



DOCTORAL PROGRAM IN MATHEMATICAL MODELS AND METHODS IN ENGINEERING

Chair:
Prof. Paolo Biscari

Equations are everywhere! Between the atmosphere and the wing of a spaceship, in the blood flowing in an artery, on the demarcation line between ice and water at the poles, in the motion of the tides, in the charge density of a semiconductor, in the compression algorithms of a signal sending images from outer space. Such equations represent real problems. The Mathematical Engineer can see and understand the nature of these equations, and can develop models in order to understand their relevant qualities and solve real problems.

This PhD program aims at training young researchers by providing them with a strong mathematical background and with ability to apply their knowledge to the solution of real-world problems that arise in various areas of science, technology, industry, finance, management, whenever advanced methods are required in analysis, design, planning, decision and control activities. PhD students carry out their research both in the development of new mathematical methods and in the implementation and improvement of advanced techniques in connection with specific contexts and applications.

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

The overall activity of the PhD students can be quantified in 180 credits. The PhD program has a duration of three years. Activity can be classified into:

introductory courses (no minimum number of credits required); main courses (at least 30 credits); specialized research training, including seminars, tutoring activity, participation to workshops/conferences, and scientific publications (at least 30 credits); development of a doctoral thesis (at least 90 credits).

At the end of each academic year, the PhD students report to the Faculty about their activity. The students report about attendance of courses and exams (and the corresponding grades), participation in various scientific activities (seminars, conferences, summer schools etc.),

planning and intermediate results on their research project and preparation of the PhD thesis, and any other relevant activity. At the annual meeting the students also receive a grade by the Faculty. A negative grade may entail repetition of the current year of doctoral study (with suspension of the grant, if any) or exclusion from the PhD program, depending on the Faculty's decision. Mobility of PhD students to other institutions is strongly encouraged and financial support is provided to this purpose.

Among others, let us mention some typical types of professional skills and possible occupations of the graduated Doctors: analytic and numerical treatment of differential models for physical and industrial problems, quantitative methods in finance and risk management, operations research and optimisation, statistical modelling and data analysis.

Placement of graduated Doctors is expected in the following positions: research and development divisions of businesses, businesses involved in innovative design activities, financial institutions such as banks or insurance companies, public or private research centres, public and/or governmental agencies for social, economical, scientific study, planning or evaluation, Universities.

Since the PhD program in Mathematical Models and Methods in Engineering (formerly, Mathematical Engineering) has been active since the year 2001, we expect that a larger number of institutions and businesses will soon become more and more aware of the professional skills and expertise of graduated doctors.

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NUMERICAL MODELLING OF FLOWS IN FRACTURED POROUS MEDIA BY THE XFEM METHOD

Alessio Fumagalli

The objective of this thesis is the development and the implementation of advanced models for the simulation of two phase flows in heterogeneous porous medium and in particular in the presence of fractures.

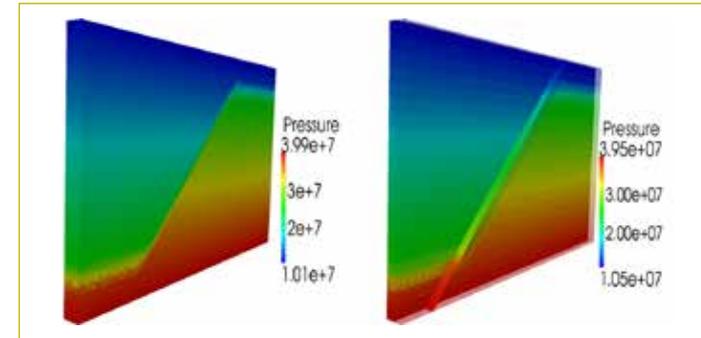
In the last few decades oil industries have resorted more and more to mathematical and numerical modelling to help locating new hydrocarbon reservoirs and to exploit the existing ones at their best. The exploration of hydrocarbons is a very expensive and risky operation, with a chance of success ranging from 30 to 80%. Accurate numerical simulation of generation and migration processes can support the tracking of hydrocarbons “from source to trap” and therefore reduce risks and costs in oil exploration.

A vast literature is present for flows of hydrocarbons in the underground in terms of both laboratory experiments and numerical models. The numerical models commonly used, like invasion percolation or flowpath modelling, are too simplistic to resolve all the physical phenomena of the problem. A major drawback is the lack of a detailed and realistic description of the fractures. Recently, thanks to new fast numerical solvers and the diffusion of super-computers, the attention of the scientific community has turned

to the direct resolution of the physical equations governing the flow, previously regarded as too computationally expensive. Usually finite elements or finite volume methods are applied to solve these equations. Even if the aforementioned technological advantages can improve the performance of a simulation some problems still remain. Both finite elements or finite volumes require a computational grid, which has to approximate the real domain. In realistic applications the creation of a mesh which resolves all the fractures is difficult even for modern mesh generation software. The resulting grid may have poor quality or involve several billions of grid cells, yielding a problem of prohibitive computational costs even in the high performance computing framework. On the other hand if the numerical model does not resolve the fractures reasonably well the solution is poorly approximated. Finally, all the data we know about the properties of the underground at the time when the secondary migration took place, i.e. several million of years ago, are affected by uncertainty and multiple scenario analysis is required to obtain a better forecast of the reservoir distribution.

In literature it was proposed a model to overcome some of

these problems, for the single-phase flow, using a domain decomposition approach where the fractures are natural interfaces between subdomains and flow within fractures is solved by a suitable reduced model. Only the twodimensional cases has been treated on simple geometries and the grids are still conforming to the fractures. This model can successfully address the problem of the high number of unknowns in the simulation, in the restricted case of non intersecting fractures acting as preferential paths or barriers, which completely cut the domain in separated sub-domains. Moreover realistic simulation in a three dimensional porous medium are presented in a sequent work where also suitable interface conditions are imposed on the intersecting fractures. These conditions do not take into account the different properties of the fractures involved in an intersection, e.g. one fracture can act as a barrier with respect to the other one, and they simply impose the conservation of mass and the continuity of the pressure. While all of the aforementioned models are written in the framework of domain decomposition and cannot handle fractures with tips, in a recent work the model is extended to admit fractures which do not cut entirely the



1. On the left, pressure field with the original model. On the right, pressure field with the reduced.

domain. To overcome the limit of the conformity between the grids of the fractures and the grid of the porous medium, the previous model is extended to the case of non matching grids between the fractures and the porous medium. The idea is based on the extended finite element method (XFEM) to allow discontinuity of the pressure and the Darcy velocity inside the cut elements of the bulk grid. With this model the problems of mesh conformity and generation disappear and the reduced model can be successfully applied to realistic problems. Finally in a recent work the authors extend the reduced model valid for the single-phase flow to the two phase flow problem.

