MECHANICAL ENGINEERING | PHYSICS | PRESERVATION OF THE ARCHITECTURAL HERITAGE | STRUCTURAL, SEISMIC AND GEOTECHNICAL ENGINEERING | URBAN PLANNING, DESIGN AND POLICY | AEROSPACE ENGINEERING | ARCHITECTURE, BUILT ENVIRONMENT AND CONSTRUCTION ENGINEERING | ARCHITECTURAL, URBAN AND INTERIOR DESIGN | BIOENGINEERING | DATA ANALYTICS AND DECISION SCIENCES | DESIGN | ELECTRICAL ENGINEERING | ENERGY AND NUCLEAR SCIENCE AND TECHNOLOGY | ENVIRONMENTAL AND INFRASTRUCTURE ENGINEERING | INDUSTRIAL CHEMISTRY AND CHEMICAL ENGINEERING | INFORMATION TECHNOLOGY | MANAGEMENT ENGINEERING | MATERIALS ENGINEERING | MATHEMATICAL MODELS AND METHODS IN ENGINEERING

PhD Yearbook | 2023

PHD COURSE IN MATHEMATICAL MODELS AND METHODS IN ENGINEERING

Chair:
Prof. Michele Correggi

Mathematics is everywhere, represented by equations. 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. The 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 PhD program has a duration of three years. Activities include: soft skills courses; specialized courses; research training, including seminars, tutoring activity, participation to workshops/conferences, and scientific publications; development of a doctoral thesis.
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.

Grants funded by external partners: IIT, Leonardo Spa, Pirelli Tyre Spa, ENI Spa, RSE, Intellicp

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MATHEMATICAL AND NUMERICAL MODELING OF THE HEART FUNCTION: INTEGRATING ELECTROPHYSIOLOGY, MECHANICS AND FLUID DYNAMICS

Michele Bucelli - Advisor: Alfio Quarteroni

Co-Advisor: Luca Dedé

Mathematical and numerical modeling of the heart is increasingly used to investigate the cardiac function in physiological and pathological settings, to better understand the physical mechanisms that regulate the heartbeat and assist in the development of innovative and personalized treatment.
The purpose of this thesis is the development of a comprehensive and fully coupled heart model, which can serve as a basis for the construction of highly accurate digital twins of the cardiac function.
To this end, I incorporate in a novel computational framework cardiac electrophysiology (through the monodomain equation and suitable biophysically detailed ionic models), contractile force generation, muscular mechanics, both active and passive, hemodynamics and the circulatory system. The presence of cardiac valves is accounted for in a simplified yet effective way by means of the Resistive Immersed Implicit Surface (RIIS) method, which allows to describe the macroscopic effect of the valves (such as their opening and closing and the formation of jets due to the leaflets) without paying the high cost of a fully fledged valve-blood FSI simulation. Finally, the model accounts for the main feedback effects existing between the different physical processes leading to the heartbeat: electro-mechanical and mechano-electrical feedback, the coupling between muscular deformation and contractile force generation, fluid-structure interaction (FSI) between the blood and the myocardium, and the coupling of the heart and the circulatory system. This gives rise to a large multiphysics and multiscale mathematical model.
Due to the complexity of the problem, suitable numerical methods must be employed for its solution. Focusing on the solution of the FSI subproblem, I compare in terms of computational efficiency and accuracy several methods, both strongly and loosely coupled, and identify a geometrically explicit monolithic method as the scheme offering the best trade-off among solver robustness, efficiency and accuracy. The geometric coupling of fluid and solid (i.e. the way the deformation of the muscle causes the fluid domain to change in shape) is addressed in the Arbitrary Lagrangian-Eulerian (ALE) framework. Due to the large displacements characterizing the heartbeat, we rely on a non-linear model representing the fluid domain as a fictitious solid material.
While more costly than the typical linear lifting operator, this approach has proven significantly more robust in dealing with the complex geometries and large deformations of heart simulations. The coupling of electrophysiology, force generation, and FSI is treated in a segregated-staggered way, so as to leverage the multiphysics nature of the problem for computational efficiency and flexibility. Numerical methods are implemented in a high-performance computing framework within lifex, a C++ high-performance library for finite element simulations tailored at cardiac applications.
I simulate a realistic human left heart (left atrium, left ventricle and ascending aorta) in physiological conditions and compare the numerical results against normal ranges for several biomarkers for ventricular volumes and pressures, flow rates through cardiac valves and the duration of heartbeat phases. The results show that the proposed model is capable of reproducing the heart function in healthy conditions, both qualitatively and quantitatively. In particular, the model can effectively reproduce all phases of the heartbeat, including the isovolumetric phases (during which ventricles contract and relax with valves closed, thus at constant volume). This is made possible by the specific choices of models and methods used in the description and simulation of the heartbeat.
Finally, a proof-of-concept simulation indicates that previous results can be extended to simulations involving all four cardiac chambers, thus providing an extremely comprehensive representation of the heart. The results show that the proposed computational model stands as a milestone towards the development of cardiac digital twins.

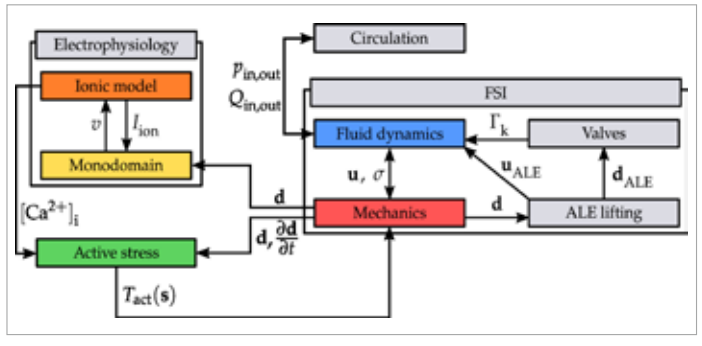

Fig. 1 - Schematic representation of the electro-mechano-fluid model of the heart.

