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PhD Yearbook | 2018

PHD COURSE IN MATHEMATICAL MODELS AND METHODS IN ENGINEERING

Chair:
Prof. Irene M. Sabadini

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 our their research both in the development of new mathematical methods and in the implementation and improvement of advanced techniques in connection with specific contexts and applications.
The Faculty of the PhD program is responsible for the organization of the training and research activities of the PhD students. Decisions of the Faculty comply with the requirements and standards of the Doctoral School of the Politecnico di Milano. A Chairman is elected within the Faculty, for representative and coordination activities. Admission of students to the PhD program is decided after examination of the candidates. Students applying to our program must provide their CV, along with reference and motivation letters. After admission, each student is assigned a tutor. The tutor is a member of the Faculty who assists the student in the early stages of his career, especially in the choice of the courses and in identifying a thesis advisor.

The 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: ENI, IIT, Karman Institut

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REGRESSION WITH PDE PENALIZATION FOR MODELLING FUNCTIONAL DATA WITH SPATIAL AND SPATIO-TEMPORAL DEPENDENCE

Eleonora Arnone - Advisor: Prof. Laura Maria Sangalli
Co-Advisor: Prof. Fabio Nobile

In this thesis we study methods that deal with spatial or spatio-temporal dependent data adopting a Functional Data Analysis approach. The methods we consider are able to include problem-specific prior information about the phenomenon under study; moreover, they handle complexities in the spatial domain, like holes or strong concavities.
Several classical and recent techniques can be applied to deal with space-dependent data. Kernel smoothing and kriging are classical methods that are suited for problems where the spatial domain on interest is very simple. Indeed, they smooth across boundaries, and do not allow for considering complex shaped domains, that influence the behavior of the field to be estimated.
Another class of methods is based on penalized regression with differential regularization. These methods define the estimator as the minimizer of a functional in a Sobolev space. In most of the cases, the estimate cannot be find analytically, and a discretized version of the solution has to be computed.
Thin plate splines and multivariate splines use, to approximate the continuous estimator, radial basis functions and tensor product basis expansion respectively, thus, they suffer from the same problem as kriging with complex domains. Recently, other techniques, based on penalized regression, that effectively deal with complex domains have been developed.
In soap film smoothing and in spatial spline regression the penalization involves the Laplacian of the function, integrated over the domain of interest.
Spatial Regression with PDE penalization (SR-PDE) generalizes the spatial spline regression method to include in the model problem-specific prior information formalized in terms of Partial Differential Equation (PDE). We concentrate on phenomena that can be described by a linear second order PDE.
SR-PDE proposes to estimate the spatial field from data observed at given spatial locations minimizing a penalized sum-of-square error functional where the penalization include the information given by the PDE, and the intensity of the penalization is regulated by a smoothing parameter. Including PDEs in the penalized regression model allows for combining a data fitting criterion and a model fitting criterion. In this framework, high values of the smoothing parameter mean a major role of the PDE model in the fitting with respect to data, and conversely. From the smoothing perspective, the smoothing parameter balances the intensity of the smoothing: large values of the parameter correspond to a high degree of smoothness while small values produce noisier estimates.
Information about the field can also be included imposing conditions at the boundary of the domain. Various kinds of boundary conditions can be considered in the model, like Dirichlet, Neuman, Robin and mixed boundary conditions. As for thin plate splines and soap film smoothing, the minimization problem cannot be solved analytically. The discretized model is based on finite element method, and efficiently deals with complex domains and boundary conditions.
The main objective of this thesis is to study the properties of SR-PDE method and extend it to more complex data. We focus on proving the consistency of the estimators, both in their infinite dimensional form and in their discretized form. Moreover, we extend the methodology to handle spatio-temporal data, considering different regularization terms.
The first chapter of the thesis is devoted to the study of consistency of SR-PDE estimators. Unfortunately, the results obtained for simpler regularized least square estimators such as univariate and multivariate splines cannot be directly extended to SR-PDE, and different approaches must be developed.
This study of the asymptotic properties of SR-PDE combines competences from statistics, analysis and numerical analysis.
We study the bias and the variance of the continuous estimator, finding the asymptotic rates for both terms with respect to the number of observations and the smoothing parameter. Thanks to these rates we have not only the consistency, but we reach also the best rate of convergence for non-parametric estimators.
We also study the properties of the discrete estimator under the hypothesis that the discretization is constrained to the data locations. The analysis is performed separately on the bias and variance term in analogy with the continuous case, and the consistency is proved. Finally, numerical simulations show evidence for the theoretical rates of convergence obtained.
The second and the third chapters instead aim at extending the methodology of SR-PDE to the estimation of spatio-temporal fields.
Spatial techniques like thin plate splines and soap film smoothing have been recently extended to space-time data with a tensorial approach. This kind of models define the estimator as the minimizer of a penalized sum-of-square errors functional with two different penalties, one for the spatial and one for the temporal dimension.
In the second chapter we study the Spatio-Temporal regression model with Partial Differential Equations regularization (ST-PDE). The method has been presented in a discretized form, for isotropic smoothing and pointwise observations. We first of all extend ST-PDE to general differential penalties, accounting for spatial anisotropy and non-stationarity of the field. Moreover, we extended the model to deal with various sampling designs, that include pointwise and areal observations in space and time. In addition, we here analyze and prove the well-posedness of the corresponding infinite dimensional estimation problem.
Two possible formalizations of the estimation problem in appropriate functional spaces are presented. The first formulation considers separately the spatial and the temporal part of the differential penalization. The second formulation considers jointly the spatial and the temporal part of the differential penalization, and is fully elliptic.
In the last chapter a third approach to deal with spatio-temporal data is presented. This method is suited for problems where we have problem specific prior information about the spatio-temporal field to estimate, that can be formulated in term of a time dependent parabolic PDE. In these cases, the tensorial approach is not appropriate, and a better strategy can be followed. Extending SR-PDE we propose a Spatio-Temporal regression model with time dependent Partial Differential Equations regularization (ST-tPDE), which estimate the spatio-temporal field with a penalized regression technique, where we have a single penalty term, that includes the parabolic PDE describing the phenomenon.
As in the SR-PDE different kinds of boundary conditions can be considered.
The model is presented for time-dependent curves corresponding to pointwise locations in the spatial domain, and is extended to a general formulation to possibly deal with different sampling designs. The well-posedness of the minimization problem is proved, and a discretized version of the estimator is derived with finite elements in space and finite differences in time. The method is compared with other classical techniques and with ST-PDE method, for pointwise and areal spatial observations.
Finally, the method is applied to estimate the blood flow velocity field in the cross section of the carotid artery, over the temporal interval of a heartbeat. Starting from Echo-Color Doppler data measured over seven beams of the carotid section, we aim to reconstruct the whole spatio-temporal field. In this context, the inclusion in the model of the problem-specific prior information concerning blood fluid dynamics and appropriate boundary conditions is fundamental to obtain physiological estimates.
The implementation of ST-PDE and ST-tPDE has been done in R and C++.

