RESEARCH CENTRE

Inria Centre at Université Côte d'Azur

IN PARTNERSHIP WITH:

Université Côte d'Azur

2023 ACTIVITY REPORT

Project-Team ACUMES

Analysis and Control of Unsteady Models for Engineering Sciences

IN COLLABORATION WITH: Laboratoire Jean-Alexandre Dieudonné (JAD)

DOMAIN

Applied Mathematics, Computation and Simulation

THEME

Numerical schemes and simulations

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Project-Team ACUMES

Creation of the Project-Team: 2016 July 01

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1 Team members, visitors, external collaborators

Research Scientists

- Paola Goatin [Team leader, INRIA, Senior Researcher, HDR]
- Mickael Binois [INRIA, Researcher]
- Régis Duvigneau [INRIA, Senior Researcher, HDR]
- Jean-Antoine Désidéri [INRIA, Emeritus, HDR]

Faculty Member

- Abderrahmane Habbal [UNIV COTE D'AZUR, Associate Professor, HDR]

Post-Doctoral Fellows

- Daniel Eduardo Inzunza Herrera [INRIA, Post-Doctoral Fellow, until Aug 2023]
- Khadija Musayeva [INRIA, Post-Doctoral Fellow]
- Enrico Siri [INRIA, Post-Doctoral Fellow]

PhD Students

- Mustapha Bahari [UNIV MOHAMMED VI POLYTECH]
- Ilaria Ciaramaglia [INRIA, from Sep 2023]
- Agatha Joumaa [IFPEN]
- Carmen Mezquita Nieto [INRIA, from Sep 2023]
- Nathan Ricard [INRIA, from Nov 2023]
- Alexandra Wuerth [INRIA]

Interns and Apprentices

- Guillaume Coulaud [INRIA, Intern, from Apr 2023 until Sep 2023]

Administrative Assistant

- Quentin Campeon [INRIA]

Visiting Scientist

- Alessandra Rizzo [UNIV DEGLI STUDI DI MESSINA, from Mar 2023 until May 2023]

2 Overall objectives

ACUMES aims at developing a rigorous framework for numerical simulations and optimal control for transportation and buildings, with focus on multi-scale, heterogeneous, unsteady phenomena subject to uncertainty. Starting from established macroscopic Partial Differential Equation (PDE) models, we pursue a set of innovative approaches to include small-scale phenomena, which impact the whole system. Targeting applications contributing to sustainability of urban environments, we couple the resulting models with robust control and optimization techniques.

Modern engineering sciences make an important use of mathematical models and numerical simulations at the conception stage. Effective models and efficient numerical tools allow for optimization before production and to avoid the construction of expensive prototypes or costly post-process adjustments. Most up-to-date modeling techniques aim at helping engineers to increase performances and safety and reduce costs and pollutant emissions of their products. For example, mathematical traffic flow models are used by civil engineers to test new management strategies in order to reduce congestion on the existing road networks and improve crowd evacuation from buildings or other confined spaces without constructing new infrastructures. Similar models are also used in mechanical engineering, in conjunction with concurrent optimization methods, to reduce energy consumption, noise and pollutant emissions of cars, or to increase thermal and structural efficiency of buildings while, in both cases, reducing ecological costs.

Nevertheless, current models and numerical methods exhibit some limitations:

- Most simulation-based design procedures used in engineering still rely on steady (time-averaged) state models. Significant improvements have already been obtained with such a modeling level, for instance by optimizing car shapes, but finer models taking into account unsteady phenomena are required in the design phase for further improvements.
- The classical purely macroscopic approach, while offering a framework with a sound analytical basis, performing numerical techniques and good modeling features to some extent, is not able to reproduce some particular phenomena related to specific interactions occurring at lower (possibly micro) level. We refer for example to self-organizing phenomena observed in pedestrian flows, or to the dynamics of turbulent flows for which large scale / small scale vortical structures interfere. These flow characteristics need to be taken into account to obtain more precise models and improved optimal solutions.
- Uncertainty related to operational conditions (e.g. inflow velocity in aerodynamics), or models (e.g. individual behavior in crowds) is still rarely considered in engineering analysis and design, yielding solutions of poor robustness.

This project focuses on the analysis and optimal control of classical and non-classical evolutionary systems of Partial Differential Equations (PDEs) arising in the modeling and optimization of engineering problems related to safety and sustainability of urban environments, mostly involving fluid-dynamics and structural mechanics. The complexity of the involved dynamical systems is expressed by multi-scale, time-dependent phenomena, possibly subject to uncertainty, which can hardly be tackled using classical approaches, and require the development of unconventional techniques.

3 Research program

3.1 Research directions

The project develops along the following two axes:

- modeling complex systems through novel (unconventional) PDE systems, accounting for multi-scale phenomena and uncertainty;
- optimization and optimal control algorithms for systems governed by the above PDE systems.

These themes are motivated by the specific problems treated in the applications, and represent important and up-to-date issues in engineering sciences. For example, improving the design of transportation means and civil buildings, and the control of traffic flows, would result not only in better performances of the object of the optimization strategy (vehicles, buildings or road networks level of service), but also in enhanced safety and lower energy consumption, contributing to reduce costs and pollutant emissions.

3.2 PDE models accounting for multi-scale phenomena and uncertainties

Dynamical models consisting of evolutionary PDEs, mainly of hyperbolic type, appear classically in the applications studied by the previous Project-Team Opale (compressible flows, traffic, cell-dynamics, medicine, etc). Yet, the classical purely macroscopic approach is not able to account for some particular phenomena related to specific interactions occurring at smaller scales. These phenomena can be of greater importance when dealing with particular applications, where the "first order" approximation given by the purely macroscopic approach reveals to be inadequate. We refer for example to self-organizing phenomena observed in pedestrian flows [117], or to the dynamics of turbulent flows for which large scale / small scale vortical structures interfere [143].

Nevertheless, macroscopic models offer well known advantages, namely a sound analytical framework, fast numerical schemes, the presence of a low number of parameters to be calibrated, and efficient optimization procedures. Therefore, we are convinced of the interest of keeping this point of view as dominant, while completing the models with information on the dynamics at the small scale / microscopic level. This can be achieved through several techniques, like hybrid models, homogenization, mean field games. In this project, we will focus on the aspects detailed below.

The development of adapted and efficient numerical schemes is a mandatory completion, and sometimes ingredient, of all the approaches listed below. The numerical schemes developed by the team are based on finite volumes or finite elements techniques, and constitute an important tool in the study of the considered models, providing a necessary step towards the design and implementation of the corresponding optimization algorithms, see Section 3.3.

3.2.1 Micro-macro couplings

Modeling of complex problems with a dominant macroscopic point of view often requires couplings with small scale descriptions. Accounting for systems heterogeneity or different degrees of accuracy usually leads to coupled PDE-ODE systems.

In the case of heterogeneous problems the coupling is "intrinsic", i.e. the two models evolve together and mutually affect each-other. For example, accounting for the impact of a large and slow vehicle (like a bus or a truck) on traffic flow leads to a strongly coupled system consisting of a (system of) conservation law(s) coupled with an ODE describing the bus trajectory, which acts as a moving bottleneck. The coupling is realized through a local unilateral moving constraint on the flow at the bus location, see [85] for an existence result and [71, 86] for numerical schemes.

If the coupling is intended to offer higher degree of accuracy at some locations, a macroscopic and a microscopic model are connected through an artificial boundary, and exchange information across it through suitable boundary conditions. See [77, 103] for some applications in traffic flow modelling, and [96, 100, 102] for applications to cell dynamics.

The corresponding numerical schemes are usually based on classical finite volume or finite element methods for the PDE, and Euler or Runge-Kutta schemes for the ODE, coupled in order to take into account the interaction fronts. In particular, the dynamics of the coupling boundaries require an accurate handling capturing the possible presence of non-classical shocks and preventing diffusion, which could produce wrong solutions, see for example [71, 86].

We plan to pursue our activity in this framework, also extending the above mentioned approaches to problems in two or higher space dimensions, to cover applications to crowd dynamics or fluid-structure interaction.

3.2.2 Micro-macro limits

Rigorous derivation of macroscopic models from microscopic ones offers a sound basis for the proposed modeling approach, and can provide alternative numerical schemes, see for example [78, 91] for the derivation of Lighthill-Whitham-Richards [129, 142] traffic flow model from Follow-the-Leader and [97] for results on crowd motion models (see also [119]). To tackle this aspect, we will rely mainly on two (interconnected) concepts: measure-valued solutions and mean-field limits.

The notion of **measure-valued solutions** for conservation laws was first introduced by DiPerna [92], and extensively used since then to prove convergence of approximate solutions and deduce existence results, see for example [98] and references therein. Measure-valued functions have been recently advocated as the appropriate notion of solution to tackle problems for which analytical results (such as existence and uniqueness of weak solutions in distributional sense) and numerical convergence are missing [59, 99]. We refer, for example, to the notion of solution for non-hyperbolic systems [105], for which no general theoretical result is available at present, and to the convergence of finite volume schemes for systems of hyperbolic conservation laws in several space dimensions, see [99].

In this framework, we plan to investigate and make use of measure-based PDE models for vehicular and pedestrian traffic flows. Indeed, a modeling approach based on (multi-scale) time-evolving measures (expressing the agents probability distribution in space) has been recently introduced (see the monograph [82]), and proved to be successful for studying emerging self-organised flow patterns [81]. The theoretical measure framework proves to be also relevant in addressing micro-macro limiting procedures of mean field type [106], where one lets the number of agents going to infinity, while keeping the total mass constant. In this case, one must prove that the *empirical measure*, corresponding to the sum of Dirac measures concentrated at the agents positions, converges to a measure-valued solution of the corresponding macroscopic evolution equation. We recall that a key ingredient in this approach is the use of the *Wasserstein distances* [151, 150]. Indeed, as observed in [136, Section 6], the usual L^1 spaces are not natural in this context, since they don't guarantee uniqueness of solutions.

This procedure can potentially be extended to more complex configurations, like for example road networks or different classes of interacting agents, or to other application domains, like cell-dynamics.

Another powerful tool we shall consider to deal with micro-macro limits is the so-called **Mean Field Games (MFG)** technique (see the seminal paper [128]). This approach has been recently applied to some of the systems studied by the team, such as traffic flow and cell dynamics. In the context of crowd dynamics, including the case of several populations with different targets, the mean field game approach has been adopted in [67, 66, 93, 127], under the assumption that the individual behavior evolves according to a stochastic process, which gives rise to parabolic equations greatly simplifying the analysis of the system. Besides, a deterministic context is studied in [138], which considers a non-local velocity field. For cell dynamics, in order to take into account the fast processes that occur in the migration-related machinery, a framework such as the one developed in [84] to handle games "where agents evolve their strategies according to the best-reply scheme on a much faster time scale than their social configuration variables" may turn out to be suitable. An alternative framework to MFG is also considered. This framework is based on the formulation of -Nash- games constrained by the **Fokker-Planck** (FP, [57]) partial differential equations that govern the time evolution of the probability density functions -PDF- of stochastic systems and on objectives that may require to follow a given PDF trajectory or to minimize an expectation functional.