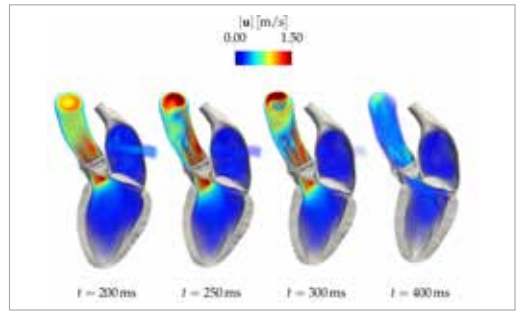

Fig. 2 - Volume rendering of the velocity magnitude for a left heart model, during the systolic ejection phase.

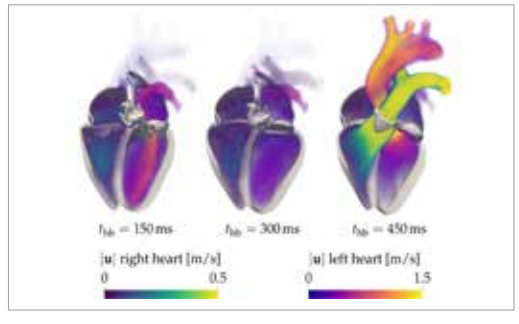

Fig. 3 - Volume rendering of the velocity magnitude for a whole heart model, during the systolic ejection phase.

WAVELET TRANSFORM AND INSTANCE-BASED METHODS FOR NON-STATIONARY TIME SERIES ANALYSIS

Antonino De Martino - Supervisor: Irene Maria Sabadini

This thesis is divided in three parts. In the first part we study the Segal-Bargmann transform and the short-Fourier transform in the quaternionic and Clifford algebra settings. This study is motivated by a recent and increasing interest in the generalization of integral transforms to the non-commutative settings. Such kind of transforms are widely studied, in general, since they help in the analysis of vector-valued signals and images. In the non-commutative settings one can deal with n-dimensional signals. Indeed, in image processing it is needed a higher-dimensional counterpart of the 1- dimensional signal. As a matter of fact, the study of hypercomplex signals can be useful in other practical fields such as optics and signal processing. The focus of the first part of the thesis is the study of the short time Fourier transform in the quaternionic and Clifford algebra settings. This integral transform can be used in several applications such as predictions of sound source position emanated by fault machine and the interpretation of ultrasonic waveforms. Furthermore, if we consider the normalized Hermite functions as window functions of the short time Fourier transform we have to deal with the theory of slice polyanalytic functions. This latter topic is a new research path that extends the theory of slice regular or slice monogenic functions to higher order. In the second part of the thesis we focus on developing new functional calculi based on the S-spectrum and related to the Fueter-Sce construction. Firstly we study the so called F-functional calculus. The crucial object to define this functional calculus is the Fueter-Sce mapping theorem in integral form. The Fueter-Sce map can be seen as an integral transform that maps slice hyperholomorphic functions into axially monogenic functions. Thus, the F -functional calculus is a monogenic functional calculus in the same spirit of McIntosh and collaborators. In this framework, we have been able to compute a resolvent equation, which is the appropriate tool to generate the Riesz projectors. It is well-known that it is possible to factorize the Fueter map in terms of the Fueter operator. Therefore one can wonder the result of applying the Fueter operator or its conjugate to a slice hyperholomorphic function. In the first case we get an axially harmonic function. On the other hand, if we apply the conjugate Fueter operator to a slice hyperholomorphic function we do not get the same result, but instead an axially polyanalytic function of order 2. We are able to write an integral representation of axially harmonic functions and axially polyanalytic functions of order 2. These are crucial tools to define the respective functional calculi, both based on the S-spectrum. In the third part we investigate the behaviour of the factorization of the Laplace operator of n+1-variables elevated to an integer power depending on n, namely the Fueter-Sce map, and we apply a chosen factorization to a slice hyperholomorphic function. Due to the various factorizations of the Fueter-Sce map, the descriptions of intermediate functional calculi are much more involved. We point out that the case of dimension five, although it is a specific case, it already shows all the possible functional calculi and function spaces that can be considered in greater dimensions. It is also important to observe that all the function spaces appear also in different contexts in the literature, but, as far as we know, they are not related each other. A natural problem is to study all the function spaces that are suggested by the Fueter-Sce theorem in complex and hypercomplex setting. Moreover, it would be a challenging problem to figure out if a similar construction holds when we deal with fractional power of the Laplace operator, namely in the case of the Fueter-Sce-Qian map, in even dimension. In this thesis we consider several problems related to the integral transforms in the hypercomplex setting and the study of the related functional calculi based on the S-spectrum. Precisely, we deal with the following topics: slice hyperholomorphic and monogenic function theories, S-functional calculus, polyanalytic function theory, Dirac operator in Clifford analysis, quaternionic Segal Bargmann-transform and Clifford Fourier transform, quaternionic short time Fourier transform with Gaussian and normalized Hermite functions as window functions, F-functional calculus and different functional calculi based on the S-spectrum. In this dissertation, under the supervision of Prof. Irene Maria Sabadini, I co-authored 10 original research papers, from which nine are already published, and one is still submitted. We give a brief summary on the results obtained in this PhD thesis.