The aim of this thesis is twofold. We introduce further extensions of the non

matching reduced model in the case of single-phase flow. In particular we address the problem of gravity effects, i.e. how the reduced model and the coupling conditions have to be modified to take into account this new feature correctly. In the framework of non matching grids, we extend the case of crossing fractures where suitable interface conditions are considered to allow jump in the pressure and in the velocity. In this case the XFEM method is applied to the porous matrix as well as to the fractures whose meshes form an arbitrary set of non matching grids which intersect and communicate. Finally using the same mathematical and numerical tools we present a reduced model for the parabolic problem governing the transport of a passive tracer in the porous medium. This

problem is very interesting as it can model pollutant transport in water-bearing strata. For all of these models we present both analytical and numerical results with an emphasis on realistic problems. The other part of the thesis consists in the parallel implementation, in the framework of the LifeV finite element library, of a three-dimensional two-phase flow solver. Modern programming and numerical techniques are used to obtain a general, robust solver. Some realistic problems are presented such as the flow of oil along a fault, as Figure 1 shows, or the trapping under an impermeable cap-rock. We also tested the scalability of the code on super-computer machines.

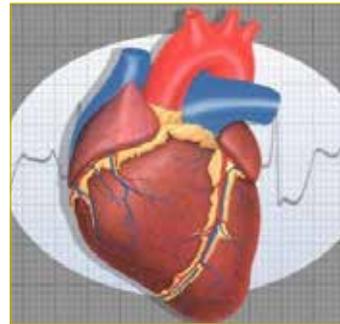
Furthermore, the effectiveness of the proposed models could be improved introducing stabilization techniques or appropriate preconditioners to obtain a condition number which is independent of the position of the fractures. In addition, for the transport of the tracer an important improvement would be the inclusion of stabilizations to handle advection-dominated problems without resorting to mesh refinement.

STATISTICAL METHODS FOR CLASSIFICATION IN CARDIOVASCULAR HEALTHCARE

Francesca Ieva

Since a strong attention has been devoted in the last decades to healthcare management for social, medical and economical reasons, over recent years also the development and the improvement of suitable tools for measuring the quality of care has become a research field of extreme importance. Within this context, since patient's outcomes enable researchers to assess the quality of care, there has been a widespread diffusion of techniques for monitoring and evaluating the underlying processes generating such outcomes. This task is nowadays unavoidable in order to get a sensible improvement of healthcare services quality, as well as to contain economical costs. In order to achieve a suitable strategy for assessing healthcare performances, it is necessary to identify suitable operating protocols, as well as the functional competence of institutions, and then to monitor them over time. In this way, a continuous collection of data proved to be mandatory. With this respect, a dataset (clinical registry and/or administrative database) describes the process underlying a disease. The more complex, structured and detailed is the dataset, the more difficult is the analysis required for its exploitation. In other words, monitoring healthcare systems through

data collections asks for careful design of experiment and high quality of collected data, shared standards of collection and strict control on filling compliance and reliability of the data. Moreover, it calls for suitable statistical methods for analysis, modelling and prediction. Only in this way it is possible to derive models which are capable of realistic interpretations of the process underlying the dataset. Statistical techniques, when applied to measurement data, can be used firstly to highlight areas that would benefit from further investigation, then to model processes relating patterns of care, patients case-mix, hospital influences and outcomes of interest, and finally to make predictions on them. Statistics enables the researchers to identify variation within the process under observation. Understanding, modelling and then quantifying this variation are the first steps towards quality improvement. An important goal of Regione Lombardia (healthcare division) is the use of performance measures for monitoring cardiovascular offer, as well as to assess institutions within the regional healthcare service in order to provide evidence for initiatives aimed at enhancing professional accountability in the public sector. Specifically, a Strategic Program, named



1.

“Sviluppo di nuove strategie conoscitive, diagnostiche, terapeutiche e organizzative in pazienti con sindromi coronariche acute”, has started in 2008 with, among others, the goals of (i) pointing out a comprehensive clinical and epidemiological picture of how Acute Myocardial Infarction (AMI) is treated in Regione Lombardia; (ii) assessing the effectiveness of patterns of care delivered at AMI patients, in order to invest in innovations starting from real epidemiological evidence and needs; (iii) exploiting administrative databanks for addressing clinical and epidemiological enquires; (iv) highlighting critical situations in healthcare delivery and then improving hospital performances; (v) providing people in charge with healthcare government with decisional support based

on statistical evidence and real time data. In order to address these issues, suitable methods to collect, analyse and model data are needed. The results of statistical analyses carried out on data arising both from clinical registries and administrative databanks may influence funding and policy decisions, and are used to generate feedback for providers. The providers' profiling based on current data collections is a new way improving quality of healthcare offer. This requires shared information-technology systems of data collection and for advanced statistical methods able to classify providers, to quantify their effect on outcomes of interest at patients' level and to make reliable predictions. Statistics is then of paramount importance in more than one step of the cardiovascular healthcare process, especially in supporting this new concept of “real-time” epidemiology based on observational clinical registries and administrative databanks. In fact, the statistician plays a central role during the design of experiment, carries out the monitoring of data collection, evaluates the process and produces a feedback for involved players, elaborates models necessary for providers' profiling, classification and outcomes prediction. The decisional

support provided by statisticians is evidence based and is based on real epidemiological evidence and needs, involving low cost data sources, i.e., real-time and sustainable from economic perspective.

In this thesis a general approach to model fitting aimed at clustering is considered, focusing on grouped (longitudinal) data arising from healthcare context, where examples of grouping factors are hospitals (and diseases) with respect to patients or patients themselves with respect to measurements carried out over time. The main goal is then to present a number of statistical techniques for the analysis of such data, in order to provide methods for supporting decisions of clinicians as well as of people in charge with healthcare government. Clinically speaking, we will focus on problems related to the improvement and optimization of patterns of care for patients affected by Acute Coronary Syndromes and on semi-automatic diagnosis of an infarction called Bundle Branch Block. On the other hand, the main statistical topics we will deal with are clustering carried out starting from random effects estimation, and unsupervised classification of multivariate functional data. Suitable statistical models and

techniques are exploited and approached both from a classical and Bayesian viewpoint. For example, we may distinguish two types of applications: those in which the individual random effects are of paramount interest for discriminating unusual performances of healthcare providers and those where functional depth measures are used for exploiting morphological features which allow for pattern recognition of different diseases. Among other benefits, these approaches provide a criterion to detect clusters of providers with unusual results or to diagnose infarction starting from a purely statistical approach.

