data is of high importance for practitioners. For instance, a test for deciding whether several groups of curves have the same (functional) mean could be applied to a wide range of situations. We may think of the case in which the curves express the movement through time of groups of subjects affected by different pathologies: in this case, a test of mean comparison between groups could provide a quantitative way to understand whether they express the same behavior. Statistical inference for

functional data is approached from two different perspectives: parametric and non-parametric inference. Non-parametric inference commonly relies on computational intensive permutation techniques. Parametric inference relies instead on distributional assumptions on functional data (e.g., normality). In the case of functional data, normality is a very demanding assumption, practically impossible to verify. For this reason, we choose to base inference on non-parametric permutation tests. For instance, suppose that we want to test for differences between two groups of curves. A permutation test can be constructed by evaluating the distribution of a test statistic measuring the distance between groups over the space of all possible permutations of data across groups. The  $p$ -value of such test can be evaluated as the proportion of permutations leading to a test statistic higher than the one evaluated with the non-permuted data. The resulting test is exact, and it does not require any distributional assumption.

## Methods

The first methodology developed in this work is a distribution-free inferential method for the mean of functional data based on a

generalization of Hotelling's  $T^2$  statistic in functional Hilbert spaces. The statistic is the natural extension in the infinite-dimensional framework of the statistical tools for testing the mean with unknown variance, from the works of Gosset (Student) and Fisher at the beginning of the twentieth century, up to the earlier extensions of Hotelling's  $T^2$  to high dimensional data. The proposed method is a global inferential procedure, i.e., it provides a unique result over the whole domain of the curves. For instance, it is able to test whether two functional populations have the same mean, but in case of rejection of the latter hypothesis, it is not able to select the parts of the domain presenting the differences. To answer this question, we developed a novel methodology, namely, the Interval Testing Procedure (ITP). This procedure is based on the expansion of data on a (possibly high-dimensional) functional basis, and provides the selection of the basis coefficients that lead to a rejection of the null hypothesis. If a local basis -such as B-splines- is used, the ITP can be used to identify regions of the domain of statistical significance. The procedure is developed for the case of testing the mean of one and two populations, and for testing

the parameters of a functional-on-scalar linear model.

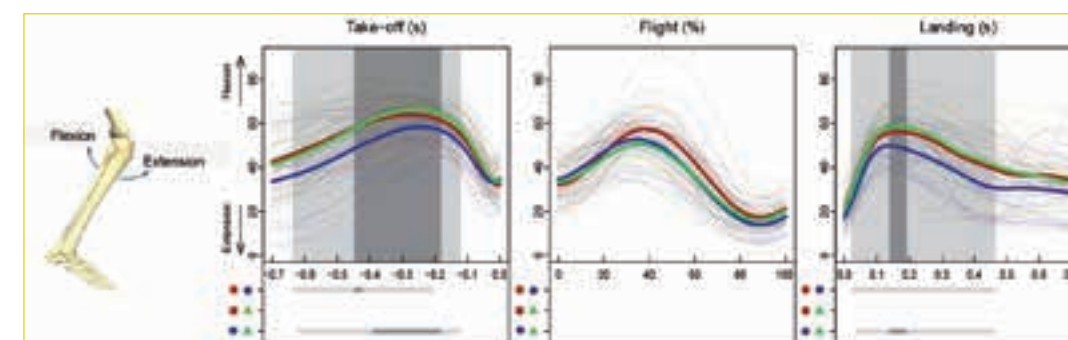
## Applications

As first application, a functional one-way ANOVA is applied to knee movement data of a follow-up study on Anterior Cruciate Ligament (ACL) ruptures. The knee movements of individuals suffering from an ACL injury, treated with surgery (first group), physiotherapy (second group), and uninjured controls (third group) are investigated. The ITP shows that individuals that were treated with physiotherapy present significantly different movement patterns with respect to the other two groups both during take-off and during landing (Fig. 1). The ITP is then applied to the remote monitoring of laser welding. A functional two-

way ANOVA is performed to investigate the effects of the gap between welded plates and the location of the laser beam on the laser emission spectra. The result of such technique is the selection of a band of wavelength in the thermal emission domain in which only the gap effect is significant. This suggests the use of emission data on this band to monitor the gap during the welding process at any possible location. Finally, the ITP for one-sample inference is applied to assess the uncertainty about solar energy generation systems. The ITP is adopted to evaluate the frequencies of a Fourier basis that are significant in the expansion of the mean function of climatic data. The result is used to evaluate relevant quantities for the installation of a residential photovoltaic plant.