- We study a special one dimensional quaternion short-time Fourier transform (QSTFT). Its construction is based on the slice hyperholomorphic Segal-Bargmann transform. We discuss some basic properties and prove different results on the QSTFT such as Moyal formula, reconstruction formula and Lieb's uncertainty principle. We provide also a formula for the reproducing kernel associated to the Gabor space considered in this setting.
- We show that it is possible to extend the previous results by considering a QSTFT with normalized Hermite functions as windows. It turns out that such a transform is based on the recent theory of slice polyanalytic functions on quaternions.
- We investigate how the short-time Fourier transform can be extended in a Clifford algebra setting. We prove some of the main properties of the Clifford short-time Fourier transform. The results show different features with respect to the classic case.
- We provide an alternative description of the Fueter-Sce-Qian theorem in terms of the generalized CK-extension, for both cases, n even and n odd
- Using the Cauchy formula of slice hyperholomorphic functions the Fueter-Sce-Qian theorem admits an integral representation for n odd. We show that the important relation between the slice monogenic Cauchy kernel and the F-kernel, that appears in the integral form of the Fueter-Sce-Qian theorem for n odd, holds also in the case we consider the fractional powers of the Laplace operator n dimension n+1, i.e., for n even.
- By writing the Fueter-Sce-Qian extension theorem in integral form and it is possible to define the F-functional calculus for n-tuples of commuting operators. This functional calculus is defined on the S-spectrum and generates a monogenic functional calculus in the spirit of McIntosh and collaborators. We show that the F-functional calculus generates the Riesz projectors. The existence of such projectors is obtained via the F-resolvent equation which was previously known only in the quaternionic setting and also its existence was under question. We prove the F-resolvent equation in the Clifford algebra setting. It is much more complicated than the one in the quaternionic case since it contains various pieces, however it still allows to nicely define the Riesz projectors.
- We introduce seminal results on the introduction of an harmonic functional calculus based on the S-spectrum and on an integral representation of axially harmonic functions. This new calculus is a bridge between harmonic analysis and the spectral theory. The resolvent operator of the harmonic functional calculus is the commutative version of the pseudo S-resolvent operator. This calculus also appears, in a natural way, in the product rule for the F-functional calculus.
- In the second step of the Fueter construction an axially monogenic function is built by applying the Laplace operator in four real variables to a slice hyperholomorphic function. We use the factorization of the Laplace operator in terms of the Fueter operator to split the previous procedure. From this splitting we get a class of functions that lies between the set of slice hyperholomorphic functions and the set of axially monogenic functions: the set of axially polyanalytic functions of order 2. We show an integral representation formula for this kind of functions. The formula obtained is fundamental to define the associated functional calculus on the S-spectrum.
- We show that the extension operator from slice hyperholomorphic functions to monogenic functions admits various possible factorizations that induce different function spaces.
- The integral representations in such spaces allows to define the associated functional calculi based on the S-spectrum. The function spaces and the associated functional calculi define the so called *fine structure of the spectral theories on the S -spectrum*. Among the possible fine structures there are the harmonic and poly-harmonic functions and the associated harmonic and poly-harmonic functional calculi. The study of the fine structures depends on the dimension considered.
- Based on the techniques developed in this thesis, we already started some new projects. We aim to tackle them in the near future. We plan to start new research investigations in the following directions: the F-resolvent equation for all dimensions, the H^∞ calculus and the Phillips functional calculus for the F-functional calculus and the for the all *fine structures*, establish a generalized Cauchy-Kovalevskaya extension for axially harmonic functions, study the function spaces that arise from the factorization of the Fueter-Sce mapping theorem, both in the complex and hypercomplex setting.

MACHINE LEARNING FOR PRECISION MEDICINE: A COMBINATION OF DATA-DRIVEN AND PHYSICS BASED MODELS

Nicola Franco Rares - Supervisor: Paolo Zunino

Co-Supervisors: Francesca Ieva, Andrea Manzoni, Anna Maria Paganoni

Precision medicine aims at improving the clinical treatment of patients by proposing subject-specific therapies, which are designed on the basis of individual characteristics, such as age and lifestyle, but also more complicated biological features. To this end, precision medicine mostly relies on biomarkers, complex indicators that characterize the genotype and phenotype of a patient. In practical applications, such biomarkers are commonly derived by synthesizing the information coming from both data-driven and physics based models.

The aim of this Thesis is to explore a unified framework for quantitative methods in precision medicine, leveraging on Machine Learning tools.

In particular, we focus on the case of personalized treatment planning of radiotherapy. Recently, many new research lines are being explored in this field, two of which are the main focus of this Thesis. The first one concerns the study of radiosensitivity as a genetic trait, and thus aims at identifying the genetic mutations associated with late toxicity in order to build suitable predictive biomarkers. The second line of research, instead, consists in the analysis of the cellular response to radiation by means of accurate and extensive numerical simulations. Both approaches present significant challenges, which in this Thesis are addressed through the development of new Machine Learning and Deep Learning algorithms.

In the first part of the Thesis, we focus on studying the connection between late toxicity and mutations in the DNA. There, the main difficulties arise from the presence of complex interactions among genetic loci and from the intrinsic class imbalance characterizing clinical data. To tackle these adversities, we take advantage of different Machine Learning tools, from deep autoencoders to data mining algorithms, ultimately developing a novel approach to polygenic risk scoring that enables the construction of interpretable interaction-aware biomarkers. Throughout the Thesis, we assess the scientific value of the proposed approach on both simulated and real data, showcasing the impact of our work on the clinical world.