CHARACTERIZATION OF DELAYED AFTER-DEPOLARIZATION IN EXTENDED FITZHUGH-NAGUMO MODELS

Chiara Lelli

In the Thesis we have studied a mathematical model that characterizes and predicts a particular type of disease in the evolution of the cardiac action potential known as delayed after-depolarization (DAD). Such a phenomenon is induced by a spontaneous depolarization of the membrane occurring before the cardiomyocytes have recovered the rest state. If the depolarized potential reaches a threshold (which is a physiological parameter peculiar to the biological system), a secondary electrical wave can be generated, and an abnormal contraction of the cell can be induced thus affecting the heart beating. In this case the after-depolarization is labeled as supra-threshold DAD, and this is the type of mechanisms we are interested in. The FitzHugh-Nagumo model provides a well-suited scheme to study this phenomenon, since, due to its flexibility, it can easily be extended in order to interpret the particular features of the system we would analyze. Although it was proposed to reproduce the transmission of the electric signal in the neuronal membrane, in the literature it is often used to model the cardiac action potential, since the physiological processes underlying the two mechanisms are generally the same. The variables involved in the dynamical system are the

membrane potential, v , and the recovery variable, w , which evolves with a slower dynamics with respect to the potential. In the present Thesis we have defined particular solutions of the FitzHugh-Nagumo dynamical system, that we have called spike-solutions. They are characterized by the number of supra-threshold turns they perform around the equilibrium point before the potential approaches the steady state. Among these trajectories, we analyzed one in particular, that acts as a separatrix in the phase plane, and we studied the behaviour of such an orbit by varying both the values of the constitutive parameters of the model and the threshold the solution has to cross. We considered that the parameters range over a set of values that ensures the presence of only one equilibrium configuration for the dynamical system, and, in particular, we proved that, for these parameters values, all the trajectories are bounded and limit cycle solutions are absent in the phase plane. A crucial property of a spike-solution is the amplitude of the first turn (spike), since it plays the role of the activation threshold. Indeed this parameter, compared with the physiological threshold, can give useful information on the nature of the DAD, and in particular it

can identify supra-threshold and sub-threshold DADs. In a first analysis we consider the minimum point of the nullcline corresponding to the potential variable as the threshold. Nevertheless this proved to be an inappropriate choice since such a minimum depends on a physiological constant, and it approaches the equilibrium point if this parameter tends to 0. Such a behaviour does not correspond to a realistic situation. Indeed the threshold should not depend on the physiological properties of the cardiac membrane, but rather it must represent an objective parameter denoting the typical physiological condition of a healthy individual. Moreover in the literature, most of the authors refer to the potential threshold as a fixed value, recovered by experimental procedure. For this reason we have considered the threshold as a constant, trying to calibrate its magnitude on the basis of the data found in the literature, and we came to fundamental results. First of all, we found that for values of the constitutive parameters large enough, the secondary spike does not occur, whatever the choice of the threshold, so that once the electrical impulse is triggered, the potential immediately stabilizes around the rest state.

Moreover, we showed that, in order to trigger a secondary action potential, the threshold of the depolarization must exceed a certain value, which cannot be too large, giving confirmation of the existence of an optimal value of the activation limit that corresponds to the physiological one. Once we have identified the correct values of the parameters ensuring the existence of DADs, we wondered under which conditions the depolarization could generate a traveling pulse that disrupts, in such a way, the contraction rhythm of the heart. In practice we investigated the occurrence of a DAD-induced traveling wave that excites again the cardiac muscle and leads to after-contractions of the fibers. Such a possibility needs the fulfilment of other parameter requirements, and, in particular, we have to restrict the admissible range of values of the constitutive parameters further on. The property that especially affects the development of the propagating pulse is the time scale difference between the evolution of the fast variable v and that of the slow recovery process. Indeed, if the dynamics of the two variables have a similar time scale, the DAD, when it arises, does not trigger a potential wave, probably because the repolarization forces do not allow the upstroke to completely develop, giving rise to a secondary action potential. Obviously, the analysis of traveling pulse solutions involves the spatial dimension of the problem and, more particularly, we must account for a potential diffusion through the tissue, that necessarily yields a dispersion of the initial impulse. Consequently, the occurrence of two-spike

solutions will be subjected to slightly different conditions on the parameters that will account for the scattering potential. Then, it is clear that the FitzHugh-Nagumo dynamical system must be refined and extended in order to obtain more precise results. A possible choice aimed at making the model more realistic requires to consider the dependence of the parameters on the potential v itself. Indeed with this correction, the model may simulate more precisely the dependence of the activation of the muscle contraction on the potential field, taking account of the so called electro-mechanical coupling. The analysis of spike-solutions for the dynamical system modified in this way produces fundamental outcomes. Indeed we proved that, by modeling the mechanical activity of the cardiac fibers, the DAD-predictive feature of the FitzHugh-Nagumo model contains also information on the nature of the extra-spike, namely on its sub-threshold or supra-threshold property. Indeed, in dependence of the magnitude of the shortening, the secondary oscillation can exceed the physiological threshold and then trigger an action potential. More particularly, if the fiber contraction is sufficiently strong, no supra-threshold DADs are generated, whereas, if it is less than a critical value, the extra-spike amplitude reaches the activation threshold and gives rise to a secondary wave. This study provides a relation between the contraction ability of the myocytes and the possible occurrence of arrhythmias, thus linking the macroscopic

environment with the molecular mechanisms that regulate the physiological processes. Our analytical results are also confirmed experimentally. Indeed in the literature some authors studied the consequences of a contractile dysfunction on the ionic environment that could establish the generation of DADs. Nevertheless, since the model itself can predict the cardiac triggered activity on the basis of the contraction magnitude, it represents a powerful tool that enables to design and predict decisive interventions in prevention of arrhythmic episodes. A natural development of the research summarized here is the extension of the DAD-predictive model presented in this work to a multidimensional setting. Indeed, as we have already said, a spatial-dependent model allows the study of the diffusion of the electric wave through the cardiac domain, and, in particular, the possible propagation of a secondary action potential, triggered by a supra-threshold DAD, that may cause the onset of abnormal heart contractions.

NON-CONFORMING HIGH ORDER METHODS FOR THE ELASTODYNAMICS EQUATION

Ilario Mazzieri

Introduction

The study of wave propagation in elastic solids has a long and distinguished history. Indeed, since the middle of the 19th century, great mathematicians as Poisson, Cauchy, Green, Lamé and Stokes developed what is now generally known as the theory of elasticity. In the latter part of the 19th century the interest in the study of wave propagations in elastic solids has increased because of applications in the field of geophysics. Currently, wave propagation in solids is still a very active area of investigation in seismology because of the need for accurate informations on earthquake phenomena, and detection of nuclear explosions. In this thesis we aim at proposing and analyzing a family of non-conforming numerical methods capable of simulating elastic wave propagations in two and three dimensional configurations, characterized by the presence of irregular interfaces, heterogeneous materials as well as the capability of predicting correctly soil-structure interaction phenomena. The use of the elastodynamics equations to model the seismic response of heterogeneous earth media with irregular topography and internal interfaces is a subject that has been intensively investigated in recent years.