## Software

Implementations of the ITP have been made freely available in the R-package `fdatest`, downloadable from CRAN, at <http://cran.r-project.org/web/packages/fdatest/index.html>. The package implements the ITP in different frameworks (i.e., one-population, two-population, ANOVA, and linear models) by means of different basis expansions (i.e., B-spline and Fourier).



1. Definition of the knee angles in the sagittal plane (left); flexion/extension curves of the physiotherapy (blue), surgery (red) and control (green) groups (right) during take-off, flight, and landing phases. Shaded areas: intervals presenting significant differences between the groups at 5% (light grey) and 1% (dark grey) levels.

# BIO-POLYMER INTERFACES FOR OPTICAL CELLULAR STIMULATION: A COMPUTATIONAL MODELING APPROACH

**Matteo Porro** - Supervisors: **Prof. Riccardo Sacco**, **Prof. Guglielmo Lanzani**,  
**Dr. Maria Rosa Antognazza**

The continuously increasing convergence of life sciences and engineering is determining an impressive expansion of novel disciplines, and a significant role among them is played by bioelectronics. In this field, innovative applications such as human-machine interfaces, wearable devices and prosthetics are able to capture enormous attention by the consumer audience and represent a huge business opportunity, attracting important investments for fundamental research and development of novel prototypes.

A dynamic and challenging branch of prosthetics is represented by the activity carried out for developing devices aimed at restoring the sight to people who lost it because of some degenerative illnesses. In this context, an important contribution is provided by the group of Prof. Guglielmo Lanzani at the Center for Nano Science and Technology @PoliMi of Istituto Italiano di Tecnologia. They recently developed a photovoltaic device made of a particular semiconducting polymer and demonstrated that this latter is able to stimulate a piece of dissected rat retina placed onto it upon illumination with visible light. This result is of great importance since polymers are characterized by an

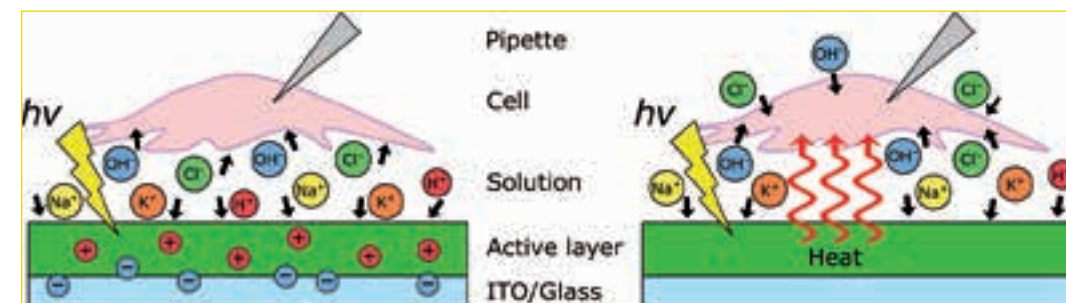
enhanced biocompatibility and superior mechanical properties compared to inorganic semiconductors, which are the reference materials for the state of the art prototypes. In particular, this thesis deals with the investigation and the mathematical description of a simplified configuration of such device. This consists in a bio-polymer interface, in which a thin slab of P3HT, a photosensitive semiconducting polymer, is contacted with a transparent electrode of Indium-Tin-Oxide, and a cell is grown onto it, the whole system being immersed in a physiological solution to allow cell survival. Despite the fact that measured cell transmembrane current and voltage clearly demonstrate that a significant electrical cellular activity is elicited with light stimulation due to absorption by the polymer, the involved physical processes are still not fully understood, with both electrical and temperature related phenomena possibly occurring in the system. For this reason, the modelling and simulation efforts have been addressed at exploring the proposed descriptions of the actual working principles of the device, and at verifying that such pictures are compatible with the experimentally observed trends. In the first part of the thesis, we focus at characterizing the