LARGE EDDY SIMULATION OF COMPRESSIBLE VARIABLE DENSITY FLOWS WITH A HIGH ORDER DG-LES MODEL

Caterina Bassi - Advisor: Prof. Luca Bonaventura

The thesis deals with Direct Numerical Simulations (DNS) and Large Eddy Simulations (LES) of turbulent gravity currents performed by means of a Discontinuous Galerkin (DG) Finite Elements method.
Numerical simulations of both two-dimensional and three-dimensional non-Boussinesq lock-exchange benchmark problems show that, in the DNS case, the proposed method allows to correctly reproduce relevant features of variable density flows with gravity.
The LES results, obtained with the LES-DG turbulence models introduced in [Abbà et al., (2015), Dynamic models for Large Eddy Simulation of compressible flows with a high order DG method, Computers & Fluids, 122:209-222], highlight, also in the gravity current context, the excessively high dissipation of the Smagorinsky model and the superiority of the dynamic models (expecially for the anisotropic version).
Some preliminar a-priori tests on the proposals in [Germano et al., (2014), On the extension of the eddy viscosity model to compressible flows, Physics of Fluids] for LES modeling of compressible variable density flows show that some terms, which are usually neglected in the common density weighting approach for compressible turbulence, are not negligible. Moreover some modifications to the approach of [Germano et al., (2014), On the extension of the eddy viscosity model to compressible flows, Physics of Fluids] are proposed, in order to better match the a-priori tests results.

DEVELOPMENT OF ADVANCED GAS-SURFACE INTERACTION MODELS FOR CHEMICALLY REACTING FLOWS FOR RE-ENTRY CONDITIONS

Georgios Bellas-Chatzigeorgis - Supervisor: Paolo F. Barbante

The design of a thermal protection system for a spaceship during its atmospheric entry is a very challenging task due to the multi-physics phenomena occurring in the shock layer of the space vehicle. These phenomena include, among many, deviation from chemical equilibrium and the interaction between the vehicle's surface and the surrounding gas (heterogeneous catalysis and ablation). The aim of this work is to develop models for catalytic and ablative materials, so that the heat fluxes experienced by a re-entry vehicle can be more accurately predicted, as well as to develop generic tools for their easy implementation in any CFD code. In order to achieve that, a module that provides proper gas-surface interaction (GSI) boundary conditions for any flow solver was developed in the Mutation++ library (www.mutationpp.org) of the von Karman Institute for Fluid Dynamics (VKI). It solves the mass and energy balances at the wall taking into account catalysis and ablation. Two different categories of models are available in the code; a phenomenological so-called gamma model and a finite-rate chemistry model. The first one treats GSI from a macroscopic point of view. It requires only the definition of a single coefficient gamma, which expresses the probability for the surface reaction to occur. Its simplicity has made the gamma model widely used in the study of thermal protection systems. The second approach is a micro-kinetic model and requires the definition of all the elementary processes that occur on the surface. Even though this approach is in principle more accurate than the previous one, these type of models still need to be better understood for aerospace applications. These two types of models are assessed based on two experiments, one for a catalytic flat plate made out of copper and one for a carbonaceous ablative material, both of them performed at the Plasmatron wind tunnel of VKI. Even though copper cannot be directly used as thermal protection material, it is very often considered as a high catalytic reference for the experimental catalytic characterisation of other materials used in real-life re-entry applications. The more we understand how copper behaves catalytically, the smaller the error margins for the actual thermal protection system are. With this aim in mind, an experiment in the Plasmatron facility, which measures the heat fluxes experienced on a copper flat plate exposed in a high temperature jet was simulated using a finite-rate chemistry model for copper. The numerical results with the micro-kinetic model were analysed showing that copper behaves very closely to a fully catalytic material, as expected. Beyond that, some unexpected interesting phenomena were observed for the material. It seems that oxygen has almost twice the catalytic activity compared to nitrogen, because it is more common in the jet and occupies most of the surface free sites. This indicates that there is competition between nitrogen and oxygen on the surface, which shows that obtaining a catalytic recombination probability in a purely nitrogen plasma and applying this value to air, a common practice for aerospace application, is not necessarily a good approach. Furthermore, even though the temperature and pressure along the surface remain constant, the equivalent recombination probability predicted by the finite-rate chemistry model changes along the flat plate. This shows that creating maps of the gamma recombination coefficient as a function of only temperature and pressure, is not sufficient for using the phenomenological catalytic models for predictive applications and instead finiterate methods should be used. As far as the values of gamma compare to experiments, the finite-rate model gives values for oxygen that are almost an order of magnitude higher compared to the experimental ones, an effect which might be associated with the oxidation phenomena of the copper surface. For this reason, further calibration of the model is still required, but the trends and overall behaviour it predicts can be trusted. The ablative properties of low-density ablators, focused on the purely carbonaceous material Carbon Fiber Preform (CBCF) were studied. When it is placed in high enthalpy conditions similar to the one experienced during re-entry, its surface ablates and it gets destroyed. This decomposition is essential for the protection of the rest of the re-entry vehicle. Mainly three processes are important on the surface, carbon oxidation, nitridation and sublimation. For nitridation and sublimation, which are the less significant processes, phenomenological models are available based on the definition of reaction probabilities. For carbon oxidation, apart from the phenomenological approach, a higher fidelity, finite-rate chemistry model (PSMM) is available. The numerical simulations performed, were compared for validation with experimental results. A spherical sample of CBCF was tested in the Plasmatron facility in a high temperature jet. Two test cases were chosen to be simulated, one at low pressure and one at high pressure. The aim of the low pressure test case was to compare the simulations with the experimental results, and a reasonable matching was found. The phenomenological models were giving a good match of the surface temperature and were predicting diffusion limited oxidation of the carbon just as expected. The discrepancies observed in the recession rate could be associated to uncertainties of the free stream experimental conditions and the density of the tested material. The influence of nitrogen catalytic recombination on the surface was also briefly tested and it was observed to increase the surface temperature and mass blowing flux. A simplistic analysis of how a real thermal protection material (carbon fiber reinforced with resin) would behave was performed including the phenomenon of resin pyrolysis. Even at steady state, pyrolysis gases increase the mass blowing flux on the surface, further reducing the wall temperature and further protecting the surface. At transient conditions, pyrolysis can be even more important. In the high pressure test case, the influence of carbon nitridation was assessed, in order to see if pure oxidation is sufficient for the prediction of the material behaviour. It was observed that even though nitridation is less significant, it is still an important process which cannot be neglected. An excellent matching of the phenomenological oxidation model with the finite-rate chemistry one was observed, showing its reliability and predictive capabilities. Since the PSMM model can predict also CO2 recombination on the surface, it was observed that almost no CO2 is produced due to GSI making our assumption to exclude it a valid one. Still its lack of the nitridation processes, makes the model less appealing for practical applications. All the simulations in this work were performed solving the multi-species Navier-Stokes equations in chemical non-equilibrium using the finite volume code Cosmic