The study and development of high-order methods for simulating elastic wave propagation in seismic regions has been subjected to a tremendous growth, occurred in the past ten years. Recent developments in computational seismology have been based on numerical strategies as finite differences, boundary element methods and, more recently, spectral element (SE) methods. SE methods are based on high-order Lagrangian interpolants sampled at the Gauss-Legendre-Lobatto quadrature points, and combine the flexibility of finite elements with the accuracy of spectral techniques. Since they are based on the weak formulation of the elastodynamics equations, they handle naturally both interface continuity and free boundary conditions, allowing very accurate resolutions of evanescent interface and surface waves. Moreover, SE methods retain a high level parallel structure, thus are well suited for massively parallel computations. The main drawback of SE methods is that they require a uniform polynomial order on the whole computational domain, and this can lead to an unreasonably large computational effort, in particular in regions where a fine mesh grid is needed already to describe accurately the domain geometry. Therefore, it can be more adequate in

some cases to use a lower order method in the small elements to reduce the CPU effort without losing much accuracy. Non-conforming high-order techniques, like the Discontinuous Galerkin Spectral Element (DGSE) or the Mortar Spectral Element (MSE) methods, allow to treat locally varying polynomial degrees of the basis functions, so-called *p*-adaptivity, as well as locally varying mesh size on the computational domain, *h*-adaptivity. The *hp*-adaptive version of these schemes is useful in complex 2 and 3-d models with small-scale features which have to be meshed with reasonably small elements to capture the necessary geometrical details of interest. In this thesis, we present a new discretization approach to combine the DGSE and MSE methods with suitable time advancing schemes for the simulation of wave propagations in heterogeneous media. To overcome the limitations of the existing approaches we will apply the non-conforming paradigm only at subdomain level. We show that the resulting formulations are stable, provide optimal approximation properties, and suffer from low dispersion and dissipation errors.

Discussion

We start describe the physical phenomenon governing seismic wave propagations and we

derive the elastodynamics weak formulation. The geometrical and functional discretization of the problem is presented in the context of non-conforming approximations and the Discontinuous Galerkin and the Mortar spectral element methods are derived starting from a common weak formulation. The computational domain is split into macro-regions called subdomains (usually associated to the earth's substrata, heterogeneous media, engineering structures) and the non-conforming approach is employed across subdomains' boundaries.

The quadrilaterals/hexahedras do not have to match between neighbouring subdomains, and different spectral approximation degrees are allowed. Therefore, the continuity of the solution at the skeleton of the decomposition is imposed weakly, either by means of a Lagrange multiplier for the MSE method, or by penalizing the jumps of the displacement in the DGSE method. Then, in each non-overlapping subdomain a conforming spectral finite element discretization is employed.

Starting from a common displacement-based weak formulation of the elastodynamics equation, we prove a priori error bounds for the non-conforming semi-discrete formulations. We also discuss the algebraic aspects

of the DGSE and MSE methods. Next we describe three different time integration schemes that could be used for the discretization of the system of ordinary differential equations resulting from the semi-discrete approximations. In particular we study the leap-frog (LF) scheme, the implicit midpoint (IM) method and the fourth order Runge-Kutta (RK4) method. Moreover we present error estimates for the fully-discrete-problem, obtained combining the non-conforming discretizations with the previous time integration methods. The semi-discrete and fully-discrete non-conforming formulations are analyzed in Chapter 4 from the point of view of the dispersion, dissipation and stability properties.

For wave propagation problems, the grid dispersion/dissipation criterion determines the lowest number of nodes per wavelength such that the numerical solution has an acceptable level of accuracy, while the stability criterion determines the largest time step allowed for explicit time integration schemes. Here, we propose a new generalized eigenvalue approach to determine sharp grid dispersion and dissipation errors as well as stability bounds for the LF and RK methods. This approach is based on the Von Neumann's method (plane wave analysis) and can be used

to determine dispersion and dissipation properties for different space and time discretizations. Then, a particular attention is devoted to the implementation aspects of the non-conforming approaches in a spectral element based code. Special emphasis is given to the description of the numerical strategies used for facing integral computations present in DGSE and the MSE discretizations.

Moreover, we propose an efficient way (in term of low memory storage and executing program velocity) to code DGSE and MSE approaches for wave propagations.

Finally, after the validation of the proposed schemes on two and three dimensional benchmarks available in literature, we addresses some real geophysical applications. At first we show the seismic response of a remarkable railway masonry bridge, and soft soil amplifications occurring on alluvial basin. Then, we present relevant earthquake scenarios, i.e., the case of the Grenoble valley (France) and the Canterbury plains near Christchurch (New Zealand). The latter results represent the state of the art in computational seismology.

MATHEMATICAL AND NUMERICAL MODELLING OF THE EVOLUTION OF MIXTURES OF SAND IN AEOLIAN DUNES

Matteo Pischiutta

The morphodynamics of desert sand dunes is due to two distinct physical mechanisms: the effect of the wind blowing on the sand surface which produces a flux of jumping sand grains said "in saltation", and the spontaneous generation of avalanches if the slope of the sand surface is steeper than the angle of repose. Given the long time scale to observe effective movement of a dune and the difficult reproducibility in wind tunnel, in the last decade mathematical modelling and numerical simulation of sand dune evolution have become an important subject of research. In the existing literature, the modelling is often based on a conservation equation for the mass of sand formulated by balancing the temporal variation of sand surface elevation with the divergence of the saltation and avalanches sand fluxes. The saltation flux is hence written in term of the shear stress exerted by the wind on the sand surface, whereas the avalanche flux depends on the local slope of the sand surface.

In this Ph.D. thesis we are interested in building a model for dune evolution when the bulk sediment is a mixture of sands with different characteristics. In particular, we consider sands which can be distinguished

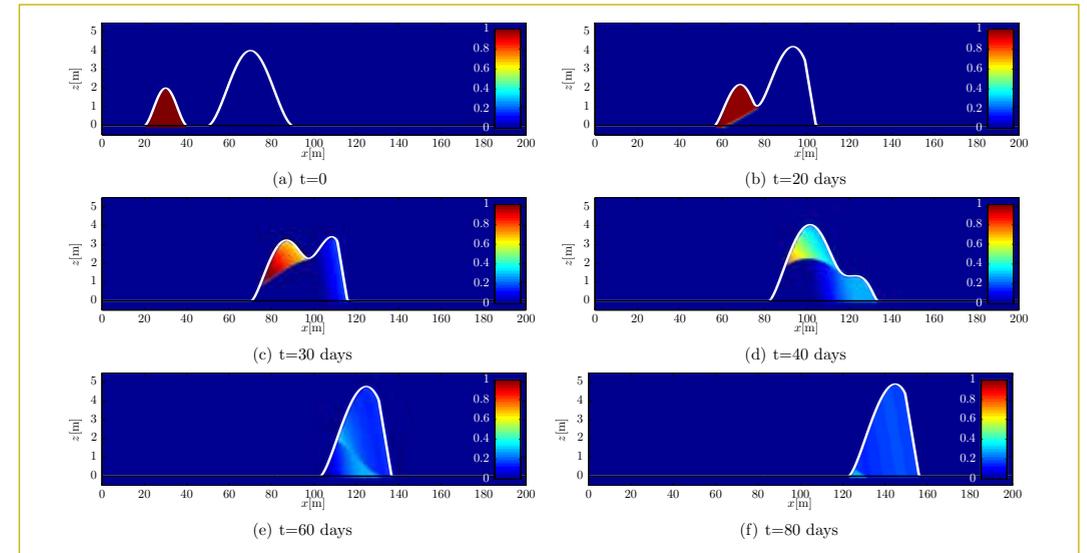
only by their appearance, but which have the same physical characteristics such as diameter and density. Hence we will refer to "marked" and "clean" sediments. The interest in the evolution of the concentration of marked sediment is motivated by the industrial problem of remote sensing for hydrocarbon microseepage. In particular situations, the light hydrocarbons can in fact seep through the seal rock of the reservoir, and hence rise to the Earth surface. This hydrocarbon microseepage can induce geochemical and geophysical alterations in the sedimentary column, and the superficial footprint of these anomalies can be further detected with remote sensing techniques. Supposing that the microseepage induced alteration is adsorbed at the sand grain level, in deserts with moving dunes the superficial footprint of the reservoir can be dispersed by the transport of sediments induced by the wind.