role of electrical effects, by considering a configuration without the cell. We carry out a systematic analysis of performed measurement and propose a sound mathematical description to describe the chain of events that lead from input light illumination to the development of an output photovoltage signal that drives cellular response. The adopted model consists in a system of partial and ordinary differential equations that represent:

- generation, diffusion, decay and dissociation into free charges of excitons, a particular type of excited state of the polymer molecules;
- electric conduction of generated free electrons and holes in the polymer according to the classical Drift-Diffusion formalism;
- trapping and release of charge carriers in localized trap states in the energy gap of the polymer;
- rearrangement of electric field inside the device according to Gauss law.

The resulting nonlinear system of equations is numerically solved using techniques including:

- time advancing with Rothe's method and Backward Differentiation Formulae;
- system linearization with the Newton method;
- spatial discretization with exponentially fitted finite



**1. Proposed device working principles. (left) Light absorption determines free charge generation and ion rearrangement in the solution, inducing cell membrane response. (right) Light absorption induces temperature variation in the environment, the cell membrane properties are modified and excitation occurs.**

elements in primal-mixed form, incorporating the classic Scharfetter-Gummel stabilization.

We perform extensive numerical simulations to corroborate and support the picture of the device working principles that we draw based on the obtained experimental evidence:

- a critical role is played by the interface between the P3HT and the ITO electrode, characterized by the presence of a depleted region and of the corresponding electric field, which drives exciton dissociation and induces charge displacement;
- charge trap dynamics determines the characteristic time scale of the device response in terms of photovoltage signal.

In the second part of the thesis, an analysis of the response upon photostimulation of cells grown onto such polymer-electrolyte interface devices is carried out using patch clamp measurements. This choice aims at demonstrating that for particular values of the illumination intensity, the observed phenomena are actually determined by a change of the local temperature. The

adopted mathematical picture of the problem consists in a system of partial and ordinary differential equations that represent:

- heat generation and diffusion in the polymer and delivery to the solution;
- the electrical response of cell membrane;
- the change of membrane capacitance, conductance and resting value due to the temperature increase.

Obtained results are in excellent agreement with measurements and support the picture which identifies the temperature induced variation of the membrane capacitance as the driving force of cellular depolarization. However, the physical interpretation of this latter membrane characteristic is still under debate, and the chapter ends with a critical discussion of the mainstream description, based on the classic Gouy-Chapman-Stern theory of double layers.

The thesis ends with a chapter devoted to a detailed description of the adopted finite element methodology, showing how the use of an exponentially fitted stabilized primal-mixed formulation

allows for an accurate and robust discretization of problem equations. Additionally we propose an extension of the method in the two-dimensional framework to account for the modified formulation of the problem in cylindrical coordinates with axial symmetry. We perform the stability and convergence analysis of the proposed methods, validating them with a series of numerical experiments.

## ON THE MATHEMATICAL MODELING OF A METAL FOAM EXPANSION PROCESS

**Elisabetta Repossi** - Advisor: **Dott. Marco Verani** - Coadvisor: **Prof. Riccardo Rosso**

Metal foams are special cases of cellular metals with closed cells. These materials attract the attention of researchers and engineers, thanks to properties like damping, high capability of energy absorption, high stiffness and low weight, that make them suitable for a wide range of applications, in particular in the automotive industry. Many different processes have been developed for producing this kind of materials. Precursor foaming is suggested in the literature as useful for filling processes and it is the method used in our research activities. It involves the heating of a solid material (called precursor) containing an embedded gas source (a blowing agent) that, upon temperature increasing, releases gas and drives the foaming process. Two processing methods can be distinguished depending on whether the precursor is prepared by a metallurgical or a melt route, which are respectively identified as Powder line or Formgrip line. In this work we have considered the powder line. Precursor foaming is characterized by a pronounced foam expansion stage in the liquid state, as it has been highlighted by the experimental work we performed at M.U.S.P. laboratory in Piacenza, in collaboration with M.U.S.P. researchers: the metal matrix is in the melted