Conversely, in the second part of the dissertation, we discuss how Deep Learning can be used to reduce the computational cost entailed by the numerical simulation of biophysical models relevant for radiotherapy, such as oxygen transfer models. In particular, we develop several strategies based on Deep Learning algorithms for replacing the original numerical solver with a cheaper, yet accurate, surrogate model. Thanks to these tools, the computational bottleneck entailed by using physics based numerical simulations in the complex workflow of biomarker discovery and validation can be completely resolved. From the methodological and, in particular, the mathematical standpoint, the proposed approaches are inspired by the flourishing literature of Reduced Order Modeling, but they also share unique benefits that distinguish them from state-of-art techniques, such as the ability of handling singularities, transport and mass propagation, in an extremely efficient way. In order to make our proposal mathematically sound, we also derive innovative theoretical results that support our reasoning. In particular, the Thesis contains innovative results about the latent dimension of autoencoders and the properties of convolutional neural networks. Finally, as a by-product of our studies, we also end up developing completely new tools, such as mesh-informed architectures, that, for their generality, stand out as independent topics of research.

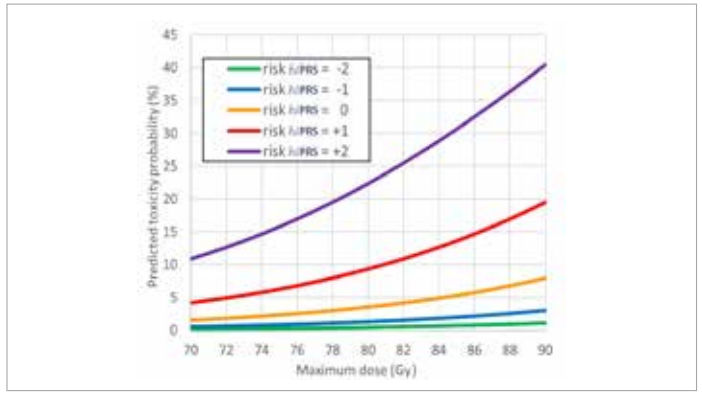

Fig. 1 - Probability of late radiotoxicity as a function of the radiation dose, for different patient genotypes.

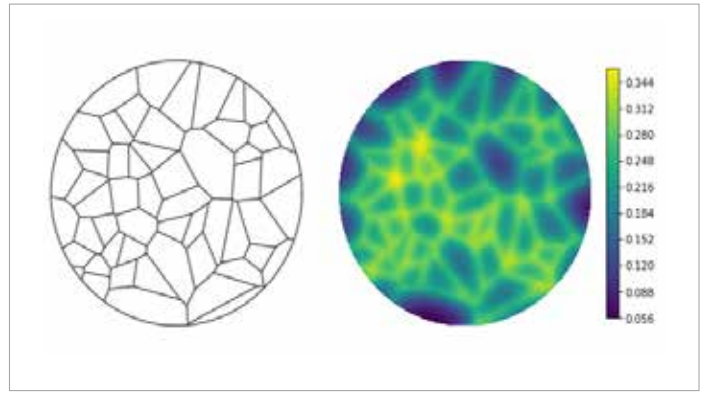

Fig. 2 - Vascular network and corresponding oxygen distribution in a simulated biological tissue.

STABILITY OF DIFFERENTIAL SYSTEMS OF MOORE-GIBSON-THOMPSON TYPE

Lorenzo Liverani - Advisor: Vittorino Pata

The present doctoral dissertation deals with the asymptotic behavior of differential systems arising in connection with the third-order, linear evolution equation

$$u_{ttt} + \alpha u_{tt} - \beta \Delta u_t - \gamma \Delta u = 0$$

known as Moore-Gibson-Thompson (MGT) equation.
Here -Δ is the Laplace-Dirichlet operator, while alpha, beta, gamma > 0 are structural parameters. From the physical viewpoint, the MGT equation is a wave-type equation arising in the context of acoustic wave propagation with the so-called second sound, being u the acoustic pressure, where the paradox of the infinite speed of propagation is eliminated by replacing the Fourier law by the Maxwell-Cattaneo one. Such a feature
explains the presence of the third-order derivative in time.
The model equation first appeared in a very old paper of Stokes, but it has received a considerable attention only in recent years, where a number of authors devised many possible applications in nonlinear acoustic and in thermal relaxation in viscous gases and fluids.

The thesis is divided into two main parts.
In the first part, we investigate systems of coupled differential equations featuring both a dissipative and a countervailing antidissipative mechanism.
There are many interesting situations where a system is made, say, by two equations, one of which dissipates through a damping mechanism, while the other one preserves the energy.
It is then natural to ask what can be said regarding the longterm behavior of the solution. In particular, from a physical and applicative standpoint, it is of utmost importance to understand whether the energy of the system vanish asymptotically and, if so, at what rate of decay. Clearly, the coupling between the two equations plays an essential role, since its action allows to transfer dissipation to the undamped equation, in such a way that the whole system usually becomes globally stable as time goes to infinity.
We may ask what happens if we couple a dissipative equation with an antidissipative one. The picture now is more intriguing, and the strength of the coupling comes into play. To hope for stability, it is necessary that the equations share their energies to a certain extent. This translates into the fact that the coupling cannot be too weak. But even if the coupling is strong enough to bypass a certain critical threshold, the system may remain unstable if the action of the antidamping is more effective than the one of the damping.
The aim of the first part of this thesis is to investigate the longterm behavior of systems of this kind,
with a special focus on the role played by the coupling in the uniform decay of the energy.
An eye of regard is, of course, given to systems involving MGT type equations. Indeed, these equations exhibit an antidissipative behavior for certain values of the structural parameters.