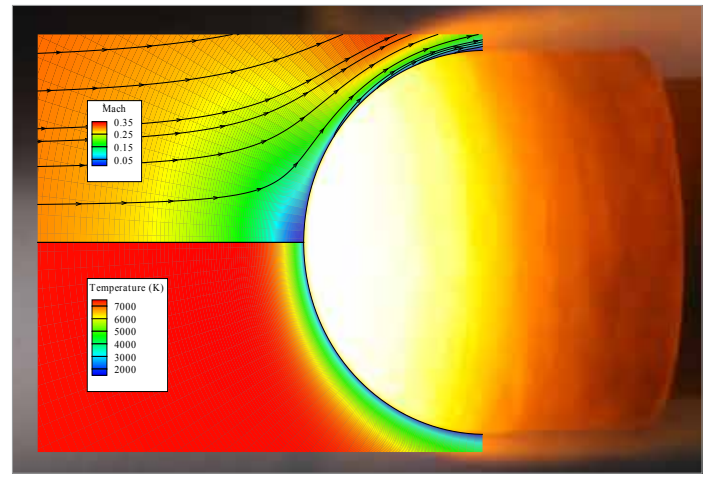

Fig. 1 - Contours around the CBCF sample for the low pressure conditions. Mach number (upper) and Temperature profiles in Kelvin (lower). Image of the experiment courtesy of Bernd Helber.

THE PROBLEM OF RANKING PLAYERS: FROM SEMIVALUES TO GAMES WITH ABSTENTION

Giulia Bernardi - Advisor: Roberto Lucchetti

In many real-life situations that are studied in voting theory or, more generally, in social choice theory, it is necessary to rank individuals or objects. For instance this problem might arise when it is necessary to have a unifying preference profile over employees in a working group, or to evaluate the power of each voter in a decision making procedure or to give different marks to some students after a workshop...
A classical approach to this problem is provided by cooperative game theory; in particular, voting situations can be modelled as simple games, a particular family of games with transferable utility and power indices, that are values restricted to the family of simple games, provide a natural ranking among players. From this classical approach many different questions may arise: is the use of a cooperative solution concept legitimate in the context of simple games? Are there any solution concepts more suitable than others? Why? Is it possible to use power indices also with different models of games, for instance in order to take into account the possibility of abstention in a voting procedure? Which indices can be generalized and what aspects of the decision process do they represent? Which different approach can be studied, besides cooperative game theory, to solve this problem?
In this thesis we analyse this topic and try to provide answers to some of these questions.
We begin our work with some new contributions to the classical cooperative game theory. Among the different solution concepts for coalitional games, the Shapley and the Banzhaf values are two of the most known and used, in particular as power indices for simple games. Both values are actually semivalues, a family of solution concepts that satisfy the linearity, anonymity and null player properties. First of all we present a theorem to characterize all semivalues by means of their behaviour on unanimity games and establish a connection between semivalues and completely monotonic sequences. Secondly, we provide a new formula to compute the Shapley value due to a different interpretation of the value, proposed by Felsenthal and Machover that is particularly interesting in the voting context.
In the central part of the thesis we examine the model of games with abstention and of multichoice games. Games with abstention are a generalization of the classical model of simple games, in which players are assumed to vote either yes or no, in order to take into account also the possibility of abstention. We generalize to the set of games with abstention some of the properties that have been provided in literature to characterize the corresponding power indices for simple games. Thus, we provide two different axiomatizations for the Banzhaf index for games with abstention and a characterization of the Shapley-Shubik index for games with abstention. We then focus on multichoice cooperative games, a generalization of the classical model of cooperative games to describe situations in which players can have different levels of participation in the cooperation (or vote among different alternatives). We analyse and compare the different models studied in literature and then define a new value for multichoice cooperative games with in the spirit of the Shapley value. The value we introduce is deduced from the Shapley-Shubik index for voting games, and extended to the class of multichoice games. As a consequence of our result, we provide an explicit formula to compute the Shapley-Shubik index for games with abstention.
In the last part of the thesis, we consider the problem of ranking players from a new perspective. We remove the structure of coalitional game and suppose that only an ordinal ranking among players is available. A similar situation can not be represented by a coalitional games and power indices can not help, since, in general, changing power index can change the ranking among players. Moreover, in many situations it is possible to have an ordinal ranking over groups, without a specific characteristic function to have a cardinal comparisons among the groups. In these situations to select a random characteristic function to represent the ordinal relation would be a bad idea, since it is well known that the same ordering on the subsets, when described by different utility functions, can provide different ranking among players. We present two functions that associate a ranking over players, given a preference profile over the subsets formed by those players. We also provide an axiomatic characterization of these two functions.
There are different directions to further develop this work. First of all, it would be interesting to find real life examples and applications for all the ideas presented in this thesis. An interesting line of application would be also to establish the connections between a ranking with power indices and with the functions we introduce in the last part. Secondly, a natural extension of our work is to provide other characterizations for power indices for games with abstention or define other values in the family of multichoice games. To reinforce the use of these indices as solution concepts, more properties can be studied and other mathematical aspects can be analysed. Lastly, the more general approach to the ranking problem given an ordinal relation among coalitions seems to be quite innovative and promising. It is clear that other properties can be defined to capture different ideas to extend the range of application of the results presented in our work.