In this work, the derivation of the complete three dimensional model of the evolution of mixtures of sands in aeolian dunes is accomplished by first assuming that sediment exchange between sand surface and superficial transport fluxes (for both the saltation and the avalanche dynamics) is limited in a superficial layer of finite

depth, called "active layer". On the one hand, this allows us to consider the substrate under the active layer as a zone where the concentration of marked sand is stored in depositional processes and remains unvaried since this zone is not involved in superficial transport processes. On the other hand, the concentration of marked sand in the active layer depends on the local balance between the mass of marked sand entrained from the surface and the mass of marked sand deposited from the superficial fluxes.

Hence, the mathematical model for dune evolution has been completely reformulated by expressing the temporal variation of sand surface elevation in term of the balance between the entrainment and deposition rates due to saltation and avalanches, instead than using the divergence of the sand fluxes as usually made so far in the aeolian literature.

We hence provide the constitutive relationship for the new variables introduced in the system. The entrainment and deposition rates due to the saltation dynamics are derived from the model of impact rate available in the literature by introducing a probability of rebound of the impacting grain. For the avalanche mechanism, we assume that erosion occurs



1. As initial condition, the first smaller dune is made of marked sand; as it's faster than the bigger one, the two dunes collide. At different time steps, we see the concentration of marked sand during dunes collision.

only if the slope exceeds the angle of repose, and introduce a probabilistic step length for avalanching grains which links the deposition rate to the upward entrainment rate. We also provide a possible characterization of the new parameters added to the system by fitting our model to experimental data existing in the literature.

Concerning the numerical simulation of the problem, at each time step we subsequently perform the update of the saltation and avalanche submodel. For the saltation dynamic, we calculate the wind field on the sand surface with a computationally efficient analytical theory of logarithmic boundary layer perturbation. Hence the system of conservation laws with source terms which describes the mass and momentum conservation of marked and cleaned sand in the saltation layer is discretized with

the conservative finite volume method, taking into account the source terms with an operator splitting technique. The results of sand dune evolution obtained with our formulation agrees well in term of dune shapes and velocities with those encountered in the literature. However, the new formulation offers the possibility for a differential evolution of sand dunes made up of a mixture of sands. Amongst the possible applications of our formulation, we can investigate the problem of dune collision from an original point of view. In fact, by assuming that one dune is made of marked sand, we can observe the evolution of the whole sedimentary structure during the collision, see Figure 1.

In the case of evolution of two dimensional dunes, we also provide a simplified formulation where the entrainment rate is written in function of the shear stress exerted by the

wind on the sand surface, while the deposition rate is linked to the upwind entrainment rate by assuming that the step length of a saltating grain is probabilistic with a given density function. Under some simple but physically based hypothesis, we show the mathematical equivalence of this formulation with a simplified model encountered in the literature. Hence this new formulation constitutes a great simplification of the problem with limited drawbacks, and it allows us to approach some large scale problems with affordable computational costs. In particular, we couple the system with a model of generation of marked sand due to hydrocarbon microseepage, and simulate the dispersions of the superficial footprint of the reservoir for large temporal and spatial scales.

EFFICIENT PARTITIONED ALGORITHMS FOR THE SOLUTION OF FLUID-STRUCTURE INTERACTION PROBLEMS IN HAEMODYNAMICS

Matteo Pozzoli

Aim of this work is to build efficient strategies for the solution of a fluid-structure interaction (FSI) problem that is a major issue in computational haemodynamics. In particular, we are interested in the FSI problem arising by the interaction between the blood flow and the vessel wall deformation. Typically, this is a strongly non-linear coupled problem, as there is a substantial amount of energy exchanged between fluid and structure in each cardiac cycle.

The main difficulties related to the numerical solution of a FSI problem are the following:

1. the fluid computational domain is an unknown of the problem (geometrical non-linearity);
2. possibly, fluid and structure are non-linear (constitutive non-linearities);
3. the FSI problem is a coupled problem, since we have to guarantee the continuity of the velocity and of the normal stresses at the fluid-structure interface (interface geometrical continuity condition);
4. numerical instability could arise for high added mass effect, that occurs whenever the density of the fluid is comparable to that of the solid.

Concerning the first point, we can mainly detect two strategies: an *implicit treatment* of the interface position, through, for example, fixed point or Newton iterations, or an *explicit treatment*, by extrapolating the solution from previous time steps. Regarding the latter treatment, several theoretical results in the last ten years have shown that this strategy is able to guarantee the stability of related algorithms in the case of the linearized equations of infinitesimal elasticity. For what concerns the accuracy of such schemes, few results have been reported so far. However, in the haemodynamic context, when dealing with three-dimensional real geometries and physiological data, it is still not clear whether the use of an explicit treatment of the FS interface is appropriate for practical purposes. Concerning the second and the third point, after a suitable linearization of the physical and geometrical non-linearities whichever of the two strategies is adopted for the treatment of the interface position (implicit or explicit) - one has to deal with a linearized FSI problem, in the sense that we have eliminated the geometrical and physical non-linearities. However, this problem is still coupled through the interface continuity conditions.

Up to now, two strategies have been proposed namely the *monolithic* and the *partitioned* approaches. In the first case, the problem is solved by building the whole FSI matrix, and then by solving the related linear system with a suitable preconditioned Krylov, domain-decomposition or multigrid method.