In the second part of the thesis, we focus on the asymptotic properties of integro-differential equations known as equations with memory.
Several interesting physical phenomena can be modeled by differential equations in which the current dynamics is influenced by the past values of one or more of the variables in play. These are known as equations with memory. Applications of these models span over many fields, including viscoelasticity, hereditary polarization in dielectrics, population dynamics or heat flow in real conductors, just to name a few. The main difficulty when treating equations with memory lies in their nonlocal character.
A way to overcome this intrinsic difficulty is to translate the equation in the so-called past history framework, which was first introduced by Dafermos in the context of viscoelasticity.
We begin by investigating an integral relaxation of the MGT equation. We prove an existence and uniqueness result removing the convexity assumption on the convolution kernel g(s), usually adopted in the literature. In the subcritical case, we establish exponential decay of the energy, only asking that g vanishes exponentially fast.
We proceed by studying a system of coupled PDEs with memory, obtained as a model for poro-thermoelasticity when microtemperatures are involved. After showing how to derive the system starting from the constitutive equations, we show that these are well posed. Furthermore, in the one dimensional case, we use linear semigroup techniques to prove that the energy of the system decays exponentially fast.
In the final chapter, we consider the abstract equation with memory known as equation of viscoelasticity. The purpose of this chapter is to provide numerical evidence for the fact that the energy of any nontrivial solution cannot decay faster than exponentially, no matter how fast the decay of the memory kernel might be.

MACHINE LEARNING-ENHANCED REFINEMENT AND AGGLOMERATION ALGORITHMS FOR POLYTOPAL FINITE ELEMENT METHODS

Enrico Manuzzi - Supervisor: Paola F. Antonietti

Many geophysical and engineering applications, such as fluid-structure interaction, crack and wave propagation problems, and flow in fractured porous media, are characterized by a strong complexity of the physical domain, possibly involving thousands of fractures, heterogeneous media, moving geometries and complex topographies. Whenever "classical" Finite Element Methods (FEMs) are employed to discretize the underlying differential model, the process of generating and handling the computational mesh can be the bottleneck of the whole simulation, as computational grids can be composed only of tetrahedral, hexahedral, or prismatic elements. To overcome this limitation, many numerical methods that support computational meshes composed of general polygonal and polyhedral (polytopal, for short) elements have been developed in the last decade, such as for example the Virtual Element Method (VEM), the Polytopal Discontinuous Galerkin method (PolyDG), the mimetic finite differences method, the hybridizable discontinuous Galerkin method and the Hybrid High-Order method. However, since elements may have any shape, there are no well-established strategies to efficiently handle polytopal mesh refinement, i.e., partitioning mesh elements into smaller elements to produce a finer grid, and agglomeration, i.e., merging mesh elements to obtain coarser grids. Refinement is used to adaptively construct the grid in order to improve the accuracy of the solution, while agglomeration is used to reduce the number of degrees of freedom or in combination with multigrid solvers, which exploit a hierarchy of grids with different resolutions to accelerate the convergence of iterative algebraic algorithms. In order to perform these operations effectively, it is therefore extremely important to preserve the geometrical structure and quality of the initial grid, at a low computational cost. In this thesis, we propose to use Machine Learning (ML) based strategies to tackle the open problems of performing effectively mesh refinement and agglomeration. In two dimensions, we develop new strategies to handle polygonal grids refinement based on Convolutional Neural Networks (CNNs). We show that CNNs can be successfully employed to identify the "shape" of a polygonal element correctly so that ad-hoc refinement criteria can be applied. In this way, CNNs can be used to enhance existing refinement strategies, at a low online computational cost. In three dimensions, we extend the two-dimensional framework for mesh refinement, combining CNNs also with the k-means clustering algorithm, to partition the points of the polyhedron to be refined, in order to make the approach more robust with respect to unstructured grids. In order to deal with the agglomeration of polygonal grids, we propose the use of Graph Neural Networks (GNNs) to partition the connectivity graph of mesh elements. GNNs can naturally and effectively process both the graph and the geometrical information, featuring strong generalisation capabilities and fast inference. The effectiveness of the proposed strategies is demonstrated in terms of quality metrics, mesh complexity, computational cost and performance when applied to VEMs, PolyDG methods and multigrid solvers. Finally, as a complementary contribution to this work, we explore the use Variational Physics-Informed Neural Networks (VPINNs) to directly solve the one-dimensional Helmholtz impedance problem, which is a mesh-less approach.