MODELING AND COMPUTATIONAL ASPECTS OF DEPENDENT COMPLETELY RANDOM MEASURES IN BAYESIAN NONPARAMETRIC STATISTICS

Ilaria Bianchini - Advisor: Alessandra Guglielmi
Co-Advisor: Raffaele Argiento

Since many scientific problems become more and more complex, models and computational methods for data analysis require more and more sophisticated statistical tools. In this sense, Bayesian nonparametric (BNP) statistics offers a framework for the development of flexible models with a broad-spectrum application. This thesis presents advances in BNP models for dealing with dependence on covariates or time from a modelling perspective; new models involving completely random measures are introduced, together with corresponding MCMC algorithms to perform posterior inference. Along the thesis, we tackle various applications where the issue of dependence arises, such as healthcare and image analysis. The building block that recurs in this work is given by completely random measures, tractable mathematical objects that might be employed for building probability random measures and also for modeling latent structures in the observations. Starting from the definition and the main properties of completely random measures, we present different modelling strategies for performing clustering and density estimation through mixture models, as well as latent feature estimation. In order to create a coherent framework for the development of the models presented in the dissertation, we include an initial chapter presenting literature review and basic concepts related to completely random measures; its reading is useful to understand the main motivations of this work. Then, we deal with nonparametric mixture models whose mixing distribution belongs to the class of normalized homogeneous completely random measures. We tackle the issue related to the infinite dimensionality of the parameter by proposing a truncation, discarding the weights of the unnormalized measure smaller than a threshold. We provide some theoretical properties about the approximation, as convergence and posterior characterization. A general conditional blocked Gibbs sampler is devised, in order to sample from the posterior of the model. Illustrative examples, including also covariate information in the location points of the random measure, show the effectiveness of the method. The following chapter illustrates the problem of predicting the next donation time for a blood donor. We consider data on blood donations provided by Milan department of AVIS (Italian Volunteer Blood-donors Association). With the goal of characterizing behaviors of donors, we analyze gap times between consecutive blood donations. In particular, we take into account population heterogeneity via model based clustering. The main contribution is given by the introduction, in an accelerated failure time model with a skew normal likelihood, of a prior on the random partition that explicitly accounts for covariate information. In particular, we consider a prior for the random partition of the form "product partition" and a term that takes into account the distance between covariates in a cluster. Another chapter deals, differently from the others, with finite mixture models, with a random number of components. Typically, when using mixture models, finite or infinite, overestimating the number of groups is quite common; hence, there is a need for models inducing We explore a class of determinantal point process (DPP) mixture models defined via spectral representation, focusing on a power exponential spectral density. In the second part of the chapter we generalize our model to account for the presence of covariates, both in the likelihood as linear regression and in the weights of the mixture by means of a mixture of experts approach. This yields a trade-off between repulsiveness of locations in the mixtures and attraction among subjects with similar covariates. This project has been developed during my stay at Pontificia Universidad Catolica de Chile, under the supervision of Prof. Fernando A. Quintana. The final chapter aims at developing a new way of flexibly modeling series of completely random measures that exhibit some temporal dependence. These processes might be fruitful in real life applications, such as latent feature model for the identification of features in images or Poisson factor analysis for topic modelling. In order to achieve a convenient mathematical tractability, namely to be able to define a flexible transition kernel for the process, we consider the large class of exponential family of completely random measures. This leads to a simple description of the process which has an AR(1)-type structure and offers a framework for generalizations to more complicated forms of time-dependence. This project was started during my stay at University of Kent, under the supervision of Prof. Jim Griffin. Each chapter includes details on the implementation of the MCMC methods employed in posterior inference. Most of the statistical analyses have been carried out using R and C++.

MOOCS AND ACTIVE LEARNING IN MATHEMATICS: EDUCATIONAL AND MATHEMATICAL MODELLING FOR CLASSROOM PRACTICES

Domenico Brunetto – Advisor: Giulio Magli

Recently, MOOCs and Flipped Classroom practices have attracted a good deal of attention for several reasons. Flipped Classroom allows to improve the student's engagement, while MOOCs provide a high quality education standard reaching a large number of students. Many issues about these two innovative pedagogical practices are still open. This work deals with some of these open problems which merge together mathematics education and mathematical modelling of social dynamics. More precisely, we study the students and teachers' attitudes towards MOOCs and Flipped Classroom: on one hand we identify some possible students' difficulties when deal with MOOC, providing three main students' profiles. On the other hand we study and design different scenarios of Flipped Classroom carried out by teachers and tutors who use instructional videos in their hybrid classroom. One of the main aspect that emerges is that Flipped Classroom facilitates group work activities in classroom because during such activities the students act, interact and communicate much more than in usual frontal lessons settings. In such a context, it is crucial to understand what are the variables which govern the student dynamics and even what is the role of the teacher during a small group activity. Thus, we designed and validate an educational model which allows to describe the students' dynamics. Such a model is based on two affective dimensions called 'I can' and 'You can' which describe the self-confidence of students and the perceived competence of their mates respectively.

Moreover, on the path of recent mathematical model of multi-agents dynamics and opinion dynamics, with the 'I can - You can' framework we propose a mathematical model for small group work activities which allows to trace the evolution of students' opinion, which is their answer to a mathematical task, and design an optimal strategy for the teacher who has a crucial role in group work activities. To this end we identify some common goals that teachers have towards their students and set a control problem of multi-agent systems, when the agents are students who are asked to solve a mathematical task working in small group. The leader of the group is represented by the teacher who is allowed to make mathematical intervention during the students' activity with the purpose of improving students' performance. Hence, the teacher opinion is the control variable of the dynamics which evolves to achieve some goals abstracted by an object function. However teachers' cognitive interventions, e.g. hints, are just one of the possible teachers' actions, indeed they may also act social interventions, such as silencing a student and prompting another to talk, a behaviour which is more effective than cognitive in certain circumstances. In order to implement such aspects, we consider a simpler problem which goes towards this direction introducing a mathematical model for the evolution of students' skill, that describes pairwise interactions and how students can improve their mathematical skill communicating and working in couple. In this setting the teachers is allowed to modify students interactions changing the couples. In this setting we design an optimal control problem to allow teachers to maximise the average skills of the class, and identify a class of optimal strategy.

To sum up, this work focuses on some aspects of students' learning to provide teachers with tools which facilitate the carrying out of innovative practices both on-line (e.g. MOOCs) and in presence (e.g. Flipped Classroom), and aid the control of group work activities thank to the proposed educational and mathematical models.

LARGE-EDDY SIMULATION OF TURBULENT REACTING FLOWS FOR INDUSTRIAL APPLICATIONS

Alessandro Della Rocca - Supervisor: Prof. Luca Bonaventura

The traditional engineering design approach relies on the Reynolds averaged Navier-Stokes (RANS) method, whose generality and predictive ability are usually limited considering the very different flows which can arise in industrial applications. Furthermore, when chemical reactions must also be accounted for, RANS methodology cannot easily capture the turbulence-chemistry interactions and its predictions must be interpreted with care. For this purpose, large-eddy simulation (LES) is an interesting alternative, providing valuable insight into the complex phenomenology of turbulent flows and, in particular, into the scale interactions between turbulence and chemical reactions typically occurring in reactive flow devices.

Since the adoption of the LES technique within a standard engineering cycle is by no means an easy task, a large portion of the activities was devoted to the relatively simple case of incompressible flow. Furthermore, since very efficient compressible pressure correction methods can be devised starting from incompressible methods, the analysis of the incompressible solvers can provide valuable insight into the stabilization techniques required for colocated finite volume schemes adopted in industrial simulation codes. In particular, all the developments pursued in this work were laid out as extensions to the open source library OpenFOAM.