Obviously, in this way the interface continuity conditions are automatically satisfied. Alternatively, in partitioned schemes one solves the fluid and structure subproblems in an iterative framework, until fulfillment of the interface continuity conditions. Since we are interested in developing modular algorithms, which allow the use of pre-existing fluid and structure codes, we do not consider the monolithic approach here. Finally, we remark that when the added mass effect is high (that is when the fluid and structure densities are similar) the performance of classical partitioned schemes, such as Dirichlet-Neumann, is very poor and a relaxation is needed to reach convergence. On the contrary, Robin-Robin (RR) schemes highlighted better convergence properties in presence of a high added-mass. In particular, it is shown that the Robin-Neumann (RN) scheme converges without relaxation and a big saving in computational time with

respect to the DN scheme is observed. Actually, the study of partitioned algorithms to solve the FSI problem with non-linear materials is still a topic of interesting. In this work, we develop partitioned algorithms to solve the FSI problem by modeling the vessel using a linear infinitesimal elastic model and a set of non-linear elastic models. In particular, we have analysed the following aspects:

1. Accuracy of non-implicit algorithms (explicit treatment of interface position).
2. Accuracy and efficiency of high order temporal schemes.
3. Introduction of hybrid implicit schemes to improve the efficiency.
4. Study of partitioned algorithms to solve FSI with non-linear materials.
5. Clinical applications.

In this work we present an *abstract* framework, in which we rewrite the FSI problem through a Lagrange multipliers formulation and we propose two families of partitioned algorithms to face the geometrical, constitutive and interface non linearities. Indeed, different treatments of such non-linearity lead to different numerical schemes. In particular, in the first family of numerical methods we apply quasi-Newton methods to the monolithic formulation of the FSI

problem, where the geometrical non-linearity is treated together with the constitutive ones, so that problem is fully linear. The second family of algorithms are based on a fixed point strategy, where the constitutive non-linearities are treated together with the continuity interface conditions. For both families different exact partitioned algorithms are generated. In order to improve the efficiency, from these schemes we derive also inexact schemes where the geometrical and/or constitutive non-linearities are not solved exactly. Moreover, we study the accuracy of this kind of schemes by proposing an analytical test case for the FSI problem in the case of the linear infinitesimal elasticity.

The second main goal of this work is to develop efficient ways to build high-order temporal schemes for the solution of the FSI problem. We consider the *Newmark scheme* for the structure in combination with the *theta-method* for the fluid, as well as BDF schemes up to fourth order for both subproblems. In particular, for inexact schemes, we study if suitable extrapolations of the interface quantities at each time step improve the time accuracy and/or reduce the number of iterations on the interface position. A significant task obtained in this work is the

fact that we are able to handle a particular haemodynamic application. More precisely, using clinical dataset of real patients, who were affected by arteriosclerosis in their carotids, we model the fluid-dynamics in the carotids pre and post thromboendarterectomy (TEA), that is a surgical procedure to remove the plaque. We also analyse the response of the vessel when it is modelled with three materials characterized by a non-linear finite elasticity. In nearly future, this kind of study could result useful for the diagnosis of such diseases.

POLYNOMIAL APPROXIMATION OF PDEs WITH STOCHASTIC COEFFICIENTS

Lorenzo Tamellini

In the last decades simulation and prediction based on computational models have become widespread tools in science and engineering practice. This process entails the selection of a suitable mathematical model for the system of interest, the tuning of the parameters involved in the model, its discretization and finally its numerical solution. Each of these steps implies some errors: in this thesis we are concerned with the errors that stem from an imperfect knowledge on the system properties. This may be due to several reasons: a) precision issues in the measurement of some physical quantities (viscosity, permeability, density); b) non-measurability of the system (the permeability of the soil cannot be measured point-wise); c) intrinsic randomness or unpredictability of some quantity (wind loads, earthquake sources). In this thesis we do not deal however with “model uncertainty”, i.e. we always assume that a suitable mathematical PDE model is available, and that the uncertainty is only affecting parameters of such model. We also assume that each uncertain parameter can be modeled as a random variable/ random field, and that the probability distribution of such random objects is known, either from experimental measures or from human expertise.

As soon as some of the parameters of the equation depend on a random event, so does the solution: each realization of the random parameters will correspond to a different solution (“input-output map”), through the evaluation of a PDE solver. In this context, the goal is usually to compute statistics of the solution, like mean, variance, probability of exceeding a threshold value (“failure probability”). Often one could also be interested in restricting such statistical analysis to functionals of the solution, hereafter called “quantities of interest”; in such case, the input-output map is usually called “response surface”. This kind of analysis is usually referred to as “Uncertainty Quantification” or “Forward Uncertainty Propagation” from the parameters to the quantity of interest of the model.

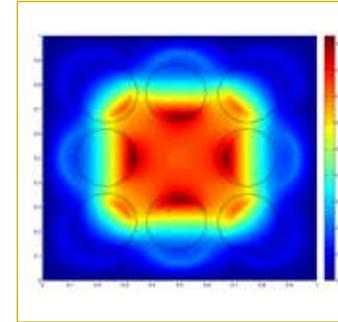
Monte Carlo sampling is the most natural approach to solve the Uncertainty Quantification problem. It only requires generating a set of independent realizations from the parameters space, and solving the equation for each sample in the set: the statistical indices are then approximated by sample averages over the obtained set of solutions. Such method has a straightforward implementation and is fully

parallelizable. Moreover, its rate of convergence is independent of the number of random parameters considered: this is a desirable feature since the number of random parameters involved can be quite large, and many methods suffer from a degradation of their performance as this number increases, a phenomenon known as “Curse of Dimensionality”. Such rate is however only proportional to S/\sqrt{M} , where M is the number of samples and S is the standard deviation of the considered quantity of interest. This may result in massive computational costs since a single evaluation of the PDE solver may be an expensive operation.

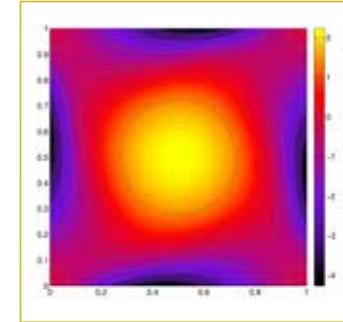
To overcome this, in this thesis we explore the possibility of reducing the computational burden taking advantage of the possible regularity of the input-output map, by computing a polynomial approximation of such map (“surrogate model”). Once the surrogate model has been computed,

statistics like mean or variance can be approximated with simple post-process with almost no computational cost.

In this thesis we mainly consider systems governed by elliptic PDEs with stochastic coefficients,



1. Standard deviation of the solution of a diffusion problem with circular inclusions with random coefficients.



2. Mean vorticity field for a Navier-Stokes problem with random Reynolds number and rotating forcing field.

for which it is possible to prove analyticity of the input-output map. Therefore looking for a global polynomial approximation is sound. Yet, the construction of the approximated response surface will be in general a difficult task, since the quantity of interest may depend on a high number of random parameters: in particular this implies that standard techniques (finite differences, finite elements) are not suitable for the approximation of the response surface, and sparse strategies need to be introduced. We have focused on two types of sparse polynomial approximations: a) interpolant schemes (Stochastic Collocation), based on sparse-grid techniques; b) spectral projection schemes (Stochastic Galerkin), using orthogonal polynomials on the parameters space. In particular we have

performed a detailed comparison of the two methods, which was missing in the state-of-the-art literature. We have then proposed some new strategies for the optimization of both methods. These strategies rely on the concept of a-priori adaptivity based on the possible anisotropy of the solution: we first individuate the parameters contributing the most to the variability of the solution and then build the polynomial approximation targeting a higher accuracy with respect to such parameters only, in order to reduce the “Curse of Dimensionality” effect. We have shown the efficiency of such improved approaches both on synthetic test cases and on a stochastic groundwater flow problem arising in the geological engineering practice.