3.2.3 Non-local flows

Non-local interactions can be described through macroscopic models based on integro-differential equations. Systems of the type

$$\partial_t u + div_{\mathbf{x}} F(t, \mathbf{x}, u, W) = 0, \qquad t > 0, \mathbf{x} \in R^d, d \geq 1, \tag{1}$$

where $u = u(t, \mathbf{x}) \in R^N$, $N \geq 1$ is the vector of conserved quantities and the variable $W = W(t, \mathbf{x}, u)$ depends on an integral evaluation of u, arise in a variety of physical applications. Space-integral terms are considered for example in models for granular flows [54], sedimentation [61], supply chains [110], conveyor belts [108], biological applications like structured populations dynamics [135], or more general problems like gradient constrained equations [56]. Also, non-local in time terms arise in conservation laws with memory, starting from [83]. In particular, equations with non-local flux have been recently introduced in traffic flow modeling to account for the reaction of drivers or pedestrians to the surrounding density of other individuals, see [62, 69, 74, 107, 146]. While pedestrians are likely to react to the presence of people all around them, drivers will mainly adapt their velocity to the downstream traffic, assigning a greater importance to closer vehicles. In particular, and in contrast to classical (without integral terms) macroscopic equations, these models are able to display finite acceleration of vehicles through Lipschitz bounds on the mean velocity [62, 107] and lane formation in crossing pedestrian flows.

General analytical results on non-local conservation laws, proving existence and possibly uniqueness of solutions of the Cauchy problem for (1), can be found in [55] for scalar equations in one space dimension ($N = d = 1$), in [75] for scalar equations in several space dimensions ($N = 1$, $d \geq 1$) and in [52], [76, 80] for multi-dimensional systems of conservation laws. Besides, specific finite volume numerical methods have been developed recently in [52, 107] and [126].

Relying on these encouraging results, we aim to push a step further the analytical and numerical study of non-local models of type (1), in particular concerning well-posedness of initial - boundary value problems, regularity of solutions and high-order numerical schemes.

3.2.4 Uncertainty in parameters and initial-boundary data

Different sources of uncertainty can be identified in PDE models, related to the fact that the problem of interest is not perfectly known. At first, initial and boundary condition values can be uncertain. For instance, in traffic flows, the time-dependent value of inlet and outlet fluxes, as well as the initial distribution of vehicles density, are not perfectly determined [68]. In aerodynamics, inflow conditions like velocity modulus and direction, are subject to fluctuations [115, 134]. For some engineering problems, the geometry of the boundary can also be uncertain, due to structural deformation, mechanical wear or disregard of some details [95]. Another source of uncertainty is related to the value of some parameters in the PDE models. This is typically the case of parameters in turbulence models in fluid mechanics, which have been calibrated according to some reference flows but are not universal [144, 149], or in traffic flow models, which may depend on the type of road, weather conditions, or even the country of interest (due to differences in driving rules and conductors behaviour). This leads to equations with flux functions depending on random parameters [145, 148], for which the mean and the variance of the solutions can be computed using different techniques. Indeed, uncertainty quantification for systems governed by PDEs has become a very active research topic in the last years. Most approaches are embedded in a probabilistic framework and aim at quantifying statistical moments of the PDE solutions, under the assumption that the characteristics of uncertain parameters are known. Note that classical Monte-Carlo approaches exhibit low convergence rate and consequently accurate simulations require huge computational times. In this respect, some enhanced algorithms have been proposed, for example in the balance law framework [133]. Different approaches propose to modify the PDE solvers to account for this probabilistic context, for instance by defining the non-deterministic part of the solution on an orthogonal basis (Polynomial Chaos decomposition) and using a Galerkin projection [115, 125, 130, 153] or an entropy closure method [90], or by discretizing the probability space and extending the numerical schemes to the stochastic components [51]. Alternatively, some other approaches maintain a fully deterministic PDE resolution, but approximate the solution in the vicinity of the reference parameter values by Taylor series expansions based on first- or second-order sensitivities [139, 149, 152].

Our objective regarding this topic is twofold. In a pure modeling perspective, we aim at including uncertainty quantification in models calibration and validation for predictive use. In this case, the choice of the techniques will depend on the specific problem considered [60]. Besides, we plan to extend previous works on sensitivity analysis [95, 131] to more complex and more demanding problems. In particular, high-order Taylor expansions of the solution (greater than two) will be considered in the framework of the Sensitivity Equation Method [63] (SEM) for unsteady aerodynamic applications, to improve the accuracy of mean and variance estimations. A second targeted topic in this context is the study of the uncertainty related to turbulence closure parameters, in the sequel of [149]. We aim at exploring the capability of the SEM approach to detect a change of flow topology, in case of detached flows. Our ambition is to contribute to the emergence of a new generation of simulation tools, which will provide solution densities rather than values, to tackle real-life uncertain problems. This task will also include a reflection about numerical schemes used to solve PDE systems, in the perspective of constructing a unified numerical framework able to account for exact geometries (isogeometric methods), uncertainty propagation and sensitivity analysis with respect to control parameters.

3.3 Optimization and control algorithms for systems governed by PDEs

The non-classical models described above are developed in the perspective of design improvement for real-life applications. Therefore, control and optimization algorithms are also developed in conjunction with these models. The focus here is on the methodological development and analysis of optimization algorithms for PDE systems in general, keeping in mind the application domains in the way the problems are mathematically formulated.

3.3.1 Sensitivity vs. adjoint equation

Adjoint methods (achieved at continuous or discrete level) are now commonly used in industry for steady PDE problems. Our recent developments [141] have shown that the (discrete) adjoint method can be efficiently applied to cost gradient computations for time-evolving traffic flow on networks, thanks to the special structure of the associated linear systems and the underlying one dimensionality of the problem. However, this strategy is questionable for more complex (e.g. 2D/3D) unsteady problems, because it requires sophisticated and time-consuming check-pointing and/or re-computing strategies [58, 109] for the backward time integration of the adjoint variables. The sensitivity equation method (SEM) offers a promising alternative [94, 120], if the number of design parameters is moderate. Moreover, this approach can be employed for other goals, like fast evaluation of neighboring solutions or uncertainty propagation [95].
Regarding this topic, we intend to apply the continuous sensitivity equation method to challenging problems. In particular, in aerodynamics, multi-scale turbulence models like Large-Eddy Simulation (LES) [143] , Detached-Eddy Simulation (DES) [147] or Organized-Eddy Simulation (OES) [64], are more and more employed to analyze the unsteady dynamics of the flows around bluff-bodies, because they have the ability to compute the interactions of vortices at different scales, contrary to classical Reynolds-Averaged Navier-Stokes models. However, their use in design optimization is tedious, due to the long time integration required. In collaboration with turbulence specialists (M. Braza, CNRS - IMFT), we aim at developing numerical methods for effective sensitivity analysis in this context, and apply them to realistic problems, like the optimization of active flow control devices. Note that the use of SEM allows computing cost functional gradients at any time, which permits to construct new gradient-based optimization strategies like instantaneous-feedback method [123] or multiobjective optimization algorithm (see section below).

3.3.2 Integration of Computer-Aided Design and analysis for shape optimization

A major difficulty in shape optimization is related to the multiplicity of geometrical representations handled during the design process. From high-order Computer-Aided Design (CAD) objects to discrete mesh-based descriptions, several geometrical transformations have to be performed, that considerably impact the accuracy, the robustness and the complexity of the design loop. This is even more critical when multiphysics applications are targeted, including moving bodies.

To overcome this difficulty, we intend to investigate *isogeometric analysis* [121] methods, which propose to use the same CAD representations for the computational domain and the physical solutions yielding geometrically exact simulations. In particular, hyperbolic systems and compressible aerodynamics are targeted.

3.3.3 Multi-objective descent algorithms for multi-disciplinary, multi-point, unsteady optimization or robust-design

In differentiable optimization, multi-disciplinary, multi-point, unsteady optimization or robust-design can all be formulated as multi-objective optimization problems. In this area, we have proposed the *Multiple-Gradient Descent Algorithm (MGDA)* to handle all criteria concurrently [88] [87]. Originally, we have stated a principle according to which, given a family of local gradients, a descent direction common to all considered objective-functions simultaneously is identified, assuming the Pareto-stationarity condition is not satisfied. When the family is linearly-independent, we have access to a direct algorithm. Inversely, when the family is linearly-dependent, a quadratic-programming problem should be solved. Hence, the technical difficulty is mostly conditioned by the number m of objective functions relative to the search space dimension n. In this respect, the basic algorithm has recently been revised [89] to handle the case where $m > n$, and even $m \gg n$, and is currently being tested on a test-case of robust design subject to a periodic time-dependent Navier-Stokes flow.

The multi-point situation is very similar and, being of great importance for engineering applications, will be treated at large.

Moreover, we intend to develop and test a new methodology for robust design that will include uncertainty effects. More precisely, we propose to employ MGDA to achieve an effective improvement of all criteria simultaneously, which can be of statistical nature or discrete functional values evaluated in confidence intervals of parameters. Some recent results obtained at ONERA [137] by a stochastic variant of our methodology confirm the viability of the approach. A PhD thesis has also been launched at ONERA/DADS.

Lastly, we note that in situations where gradients are difficult to evaluate, the method can be assisted by a meta-model [155].

3.3.4 Bayesian Optimization algorithms for efficient computation of general equilibria

Bayesian Optimization (BO) relies on Gaussian processes, which are used as emulators (or surrogates) of the black-box model outputs based on a small set of model evaluations. Posterior distributions provided by the Gaussian process are used to design acquisition functions that guide sequential search strategies that balance between exploration and exploitation. Such approaches have been transposed to frameworks other than optimization, such as uncertainty quantification. Our aim is to investigate how the BO apparatus can be applied to the search of general game equilibria, and in particular the classical Nash equilibrium (NE). To this end, we propose two complementary acquisition functions, one based on a greedy search approach and one based on the Stepwise Uncertainty Reduction paradigm [101]. Our proposal is designed to tackle derivative-free, expensive models, hence requiring very few model evaluations to converge to the solution.

3.3.5 Decentralized strategies for inverse problems

Most if not all the mathematical formulations of inverse problems (a.k.a. reconstruction, identification, data recovery, non destructive engineering,...) are known to be ill posed in the Hadamard sense. Indeed, in general, inverse problems try to fulfill (minimize) two or more very antagonistic criteria. One classical example is the Tikhonov regularization, trying to find artificially smoothed solutions close to naturally non-smooth data.

We consider here the theoretical general framework of parameter identification coupled to (missing) data recovery. Our aim is to design, study and implement algorithms derived within a game theoretic framework, which are able to find, with computational efficiency, equilibria between the "identification related players" and the "data recovery players". These two parts are known to pose many challenges, from a theoretical point of view, like the identifiability issue, and from a numerical one, like convergence, stability and robustness problems. These questions are tricky [53] and still completely open for systems like coupled heat and thermoelastic joint data and material detection.

4 Application domains

4.1 Active flow control for vehicles

The reduction of CO_2 emissions represents a great challenge for the automotive and aeronautic industries, which committed respectively a decrease of 20% for 2020 and 75% for 2050. This goal will not be reachable, unless a significant improvement of the aerodynamic performance of cars and aircrafts is achieved (e.g. aerodynamic resistance represents 70% of energy losses for cars above 90 km/h). Since vehicle design cannot be significantly modified, due to marketing or structural reasons, active flow control technologies are one of the most promising approaches to improve aerodynamic performance. This consists in introducing micro-devices, like pulsating jets or vibrating membranes, that can modify vortices generated by vehicles. Thanks to flow non-linearities, a small energy expense for actuation can significantly reduce energy losses. The efficiency of this approach has been demonstrated, experimentally as well as numerically, for simple configurations [154].