Monotonicity preserving time integrators

In this framework, the first outcome of this research was the analysis of time integrators with monotonicity preserving properties. One-step time discretization methods were analyzed using the nonlinear analysis tools developed for SSP (strong stability preserving) time discretizations. Several well-known time integrators were compared together with the TR-BDF2 method, and their monotonicity, strong stability and positivity properties were analyzed, interpreting them in the framework of absolute monotonicity. In order to achieve unconditional monotonicity, hybrid variants of TR-BDF2 were proposed, that reduce the formal order of accuracy, while keeping the native L-stability property which is useful for the application to stiff problems.

Analysis of cell centered finite volume schemes

Following some recent developments in the interpretation of finite volume schemes as weak formulations in suitable discrete spaces, also in the light of the current development of the gradient schemes, an analysis was proposed for an isotropic diffusion problem operator on non-orthogonal meshes. This operator is currently implemented in a variety of finite volume codes, providing good results on non-orthogonal meshes of industrial quality, but to the author's knowledge its numerical analysis was never attempted before. By relying on the analysis tools recently introduced for finite volume schemes, the convergence analysis for this specific diffusion scheme was carried out.

Low-dissipative projection methods

By using the cell centered diffusion scheme, a stabilized projection method for colocated finite volume discretizations was analyzed. This method has previously been shown to be well suited to LES at large Reynolds numbers, due to its limited artificial dissipation and robustness. By identification of the similarities with a coupled discretization proposed for orthogonal meshes, after a proper reformulation of the stabilization term with the results for the diffusion operator, a convergence analysis was outlined. Interestingly, it turns out that the empirically proposed methodology relies on a Brezzi-Pitkäranta stabilization technique, in which a consistent stabilization term is added to the divergence constraint to circumvent the inf-sup stability condition, thus allowing the use of colocated pressure and velocity variables. Finally, global and local kinetic energy inequalities allowed to explain the good performance of the projection method in the context of LES, where minimal kinetic energy dissipation is a key issue to allow different subgrid models to be active, without their dissipative action being overwhelmed by the artificial damping from the use of flux-limiters or other extra-dissipative stabilizations.

Pressure-correction for compressible and reactive flows

Successively, the same stabilized pressure-correction technique was extended to the cases of compressible and reactive flows, where a non-iterative scheme was devised. This pressure-implicit strategy is able to limit the thermodynamic drift of the solution within the tolerance bounds of the linear solver. In the limit of low Mach number and arbitrarily high Reynolds number, this variable density pressure-correction method was shown to limit the artificial kinetic energy dissipation below the theoretical power law exponent provided by the eddy-damping quasi-normal Markovian (EDQNM) closure, hence allowing to identify it as a good candidate for performing LES of turbulent flows in realistic applications.

LES applications

Several LES cases complemented this work, ranging from incompressible, to compressible and finally to reactive flows. Particular attention was devoted to the post-processing techniques able to extract the vast amount of information provided from LES runs. Finally, the application of the proposed methods to reactive flow configurations of industrial interest was demonstrated. The detailed representation of the complex effects involved allows to classify the numerical techniques here developed as effective tools to analyze the rich phenomenology occurring in turbulent reactive flows of industrial interest.

This research work has been developed as an Executive PhD Programme between Tenova S.p.A. and the MOX – Modeling and Scientific Computing, Politecnico di Milano.

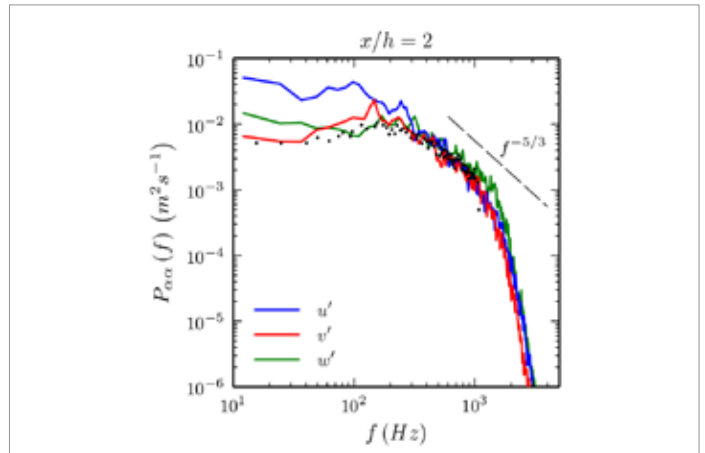

Fig. 1 - Velocity spectra in the shear layer from LES of an isothermal backward step, with black dots representing the experimental v' spectrum.

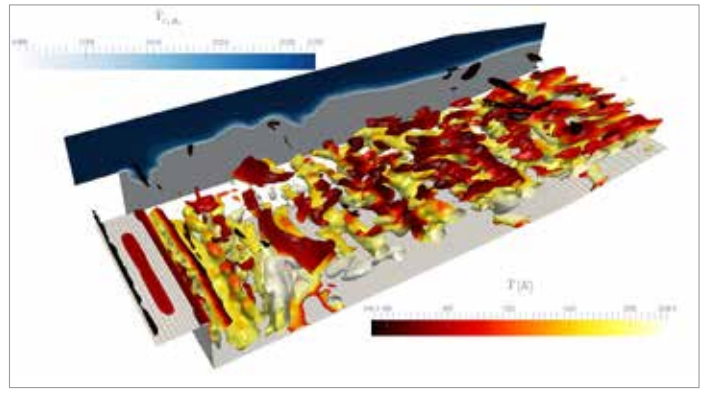

Fig. 2 - Coherent vortices in a reacting backward step colored by temperature, with contours of propane mass fraction shown on the section plane.

CONTRIBUTIONS TO QUATERNIONIC OPERATOR THEORY AND APPLICATIONS

Jonathan Gantner - Supervisor: Prof. Fabrizio Colombo

This thesis generalises classical techniques for complex linear operators to quaternionic linear operators and explores their possible applications. The following results have been obtained:

1) The S-functional calculus, the generalisation of the holomorphic Riesz-Dunford functional calculus, is defined for unbounded operators directly via an integral formula. This extends the class of admissible operators as compared to the existing approaches in the literature. Furthermore its properties, in particular the generation of Riesz projectors and the compatibility with polynomials are studied in detail.

2) The Phillips functional calculus for infinitesimal generators of strongly continuous groups, which is based on the Laplace-Stieltjes transform, is extended to the quaternionic setting.

3) The H-Infinity-functional calculus is introduced in its full generality (a version making stronger assumptions on the operator has already been studied in the literature). In particular precise proofs of the spectral mapping theorem and the composition rule of this functional calculus are developed.