state upon heat treatment of the foaming precursor(s). In fact, during the heat treatment, at temperatures near the melting point of the matrix material, the blowing agent decomposes and the released gas forces the compacted precursor material to expand. In the process, the resulting foam expansion depends, therefore, on the content of blowing agent, temperature, time, pressure, heating rate, size of the precursor, etc. Furthermore, other physical variables govern the dynamics of the gas bubbles in the foamed matrix of a precursor, such as the matrix state (solid, semi-solid or liquid), the presence of solid particles on the bubble walls, fluid viscosity, etc. The high costs and the lack of control in the manufacturing process (in order to avoid foam-decay phenomena like drainage and coarsening) prevent the industrial production of metal foams. A mathematical model describing the manufacturing route of metal foams could help engineers in the study of the physical parameters that are involved in the evolution of the foam. We are interested in the study of the expansion stage of the foam within a hollow mold. The mathematical modeling of the foam expansion stage can be reduced to the mathematical modeling of two-phase

incompressible-compressible fluids: the incompressible part is the liquid metal, while the compressible part is the gas inside bubbles. The literature of multiphase flows includes many types of differential models. In a sharp-interface approach, the thickness of the interface between the two phases is small compared with other characteristic scales of the fluids. In recent years, diffuse interface models have been successfully used to describe the flow of two or more immiscible fluids both for theoretical studies and numerical simulations. In this situation, the transition between the two phases takes place smoothly across an appropriate diffuse interface or layer (in contrast with the sharp-interface approach, in which the physical parameters characterizing the flow are discontinuous across the interface). These models are based on the observation that even for two (macroscopically) immiscible fluids there is a very thin interfacial region in which partial mixing of the two fluids occurs. Phase-field models belong to the diffuse-interface family of models. They have been used to describe a variety of physical problems in which phase transitions play a role, namely condensation, evaporation, crystallization, etc. The importance of phase-field techniques has grown

considerably as they can be implemented numerically in an effective way. They are characterized by a scalar parameter, called order parameter, which differs in the two phases. There are different choices for the order parameter: for example, the average volume fraction of a phase or the mass concentration of a phase. In both cases, the order parameter has a clear physical meaning and its evolution is described by a nonlinear diffusion equation. We have derived a thermodynamically consistent phase-field model for the description of the expansion stage of the foam. We have adopted mass concentration of the liquid phase as phase-field variable.

The system of equations associated the phase-field model for metal foams is an incompressible-compressible version of a Navier-Stokes-Cahn-Hilliard (NSCH) system. Several numerical approximations of the NSCH system have been proposed in literature in the case of incompressible two-phase fluids, but, up to our knowledge, the numerical analysis in the incompressible-compressible case is missing. Very recently numerical techniques have been developed for quasi-incompressible fluids, i.e., fluids in which both phases are incompressible, but the

mixing is compressible. The main difficulties in the numerical approximation of these systems are represented by the presence of the pressure in the chemical potential definition and by the velocity field that is no longer divergence-free. The idea is to build a numerical scheme that, at the discrete level, preserves mass conservation and the energy dissipation law associated to the original system. The system of equations derived by Lowengrub and Truskinovsky (LT system) for quasi-incompressible fluids has many similarities with the NSCH system associated to the metal foaming model: for this reason, first we have derived a numerical discretization for the LT system and then we extended this numerical method to the case of the NSCH system for incompressible-compressible fluids (i.e., the metal foam model case). We proved that these discretizations satisfy mass conservation and an energy dissipation property at the discrete level.