However, the lack of efficient and flexible numerical tools, that allow to simulate and optimize a large number of such devices on realistic configurations, is still a bottleneck for the emergence of this technology in industry. The main issue is the necessity of using high-order schemes and complex models to simulate actuated flows, accounting for phenomena occurring at different scales. In this context, we intend to contribute to the following research axes:

- *Sensitivity analysis for actuated flows.* Adjoint-based (reverse) approaches, classically employed in design optimization procedure to compute functional gradients, are not well suited to this context. Therefore, we propose to explore the alternative (direct) formulation, which is not so much used, in the perspective of a better characterization of actuated flows and optimization of control devices.

- *Isogeometric simulation of control devices.* To simulate flows perturbed by small-scale actuators, we investigate the use of isogeometric analysis methods, which allow to account exactly for CAD-based geometries in a high-order hierarchical representation framework. In particular, we try to exploit the features of the method to simulate more accurately complex flows including moving devices and multiscale phenomena.

4.2 Vehicular and pedestrian traffic flows

Intelligent Transportation Systems (ITS) is nowadays a booming sector, where the contribution of mathematical modeling and optimization is widely recognized. In this perspective, traffic flow models are a commonly cited example of "complex systems", in which individual behavior and self-organization phenomena must be taken into account to obtain a realistic description of the observed macroscopic dynamics [116]. Further improvements require more advanced models, keeping into better account interactions at the microscopic scale, and adapted control techniques, see [65] and references therein.

In particular, we will focus on the following aspects:

- *Junction models.* We are interested in designing a general junction model both satisfying basic analytical properties guaranteeing well-posedness and being realistic for traffic applications. In particular, the model should be able to overcome severe drawbacks of existing models, such as restrictions on the number of involved roads and prescribed split ratios [79, 104], which limit their applicability to real world situations. Hamilton-Jacobi equations could be also an interesting direction of research, following the recent results obtained in [122].

- *Data assimilation.* In traffic flow modeling, the capability of correctly estimating and predicting the state of the system depends on the availability of rich and accurate data on the network. Up to now, the most classical sensors are fixed ones. They are composed of inductive loops (electrical wires) that are installed at different spatial positions of the network and that can measure the traffic flow, the occupancy rate (i.e. the proportion of time during which a vehicle is detected to be over the loop) and the speed (in case of a system of two distant loops). These data are useful / essential to calibrate the phenomenological relationship between flow and density which is known in the traffic literature as the Fundamental Diagram. Nowadays, thanks to the wide development of mobile internet and geolocalization techniques and its increasing adoption by the road users, smartphones have turned into perfect mobile sensors in many domains, including in traffic flow management. They can provide the research community with a large database of individual trajectory sets that are known as Floating Car Data (FCD), see [118] for a real field experiment. Classical macroscopic models, say (hyperbolic systems of) conservation laws, are not designed to take into account this new kind of microscopic data. Other formulations, like Hamilton-Jacobi partial differential equations, are most suited and have been intensively studied in the past five years (see [72, 73]), with a stress on the (fixed) Eulerian framework. Up to our knowledge, there exist a few studies in the time-Lagrangian as well as space-Lagrangian frameworks, where data coming from mobile sensors could be easily assimilated, due to the fact that the Lagrangian coordinate (say the label of a vehicle) is fixed.

- *Control of autonomous vehicles.* Traffic flow is usually controlled via traffic lights or variable speed limits, which have fixed space locations. The deployment of autonomous vehicles opens new perspectives in traffic management, as the use of a small fraction of cars to optimize the overall traffic. In this perspective, the possibility to track vehicles trajectories either by coupled micro-macro models [85, 103] or via the Hamilton-Jacobi approach [72, 73] could allow to optimize the flow by controlling some specific vehicles corresponding to internal conditions.

4.3 Combined hormone and brachy therapies for the treatment of prostate cancer

The latest statistics published by the International Agency for Research on Cancer show that in 2018, 18.1 million new cancer cases have been identified and 9.6 million deaths have been recorded worldwide making it the second leading cause of death globally. Prostate cancer ranks third in incidence with 1.28 million cases and represents the second most commonly diagnosed male cancer.

Prostate cells need the hormone androgen to survive and function properly. For this to happen, the androgens have to bind to a protein in the prostate cells called Androgen Receptor and activate it. Since androgens act as a growth factor for the cells, one way of treating prostate cancer is through the antihormone therapy that hinder its activity. The Androgen Deprivation Therapy (ADT) aims to either reduce androgen production or to stop the androgens from working through the use of drugs. However, over time, castration-resistant cells that are able to sustain growth in a low androgen environment emerge. The castration-resistant cells can either be androgen independent or androgen repressed meaning that they have a negative growth rate when the androgen is abundant in the prostate. In order to delay the development of castration resistance and reduce its occurrence, the Intermittent Androgen Deprivation Therapy is used.

On the other hand, brachytherapy is an effective radiation therapy used in the treatment of prostate cancer by placing a sealed radiation source inside the prostate gland. It can be delivered in high dose rates (HDR) or low dose rates (LDR) depending on the radioactive source used and the duration of treatment.

In the HDR brachytherapy the source is placed temporarily in the prostate for a few minutes to deliver high dose radiation while for the LDR brachytherapy low radiations dose are delivered from radioactive sources permanently placed in the prostate. The radioactivity of the source decays over time, therefore its presence in the prostate does not cause any long-term concern as its radioactivity disappears eventually. In practice, brachytherapy is prescribed either as monotherapy, often for localized tumors, or combined with another therapy such as external beam radiation therapy for which the total dose prescribed is divided between internal and external radiation. Brachytherapy can also be prescribed in combination with hormone therapy.

However, in the existing literature there is currently no mathematical model that explores this combination of treatments. Our aim is to develop a computational model based on partial differential equations to assess the effectiveness of combining androgen deprivation therapy with brachytherapy in the treatment of prostate cancer. The resulting simulations can be used to explore potential unconventional therapeutic strategies.

4.4 Other application fields

Besides the above mentioned axes, which constitute the project's identity, the methodological tools described in Section have a wider range of application. We currently carry on also the following research actions, in collaboration with external partners.

- **Game strategies for thermoelastography.** Thermoelastography is an innovative non-invasive control technology, which has numerous advantages over other techniques, notably in medical imaging [132]. Indeed, it is well known that most pathological changes are associated with changes in tissue stiffness, while remaining isoechoic, and hence difficult to detect by ultrasound techniques. Based on elastic waves and heat flux reconstruction, thermoelastography shows no destructive or aggressive medical sequel, unlike X-ray and comparables techniques, making it a potentially prominent choice for patients.

  Physical principles of thermoelastography originally rely on dynamical structural responses of tissues, but as a first approach, we only consider static responses of linear elastic structures.

The mathematical formulation of the thermoelasticity reconstruction is based on data completion and material identification, making it a harsh ill-posed inverse problem. In previous works [111, 124], we have demonstrated that Nash game approaches are efficient to tackle ill-posedness. We intend to extend the results obtained for Laplace equations in [111], and the algorithms developed in Section 3.3.5 to the following problems (of increasing difficulty):
- Simultaneous data and parameter recovery in linear elasticity, using the so-called Kohn and Vogelius functional (ongoing work, some promising results obtained).
- Data recovery in coupled heat-thermoelasticity systems.
- Data recovery in linear thermoelasticity under stochastic heat flux, where the imposed flux is stochastic.
- Data recovery in coupled heat-thermoelasticity systems under stochastic heat flux, formulated as an incomplete information Nash game.
- Application to robust identification of cracks.

- **Constraint elimination in Quasi-Newton methods.** In single-objective differentiable optimization, Newton's method requires the specification of both gradient and Hessian. As a result, the convergence is quadratic, and Newton's method is often considered as the target reference. However, in applications to distributed systems, the functions to be minimized are usually "functionals", which depend on the optimization variables by the solution of an often complex set of PDE's, through a chain of computational procedures. Hence, the exact calculation of the full Hessian becomes a complex and costly computational endeavor.

  This has fostered the development of *quasi-Newton's methods* that mimic Newton's method but use only the gradient, the Hessian being iteratively constructed by successive approximations inside the algorithm itself. Among such methods, the Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm is well-known and commonly employed. In this method, the Hessian is corrected at each new iteration by rank-one matrices defined from several evaluations of the gradient only. The BFGS method has "super-linear convergence".

  For constrained problems, certain authors have developed so-called *Riemannian BFGS*, e.g. [140], that have the desirable convergence property in constrained problems. However, in this approach, the constraints are assumed to be known formally, by explicit expressions.

  In collaboration with ONERA-Meudon, we are exploring the possibility of representing constraints, in successive iterations, through local approximations of the constraint surfaces, splitting the design space locally into tangent and normal subspaces, and eliminating the normal coordinates through a linearization, or more generally a finite expansion, and applying the BFGS method through dependencies on the coordinates in the tangent subspace only. Preliminary experiments on the difficult Rosenbrock test-case, although in low dimensions, demonstrate the feasibility of this approach. On-going research is on theorizing this method, and testing cases of higher dimensions.

- **Multi-objective optimization for nanotechnologies.** Our team takes part in a larger collaboration with CEA/LETI (Grenoble), initiated by the Inria Project-Team Nachos (now Atlantis), and related to the Maxwell equations. Our component in this activity relates to the optimization of nanophotonic devices, in particular with respect to the control of thermal loads. We have first identified a gradation of representative test-cases of increasing complexity:
  - infrared micro-source;
  - micro-photoacoustic cell;
  - nanophotonic device.

  These cases involve from a few geometric parameters to be optimized to a functional minimization subject to a finite-element solution involving a large number of degrees of freedom. CEA disposes of such codes, but considering the computational cost of the objective functions in the complex cases, the first part of our study is focused on the construction and validation of meta-models, typically of RBF-type. Multi-objective optimization will be carried out subsequently by MGDA, and possibly Nash games.

5 Social and environmental responsibility

5.1 Impact of research results

The research conducted with the startup Mycophyto aims at reducing the use of chemical fertilisers and phytopharmaceutical products by developing natural biostimulants (mycorrhyzal fungi). It started with the arrival of Khadija Musayeva in October 2020.

Acumes's research activity in traffic modeling and control is intended to improve road network efficiency, thus reducing energy consumption and pollutant emission.

Regarding the impact on health care, our research activity and preliminary results on hormono-radio therapies for prostate cancer show that combining hormone therapy with brachytherapy allowed us to reduce the radiative dose used from 120Gy to 80Gy. When the treatments are given at the same time, the final tumor volume is significantly reduced compared to using each therapy separately. The outcomes for public health in terms of financial cost and limitations of undesired side effects is of very high potential.

The research activities related to isogeometric analysis aim at facilitating the use of shape optimization methods in engineering, yielding a gain of efficiency, for instance in transportation industry (cars, aircrafts) or energy industry (air conditioning, turbines).

6 New software, platforms, open data

6.1 New software

6.1.1 MGDA

Name: Multiple Gradient Descent Algorithm

Keywords: Descent direction, Multiple gradients, Multi-objective differentiable optimization, Prioritized multi-objective optimization

Scientific Description: The software relies upon a basic MGDA tool which permits to calculate a descent direction common to an arbitrary set of cost functions whose gradients at a computational point are provided by the user, as long as a solution exists, that is, with the exclusion of a Pareto-stationarity situation.

More specifically, the basic software computes a vector d whose scalar product with each of the given gradients (or directional derivative) is positive. When the gradients are linearly independent, the algorithm is direct following a Gram-Schmidt orthogonalization. Otherwise, a sub-family of the gradients is identified according to a hierarchical criterion as a basis of the spanned subspace associated with a cone that contains almost all the gradient directions. Then, one solves a quadratic programming problem formulated in this basis.