NON-CONFORMING METHODS FOR THE SIMULATION OF INDUSTRIAL POLYMER MIXING PROCESSES

Giorgio Negrini - Supervisor: Nicola Parolini

This work focuses on the numerical modelling of polymer mixing processes. These processes are performed with the aid of devices (single- and twin- screw extruders, planetary extruders, Banbury mixers, etc.) characterized by complex geometries in which body-fitted simulations can hardly be performed. Non-conforming approaches, like diffuse interface, fictitious domain, immersed boundary or volume penalty methods, represent the best alternative to simulate these types of processes, that may also involve complex kinematics. In this work, we present an implementation of an Immersed Boundary method (IBM) to deal with this type of simulations and with realistic industrial screw geometries.
The flow of a polymer inside a mixing device is described by the incompressible Navier-Stokes equations. Moreover, the polymer is modelled as a non-Newtonian fluid with temperature dependent viscosity. Particular attention is paid to the description of rheological models of polymer viscosity, that depends on shear rate, temperature and filler fraction. To solve numerically this problem, we consider the Finite Volume method (FVM), widely adopted in industry because of its built-in conservation properties, its ability to deal with arbitrary mesh and its computational efficiency. In this context, a variational analysis of the FVM as a Box method (BM) applied to the Stokes problem is carried out. The BM is a piecewise linear Petrov-Galerkin formulation on the Voronoi dual mesh of a Delaunay triangulation. To recover the inf-sup stability of the Stokes problem discretized by the Box method, we resort to the Rhie-Chow stabilization, for which a convergence analysis is presented. Then, we consider the linear Stokes problem discretized using the Box method combined with a Diffuse Interface method (DIM). The application of DIM to approximate non-conforming boundaries leads to error convergence rates that are suboptimal with respect to the ones of the conforming solution. To overcome the limited convergence properties of the Diffuse Interface Box method, we introduce an improved non-conforming approach based on the Immersed Boundary method. It consists in a discrete-forcing direct-imposition method where a mesh subset is selected and then the solution on this subset is computed with respect to the original boundary condition. The solution imposed is then corrected using a quadratic weighted least squares interpolation, that allows to significantly improve accuracy and recover optimal convergence rates. Moreover, since the pressure-velocity coupling is solved with a projection algorithm (SIMPLE), a Neumann boundary condition for pressure that is consistent with the velocity profile has been developed.
Finally, several applications to real industrial devices complete this work, in particular we considered single- and twin-screw extruders and planetary roller extruders (Figures 1, 2 and 3). In general, extruders are made by an external shell, called barrel, and internal parts, called screws or rotors. While the barrel has often simple shape, screws present different geometric features and sharp edges. Moreover, the gaps between the barrel and the internal screws are narrow, four orders of magnitude smaller than the machine dimensions, which make the problem multi-scale. Here, the strategies that have been developed to deal with these complex objects are exposed, in particular for anisotropic grids or graded grids, multiple interacting and adjacent immersed geometries, moving objects, small gaps and the high non-linearity of the problem.

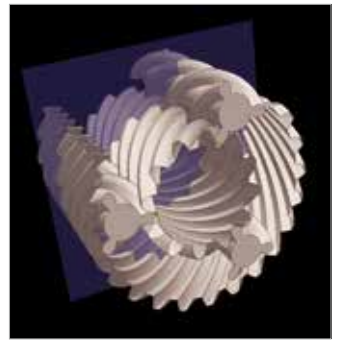

Fig. 1 - PRE rendering and position of the slice.

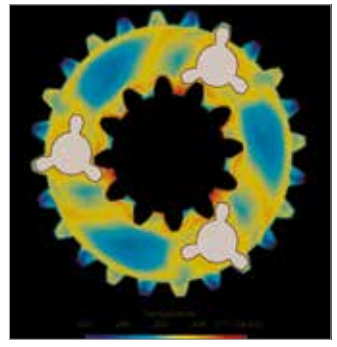

Fig. 2 - Temperature distribution on the axial slice.

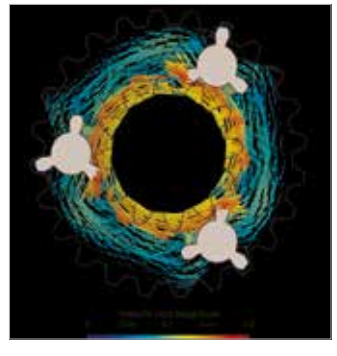

Fig. 3 - Velocity field on the axial slice.

MODELLING AND SIMULATIONS OF TWO-PHASE FLOWS INCLUDING GEOMETRIC VARIABLES

Giuseppe Orlando – Supervisor: Luca Bonaventura

Co-Supervisor: Paolo Francesco Barbante

In this thesis, we analyze two-phase flows with emphasis on geometric variables that arise in their description. Two-phase flows play an important role in several natural processes and engineering systems and their modelling is thus a highly interdisciplinary research topic. They are characterized by the presence of an interface which separates the bulk regions of the single phases. Two-phase flows are classified into two main regimes: separated and disperse flows. However, independently of the specific regime, the exchanges between two phases occur at the interface and phase exchange terms are proportional to the interface area. Hence, the computation of this quantity is a prerequisite in order to obtain an accurate description of the phase exchanges themselves. Evolution equations for the interface area density are typically obtained by means of empirical approaches. One of the main goals of this thesis is the derivation of dynamic equations for the interface area density through the Stationary Action Principle (SAP). Moreover, the addition of source terms compatible with the second principle of thermodynamics allows to obtain, in appropriate limiting regimes, the classical pressure relaxation associated to the transport of the volume fraction. Furthermore, thanks to a suitable interpretation of some parameters, it is also possible to derive semi-empirical relationships for the interface area density already known in the literature.