# EFFICIENT SOLUTION TECHNIQUES FOR HP-VERSION DISCONTINUOUS GALERKIN APPROXIMATION OF ELLIPTIC PROBLEMS

**Marco Sarti** - Advisor: **Dr. Paola F. Antonietti** - Co-Advisor: **Dr. Marco Verani**

In this thesis, we address the study and design of efficient solution techniques for the linear system of equations arising from the high-order version of the Discontinuous Galerkin (DG) discretization of elliptic equations. Since they were first introduced in 1973 by Reed and Hill for parabolic problems, DG methods have undergone huge developments and a variety of schemes have been designed for the discretization of a wide range of equations. The main reason behind the success of DG methods lies in their inherent advantages compared to standard (conforming) discretizations, such as:

- the limited number of inter-element communications, restricted only to neighboring elements, which makes the method suitable for parallelization;
- the intrinsic local conservativity property;
- the simplicity in treating non-matching grids;
- the natural flexibility in handling high-order polynomial approximations, which allows to employ an elementwise varying polynomial order over the computational domain;
- the simplicity in imposing weakly boundary conditions and in handling possible discontinuities in the coefficients of the physical model.

In addition to the above mentioned advantages, it has recently been shown that DG schemes are suitable to be built in the physical frame, avoiding traditional polynomial spaces mapped from a reference frame. This property allows to deal with general-shaped elements, including polygonal/polyhedral elements. The flexibility of DG methods in handling general meshes has no counterpart in the conforming framework, where the design of suitable finite element space for meshes of polygons/polyhedra is far from being a trivial task. Several examples are represented by the Composite Finite Element Method, the Polygonal Finite Element Method, the Mimetic Finite Difference method, the Extended Finite Element Method, and the most recent Virtual Element Method. It is recognized that the main drawback of discontinuous discretizations is the larger number of degrees of freedom for a given computational finite element mesh and polynomial approximation order, compared to their conforming counterpart. Moreover, for second order elliptic problems with smooth solutions, it is usually observed that, for fixed discretization parameters, the discretization error resulting from DG and conforming discretizations is roughly comparable, which

implies that the practical utility of this class of methods is strictly related to the availability of fast solution techniques for the (linear) system of equations resulting from the discretization. The recent trend in this direction is focused on multilevel techniques, including Schwarz domain decomposition methods and two-level and multigrid techniques.

In this doctoral work, we analyze W-cycle multigrid algorithms in the case of standard computational grids, following the abstract theoretical framework for this class of multilevel solvers. We prove that the W-cycle multigrid scheme converges uniformly with respect to the granularity of the underlying mesh, the polynomial approximation degree and the number of levels, provided the number of smoothing steps is large enough, and properly chosen as a function of the polynomial degree. The numerical experiments confirm our theoretical results and also demonstrate that our multigrid methods converge even if the assumption on the minimum number of smoothing steps is not satisfied, but in this case the convergence factor deteriorates when the polynomial order increases. We also discuss in detail the effects of employing non-inherited or inherited sublevel solvers, and show that

our W-cycle algorithms converge uniformly with respect to the number of levels if non-inherited sublevel solvers are employed (*i.e.*, the coarse solvers are constructed discretizing our original problem at each level), whereas convergence cannot be independent of the number of levels if inherited bilinear forms are considered (*i.e.*, the coarse solvers are the restriction of the stiffness matrix constructed on the finest grid).

The same theoretical tools are employed to develop the multigrid framework for the case of polygonal/polyhedral grids, thus retrieving similar convergence estimates. The analysis is based on suitable geometrical assumptions on the set of underlying grids, which cause the convergence result for the W-cycle multigrid scheme to hold only if the number of levels is kept limited. Moreover, unlike the case of standard grids, where the set of nested grids is obtained from successive refinements of an initial partition, here the grids are obtained by successive agglomerations of the finest partition where the problem is meant to be solved. The flexibility of the DG method in handling general-shaped elements allows to fully exploit this agglomeration-based strategy, which can be considered a more natural