This basic tool admits the following extensions: - constrained multi-objective optimization - prioritized multi-objective optimization - stochastic multi-objective optimization.

Functional Description: Chapter 1: Basic MGDA tool Software to compute a descent direction common to an arbitrary set of cost functions whose gradients are provided in situations other than Pareto stationarity.

Chapter 2: Directions for solving a constrained problem Guidelines and examples are provided according the Inria research report 9007 for solving constrained problems by a quasi-Riemannian approach and the basic MGDA tool.

Chapter 3: Tool for prioritized optimization Software permitting to solve a multi-objective optimization problem in which the cost functions are defined by two subsets: - a primary subset of cost functions subject to constraints for which a Pareto optimal point is provided by the user (after using the previous tool or any other multiobjective method, possibly an evolutionary algorithm) - a secondary subset of cost functions to be reduced while maintaining quasi Pareto optimality of the first set. Procedures defining the cost and constraint functions, and a small set of numerical parameters are uploaded to the platform by an external user. The site returns an archive containing datafiles of results including graphics automatically generated.

Chapter 4: Stochastic MGDA Information and bibliographic references about SMGDA, an extension of MGDA applicable to certain stochastic formulations.

Concerning Chapter 1, the utilization of the platform can be made via two modes : – the interactive mode, through a web interface that facilitates the data exchange between the user and an Inria dedicated machine, – the iterative mode, in which the user downloads the object library to be included in a personal optimization software. Concerning Chapters 2 and 3, the utilizer specifies cost and constraint functions by providing procedures compatible with Fortran 90. Chapter 3 does not require the specification of gradients, but only the functions themselves that are approximated by the software by quadratic meta-models.

URL: https://mgda.inria.fr

Publications: hal-01139994, hal-01414741, hal-01417428, hal-02285197, hal-02285899

Contact: Jean-Antoine Désidéri

Participant: Jean-Antoine Désidéri

6.1.2 Igloo

Name: Iso-Geometric anaLysis using discOntinuOus galerkin methods

Keywords: Numerical simulations, Isogeometric analysis

Scientific Description: Igloo contains numerical methods to solve partial differential equations of hyperbolic type, or convection-dominant type, using an isogeometric formulation (NURBS bases) with a discontinuous Galerkin method.

Functional Description: Simulation software for NURBS meshes

URL: https://gitlab.inria.fr/igloo/igloo/-/wikis/home

Author: Régis Duvigneau

Contact: Régis Duvigneau

6.1.3 BuildingSmart

Name: BuildingSmart interactive visualization

Keywords: Physical simulation, 3D rendering, 3D interaction

Scientific Description: The aim of the BuildingSmart project is to develop a software environment for the simulation and interactive visualisation for the design of buildings (structural safety, thermal confort).

Functional Description: The main task of the project is to study and develop solutions dedicated to interactive visualisation of building performances (heat, structural) in relation to the Building Information Modeling BIM framework, using Occulus Rift immersion.

URL: https://youtu.be/MW_gIF8hUdk

Contact: Abderrahmane Habbal

Participants: Régis Duvigneau, Jean-Luc Szpyrka, David Rey, Clément Welsch, Abderrahmane Habbal

6.1.4 RoadNetwork

Keywords: Road traffic, Road network, Python, Numerical simulations

Functional Description: Python library dedicated to create, manipulate and simulate ODE traffic equations on networks

Release Contributions: First version. Some fixing of module names and comments is ongoing.

Contact: Abderrahmane Habbal

Partner: Université Côte d'Azur (UCA)

6.1.5 pinnacle

Name: Physics-Informed Neural Networks Computational Library and Environment

Keywords: Neural networks, Partial differential equation, Physical simulation, Data assimilation, Inverse problem, Multiphysics modelling

Scientific Description: Set of methods for rapid implementation of physics-informed neural networks to solve direct and inverse problems: space-time sampling with refinement algorithms, dense multi-layer neural networks, library of physical models (mechanics, fluid, heat transfer, electromagnetics), optimisation algorithms, import/export tools for meshes and solutions.

Functional Description: Software library for implementation of physics informed neural networks.

Contact: Régis Duvigneau

Participants: Régis Duvigneau, Stéphane Lanteri, Alexis Gobe, Maxime Le

7 New results

7.1 Macroscopic traffic flow models on networks

Participants: Mickaël Binois, Paola Goatin, Alexandra Würth, Chiara Daini *(KOPERNIC Project-Team, INRIA Paris)*, Maria Laura Delle Monache *(UC Berkeley, USA)*, Antonella Ferrara *(Univ. Pavia, Italy)*, Adriano Festa *(Polytechnic of Turin, Italy)*, Alessandra Rizzo *(Univ. Messina, Italy)*, Enrico Siri, Fabio Vicini *(Polytechnic of Turin, Italy)*.

Traffic control by Connected and Automated Vehicles

We rely on a multi-scale approach to model mixed traffic composed of a small fleet of CAVs in the bulk flow. In particular, CAVs are allowed to overtake (if on distinct lanes) or queuing (if on the same lane). Controlling CAVs desired speeds allows to act on the system to minimize the selected cost function. For the proposed control strategies, we apply both global optimization and a Model Predictive Control approach. In particular, we perform numerical tests to investigate how the CAVs number and positions impacts the result, showing that few, optimally chosen vehicles are sufficient to significantly improve the selected performance indexes, even using a decentralized control policy. Simulation results support the attractive perspective of exploiting a very small number of vehicles as endogenous control actuators to regulate traffic flow on road networks, providing a flexible alternative to traditional control methods. Moreover, we compare the impact of the proposed control strategies (decentralized, quasi-decentralized, centralized). See [43].

In the aim of modeling the formation of stop-and-go waves (to be controlled employing CAVs), in [46] we prove the existence of weak solutions for a class of second order traffic models with relaxation, without requiring the sub-characteristic stability condition to hold. Therefore, large oscillations may arise from small perturbations of equilibria, capturing the formation of stop-and-go waves observed in reality. An analysis of the corresponding travelling waves completes the study.

Traffic flow predictions by statistical approaches

In the framework of A. Würth's PhD thesis [40], we propose a physics informed statistical framework for traffic travel time prediction. On one side, the discrepancy of the considered mathematical model is represented by a Gaussian process. On the other side, the traffic simulator is fed with boundary data predicted by a Gaussian process, forced to satisfy the mathematical equations at virtual points, resulting in a multi-objective optimization problem. This combined approach has the merit to address the shortcomings of the purely model-driven or data-driven approaches, while leveraging their respective advantages. Indeed, models are based on physical laws, but cannot capture all the complexity of real phenomena. On the other hand, pure statistical outputs can violate basic characteristic dynamics. We validate our approach on both synthetic and real world data, showing that it delivers more reliable results compared to other methods, see [36]. This approach is further extended to traffic prediction in [48], showing promising results on both synthetic and real world data.

Besides, in [49] we extend the finite volume numerical scheme proposed by Hilliges and Weidlich to second order traffic flow models consisting in 2×2 systems of non strictly hyperbolic conservation laws of Temple class. The scheme is shown to satisfy some maximum principle properties on the density. We provide numerical tests illustrating the behaviour at vacuum and the gain in computational time when dealing with optimization algorithms.

Routing strategies in traffic flows on networks

In the framework of A. Joumaa's PhD thesis, [33] presents a macroscopic multi-class traffic flow model on road networks that accounts for an arbitrary number of vehicle classes with different free flow speeds. A comparison of the Eulerian and Lagrangian formulations is proposed, with the introduction of a new Courant-Friedrichs-Lewy condition. In particular, the L^1-error and the computational times are used to compare the performance of the two formulations and show that the Eulerian formulation outperforms the Lagrangian. The paper then extends the Eulerian formulation to traffic networks, providing a general implementation of the dynamics at junctions. We finally simulate the effect of traffic measures and policies, such as route guidance and modal shift, on total travel time and network throughput, which shows that the proposed multi-class model correctly depicts the interactions among classes and it can be used to model such behaviors in complex networks.

In [26], we introduce a macroscopic differential model coupling a conservation law with a Hamilton-Jacobi equation to respectively model the nonlinear transportation process and the strategic choices of users. Furthermore, the model is adapted to the multi-population case, where every population differs in the level of traffic information about the system. This enables us to study the impact of navigation choices on traffic flows on road networks.

In [34], we address a pseudo-System Optimum Dynamic Traffic Assignment optimization problem on road networks relying on trajectory control over a portion of the flows and limited knowledge on user response. The fractions of controlled flow moving between each origin-destination couple are defined as "compliant", while the remaining portions, consisting of users free to make their own individual choices, are defined as "non-compliant". The objective is to globally improve the state of the network by controlling a varying subset of compliant traffic flows. On one hand, the selfish response of non-compliant users to changing traffic conditions is computed at each time step by updating the class related turn ratios accordingly to a discrete-choice multinomial Logit model to represent users imperfect information. On the other hand, the control action is actuated by varying the flow rates over a precomputed set of routes while the coupled optimization problem takes into account an a priori fixed distribution of users at the nodes. We show how the effectiveness of the resulting finite horizon optimal control problem degrades by not considering the dynamic response of non-compliant users and how it varies according to the fraction of compliant ones. The goal of the the partial control optimization problem is to globally improve the network congestion level by rerouting a variable fraction of flows over a set of pre-computed routes. The fraction of controlled users varies according to the trade-off between the rerouting effort and the network status improvement. Results on a synthetic network are then presented and discussed in [35].

7.2 Nonlocal pedestrian flow models

Participants: Paola Goatin, Daniel Inzunza, Luis Miguel Villada *(U Bìo Bìo, Chile)*.

In the framework of the MathAmSud project NOTION, we propose a nonlocal macroscopic pedestrian flow model for two populations with different destinations trying to avoid each other in a confined environment, where the nonlocal term accounts for anisotropic interactions, mimicking the effect of different cones of view, and the presence of walls or other obstacles in the domain. In particular, obstacles can be incorporated in the density variable, thus avoiding to include them in the vector field of preferred directions. In order to compute the solution, we propose a Finite Difference scheme that couples highorder WENO approximations for spatial discretization, a multi-step TVD method for temporal discretization, and a high-order numerical derivative formula to approximate the derivatives of nonlocal terms, and in this way avoid excessive calculations. Numerical tests confirm that each population manages to evade both the presence of the obstacles and the other population. The evacuation time problem is studied, in particular, the optimal position of the obstacles is obtained using a total travel time optimization processes, see [45, 44].

7.3 MFG for two-class traffic flows

Participants: Abderrahmane Habbal, Amal Machtalay *(U Mohamed VI Polytech, Morocco)*(UM6P) , Imad Kissami *(UM6P)*, Ahmed Ratnani *(UM6P)*.

We have explored a multi-class traffic model and examined the computational feasibility of mean-field games (MFG) in obtaining approximate Nash equilibria for traffic flow games involving a large number of players. We introduced a two-class traffic mean-field game framework, building upon classical multi-class formulations. To facilitate our analysis, we employed various numerical techniques, including high-performance computing and regularization of LGMRES solvers. By utilizing these tools, we conducted simulations at significantly larger spatial and temporal scales.

We led extensive numerical experiments considering three different scenarios involving cars and trucks, as well as three different cost functionals. Our results primarily focused on the dynamics of autonomous vehicles (AVs) in traffic, yielding results which support the effectiveness of the approach.

Moreover, we conducted original comparisons between macroscopic Nash mean-field speeds and their microscopic counterparts. These comparisons allowed us to computationally validate the $\epsilon-$Nash approximation, demonstrating a slightly improved convergence rate compared to theoretical expectations.