The other main goal of the thesis is the development of an effective computational environment for the simulation of two-phase flows. More specifically, we propose a Discontinuous Galerkin (DG) discretization suitable for a range of fluid dynamical models in the framework of the *deal.II* library, which is based on matrix-free approach and provides Adaptive Mesh Refinement (AMR) tools. We first present an implicit solver for the incompressible Navier-Stokes equations using an artificial compressibility formulation. We then derive an extension for single-phase weakly compressible flows with an implicit coupling between momentum and energy balance. A second order IMEX scheme is employed for the time discretization, with the implicit part coinciding with the TR-BDF2 scheme used for the incompressible Navier-Stokes equations, providing thus ample guarantees of robustness in the low Mach regime. The proposed technique allows us the use of rather general Equations of State (EOS) for non-ideal gases. More specifically, we propose a non straightforward extension of existing semi-implicit approaches for the ideal gas law for the Stiffened Gas (SG-EOS) and for the general cubic equation of state and we develop suitable refinement indicators for real gases.

Finally, we provide an extension for the full non-equilibrium two-phase Baer-Nunziato models, developing also a filtering monotonization procedure in order to avoid, or at least reduce, the under- and over-shoots that arise in presence of discontinuities using high order discretizations. The effectiveness of all the proposed methods is shown in a number of significant benchmarks.

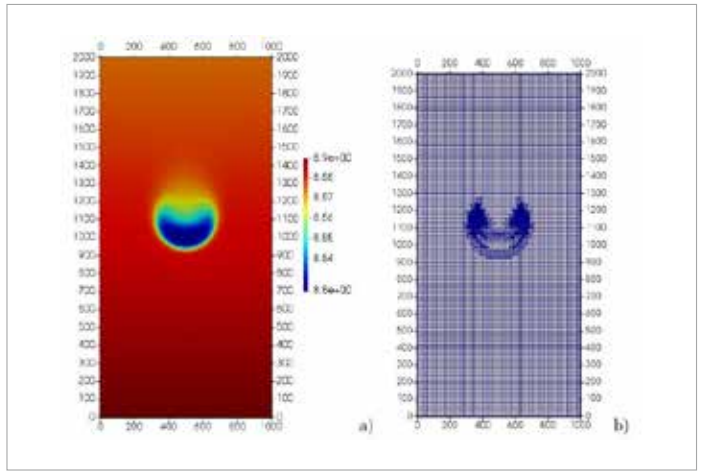

Fig. 1 - Cold bubble test case, van der Waals EOS, adaptive simulation a) Contour plot b) Computational grid

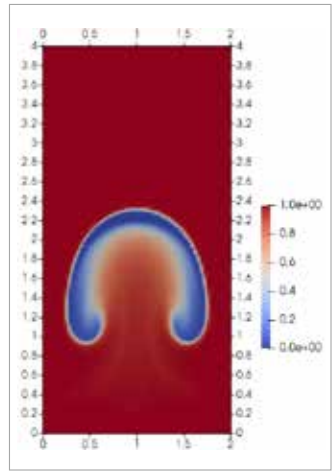

Fig. 2 - Rising bubble test case, volume fraction.

ANALYSIS OF SOME FLUID-STRUCTURE INTERACTION PROBLEMS IN CHANNELS

Clara Patriarca - Supervisor: Filippo Gazzola

This thesis is concerned with the analysis of some fluid-structure interaction problems in channels. The physical motivations mostly stem from the phenomenon of wind interacting with suspension bridges. In particular, our attention focuses on the instabilities which might affect the deck, which is the most sensitive part of the structure. Beside inducing on the deck some static effects, such as *lift* and *drag* forces, the wind generates dynamical instabilities, among which we count vortex-induced *vibrations*, *buffeting*, *one-degree of freedom instability* and *flutter*. This type of instabilities occurs in general during the interaction between a fluid and a structure, whenever the fluid's dynamic loading excites the natural modes of the structure. While the motivations come from physics, the nature of our analysis is essentially theoretical. Starting from some models apt to describe the desired phenomena, we investigate their purely analytical properties. First, we establish some existence and uniqueness results. Beside serving as a preliminary step, these results are interesting per se, since we treat the case of fluid-structure problems with non-homogeneous boundary conditions, still partially unexplored in the existing literature, both in a stationary framework and in a full evolutionary fluid-structure interaction framework. In particular, in the static case we study the connection between the multiplicity of solutions generating under large enough data and the apperance of forces acting on the fixed obstacle.
In the dynamic case, we adapt some existing techniques for well-posedness to the non-homogeneous case, also dealing with the issue of collisions.
Then, we dig into the longterm dynamics of fluid-structure interaction problems. In this way, we directly approach through a theoretical strategy fluid-structure instabilities.
In this context, we will use notions from the theory of infinite-dimensional dynamical systems, like the one of global attractor, showing how it can be extended to the field of fluid-structure interaction. The purely theoretical description of the long time behaviour is partially combined with a numerical investigation, aiming at enriching the picture.