approach in the context of a multigrid philosophy. Space decomposition techniques are also considered, and we design and analyze a two-level additive preconditioner, which is uniform with respect to the discretization parameters, *i.e.*, the mesh size, the polynomial approximation degree, and the penalization coefficient appearing in the bilinear form. The proposed method is based on the splitting of the high-order DG space into the high-order conforming finite element space plus a correction. Then, in the context of Parallel Subspace Correction method, we prove that the uniformity of the preconditioner on the DG space results from the uniformity of two distinct preconditioners on the corresponding subspaces. In particular, our operator is a combination of a two-level overlapping Schwarz method, built on the high-order conforming subspace, and of a pointwise Jacobi method, built on the remaining DG subspace. The two-level setting is then further developed into a V-cycle multigrid algorithm, which is uniformly convergent with respect to the number of levels and the discretization parameters. In this case, the highorder DG finest space is paired with a hierarchy of nested linear conforming finite element spaces, and the convergence

analysis is carried out following the standard multigrid theory for the V-cycle method. We underline, that unlike the W-cycle multigrid scheme we have previously studied, here we do not require any lower bound on the number of smoothing steps to guarantee a convergence iteration, and this is due to the choice of conforming finite element spaces for the coarser levels. For any solution technique proposed, we show extensive numerical tests which underpin our theoretical predictions, and for the W-cycle multigrid algorithm we also include the numerical study of several variants of the method not explicitly treated in the analysis.



# DISCONTINUOUS FINITE ELEMENT APPROXIMATION OF CALM-HILLIARD PROBLEMS

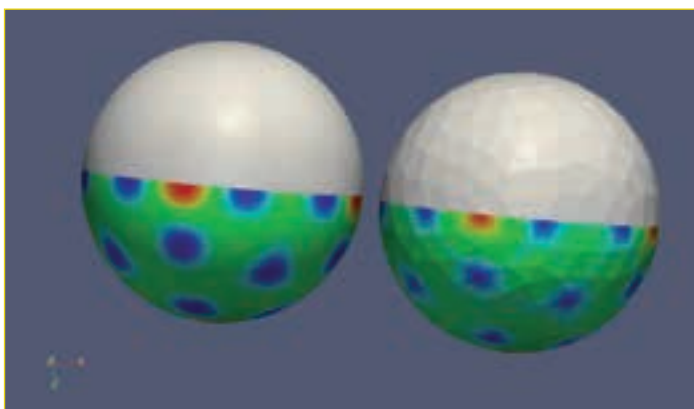
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This thesis is devoted to the design of a new discontinuous Galerkin (DG) approximation of Cahn-Hilliard (CH) equation with dynamic boundary conditions. To achieve this goal we focus on a set of subproblems that represent crucial steps towards the achievement of the final goal.

The first chapter is the introduction of the thesis. It is presented the process of phase separation in a binary alloy and the importance of the CH equation as a model of such a process. The interest of dynamic boundary conditions is also underlined: such conditions take into account the interaction of the alloy with the walls. Finally, are reported several advantages related to the choice of DG methods for the numerical resolution of CH type problems. Chapter 2 deals with high order DG methods for elliptic problems on surfaces. A second order linear elliptic model problem is considered on a compact, smooth and oriented surface  $\Gamma$  embedded in  $\mathbb{R}^3$ . First, a family of polynomial approximations to  $\Gamma$  of degree  $k \geq 1$  is built, as well as an isoparametric DG space of degree  $k$ ; associated to this family. Then, a unified (so-called “primal”) formulation is given for the DG approximation of the model problem, using the elements of degree  $k$ . The primal formulation is based

on numerical fluxes: different choices of the fluxes lead to different classical formulations of V surface DG methods. Up to seven examples which fit into this general framework are provided. A unified analysis is then performed and provides optimal error estimates in  $L^2$  norm and  $H^1$ -like mesh-dependent norms. Numerical simulations on the unit sphere with linear, quadratic and quartic elements illustrate the theoretical results. In Chapter 3, the DG approximation of a parabolic problem with dynamic boundary conditions is considered. A second order linear elliptic problem is first studied on a rectangular domain  $\Omega$ , with generalized Robin boundary conditions on the bottom and top edges (denoted