Future directions encompass second order traffic models, the multi-lane case, particularly prone to non-cooperative game considerations, and addressing some theoretical issues, see [113].

7.4 Learning strategies for PDEs

Participants: Guillaume Coulaud, Régis Duvigneau, Paola Goatin, Daniel Inzunza, Nathan Ricard, Maxime Le *(SED Centre Inria d'Université Côte d'Azur)*, Adrien Bousseau *(GraphDeco Project-Team)*, Guillaume Cordonnier *(GraphDeco Project-Team)*, Nicolas Rosset *(GraphDeco Project-Team)*.

We investigate the use of novel machine learning paradigms in the context of complex PDE systems, including the following research axes:

- **Interactive car design using data-driven flow model**
  The design of car shapes requires a delicate balance between aesthetic and performance. While fluid simulation provides the means to evaluate the aerodynamic performance of a given shape, its

computational cost hinders its usage during the early explorative phases of design, when aesthetic is decided upon. We present an interactive system to assist designers in creating aerodynamic car profiles. Our system relies on a neural surrogate model, trained using a simulation database, to predict fluid flow around car shapes, providing fluid visualization and shape optimization feedback to designers as soon as they sketch a car profile. We architectured our model to support gradient-based shape optimization within a learned latent space of car profiles [31]. This work is carried out in collaboration with GraphDeco Project-Team, in the context of Nicolas Rosset's PhD thesis.

- **A PINN approach for traffic state estimation and model calibration based on loop detector flow data**
  In [32], we analyze the performances of a Physics Informed Neural Network (PINN) strategy applied to traffic state estimation and model parameter identification in realistic situations. The traffic dynamics is modeled by a first order macroscopic traffic flow model involving two physical parameters and an auxiliary one. Besides, observations consist of (averaged) density and flow synthetic data computed at fixed space locations, simulating real loop detector measurements. We show that the proposed approach is able to give a good approximation of the underlying dynamics even with poorer information. Moreover, the precision generally improves as the number of measurement locations increases.

- **Multiphysics coupling using physics-informed neural networks**
  Physics-Informed Neural Networks (PINNs) have emerged as a promising paradigm for modeling complex physical phenomena, offering the potential to handle diverse scenarios to simulate coupled systems. This is a supervised or unsupervised deep learning approach that aims at learning physical laws described by partial differential equations. We consider an exploration of PINNs for multiphysics applications, by embedding the different PDE models and coupling conditions in a single learning task, through three distinct test cases: heat transfer, and conjugate heat transfer, with forced and natural convection. The investigations reveal PINNs' proficiency in accommodating parameterized resolution, addressing piecewise constant conditions, and enabling multiphysics coupling. Despite their versatility, challenges emerged, including difficulties in achieving high accuracy, error propagation near singularities, and limitations in scenarios with high Rayleigh values [42]. This activity is part of Guillaume Coulaud's Master thesis and Nathan Ricard's PhD thesis.

- **Turbulence characterization using physics-informed neural networks**
  Turbulence modeling is still a major issue in complex flow simulations, due to the limitations of turbulence models in terms of application range. Physics informed neural networks offer a promising framework to overcome this difficulty, by allowing to build simulation tools based on both PDE models and experimental data. Thus, we investigate this approach to simulate turbulent flows including data in replacement to classical turbulence closures.

The two latter activities benefit from SED support for the development of pinnacle software (6.1.5) devoted to PINNs.

7.5 Advanced Bayesian optimization

Participants: Mickaël Binois, Nicholson Collier *(Argonne, USA)*, Régis Duvigneau, Mahmoud Elsawy *(Atlantis team)*, Patrice Genevet *(Colorado School of Mines, USA)*, Enzo Isnard *(Atlantis team)*, Stéphane Lanteri *(Atlantis team)*, Jonathan Ozik *(Argonne, USA)*, Victor Picheny *(SecondMind, GB)*
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Bayesian optimization of nano-photonic devices

In collaboration with Atlantis Project-Team, we consider the optimization of optical meta-surface devices, which are able to alter light properties by operating at nano-scale. In the context of Maxwell equations, modified to account for nano-scale phenomena, the geometrical properties of materials are optimized to achieve a desired electromagnetic wave response, such as change of polarization, intensity or direction. This task is especially challenging due to the computational cost related to the 3D time-accurate simulations, the difficulty to handle the different geometrical scales in optimization and the presence of uncertainties [50].

Massively parallel Bayesian optimization

Motivated by a large scale multi-objective optimization problem for which thousands of evaluations can be conducted in parallel, we develop an efficient approach to tackle this issue in [41].

One way to reduce the time of conducting optimization studies is to evaluate designs in parallel rather than just one-at-a-time. For expensive-to-evaluate black-boxes, batch versions of Bayesian optimization have been proposed. They work by building a surrogate model of the black-box that can be used to select the designs to evaluate efficiently via an infill criterion. Still, with higher levels of parallelization becoming available, the strategies that work for a few tens of parallel evaluations become limiting, in particular due to the complexity of selecting more evaluations. It is even more crucial when the black-box is noisy, necessitating more evaluations as well as repeating experiments. Here we propose a scalable strategy that can keep up with massive batching natively, focused on the exploration/exploitation trade-off and a portfolio allocation. We compare the approach with related methods on deterministic and noisy functions, for mono- and multi-objective optimization tasks. These experiments show similar or better performance than existing methods, while being orders of magnitude faster.

A game theoretic perspective on Bayesian multi-objective optimization

In [38], a book chapter, we address the question of how to efficiently solve many-objective optimization problems in a computationally demanding black-box simulation context. We motivate the question by applications in machine learning and engineering, and discuss specific harsh challenges in using classical Pareto approaches when the number of objectives is four or more. Then, we review solutions combining approaches from Bayesian optimization, e.g., with Gaussian processes, and concepts from game theory like Nash equilibria, Kalai-Smorodinsky solutions and detail extensions like Nash-Kalai-Smorodinsky solutions. We finally introduce the corresponding algorithms and provide some illustrating results.

7.6 Complex data analysis

Participants: Mickaël Binois, Khadija Musayeva.

In the context of the analysis of complex data sets, such as those appearing in biology, we considered two different questions. The first one is related to label learning, that is, learning missing labels from other available variables and labels. The second considers dimension reduction, to find a common set of new variables when many outputs are present.

In [39], the work focuses on multi-label learning from small number of labelled data. We demonstrate that the straightforward binary-relevance extension of the interpolated label propagation algorithm, the harmonic function, is a competitive learning method with respect to many widely-used evaluation measures. This is achieved mainly by a new transition matrix that better captures the underlying manifold structure. Furthermore, we show that when there exists label dependence, we can use the outputs of a competitive learning method as part of the input to the harmonic function to provide improved results over those of the original model. Finally, since we are using multiple metrics to thoroughly evaluate the performance of the algorithm, we propose to use the game-theory based method of Kalai and Smorodinsky to output a single compromise solution. This method can be applied to any learning model irrespective of the number of evaluation measures used.

In [47], we propose several approaches as baselines to compute a shared active subspace for multivariate vector-valued functions. The goal is to minimize the deviation between the function evaluations on the original space and those on the reconstructed one. This is done either by manipulating the gradients or the symmetric positive (semi-)definite (SPD) matrices computed from the gradients of each component function so as to get a single structure common to all component functions. These approaches can be applied to any data irrespective of the underlying distribution unlike the existing vector-valued approach that is constrained to a normal distribution. We test the effectiveness of these methods on five optimization problems. The experiments show that, in general, the SPD-level methods are superior to the gradient-level ones, and are close to the vector-valued approach in the case of a normal distribution. Interestingly, in most cases it suffices to take the sum of the SPD matrices to identify the best shared active subspace.

7.7 Pareto optimality and Nash games

Participants: Mickaël Binois, Jean-Antoine Désidéri, Sébastien Defoort *(ONERA/DTIS, Université de Toulouse)*, Nathalie Bartoli *(ONERA/DTIS, Université de Toulouse)*, Christophe David *(ONERA/DTIS, Université de Toulouse)*, Julien Wintz *(SED, INRIA Sophia Antipolis)*.

In the multi-objective optimization of a complex system, establishing the Pareto front associated with the whole set of cost functions is usually a computationally demanding task, whose results are not always easy to analyze, while the final decision still remains to be made among Pareto-optimal solutions. These observations had led us to propose a prioritized approach in which the Pareto front is calculated only for a subset of primary cost functions, those of preponderant importance, followed by an economical and decisive step in which a continuum of Nash equilibria accounting for secondary functions is calculated [8].

The method had been applied to the multi-objective optimization of the flight performance of an Airbus-A320-type aircraft in terms of take-off fuel mass and operational empty weight (primary cost functions) concurrently with ascent-to-cruise altitude duration (secondary) [12]. These results have been presented at a Conference on “New Greener and Digital Modern Transport” (JyU., Finland, May 2023), and recently completed by Bayesian optimization and are currently in press for proceedings,

That work reflects our cooperation with the Information Processing and Systems Department (DTIS) of Onera Toulouse. It will be continued to account for additional criteria related to environmental impact and operational performance.

7.8 Inverse Cauchy-Stokes problems solved as Nash games

Participants: Abderrahmane Habbal, Marwa Ouni *(PhD, LAMSIN, Univ. Tunis Al Manar)*, Moez Kallel *(LAMSIN, Univ. Tunis Al Manar)*.

We extend in two directions our results published in [112] to tackle ill-posed Cauchy-Stokes inverse problems as Nash games. First, we consider the problem of detecting unknown pointwise sources in a stationary viscous fluid, using partial boundary measurements. The considered fluid obeys a steady Stokes regime, the boundary measurements are a single compatible pair of Dirichlet and Neumann data, available only on a partial accessible part of the whole boundary. This inverse source identification for the Cauchy-Stokes problem is ill-posed for both the sources and missing data reconstructions, and designing stable and efficient algorithms is challenging. We reformulate the problem as a three-player Nash game. Thanks to a source identifiability result derived for the Cauchy-Stokes problem, it is enough to set up two Stokes BVP, then use them as state equations. The Nash game is then set between 3 players, the first two targeting the data completion while the third one targets the detection of the number, location and magnitude of the unknown sources. We provided the third player with the location and magnitude parameters as strategy, with a cost functional of Kohn-Vogelius type. In particular, the location is obtained through the computation of the topological sensitivity of the latter function. We propose an original algorithm, which we implemented using Freefem++. We present 2D numerical experiments for many different test-cases.The obtained results corroborate the efficiency of our 3-player Nash game approach to solve parameter or shape identification for Cauchy-Stokes problems [30]

The second direction is dedicated to the solution of the data completion problem for non-linear flows. We consider two kinds of non linearities leading to either a non Newtonian Stokes flow or to Navier-Stokes equations. Our recent numerical results show that it is possible to perform a one-shot approach using Nash games : players exchange their respective state information and solve linear systems. At convergence to a Nash equilibrium, the states converge to the solution of the non linear systems. To the best of our knowledge, this is the first time where such an approach is applied to solve inverse problems for nonlinear systems [114].

7.9 Combined therapies for the treatment of prostate cancer

Participants: Abderrahmane Habbal, Salma Chabbar *(PhD, ACUMES and EMI, Univ. Mohammed V)*, Rajae Aboulaich *(EMI, Univ. Mohammed V)*, Nabil Ismaili *(PhD.MD., Univ Mohamed VI for health sciences, Casablanca)*, Sanae EL Mejjaoui *(PhD.MD., Institute for Oncology, Avicenne Hospital, Rabat)*.