4) Using the above techniques, three different approaches for defining fractional powers of operators are extended to the quaternionic setting. One of them is an application of the previously studied H-Infinity-functional calculus. It allows to deduce the famous Balakrishnan-formula, which is essential for possible applications in the field of fractional diffusion mentioned below.

5) The minimal structure necessary for developing quaternionic operator theory is identified. Usually quaternionic operator theory is, for technical reasons, developed under the assumption that vectors can be multiplied with quaternionic scalars from both sides. A quaternionic right linear operator is however only associated with the right linear structure on the space, that is with the multiplication of vectors with scalars from the right. We show that the essential concepts and functional calculi of quaternionic operator theory do actually not depend on the left multiplication. They can be expressed only in terms of the right linear structure of the space. As a byproduct we obtain that the quaternionic theory is consistent with the complex linear theory under each imbedding of the complex numbers into the quaternions.

6) A concise theory of spectral integration is developed. It unifies the different existing approaches and removes some of their problems (in particular the requirement to randomly introduce structures that are not determined by any of the given mathematical objects). Furthermore, it also extends smoothly to the Banach space setting and has a clear interpretation in terms of the right linear structure of the space.

7) Based on the above theory of spectral integration, the theory of bounded quaternionic linear spectral operators is developed. We study the spectral decomposition and the canonical decomposition of such operators and their behaviour under the S-functional calculus.

8) We develop the spectral theory of the nabla operator – the quaternionification of the gradient. This allows us to deduce the fractional heat equation by applying quaternionic techniques to the gradient operator. The used techniques provide a tool for deducing new fractional evolution equations in the future. In particular these equations might be derived from Fourier's laws with non-constant thermal conductivity coefficients, which could model non-homogenous materials.

9) Quaternionic operators were originally studied because of their applications in quaternionic quantum mechanics. This formulation of quantum mechanics seemed to be not equivalent to the usual complex formulation. We conjecture that this is not correct and provide an idea how quaternionic quantum systems can be considered simply as the quaternionification of complex quantum systems so that both formulations turn out to be equivalent. For relativistic elementary systems, we show that the reduction of the quaternionic to a complex system is always possible.

MATHEMATICAL ANALYSIS OF SOME DIFFUSE INTERFACE MODELS FOR BINARY FLUIDS

Andrea Giorgini - Supervisor: Maurizio Grasselli

The mathematical description of the motion of immiscible fluids is a longstanding problem in Fluid Dynamics starting at the beginning of the 19th century. Since then, a vast literature has been devoted to finding macroscopic models which comply the physical laws and lead to efficient numerical calculations. The mutual interaction between the interface and the surrounding fluid is a complex phenomenon, depending also on surface tension effects, topological changes, viscosity ratios, temperature gradients and imposed flow at the boundary. The main common goal among these investigations has been understanding the nature of the interface separating the binary mixture. In the classical attempt, the interface is assumed to be an evolving in time surface with zero thickness, across which physical quantities must satisfy suitable boundary conditions. Instead, a more recent and powerful approach treats the interface as a narrow zone with finite thickness. This is the so-called diffuse interface method. In this case, the interface evolution is described through the concentration variable which is uniform in bulk phases and varies steeply but continuously across the interface.

The subject of this dissertation is the mathematical analysis of some diffuse interface models describing the motion of two globally immiscible, incompressible and viscous fluids. Depending on the interplay between inertial and viscous forces, we consider two classes of equations governing the velocity field, known in the literature as:

- the model H,
- the Hele-Shaw approximation.

In such models a crucial role is played by the choice of the free energy. In the first part of this contribution we study *local* models originating from the Ginzburg-Landau free energy. In the second part we consider *nonlocal* models related to the Helmholtz free energy, taking more general long-range interactions into account. Both of them penalize concentration variations. This twofold choice is motivated by the classical literature and leads to different Cahn-Hilliard type equations for the order parameter.

The common denominator throughout this investigation is the presence of the physically relevant free energy density which consists of a logarithmic function. The main advantage is the possibility to show the existence of *physical* solutions, meaning that the order parameter (i.e. the difference of concentrations) is forced to take physically admissible values. Thus, the order parameter maintains its original meaning. On the other hand, the study of a logarithmic potential requires non classical mathematical methods. Indeed, by virtue of the different behaviour between the logarithmic potential and its derivatives close to the singular points, high order estimates involving the order parameter are hard to get.

The main results herein concern the uniqueness and regularity of weak solutions as well as the existence of strong solutions. Particular attention is given to the so-called *separation property.* The latter means that, if the initial datum is not a pure phase, then the order parameter eventually stays away from the pure states with a uniform in time displacement. In the two dimensional setting, we present two different methods in order to handle local or nonlocal models leading to the *instantaneous* separation property, namely the separation occurs for any positive time with a parameter depending (explicitly) only on the initial energy value and the total mass of the initial datum. As an interesting application of the regularity properties, we discuss the asymptotic behaviour of solutions.

Let us now describe a summary of the main results contained in this thesis. First, the Navier-Stokes-Cahn-Hilliard-Oono system is studied in dimension two. This model is a generalization of the classical model H accounting for (reversible) chemical reactions. In the matched viscosities case, we show the uniqueness and the instantaneous regularization in time of weak solutions as well as the validity of the separation property. The latter has been obtained by combining high order Sobolev estimates with a regularity theory for an elliptic problem with logarithmic nonlinear term, for which the Trudinger-Moser inequality plays an essential role. The same results also goes for the Navier-Stokes-Cahn-Hilliard system.

The Hele-Shaw-Cahn-Hilliard system with matched viscosities is analyzed in both two and three dimensions. We first prove the existence of a global weak solution. Then, in dimension two we demonstrate the uniqueness of weak solutions, their regularity propagation in time and the separation property. Instead, in dimension three we show the global existence of strong solutions provided that the initial datum is regular enough and sufficiently close to any local minimizer of the Gindzburg-Landau free energy.

We also investigate the Brinkman-Cahn-Hilliard system in dimension two. In particular, we address the unmatched viscosities case. We show the existence and uniqueness of weak solutions, their regularity properties and the separation property.

Next, we study the nonlocal model H. First, we provide a comprehensive analysis of the nonlocal Cahn-Hilliard equation. In particular, we introduce a novel technique for the separation property which differs from the one employed in the local case. The proposed argument is based on an Alikakos-Moser iteration argument combined with the Trudinger-Moser inequality. Then, the analysis has been extended to the nonlocal Navier-Stokes-Cahn-Hilliard system in dimension two.

Finally, the nonlocal Hele-Shaw-Cahn-Hilliard system is considered in two and three space dimensions. In both cases we show existence and uniqueness of weak solutions, existence of strong solutions and their regularity properties.