$\Gamma_1$ ), and periodic boundary conditions on the left and right edges. An interior penalty DG approximation of the problem is proposed with elements of order  $p \geq 1$ , and optimal error estimates are derived in the  $L^2(\Omega)$  norm and a mesh-dependent  $H^1(\Omega) \times H^1(\Gamma_1)$ -like norm; the error estimates take into account the regularity of the solution and the degree of the element. The parabolic version of the problem is then considered on the same domain, with dynamic boundary conditions. A fully discrete approximation of the parabolic problem is proposed. Optimal error estimates are provided in  $L^\infty(0,T; L^2(\Omega))$  norm and mesh-dependent  $L^2(0,T; H^1(\Omega) \times H^1(\Gamma_1))$  norm, assuming enough regularity and compatibility conditions for



Paraview plots of the linear (right) and quartic (left) DG approximations

the solution of the continuous problem. Numerical experiments using various time steps, various space steps and various orders  $p$  confirm the theoretical rates of convergence. A numerical example with Dirichlet boundary conditions instead of periodic boundary conditions is also performed, exhibiting similar convergence rates.

Chapter 4 presents a numerical comparison of several multigrid methods for the numerical resolution of the (classical) CH equation by a DG method. For the numerical simulation of the CH equation, many time steps are usually required, so that the fast resolution of the nonlinear problem at every time step is a crucial point for accelerating the computation. Four examples on long time scales with linear and quadratic elements are first presented in two space dimensions: they illustrate the efficiency of the approach. Then, two multigrid methods are presented and compared on a few time steps. The first method is a classical multigrid method applied to the Newton linearization of the fully discrete problem, and the second method is a nonlinear multigrid method (Fully Approximation Scheme, or FAS). Various numerical experiments are presented, with different initial conditions, different time steps, different number

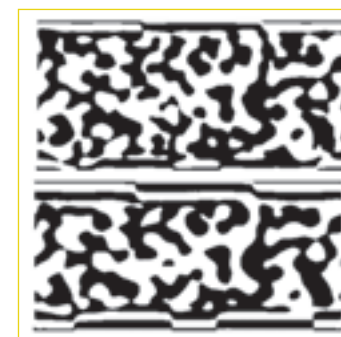
of levels. In several situations, the FAS algorithm is shown to behave faster than the Newton linearized algorithm.

In Chapter 5, is presented a new family of smoothers involved in the FAS algorithm from Chapter 4, the so-called “collective block Gauss-Seidel smoothers”. The local blocks are composed by degrees of freedom associated either to one or more elements (element-wise blocks) or to one or more interfaces (interface-wise blocks). The smoothers are stated in one space dimension in the context of a reaction diffusion equation and of a linearized CH equation.

A local Fourier analysis is performed, and the resulting spectrum of the smoothers is presented in a great variety of situations, with various discrete parameters. The smoothers are then considered in a two-level multigrid algorithm. Numerical tests clearly show that the interface-wise block smoothers behave better than the element-wise block smoothers in such a situation. The efficiency of these smoothers regarding the computational cost is finally shown in several tests.

In the last chapter, Chapter 6, is proposed and implemented a DG approximation of the CH equation with dynamic boundary conditions in two space dimensions. The space discretization is similar to the

one introduced in Chapter 3 and the time discretization is an implicit Euler scheme. Three numerical examples compare the new DG method with a classical conforming finite element approach from the literature. In the first two examples, a rectangular domain is chosen, and in the last one, an annulus-like domain is chosen. The results are similar to those obtained with the conforming finite element method. The results in this chapter illustrate the adaptability and the efficiency of the DG approach chosen here.



Snapshots of the computed solutions using DG discretization of CH problem. We notice the typical behaviour of the solution on the edge where dynamic boundary conditions are imposed.