Prostate cancer is a hormone-dependent cancer characterized by two types of cancer cells, androgen-dependent cancer cells and androgen-resistant ones. The objective of this work is to present a novel mathematical model for the treatment of prostate cancer under combined hormone therapy and brachytherapy. Using a system of partial differential equations, we quantify and study the evolution of the different cell densities involved in prostate cancer and their responses to the two treatments. The numerical simulations are carried out on FreeFem++ using a 2D finite element method. Numerical simulations of tumor growth under different therapeutic strategies are explored and discussed. Combining hormone therapy with brachytherapy allowed us to reduce the dose used from 120Gy to 80Gy. When the treatments are given at the same time, the final tumor volume is significantly reduced compared to using each therapy separately. However, starting with hormone therapy gave better results. When using intermittent hormone therapy combined with brachytherapy, we found that once the PSA level drops below the critical level, it stays at reasonable levels and therefore the hormone therapy does not reactivate. When we use continuous hormone therapy instead, the prostate is unnecessarily deprived of androgen for an almost non-existent reduction in tumor volume compared to intermittent deprivation. The use of hormone therapy over a short period of time is therefore sufficient to give good results. The results also showed that the dose used in the combined treatments affects the tumor relapse. See [70] and [24].

7.10 Optimal transport and isogeometric analysis

Participants: Abderrahmane Habbal, Mustapha Bahari *(U Mohamed VI Polytech, Morocco)*(UM6P) , Ahmed Ratnani *(UM6P)*, Eric Sonnendrücker *(Max Planck Institute)*.

In this work, we devise fast solvers and adaptive mesh generation procedures based on the Monge–Ampère Equation using B-Splines Finite Elements, within the Isogeometric Analysis framework. Our approach ensures that the constructed mapping is a bijection, which is a major challenge in Isogeometric Analysis. First, we use standard B-Splines Finite Elements to solve the Monge–Ampère Equation. An analysis of this approach shows serious limitations when dealing with high variations near the boundary. In order to solve this problem, a new formulation is derived using compatible B-Splines discretization based on a discrete DeRham sequence. A new fast solver is devised in this case using the Fast Diagonalization method. Different tests are provided and show the performance of our new approach, see [23].

8 Bilateral contracts and grants with industry

8.1 Bilateral contracts with industry

- **Mycophyto** (2020-...): this research contract involving Université Côte d'Azur is financing the post-doctoral contract of Khadija Musayeva. The goal is to develop prediction algorithms based on environmental data.

  Participants: Mickaël Binois, Khadija Musayeva.

9 Partnerships and cooperations

9.1 International initiatives

9.1.1 STIC/MATH/CLIMAT AmSud projects

NOTION

Title: Non-local conservation laws for engineering, biological and epidemiological applications: theory and numerics

Program: MATH-AmSud

Duration: January 1, 2022 – December 31, 2023

Local supervisor: Paola Goatin

Partners:

- Universidad del Bio Bio
- Universidad de Concepcion
- Universidad de Cordoba

Inria contact: Paola Goatin

Summary: Conservation laws with flux function depending on integral evaluations of the conserved quantities arise in several models describing engineering, biological and epidemiological applications. The presence of non-local terms makes the classical techniques developed for hyperbolic systems of conservation laws inapplicable as such, thus requiring the development of novel analytical and numerical tools. Moreover, the presence of integral terms has a huge impact on the cost of numerical simulations, motivating the design of efficient approximation schemes. This project aims to tackle the above mentioned analytical and numerical challenges, focusing on engineering applications (sedimentation, traffic, population dynamics, etc) and biological and epidemiological phenomenon.

9.2 International research visitors

9.2.1 Visits of international scientists

Other international visits to the team

Alessandra Rizzo

Status: PhD student

Institution of origin: Università di Messina

Country: Italy

Dates: March-May, 2023 (3 months)

Context of the visit: collaboration on second order traffic models with relaxation

Mobility program/type of mobility: research stay

Elena Rossi

Status: Associate Professor

Institution of origin: Università di Modena - Reggio Emilia

Country: Italy

Dates: April and September, 2023 (1 week each)

Context of the visit: collaboration on applications of conservation laws to traffic problems

Mobility program/type of mobility: research stay

9.3 European initiatives

9.3.1 Horizon Europe

DATAHYKING

Participants: Paola Goatin, Ilaria Ciaramaglia, Carmen Mezquita Nieto.

DATAHYKING project on cordis.europa.eu

Title: Data-driven simulation, uncertainty quantification and optimization for hyperbolic and kinetic models

Duration: From March 1, 2023 to February 28, 2027

Partners:

- TRANSPORT & MOBILITY LEUVEN NV (TML), Belgium
- Autovie Venete S.p.A., Italy
- INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET AUTOMATIQUE (INRIA), France
- UNIVERSITE COTE D'AZUR, France
- RHEINISCH-WESTFAELISCHE TECHNISCHE HOCHSCHULE AACHEN (RWTH AACHEN), Germany
- ESI GROUP (ESI SOFTWARE PAM SYSTEM INTERNATIONAL PSI), France
- Cassa di Compensazione e Garanzia s.p.a. (CC&G), Italy
- NEOVYA Mobility by Technology (NEOVYA Mobility by Technology), France
- INCICO (INICIO SPA), Italy

- SIEMENS INDUSTRY SOFTWARE NETHERLANDS BV (Siemens Industry Software Netherlands B.V.), Netherlands
- RHEINLAND-PFALZISCHE TECHNISCHE UNIVERSITAT, Germany
- CENTRE DE RECHERCHE EN AERONAUTIQUE ASBL - CENAERO (CENAERO), Belgium
- UNIVERSITE DE LILLE (UNIVERSITE DE LILLE), France
- ZENSOR (ZENSOR), Belgium
- KATHOLIEKE UNIVERSITEIT LEUVEN (KU Leuven), Belgium
- UNIVERSITA DEGLI STUDI DI ROMA LA SAPIENZA (UNIROMA1), Italy
- UNIVERSITA DEGLI STUDI DI FERRARA (Unife), Italy

Inria contact: Paola Goatin

Coordinator: Giovanni Samaey (KU Leuven)

Summary: Europe faces major challenges in science, society and industry, induced by the complexity of our dynamically evolving world. To tackle these challenges, mathematical models and computer simulations are indispensable, for instance to design and optimize systems using virtual prototypes. Moreover, while the big data revolution provides additional possibilities, it is currently unclear how to optimally combine simulation results with observation data into a digital. Many systems of interest consist of large numbers of particles with highly non-trivial interaction (e.g., fine dust in pollution, vehicles in mobility).

However, to date, computer simulation of such systems is usually done with highly approximate (macroscopic) models to reduce computational complexity. Facing these challenges without sacrificing the complexity of the underlying particle interactions requires a fundamentally new type of scientist that uses an interdisciplinary approach and a solid mathematical underpinning. Hence, we aim at training a new generation of modeling and simulation experts to develop virtual experimentation tools and workflows that can reliably and efficiently exploit the potential of mathematical modeling and simulation of interacting particle systems.

To this end, we create a data-driven simulation framework for kinetic models of interacting particle systems, and define a common methodology for these future modeling and simulation experts. The network focuses on (i) reliable and efficient simulation; (ii) robust consensus-based optimization, also for machine learning; (iii) multifidelity methods for uncertainty quantification and Bayesian inference; and (iv) applications in fluid flow, traffic flow, and finance, also in collaboration with industry. Moreover, the proposed EJD program will create a closely connected new generation of highly demanded European scientists, and initiate long-term partnerships to exploit synergy between academic and industrial partners.

9.3.2 Other european programs/initiatives

Program: COST

Project acronym: CA18232

Project title: Mathematical models for interacting dynamics on networks

Duration: October 2019 - September 2023

Coordinator: University of Ljubljana (Prof. Marjeta Kramar Fijavz)

Partners: see website

Inria contact: Paola Goatin

Summary: Many physical, biological, chemical, financial or even social phenomena can be described by dynamical systems. It is quite common that the dynamics arises as a compound effect of the interaction between sub-systems in which case we speak about coupled systems. This Action shall study such interactions in particular cases from three points of view:

- the abstract approach to the theory behind these systems,
- applications of the abstract theory to coupled structures like networks, neighbouring domains divided by permeable membranes, possibly non-homogeneous simplicial complexes, etc.,
- modelling real-life situations within this framework.

The purpose of this Action is to bring together leading groups in Europe working on a range of issues connected with modeling and analyzing mathematical models for dynamical systems on networks. It aims to develop a semigroup approach to various (non-)linear dynamical systems on networks as well as numerical methods based on modern variational methods and applying them to road traffic, biological systems, and further real-life models. The Action also explores the possibility of estimating solutions and long time behaviour of these systems by collecting basic combinatorial information about underlying networks.

Participants: Paola Goatin.

9.4 National initiatives

9.4.1 ANR

- **Institute 3IA Côte d'Azur**: The 3IA Côte d'Azur is one of the four "Interdisciplinary Institutes of Artificial Intelligence" that were created in France in 2019. Its ambition is to create an innovative ecosystem that is influential at the local, national and international levels, and a focal point of excellence for research, education and the world of AI.
  ACUMES is involved with the project "Data driven traffic management" in the axis *AI for smart and secure territories* (2020-2024), for which P. Goatin is chair holder. This project aims at contributing to the transition to intelligent mobility management practices through an efficient use of available resources and information, fostering data collection and provision. We focus on improving traffic flow on road networks by using advanced mathematical models and statistical techniques leveraging the information recovered by real data.

  Participants: Paola Goatin, Daniel Inzunza, Alexandra Würth.

- **COSS - COntrol on Stratified Structures** (ANR-22-CE40-0010, PI Nicolas Forcadel, INSA Rouen): The central theme of this project lies in the area of control theory and partial differential equations (in particular Hamilton-Jacobi equations), posed on stratified structures and networks. These equations appear very naturally in several applications. Indeed, many practical optimal control problems, such as traffic flow modeling or energy management in smart-grids networks or sea-land trajectories with different dynamics, involve a state space in a stratified form (a collection of manifolds with different dimensions and associated to different dynamics). These control problems can be studied within the framework of Hamilton Jacobi equations theory; in particular, they involve admissible trajectories that have to stay in the stratified domain.

  Participants: Paola Goatin.

10 Dissemination

10.1 Promoting scientific activities

10.1.1 Scientific events: organisation

General chair, scientific chair Paola Goatin was member of the scientific committee of the following events:

- *"PED2023 - Conference on Pedestrian and Evacuation Dynamics"*, Eindhoven (Nederlands), 2023.
- Maathrafic - *"Modélisation mathématique, analyse et approximation des dynamiques routières et piétonnières"*, Tours (France), June 2023.
- MT-ITS 2023 *"8th International Conference on Models and Technologies for Intelligent Transportation Systems"*, Nice (France), June 2023.

Member of the organizing committees

- Abderrahmane Habbal is member of the organizing committee of the *Winter-School on Model Reduction Methods for Control and Machine Learning* February 26-29, 2024 The UM6P Vanguard Center, Benguerir, Morocco.

10.1.2 Scientific events: selection

Member of the conference program committees

- Mickael Binois was part of the program committee of the Evolutionary Multiobjective Optimization (EMO) Track of the Genetic and Evolutionary Computation Conference (GECCO-2023) that was held in Lisbonne as well as the Neuro-Explicit AI and Expert-informed Machine Learning for Engineering and Physical Sciences workshop at ECML PKDD which was held in Turin.
- Régis Duvigneau was part of the program committee of the 3rd Inria-DFKI European Summer School on AI (IDESSAI 2023).
- Paola Goatin was member of the program committee of the 26th IEEE International Conference on Intelligent Transportation Systems (IEEE ITSC 2023).