We have also considered equations other than elliptic. In particular, we have tackled a Navier-Stokes problem with uncertain viscosity and forcing term with an alternative projection approach, the so-called “Proper Generalized Decomposition”, that can be ascribed to the field of “Reduced Order Modeling”. Such method is appealing since it improves the Galerkin method considered before: the adaptivity is “automatically” performed, i.e. the user does not need to run a preliminary analysis to detect the more important parameters, and the algorithm decouples the problems in the deterministic and stochastic domain, thus allowing for low computational costs and significant reuse of preexisting deterministic solvers. Finally, we have also addressed a second geological problem, namely, the geochemical compaction of a sedimental basin. For such problem we have proposed a hybrid interpolation/projection strategy to perform a Sensitivity Analysis study, by computing the so-called Sobol’ indices.

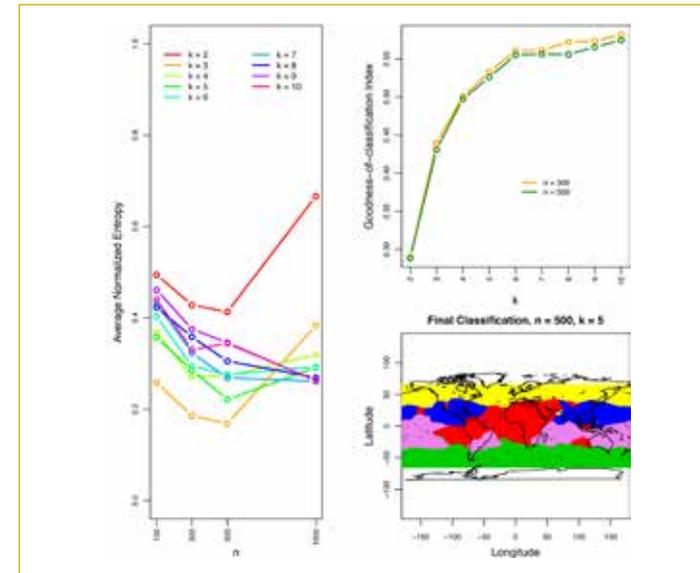
CLASSIFICATION OF FUNCTIONAL DATA IN THE PRESENCE OF SPATIAL DEPENDENCE

Valeria Vitelli

The general framework of the PhD thesis is the analysis of high dimensional and complex data. The peculiarity of all the considered problems and case studies is the combination of different sources of complexity: high – dimensionality, spatial dependence, geo – referencing, high sample size. The main aim is performing data classification, i.e. reconstructing a latent field of labels which influences the distribution of the observed (functional) signal. This classification problem motivates the first part and most of the second part of the thesis. Indeed, the general paradigm here discussed, at least in the framework of spatially dependent functional data, can be adapted to different problems arising in the applications, and to different purposes: dimensional reduction, regression... but the main focus remains on the development of methods and algorithms for the classification of functional data. The PhD thesis is articulated in three parts: the first part concerns the classification of functional data when spatial dependence is not present, while with the second one we enter the more general framework of spatially dependent functions. Here, innovative classification and dimensional reduction methods, suited for the case of functional data indexed by

the sites of a spatial lattice, are presented. In the third part of the dissertation, all the analyses we have conducted and all the results we have attained within the eni project that funded the PhD grant are detailed: this scientific endeavour has motivated the development of many of the methods described in the first two parts of the dissertation. While the first two parts of the dissertation correspond to its public part, the third one is subject to confidentiality constraints, and can not be disclosed. In Chapter 1, an introduction to many issues arising in the treatment of functional data is given. The focus is on the problem of clustering functional data, which in this Chapter are assumed to be an independent sample. The problem of data misalignment is also introduced and discussed as a further source of complexity in the analysis of functional data. The most interesting and innovative part of this Chapter is not the methodology, since it serves only as an introduction to techniques that will be useful in the subsequent Chapters, but the case study: it shows the application of functional data classification techniques to a very complex dataset of ECG curves, with the aim of automatically detecting different coronary ischemic diseases

on the basis of the sole ECG morphology, without relying on any clinical information. To our knowledge, this is the first attempt to apply functional data analysis techniques to the automatic diagnosis of heart pathologies. Chapter 2 focuses on the problem of jointly clustering and aligning a sample of independent functional data. Indeed, when treating functional data, one has to take into account a very specific source of variability, which can confound the results of the classification: phase variability. Starting from the methods discussed in Chapter 1, an innovative joint solution to the two problems of clustering and alignment of functional data is described. This novel procedure proves to be very effective in real data applications, when no a-priori information is available on data misalignment (e.g. landmarks). The proposed framework for performing joint clustering and alignment is tested on a benchmark dataset for functional data analysis: the Berkeley Growth Study dataset. In Chapter 3 we further discuss the problem of clustering functional data, by also considering the issue of feature selection. The definition of a proper methodology able to cluster functional data and jointly to select the features



1. Results of clustering of spatially dependent functional data from the Surface meteorology and Solar Energy database: in the left panel, average normalized entropy obtained with different choices of K and for $n = 100, 300, 500, 1000$; in the top – right panel, goodness – of – classification index associated to the final classification with $K = 2, \dots, 10$, and for $n = 300$ and $n = 500$; in the bottom – right panel, final classification map obtained via a majority vote on frequencies of assignment to clusters, and by setting $K = 5$.

which are the most relevant to the clustering scope is urgent in the infinite dimensional context, due to the high data dimensionality: in many applications, having a sparse clustering solution can lead to more reliable, interpretable, and robust results. We propose an innovative generalization of the problem of sparse clustering to the infinite dimensional setting: it is stated as an optimization problem, whose solution exists under reasonable assumptions. The method is again tested on the Berkeley Growth Study dataset, and a comparison with the analysis described in Chapter 2 is also discussed. With Chapter 4 we enter the second part of the thesis. In this Chapter, the innovative methodology proposed for the classification of functional

data with spatial dependence, indexed by the sites of a huge lattice, is fully introduced and described. To our knowledge, the problem of treating functional data indexed by a lattice had never been taken into account in the statistical literature on functional data. A common approach to treat such a kind of data is to resort to spatio – temporal modelling, often relying on very restrictive assumptions on the stationarity of the process with respect to the spatial component. The proposed innovative clustering technique is instead non – parametric: it is based on the bagging of coarse classifiers, which are obtained by repeatedly accounting for spatial dependence via random systems of neighbourhoods (random Voronoi tessellations). The

method has been extensively tested via a battery of simulation studies. The application to a real data set, concerning clustering of irradiance patterns for solar power applications, is also reported. One of the attained results is shown in Figure 1. Finally, focus of Chapter 5 is the generalization of the strategy proposed in Chapter 4 to a problem of dimensional reduction. This generalization is motivated by a case study concerning functional mobile – network patterns in time, geo-referenced on the metropolitan area of Milan: the analysis of these data has a possible innovative impact on a city planning analysis of Milan, and it can provide information about people mobility and behaviour. The generalization of the Bagging Voronoi strategy to a different problem with respect to classification is not trivial, since the aggregation part of the algorithm has to be carefully modified: for this particular application, the aggregation strategy is obtained through a novel 1-median alignment algorithm. The results of the analysis are disclosing patterns amenable of a clear spatiotemporal interpretation, e.g. average population density, working and residential activities, universities, shopping, leisure, and morning/evening road/railways commuting.