NON-PARAMETRIC CLASSIFICATION AND REGRESSION TECHNIQUES FOR THE CHARACTERISATION OF THE DISEASE SUBTYPES AND THE ASSESSMENT OF THE TEMPORAL EVOLUTION OF IMAGE-BASED BIOMARKERS

Riccardo Pascuzzo - Advisor: Prof. Simone Vantini
Co-Advisor: Dr. Aymeric Stamm

The concept of biomarker has evolved during time, from the inclusion of only biological molecules, to the recently updated definition given by the Food and Drug Administration in collaboration with the National Institutes of Health of the US: "a defined characteristic that is measured as an indicator of normal biological processes, pathogenic processes, or responses to an exposure or intervention, including therapeutic interventions. Molecular, histologic, radiographic, or physiologic characteristics are types of biomarkers". Thus, a biomarker can originate from different modalities (e.g., biological samples, medical images), be qualitatively or quantitatively measured, and used for several purposes (e.g. diagnosis, prognosis, treatment assessment). In addition, according to the aim of the study, the specific research design guides how to collect biomarker measurements (e.g., cross-sectional study, longitudinal study). From the last decades, all these types of biomarker have become more and more commonly adopted in the clinical practice and research, and this has also stimulated in the statistical science an increasing interest in the development of new and advanced tools to properly handle the structure of each dataset. In this thesis, we present some non-parametric statistical models and methods that have been developed and adapted to deal with different types of biomarker.
In particular, the first part describes the assessment of the respiratory function evolution of Duchenne Muscular Dystrophy (DMD) patients from childhood to adulthood. DMD is an X-linked myopathy resulting in progressive wasting of locomotor and respiratory muscles, with consequent chronic ventilatory failure that is the main cause of death. In these patients it is extremely important, therefore, to measure lung function and respiratory muscle action in order to monitor the progression of the disease, to identify early signs of ventilatory insufficiency, to plan optimal interventions for improving the quality of life and to quantify the effects of novel gene-modifying strategies and pharmacological therapies. A dataset that comprises spirometric and opto-eletronic plethysmographic biomarker measurements is collected longitudinally at different time points for each subject. We deal with this irregular and subject-specific timing by adopting a regression model based on natural cubic splines with mixed effects, that allows to identify specific time points of respiratory impairment during disease progression, and to investigate possible effects of scoliosis, nocturnal non-invasive mechanical ventilation and steroid therapy.
In the second part, we characterise the subtypes of the most common form of prion disease, the sporadic Creutzfeldt-Jakob disease (sCJD), with imaging biomarkers collected in a cross-sectional design. The clinical diagnosis of prion diseases is compounded by the diversity of their phenotypes. Sporadic CJD alone comprises five distinct clinical and histopathological phenotypes or subtypes, which are associated with distinctive pairings of the genotypes at the methionine (M) and valine (V) polymorphic codon 129 (MM, MV, and VV) with the disease-associated prion protein (PrPD) types 1 and 2. The five histopathological phenotypes are characterised by the anatomical distribution and/or type of the spongiform change, distribution and shape of PrPD deposits and severity of astrogliosis and loss of neurons. The only way to have a confirmation of the sCJD subtype is by tissue examination either at biopsy or, more definitely, at autopsy. Establishing in vivo biomarkers that could predict sCJD subtype would thus be relevant for patient management and clinical trials. Magnetic resonance imaging (MRI) has recently gained a high degree of reliability in the diagnosis of prion diseases with the introduction of diffusion-weighted imaging (DWI) in the diagnostic criteria. MRI remains the test of choice at the initial clinical evaluation when the diagnosis is open and requires timely identification of treatable conditions. Moreover, MRI is an ideal candidate for providing in vivo biomarkers, because it evaluates the whole brain rather than just a few small specimens, as neuropathology does. Thus, MRI has great potential to be established as the method of choice to assess regional extension of brain lesions in the early stage of prion diseases. Among different MRI modalities, diffusion MRI (dMRI) has been shown the most sensitive to peculiar brain microstructural alterations such as spongiosis and PrPD deposition. Diffusion MRI measures microstructure by using the random walk of water molecules as a probe. Entrapment of water within vacuoles and/or slowing of water diffusivity in the interstitium enriched with prion protein aggregates is likely responsible for the signal hyperintensity detected with DWI in affected regions of the brain. In our work, variations of the MRI signal were rated and compared over 12 brain anatomical regions in a cohort of more than 300 patients in which the histological, genetic and PrPD examinations allowed for the definitive diagnoses of prion diseases as for form, type and subtype of prion disease.
The MRI rating profiles generated with this procedure revealed significant differences which enable the diagnosis of individuals CJD subtypes, classifying the sCJD patients into their most compatible subtype according to their biomarker measurements, with a classification tree-based method.
In the third part, we describe the disease progression in each sCJD subtype by finding the sequence of brain regions that become detectably hyperintense in DWI. Based on the results of the previous part, we have seen that each subtype has distinctive features that should be always considered when analysing the whole spectrum of sCJD. Thus, to move further and explore the disease progression in sCJD with the use of imaging biomarkers such as signal abnormalities on DWI, it is clear that each sCJD suptype has to be considered separately, since it is likely that in different strains the propagation could be different. Recent studies have dealt with the assessment of the disease evolution in sCJD using DWI signal abnormalities as biomarkers of the disease. However, they did not take into account the subtype classification in the analysis, nor provided a real staging of the disease based on the signal abnormalities. Therefore, to go beyond these preliminary studies and to overcome the missing temporal dependency that is intrinsic in any cross-sectional design, we adapt the recently introduced event-based model (EBM), a data-driven statistical model that assess the disease evolution in terms of its characterising biomarkers, without relying on a longitudinal dataset. Our results of the EBM provide for the first time data-driven models of sCJD progression within each pure subtype: the characteristic orderings are based on a cross-sectional dataset and their longitudinal consistency has been validated comparing the stages at follow-ups with the baseline.
Finally, we outline a work aimed at developing a function-on-function regression model that can deal with temporal dependent biomarkers (e.g., from functional magnetic resonance imaging data). We model a functional response in terms of several functional covariates, and we propose a permutation test to identify sub-regions that exhibit similar statistical differences. Moreover, in case of multiple tests performed at different locations in the same domain (e.g., the voxels of the brain MR image), we extend to a three-dimensional setting the closure multiplicity adjustment method to control the family-wise error rate of the proposed procedure.