Reviewer

- Mickael Binois reviewed for the following conferences: AISTATS 2024, ICLR24, ICML 2023 and NeurIPS 2023.
- Paola Goatin reviewed for ACC 2024.

10.1.3 Journal

Member of the editorial boards

- Mickael Binois is Associate Editor of *ACM Transactions on Evolutionary Learning and Optimization*
- Paola Goatin is Managing Editor of *Networks and Heterogeneous Media* and Associate Editor of *SIAM Journal on Applied Mathematics* and *ESAIM: Mathematical Modelling and Numerical Analysis*.

Reviewer - reviewing activities

- Mickael Binois is a reviewer for the following international journals: European J. Oper. Res, J. Mach. Learn. Res, J Glob Optim, SIAM-ASA J Uncertain, Int J Numer Methods Eng, Struct Multidiscipl Optim, SIAM J Sci Comput, Technometrics, ACM Transactions on Evolutionary Learning and Optimization, IEEE Trans. Evol. Comput., Transactions on Machine Learning Research.
- Régis Duvigneau is a reviewer for the following international journals: Comp. & Fluids, Comp. Meth. Appl. Mech. Eng., J. Fluids & Struct., J. Opt. Soc. of America, Trans. on Elec. Comp.
- Paola Goatin reviewed for: Advances in Computational Mathematics, Comm. Math. Sci., EURO Journal on Transportation and Logistics, Journal of Differential Equations, Mathematical Methods in the Applied Sciences, SIAM J. Num. Anal., Transportation Science.
- Abderrahmane Habbal reviewed for the following international journals: J. of Math. Biology, Asian J. of Control, ARIMA, J. of Scientific Computing

10.1.4 Invited talks

- Mickael Binois: SIAM conference on Computational Science and Engineering 23, Amsterdam (Netherlands), March 2023. Symposium talk: Massively Parallel Bayesian Optimization.
- Mickael Binois and Régis Duvigneau: hybrid EOLIS workshop, January 2023. Talk: Multi-Fidelity Models and Optimization using Gaussian Processes.
- Mickael Binois: SIAM Conference on Optimization, Seattle (USA), June 2023. Symposium talk: Scalable Bayesian optimization for noisy problems.
- Mickael Binois: LIKE23 workshop, Bern (Switzerland), June 2023. Invited talk: Kernels for high-dimensional Gaussian Process modeling
- Paola Goatin: Workshop "Control Methods in Hyperbolic Partial Differential Equations", Mathematisches Forschungsinstitut, Oberwolfach (Germany), November 2023. Invited talk: *Nonlocal macroscopic models of multi-population pedestrian flows forwalking facilities optimization*.
- Paola Goatin: Hirschegg Workshop on Conservation Laws, Hirschegg (Austria), September 2023. Invited talk: *Macroscopic traffic flow models for new mobility paradigms*.
- Paola Goatin: Traffic and Autonomy Conference, Maiori (Italy), June 2023. Plenary talk: *Traffic flow models for new mobility paradigms*.
- Paola Goatin: Math 2 Product (M2P) 2023 - Emerging Technologies in Computational Science for Industry, Sustainability and Innovation, Taormina (Italy), May 2023. Plenary lecture: *Traffic flow models for current and future mobility challenges*.
- Abderrahmane Habbal: Mathematics Würzburg Colloquium (GE), May 2023. Plenary lecture *Game formulation of coupled data recovery and shape identification for Stokes problems*.
- Abderrahmane Habbal: ICIAM 2023, Tokyo : August 20-25, 2023. Minisymposium on *Modern numerical methods for PDE-constrained optimization and control* contributed talk *Decentralized strategies for coupled shape and parameter inverse problems*
- Abderrahmane Habbal: Euro-Maghreb conference at Levico (IT) October 2023, *A game theoretic viewpoint on boundary data recovery coupled to shape identification problems*

10.1.5 Scientific expertise

- Paola Goatin was member of the committee of the *"Fausto Saleri"* prize from SIMAI for young researchers.
- Abderrahmane Habbal was sollicitated for the evaluation of a Call for Project INRAE-ANSES on Mathematical Obesity. November 2023.

10.1.6 Research administration

- Régis Duvigneau is head of the Scientific Committee of Platforms (cluster and immersive space) for Inria Centre at Université Côte d'Azur.
- Régis Duvigneau is member of the Scientific Committee of OPAL computing Platform at Université Côte d'Azur
- Régis Duvigneau is member of the Steering Committee of "Maison de la Simulation et Interactions" at Université Côte d'Azur.
- Paola Goatin is adjunct director of the Doctoral School of Fundamental and Applied Sciences (ED SFA) of Université Côte D'Azur.
- Paola Goatin was member of the Junior Professor Chair (JPC) hiring committee of École des Ponts ParisTech in Applied Mathematics.
- Abderrahmane Habbal was member of the hiring committee for Affiliate Professors (April, November 2023) at University Mohammed VI Polytechnic (Morocco).
- Abderrahmane Habbal is member of the local PhD committee CSD (comité de suivi doctoral) at Inria d'Université Côte d'Azur.

10.2 Teaching - Supervision - Juries

10.2.1 Teaching

- Master: M. Binois, Optimisation bayésienne, 9 hrs, M2, Polytech Nice Sophia - Université Côte d'Azur.
- Master: M. Binois, Optimization, 24 hrs, M1, Polytech Nice Sophia - Université Côte d'Azur.
- Master: M. Binois, Bayesian optimization, 9 hrs, M2, Mohammed VI Polytechnic University, Morocco.
- Master: J.-A. Désidéri, Multidisciplinary Optimization, ISAE Supaéro (Toulouse), 5 hrs.
- Master: R. Duvigneau, Advanced Optimization, 28 hrs, M2, Polytech Nice Sophia - Université Côte d'Azur.
- Advanced course: R. Duvigneau, 3 hrs, 3rd Inria-DFKI European Summer School on AI (IDESSAI 2023) , Sophia-Antipolis (France), September 2023: *"Physics-informed neural networks for simulation"*.
- Master: P. Goatin, projets M1 and M2, 17 hrs, Polytech Nice Sophia - Université Côte d'Azur.
- Master: P. Goatin, Optimization, 24 hrs, M1, Polytech Nice Sophia - Université Côte d'Azur.
- Master: J.-A. Désidéri, Multidisciplinary Optimization, 22.5 hrs, joint *Institut Supérieur de l'Aéronautique et de l'Espace* (ISAE Supaéro, "Complex Systems") and M2 (Mathematics), Toulouse.
- Master: A. Habbal, Optimization, 18 hrs, M1, Polytech Nice Sophia - Université Côte d'Azur.
- Master: A. Habbal, Numerical methods for PDEs, 24 hrs, M1, Polytech Nice Sophia - Université Côte d'Azur.
- Master: A. Habbal, Stochastic Processes, 24 hrs, M1, Polytech Nice Sophia - Université Côte d'Azur.
- Master: A. Habbal, Introduction to optimization, 15 hrs, M1, Mohammed VI Polytechnic University, Morocco.
- Master: A. Habbal, Fall projects M1, 20 hrs, Polytech Nice Sophia - Université Côte d'Azur.

- Licence (L3): A. Habbal, Mathematical model of addiction, 48 hrs, L3 Semester Project, Polytech Nice Sophia - Université Côte d'Azur.
- Licence (L1): A. Habbal, Mathematics reinforcement, 36 hrs, Polytech Nice Sophia - Université Côte d'Azur.

10.2.2 Supervision

- PhD defense: A. Würth, *AI for road traffic modeling and management*, Univ. Côte d'Azur/3IA, December 6, 2023. Supervisors: P. Goatin, M. Binois.
- PhD in progress: A. Joumaa, *Pseudo-real-time optimization of the environmental performance of urban mobility using macroscopic and multimodal modeling approaches*, Univ. Côte d'Azur/IFPEN. Supervisors: P. Goatin, G. De Nunzio.
- PhD in progress: I. Ciaramaglia, *Interactions between microscopic and macroscopic models for autonomous vehicles in human-driven environments*, Univ. Côte d'Azur and Univerità di Roma La Sapienza. Supervisors: P. Goatin, G. Puppo.
- PhD in progress: C. Mezquita Nieto, *Modeling and optimization of multi-modal transportation networks based on kinetic and hyperbolic equations*, Univ. Côte d'Azur and RPTU Kaiserslautern. Supervisors: P. Goatin, A. Klar.
- PhD in progress: N. Rosset, *Flow prediction from sketches*, Univ. Côte d'Azur. Supervisors: A. Bousseau, G. Cordonnier, R. Duvigneau
- PhD in progress: N. Ricard, *Physics-informed neural networks for multiphysics design*, Univ. Côte d'Azur. Supervisor: R. Duvigneau
- PhD in progress: M. Bahari, *Optimal-Mass Transportation for Adaptive Mesh Generation and r-Refinement.* Univ. Côte d'Azur and Univ. Mohammed VI Polytechnic. Supervisors: A. Habbal, A. Ratnani.
- PhD in progress: A. Machtalay, *From Mean Field Games to Agent-based Models and back* Univ. Côte d'Azur and Univ. Mohammed VI Polytechnic. Supervisors: A. Habbal, A. Ratnani.
- Master Thesis project (5 months) Amal Amhamdi, Prise en compte de la dépendance en optimisation multi-objectif (Master 2, Polytech Nice Sophia - Université Côte d'Azur). Supervisor: Mickael Binois
- Master Thesis project (6 months) Guillaume Coulaud, ENSEIHT, Physics informed neural networks for multiphysics coupling, Advisor : R. Duvigneau

10.2.3 Juries

- Paola Goatin was referee of A. Hayat's Habilitation thesis *"Stabilization of 1D evolution systems"*, Université Paris Dauphine, February 8th, 2023.
- Paola Goatin was president of the committee of V.K. Lakshmanan's PhD thesis *"Cooperative control of eco-driving trajectories for a fleet of electric connected and autonomous vehicles"*, Université Paris-Saclay May 23rd, 2023.
- Paola Goatin was referee of N. De Nitti's PhD thesis *Analysis, control, and singular limits for hyperbolic conservation laws*, Friedrich-Alexander-Universität Erlangen-Nürnberg, July 24th, 2023.
- Paola Goatin was member of the committee of L. Monasse's Habilitation thesis *"Contributions to the simulation of hyperbolic systems in fluid and solid mechanics using computational geometry"*, Université Côte d'Azur, October 12th, 2023.
- Paola Goatin was referee of C. Donadello's Habilitation thesis *"Some contributions to the analysis of hyperbolic conservation laws"*, Université de Franche-Comté, December 21st, 2023.

11 Scientific production

11.1 Major publications

[1] A. Aggarwal, R. M. Colombo and P. Goatin. 'Nonlocal systems of conservation laws in several space dimensions'. In: *SIAM Journal on Numerical Analysis* 52.2 (2015), pp. 963–983. URL: https://hal.inria.fr/hal-01016784.

[2] B. Andreianov, P. Goatin and N. Seguin. 'Finite volume schemes for locally constrained conservation laws'. In: *Numer. Math.* 115.4 (2010). With supplementary material available online, pp. 609–645.

[3] S. Blandin and P. Goatin. 'Well-posedness of a conservation law with non-local flux arising in traffic flow modeling'. In: *Numerische Mathematik* (2015). DOI: 10.1007/s00211-015-0717-6. URL: https://hal.inria.fr/hal-00954527.