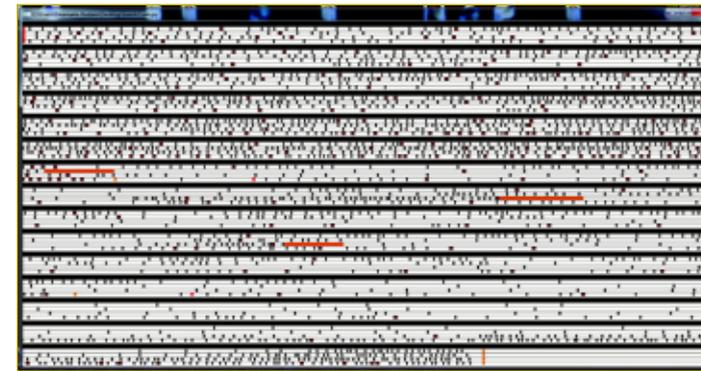
A STOCHASTIC CONTINUOUS CELLULAR AUTOMATA TRAFFIC MODEL WITH FUZZY DECISION RULES

Oznur Yeldan (ex Mathematical Engineering)

In recent decades, growing traffic congestion has become one of the most prior problem of the society. Traffic models are thus fundamental resources in the management of road network. There is a wide range of alternative modeling approaches now available which can be roughly divided into three categories: macroscopic, mesoscopic and microscopic models depending on the level of detail. Microscopic models are promising models for their ability to simulate detailed phenomena (each individual vehicle) in traffic which yields to an accurate representation of traffic flow, and macroscopic ideas can also be studied with microscopic models. On the other hand, these models have the disadvantage of the computational requirements and their associated costs (e.g., parallel computing) requiring modern computer power. Among microscopic traffic flow models, cellular automata (CA) models have the ability of being easily implemented for parallel computing because of their intrinsic synchronous behavior. A cellular automaton is a collection of cells (sites) on a grid of specified shape (lattice) that evolves through a number of discrete time steps according to a set of local rules based on the states of neighboring cells. The models based on CA are conceptually simple, thus it can

be used a set of simple rules to simulate a complex behavior. In other words, the simplicity of these models make them numerically very efficient and can be used to simulate large road networks in real-time or even faster. CA models are capable of capturing micro-level dynamics and relating these to macro-level traffic flow behavior. However, these models are lack of the accuracy of other microscopic traffic models such as the car-following models. A basic one-dimensional CA model for highway traffic flow was first introduced by Wolfram (R184), where he gave an extensive classification of CA models as mathematical models for self-organizing dynamic systems. Nagel and Schreckenberg proposed the first nontrivial stochastic traffic model (the NaSch model) based on CA to simulate single-lane traffic with closed boundary conditions in 1992, which is a variant of R184. In literature, there are many attempts in that direction and in all these models the cells represent the space as it is in the NaSch model, so we call them as "NaSch-type" models. In this dissertation, we propose a new stochastic traffic model using continuous cellular automata (CCA), CA where the set of states is infinite. By defining a new class of CA traffic model, we get closer to

the car-following models where we introduce some continuity without losing the computational advantages which are typical of CA models. Therefore, to define a CA traffic model where the space is a continuous variable, we abandon the idea "the space is discretely represented by cells" and we embrace a new philosophy where we assume that cells represent vehicles. This gives the immediate advantage of having less cells to compute compared to the previous CA traffic models. Moreover, the continuity in space gives us the possibility to refine the microscopic rules that govern the traffic dynamic by using fuzzy reasoning (fuzzy logic) to mimic different driver behaviors. Therefore, in our open boundary CA model, we apply a multi-agent fuzzy system where all parameters of the decision process of the drivers are modeled individually by means of fuzzy subsets, thus various types of drivers can be taken into consideration. In this way, we study how the heterogeneity (the different composition of vehicles) influences the traffic macroscopically. The CCA model proposed here is defined first for a single-lane road and then the model is extended to the multi-lane case where the extension is not as natural as "NaSch-type" models. Thus, we present the multi-lane model as a union



1. A screenshot of the real-time simulator.

of interacting single-lane CCA where the interaction is given by a transfer operation. The decision for lane-changing in the multi-lane model is depending on a stress parameter representing how much the driver is above or below of his optimal velocity (the velocity specified for each kind of vehicle with which they feel comfortable in traffic). Furthermore, the process of lane-changing is based on some safety criteria which check the possibility of executing a lane-changing by considering the situation on the target lane. These criteria guarantee that after the lane-changing there will be no danger (avoidance of collision) with the vehicles on the target lane. We assume that the precedence for the lane-changing is given to the vehicles moving from left to right, since on the highways that apply European rules where

the overtaking is only allowed on the left, the right-most lane is the slowest and the left-most lane is the fastest lane. After we describe our multi-lane model, we prove that it can actually be simulated by a suitable CCA. In this way, we have framed the model inside the class of CCA. For a first test, we have implemented our model using Python with an object-oriented philosophy of programming and we have simulated a piece of highway with an on- and off-toll plaza and an obstacle. Using a questionnaire we have set up two kinds of vehicles (passenger vehicles and long vehicles) which we have used to run a series of experiments. In all the experiments carried out, we have noticed that the heterogeneity is an important factor in influencing the flow. In the fundamental diagram, we have seen that adding even a small amount of

long vehicles to the traffic stream changes the diagram significantly. The experiments also show that the model reproduces the typical traffic flow phenomena such as the transition between the flow phases, the metastable states and the back propagation wave effect. The code written in Python does not take advantage of the CA and its typical synchronous behavior. For this reason, we have also adapted the code using PyCuda to partially parallelize the model on GPU's and we have seen that it is possible to boost the speed of execution by a factor of ~10 (on a laptop equipped with a processor i7 intel and with a graphic card NVIDIA GeForce GT 555M). By partial parallelization, we mean that the lane-changing process performed using the transfer operations is done sequentially, and the only parts that can be run in parallel is the global transition function. Therefore the model can be completely parallelized only if we decide not to apply the precedence rules and assume a concurrent strategy of lane-changing. A screenshot of the real-time simulator can be seen in Figure 1 where we have generated a random four-lane highway of length 22000 m. with an on-toll plaza, an off-toll plaza, two on-toll ramps, two off-toll ramps and three obstacles.