UNFITTED NUMERICAL METHODS FOR FLUID-STRUCTURE INTERACTION ARISING BETWEEN AN INCOMPRESSIBLE FLUID AND AN IMMERSED THICK STRUCTURE

Stefano Zonca - Supervisors: Prof. Christian Vergara, Prof. Luca Formaggia

The interaction between an incompressible fluid and a flexible immersed structure may be significant in many engineering applications, for example in aeronautic engineering to study the response of the air on the aircraft, in civil engineering to understand how the wind affects the stability and produces vibrations on bridges, towers and suspended cables, in energy engineering to study the modeling of wind-turbines, in sport engineering to investigate the impact of the waves over a rowing boat, and so on. The employment of fluid-structure interaction (FSI) models is not limited to engineering applications. In fact the modeling of deformable solids interacting with fluids is also applied in biomedical applications, for instance in haemodynamics to study the stresses exerted by blood flow to the vessel wall, to analyze how the blood interacts with the leaflets of a heart valve or to study the blood pressure to the retinal vessels walls, and in many other applications such as phonation, drug delivery in arteries and red blood cell aggregation, just to cite a few of them. It is easy to understand that, both from the modeling and computational point of view, FSI problems are very challenging since they require to consider and combine more than one physical aspect, resulting in a multiphysics problem. In case of soft materials, the deformation of the structure may become very large resulting in a very challenging situation. Moreover, in some applications the thickness of the structure is small with respect to the characteristic size of the domain, leading to a complex geometry. In some cases a 2D or 1D geometric reduced order model is enough to describe the behaviour with an adequate accuracy. However in other cases it may be interesting to study a geometric full three-dimensional model also for the structure, even though the structure is thin. For example, in the simulation of the heart valves, an interesting application is the interaction between the blood and the leaflets of the valve. The leaflets are thin flexible tissues that regulate blood flow between the chambers of the heart. They play a key role since they have a major influence on the blood fluid dynamics in the proximity of the valve. However, it is not only important to predict their movement, but also to accurately evaluate their internal stresses, which can be recovered only by means of a full geometric model.

The purpose of this thesis is to propose innovative numerical methods for the simulation of FSI problems in the case of an immersed structure that interacts with an incompressible fluid. In particular, we address the case of structures represented via a full three-dimensional model, though its thickness in smaller than its characteristic size, and that undergo large displacements with the final aim to simulate the dynamics of heart valves. To this aim, we consider unfitted methods that, differently from the standard Finite Element Method, rely on the fact that the computational domains are unfitted, i.e. the mesh for the fluid and the solid are generated independently of one another so that they are not conforming at the fluid-structure interface. Moreover, we consider the case of a solid mesh that overlaps the fluid one. These features are very useful when the displacement of the structure is very large, since they avoid the fluid mesh to follow the structure one, to maintain the matching between them, and to remesh the fluid grid when the deformation is too large. We propose two new unfitted methods: the first one is based on the Extended Finite Element Method, while the second one is based on a Discontinuous Galerkin method on polygonal grids. Their peculiarity is that, due to the overlapping of the fluid and structure meshes, this generates polyhedral elements in the fluid mesh that require to be properly managed. The thesis starts by presenting the state-of-the-art regarding the FSI problem by focusing on the methodological point of view. We report a brief overview about the numerical methods that have been employed in the literature to tackle this kind of problems. We highlight the advantages and the drawbacks of these methods, especially in the case of i) a full three-dimensional model for the immersed structure ii) that undergoes large displacements. By considering these two key points, we propose two possible approaches, based on two recent methodologies, to numerically solve the considered fluid-structure interaction problems: i) the eXtended Finite Element Method (XFEM) coupled with a Discontinuous Galerkin (DG) approach and ii) the Polygonal Discontinuous Galerkin (PolyDG) method. The XFEM/DG method allows to describe a discontinuous solution within a fluid element that is split by the structure. The idea of XFEM is to double the degrees of freedom to enrich the numerical approximation of the solution, by considering the classical shape functions defined on the tetrahedron of the Finite Element Method. The DG approach is used to couple the fluid and structure problems at the fluid-structure interface. We first apply the method to the Poisson problem and then to the FSI one, both in the case of a fixed and moving structure. We describe the major technical issues with a close attention to the implementation aspects, and we assess the optimality of the method by performing several 3D simulations and by validating the numerical results with respect to analytical solutions or the classical Finite Element Method. The PolyDG method allows to directly treat the resulting polygonal elements that appear in the fluid mesh, by generating suitable shape functions and degrees of freedom on the polygon itself. We show some numerical results for a fluid-structure interaction problem in the case of an immersed and moving structure. Finally, we employ the XFEM/DG approach to the case of a specific biomedical application, i.e. a 3D heart valve under the conditions of high Reynolds numbers with moving leaflets. To conclude, we present a critical discussion of the results and possible further developments of this work. The numerical results highlight the effectiveness of the proposed methods in solving fluid-structure interaction problems in the case of moving immersed structure.

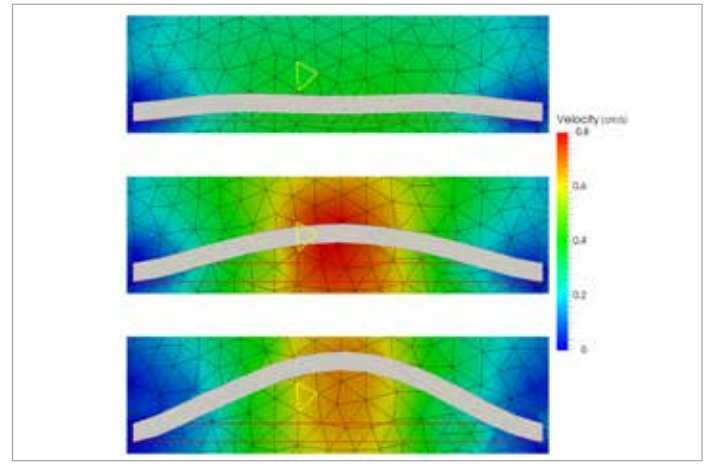

Fig. 1 - Evolution of an immersed structure. FSI simulation obtained with the PolyDG method.

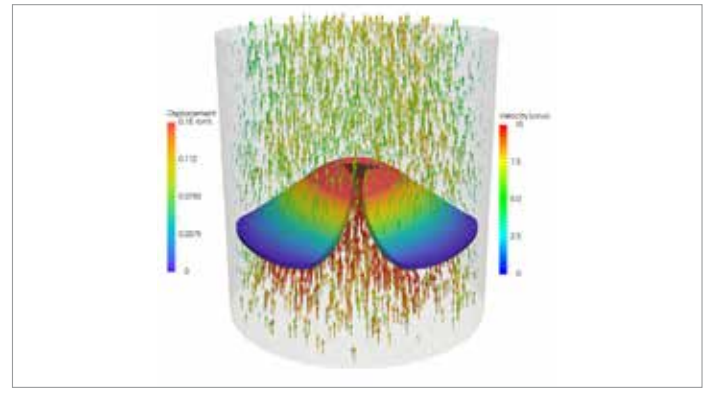

Fig. 2 - FSI simulation of an ideal valve obtained with the XFEM/DG method.