[4] R. M. Colombo and P. Goatin. 'A well posed conservation law with a variable unilateral constraint'. In: *J. Differential Equations* 234.2 (2007), pp. 654–675.

[5] M. L. Delle Monache and P. Goatin. 'Scalar conservation laws with moving constraints arising in traffic flow modeling: an existence result'. In: *J. Differential Equations* 257.11 (2014), pp. 4015–4029.

[6] M. L. Delle Monache, J. Reilly, S. Samaranayake, W. Krichene, P. Goatin and A. Bayen. 'A PDE-ODE model for a junction with ramp buffer'. In: *SIAM J. Appl. Math.* 74.1 (2014), pp. 22–39.

[7] J.-A. Desideri and R. Duvigneau. 'Parametric optimization of pulsating jets in unsteady flow by Multiple-Gradient Descent Algorithm (MGDA)'. In: *Numerical Methods for Differential Equations, Optimization, and Technological Problems, Modeling, Simulation and Optimization for Science and Technology*. 1st Jan. 2017. URL: https://hal.inria.fr/hal-01414741.

[8] J.-A. Désidéri. 'Adaptation by Nash games in gradient-based multi-objective/multi-disciplinary optimization'. In: JANO13 - Mathematical Control and Numerical Applications. Vol. 372. Springer Proceedings in Mathematics & Statistics Series. Khouribga, Morocco, 22nd Feb. 2021. URL: https://hal.inria.fr/hal-03430972.

[9] J.-A. Désidéri. 'COOPERATION AND COMPETITION IN MULTIDISCIPLINARY OPTIMIZATION Application to the aero-structural aircraft wing shape optimization'. In: *Computational Optimization and Applications* 52.1 (2012), pp. 29–68. DOI: 10.1007/s10589-011-9395-1. URL: https://hal.inria.fr/hal-00645787.

[10] J.-A. Désidéri. 'Multiple-gradient descent algorithm (MGDA) for multiobjective optimization / Algorithme de descente à gradients multiples pour l'optimisation multiobjectif'. In: *Comptes Rendus. Mathématique* Tome 350.Fascicule 5-6 (20th Mar. 2012), pp. 313–318. DOI: 10.1016/j.crma.2012.03.014. URL: https://hal.inria.fr/hal-00768935.

[11] J.-A. Désidéri and R. Duvigneau. 'Prioritized optimization by Nash games : towards an adaptive multi-objective strategy'. In: *ESAIM: Proceedings and Surveys* 71 (Aug. 2021), pp. 54–63. DOI: 10.1051/proc/202171106. URL: https://hal.inria.fr/hal-03430912.

[12] J.-A. Désidéri, J. Wintz, N. Bartoli, C. David and S. Defoort. *Combining Pareto Optimality with Nash Games in Multi-Objective Prioritized Optimization of an Aircraft Flight Performance*. RR-9490. Inria - Sophia Antipolis; Acumes, 17th Oct. 2022, p. 29. URL: https://inria.hal.science/hal-03817789.

[13] R. Duvigneau and P. Chandrashekar. 'Kriging-based optimization applied to flow control'. In: *Int. J. for Numerical Methods in Fluids* 69.11 (2012), pp. 1701–1714.

[14] A. Habbal and M. Kallel. 'Neumann-Dirichlet Nash strategies for the solution of elliptic Cauchy problems'. In: *SIAM J. Control Optim.* 51.5 (2013), pp. 4066–4083.

[15] M. Kallel, R. Aboulaich, A. Habbal and M. Moakher. 'A Nash-game approach to joint image restoration and segmentation'. In: *Appl. Math. Model.* 38.11-12 (2014), pp. 3038–3053. DOI: 10.1016/j.apm.2013.11.034. URL: http://dx.doi.org/10.1016/j.apm.2013.11.034.

[16] M. Martinelli and R. Duvigneau. 'On the use of second-order derivative and metamodel-based Monte-Carlo for uncertainty estimation in aerodynamics'. In: *Computers and Fluids* 37.6 (2010).

[17] Q. Mercier, F. Poirion and J.-A. Desideri. 'A stochastic multiple gradient descent algorithm'. In: *European Journal of Operational Research* (31st May 2018), p. 10. DOI: 10.1016/j.ejor.2018.05.064. URL: https://hal.archives-ouvertes.fr/hal-01833165.

[18] S. Roy, A. Borzì and A. Habbal. 'Pedestrian motion modelled by Fokker–Planck Nash games'. In: *Royal Society open science* 4.9 (2017), p. 170648.

[19] G. Todarello, F. Vonck, S. Bourasseau, J. Peter and J.-A. Desideri. 'Finite-volume goal-oriented mesh adaptation for aerodynamics using functional derivative with respect to nodal coordinates'. In: *Journal of Computational Physics* 313 (15th May 2016), p. 21. DOI: 10.1016/j.jcp.2016.02.063. URL: https://hal.inria.fr/hal-01410153.

[20] M. Twarogowska, P. Goatin and R. Duvigneau. 'Macroscopic modeling and simulations of room evacuation'. In: *Appl. Math. Model.* 38.24 (2014), pp. 5781–5795.

[21] G. Xu, B. Mourrain, A. Galligo and R. Duvigneau. 'Constructing analysis-suitable parameterization of computational domain from CAD boundary by variational harmonic method'. In: *J. Comput. Physics* 252 (Nov. 2013).

[22] B. Yahyaoui, M. Ayadi and A. Habbal. 'Fisher-KPP with time dependent diffusion is able to model cell-sheet activated and inhibited wound closure'. In: *Mathematical biosciences* 292 (2017), pp. 36–45.

11.2 Publications of the year

International journals

[23] M. Bahari, A. Habbal, A. Ratnani and E. Sonnendrücker. 'Adaptive isogeometric analysis using optimal transport and their fast solvers'. In: *Computer Methods in Applied Mechanics and Engineering* 418 (Jan. 2024), p. 116570. DOI: 10.1016/j.cma.2023.116570. URL: https://inria.hal.science/hal-03936627.

[24] S. Chabbar, A. Habbal, R. Aboulaich, N. Ismaili and S. El Majjaoui. 'Combined Hormone and Brachy Therapies for the Treatment of Prostate Cancer'. In: *Mathematical Modelling of Natural Phenomena* (17th Nov. 2023). DOI: 10.1051/mmnp/. URL: https://inria.hal.science/hal-03936301.

[25] F. A. Chiarello and P. Goatin. 'A non-local system modeling bi-directional traffic flows'. In: *SEMA SIMAI Springer Series*. SEMA SIMAI Springer Series 32 (2023), pp. 49–66. DOI: 10.1007/978-3-031-29875-2_3. URL: https://hal.science/hal-03722225.

[26] A. Festa, P. Goatin and F. Vicini. 'Navigation system based routing strategies in traffic flows on networks'. In: *Journal of Optimization Theory and Applications* 198.3 (Sept. 2023), pp. 930–957. DOI: 10.1007/s10957-023-02250-z. URL: https://hal.science/hal-03712945.

[27] P. Goatin. 'Macroscopic traffic flow modelling: from kinematic waves to autonomous vehicles'. In: *Communications in Applied and Industrial Mathematics* 14.1 (1st Jan. 2023), pp. 1–16. DOI: 10.2478/caim-2023-0001. URL: https://hal.science/hal-04337318.

[28] P. Goatin, C. Daini, M. L. Delle Monache and A. Ferrara. 'Interacting moving bottlenecks in traffic flow'. In: *Networks and Heterogeneous Media* 18.2 (2023), pp. 930–945. DOI: 10.3934/nhm.2023040. URL: https://hal.science/hal-04337346.

[29] P. Goatin and A. Würth. 'The initial boundary value problem for second order traffic flow models with vacuum: existence of entropy weak solutions'. In: *Nonlinear Analysis: Theory, Methods and Applications* 233 (Aug. 2023), p. 113295. DOI: 10.1016/j.na.2023.113295. URL: https://hal.science/hal-03828079.

[30] M. Ouni, A. Habbal and M. Kallel. 'A Three-player Nash game for point-wise source identification in Cauchy-Stokes problems'. In: *Journal of Computational and Applied Mathematics* 417 (Jan. 2023), p. 23. DOI: 10.1016/j.cam.2022.114613. URL: https://inria.hal.science/hal-03523088.

[31] N. Rosset, G. Cordonnier, R. Duvigneau and A. Bousseau. 'Interactive design of 2D car profiles with aerodynamic feedback'. In: *Computer Graphics Forum* 42.2 (8th Feb. 2023). DOI: 10.1111/cgf.14772. URL: https://inria.hal.science/hal-03975369.

International peer-reviewed conferences

[32] P. Goatin and D. Inzunza. 'A PINN approach for traffic state estimation and model calibration based on loop detector flow data'. In: MT-ITS 2023 - 8th International Conference on Models and Technologies for Intelligent Transportation Systems. Saint-Laurent-Du-Var, France, 14th June 2023. URL: https://hal.science/hal-04206224.

[33] A. Joumaa, P. Goatin and G. de Nunzio. 'A Macroscopic Model for Multi-Modal Traffic Flow in Urban Networks'. In: ITSC 2023 - 26th IEEE International Conference on Intelligent Transportation Systems. Bilbao, Spain, 2023. URL: https://hal.science/hal-04206252.

[34] E. Siri and P. Goatin. 'Assessing the impact of non-compliant users response to System-Optimal Dynamic Traffic Assignment'. In: CDC 2023 - 62nd IEEE Conference on Decision and Control. Singapore, Singapore, 13th Dec. 2023. URL: https://hal.science/hal-04206328.

[35] E. Siri and P. Goatin. 'System-Optimal Dynamic Traffic Assignment with partial users control: an analysis of different strategies'. In: ITSC 2023 - 26th IEEE International Conference on Intelligent Transportation Systems. Bilbao, Spain, 24th Sept. 2023. URL: https://hal.science/hal-04206281.

[36] A. Würth, M. Binois and P. Goatin. 'Validation of calibration strategies for macroscopic traffic flow models on synthetic data'. In: *IEEE PDF eXpress*. 8th International Conference on Models and Technologies for Intelligent Transportation Systems (MT-ITS 2023). Saint-Laurent-Du-Var, France, 14th June 2023. URL: https://hal.science/hal-04197769.

Scientific book chapters

[37] D. Amadori, B. Andreianov, M. Di Francesco, S. Fagioli, T. Girard, P. Goatin, P. Markowich, J. F. Pietschmann, M. D. Rosini, G. Russo, G. Stivaletta and M.-T. Wolfram. 'The mathematical theory of Hughes' model : a survey of results'. In: *Crowd Dynamics, Volume 4 : Analytics and Human Factors in Crowd Modeling*. Modeling and Simulation in Science, Engineering and Technology. Springer, 25th Dec. 2023. URL: https://hal.science/hal-04087181.

[38] M. Binois, A. Habbal and V. Picheny. 'A game theoretic perspective on Bayesian multi-objective optimization'. In: *Many-Criteria Optimization and Decision Analysis: State-of-the-Art, Present Challenges, and Future Perspectives*. 2023. DOI: 10.1007/978-3-031-25263-1_11. URL: https://inria.hal.science/hal-03206174.

Edition (books, proceedings, special issue of a journal)

[39] K. Musayeva and M. Binois, eds. *Improved Multi-Label Propagation for Small Data with Multi-Objective Optimization*. ECML PKDD 2023. Lecture Notes in Computer Science. 18th Sept. 2023, pp. 284–300. DOI: 10.1007/978-3-031-43421-1_17. URL: https://inria.hal.science/hal-03914733.

Doctoral dissertations and habilitation theses

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