MATHEMATICAL MODELS AND METHODS OF MULTI-PHYSICS BIOLOGICAL SYSTEMS

Giulia Pozzi – Supervisor: Pasquale Ciarletta

Mathematical models, due to their ability of unveiling biological mechanisms and their utility in studying new therapies, are of great importance in life sciences and medicine. In particular, mathematical-physical modeling is extremely effective in describing the peculiar nonlinear and non-equilibrium response of biological and bio-engineered tissues and, more generally, of soft matter. This thesis focuses on mathematical models and methods of multi-physics systems through their application to several biological problems.
We set our theoretical framework in the field of nonlinear partial differential models to capture the complex behavior of such open thermomechanical systems both from the perspective of their spatio-temporal evolution and of their quasi-static equilibrium states.
In the first part, we propose evolutive partial differential equation (PDE) models for the description of open multi-physics systems that are out of thermodynamic equilibrium, characterized by the presence of mass and energy fluxes through the interfaces, and evolving according to maximum dissipation principles. Within this framework, we exploit a diffuse interface approach to study the evolution of systems described as multiphasic mixtures of immiscible components. We recur to perturbation techniques to perform a qualitative analysis on the behavior of the solution. Furthermore, we propose robust schemes for their numerical approximation, integrating experimental data to quantitatively test the reliability of the predictions. In this regard, the major contributions concern two novel models for describing the healing of an epithelial wound (see Fig. 1) and the response of murine models of prostatic cancer to a new protocol of immunotherapy.
In the second part, we address three distinct bio-inspired boundary values problems in non-linear elasticity for prestressed and active matter. We exploit perturbation techniques to study the dimensional reduction and the morphological transitions in the solution of non-standard classes of nonlinear elastic materials, i.e. Foppl-von Karman equations for prestressed elastic plates and the active response of axons to chemo-mechanical stimuli. Moreover, we develop a new numerical approach to the creasing instability that underlies the formation of sulci in the brain cortex, proposing a new and robust framework to simulate in a quasi-static manner the onset and development of self-contact in a free surface subjected to a critical compression (see Fig. 2).

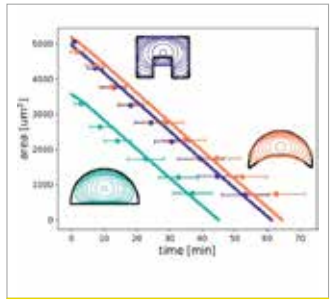

Fig. 1 - Gap closure dynamics for three different wound shapes.

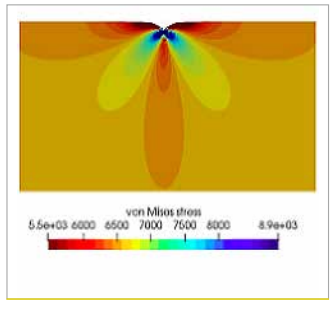

Fig. 2 - Stress pattern in proximity of the self-contacting fold.

NUMERICAL METHODS FOR THE MATHEMATICAL HEART-TORSO MODEL: TOWARD THE EFFICIENT GENERATION OF ELECTROCARDIOGRAMS

Elena Zappon - Advisor: Alfio Quarteroni
Co-Advisor: Andrea Manzoni

Computer-based numerical simulations of the cardiac electrical activity can play an important role in understanding cardiac events, diagnosing heart diseases, and generating additional clinical data. They are based on rigorous and accurate mathematical models able to faithfully reproduce physical phenomena at different scales, and can match clinical outputs such as electrocardiograms (ECGs). The intrinsic multi-scale and multi-physics nature of cardiac electrophysiology requires however to achieve a trade-off between the accuracy of the models and their computational efficiency.

In this thesis, I propose a rigorous mathematical setting for simulating cardiac electrophysiology, as well as clinical outputs of interest like the most widely used 12-lead ECG system. The latter is modeled by means of a coupled multi-physics system, termed heart-torso model. I investigate the solution of this coupled problem in terms of numerical performances and accuracy by employing both Domain-Decomposition iterations and monolithic scheme, for a range of different anatomical geometries. Since the ECG is strongly dependent on the geometrical shape and position of the heart within the human body, I address the problem - almost never tackled before in a systematic way - of evaluating the impact of the geometrical properties of the torso domain on the ECGs. To this end (i) I introduce a set of geometrical transformations on the cardiac geometry to simulate the uncertainty due to the imaging acquisition process, and compute the ECG while prescribing the solution of the electrophysiology problem, and (ii) I develop an electromechanical model for both the heart and the torso, able to account for the myocardial contraction in the ECG.

In this thesis I also develop and implement efficient reduced order strategies to enhance numerical efficiency in cardiac electrophysiology, e.g. when multi-query simulations are carried out to assess the ECG dependency from electrophysiological parameters. Model order reduction of coupled problems has rarely been addressed. I first propose, verify and test a reduced basis method relying on Proper Orthogonal Decomposition and Discrete Empirical Interpolation to reduce coupled problems when both conforming and non-conforming finite element approximations are used as full-order models. Finally, I test the proposed reduced order strategies on the cardiac electrophysiology problem, as well as in the case of a coupled heart-torso model, where capturing the sharp traveling front due to the electrical activation in a parameter-dependent scenario is a challenging task.

The mathematical approach that I propose in this thesis can represent an important step towards the construction of personalized models in cardiac electrophysiology, that require the synergistic use of trustworthy mathematical models with efficient and scalable numerical strategies.

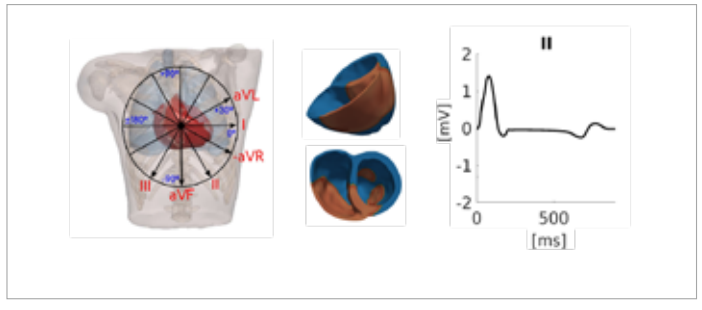

Fig. 1 - Realistic human torso with the 12-lead ECG system representation (left), transmembrane potential resulting from a cardiac electrophysiology simulation on a realistic biventricular geometry (center), and simulated and realistic II lead (left).