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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

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1 Team members, visitors, external collaborators

Research Scientists

- Paola Goatin [Team leader, Inria, Senior Researcher, HDR]
- Mickael Binois [Inria, Researcher]
- Jean-Antoine Desideri [Inria, Emeritus, HDR]
- Regis Duvigneau [Inria, Researcher, HDR]

Faculty Member

- Abderrahmane Habbal [Univ Côte d'Azur, Associate Professor, HDR]

Post-Doctoral Fellow

- Khadija Musayeva [Univ de Nice - Sophia Antipolis, from Oct 2020]

PhD Students

- Salma Chabbar [Ecole Mohammedia d'Ingénieurs, Université Mohamed V, Rabat, 01/01/2020 - 31/12/2022, co-advise EIFFEL Scholarship]
- Marwa Ouni [Ecole Nationale d'ingénieurs de Tunis, Université Tunis al Manar, Tunis, 01/10/2017 - 31/03/2021, PHC Utique co-advise]
- Stefano Pezzano [Inria]

Interns and Apprentices

- Alexandra Wuerth [Inria, from Apr 2020 until Sep 2020]

Administrative Assistant

- Montserrat Argente [Inria]

Visiting Scientist

- Brahim El Alaoui [Université Mohamed V, , until Aug 2020, Erasmus++ doctoral]

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 [111], or to the dynamics of turbulent flows for which large scale / small scale vortical structures interfere [139].

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 [79] for an existence result and [64, 80] 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 [70, 98] for some applications in traffic flow modelling, and [90, 95, 97] 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 [64, 80].

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 [71, 85] for the derivation of Lighthill-Whitham-Richards [122, 138] traffic flow model from Follow-the-Leader and [91] for results on crowd motion models (see also [113]). 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 [86], and extensively used since then to prove convergence of approximate solutions and deduce existence results, see for example [92] 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 [52, 94]. We refer, for example, to the notion of solution for non-hyperbolic systems [100], 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 [94].

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 [75]), and proved to be successful for studying emerging self-organised flow patterns [74]. The theoretical measure framework proves to be also relevant in addressing micro-macro limiting procedures of mean field type [101], 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* [148, 147]. Indeed, as observed in [131, 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 [121]). 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 [61, 60, 87, 120], 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 [134], 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 the one developed in [78] 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, [50]) 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 [47], sedimentation [54], supply chains [105], conveyor belts [103], biological applications like structured populations dynamics [130], or more general problems like gradient constrained equations [49]. Also, non-local in time terms arise in conservation laws with memory, starting from [77]. 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 [56, 63, 67, 102, 142]. 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 [56, 102] and lane formation in crossing pedestrian flows.

General analytical results on non-local conservation laws, proving existence and eventually uniqueness of solutions of the Cauchy problem for 1, can be found in [48] for scalar equations in one space dimension ($N = d = 1$), in [68] for scalar equations in several space dimensions ($N = 1$, $d \geq 1$) and in [43], [69, 73] for multi-dimensional systems of conservation laws. Besides, specific finite volume numerical methods have been developed recently in [43, 102] and [119].

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 - regularity of solutions, boundary value problems 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 [62]. In aerodynamics, inflow conditions like velocity modulus and direction, are subject to fluctuations [109, 129]. For some engineering problems, the geometry of the boundary can also be uncertain, due to structural deformation, mechanical wear or disregard of some details [89]. 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 [140, 146], 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 [141, 144], 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 [126]. 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 [109, 118, 123, 151] or an entropy closure method [84], or by discretizing the probability space and extending the numerical schemes to the stochastic components [42]. 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 [135, 146, 149].

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 [53]. Besides, we plan to extend previous works on sensitivity analysis [89, 124] 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 [57] (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 [146]. 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 w.r.t. 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 [137] 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 [51, 104] for the backward time integration of the adjoint variables. The sensitivity equation method (SEM) offers a promising alternative [88, 114], 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 [89].
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) [139] , Detached-Eddy Simulation (DES) [143] or Organized-Eddy Simulation (OES) [58], are more and more employed to analyse 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 [116] or multiobjective optimization algorithm (see section below).

3.3.2 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 [82] [81]. Originally, we have stated a principle according 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 dispose of 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 [83] 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 [132] 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 [153].

3.3.3 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 [96].

Our proposal is designed to tackle derivative-free, expensive models, hence requiring very few model evaluations to converge to the solution.

3.3.4 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 [44] and still completely open for systems like e.g. coupled heat and thermoelastic joint data and material detection.

4 Application domains

4.1 Active flow control for vehicles

The reduction of CO2 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 [152].

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 [110]. Further improvements require more advanced models, keeping into better account interactions at the microscopic scale, and adapted control techniques, see [59] 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 [72, 99], 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 [115].

- *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 [112] 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 [65, 66]), 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 [79, 98] or via the Hamilton-Jacobi approach [65, 66] could allow to optimize the flow by controlling some specific vehicles corresponding to internal conditions.

4.3 Virtual Fractional Flow Reserve in coronary stenting

Atherosclerosis is a chronic inflammatory disease that affects the entire arterial network and especially the coronary arteries. It is an accumulation of lipids over the arterial surface due to a dysfunction of this latter. The objective of clinical intervention, in this case, is to establish a revascularization using different angioplasty techniques, among which the implantation of stents is the most widespread. This intervention involves introducing a stent into the damaged portion in order to allow the blood to circulate in a normal way over all the vessels. Revascularization is based on the principle of remedying ischemia, which is a decrease or an interruption of the supply of oxygen to the various organs. This anomaly is attenuated by the presence of several lesions (multivessel disease patients), which can lead to several complications. The key of a good medical intervention is the fact of establishing a good diagnosis, in order to decide which lesion requires to be treated. In the diagnosis phase, the clinician uses several techniques, among which angiography is the most popular. Angiography is an X-ray technique to show the inside (the lumen) of blood vessels, in order to identify vessel narrowing: stenosis. Despite its widespread use, angiography is often imperfect in determining the physiological significance of coronary stenosis. If the problem remains simple for non significant lesions ($\leq 40\%$) or very severe ($\geq 70\%$), a very important category of intermediate lesions must benefit from a functional evaluation which will determine the strategy of treatment [76].

The technique of the Fractional Flow Reserve (FFR) has derived from the initial coronary physical approaches decades ago. Since then, many studies have demonstrated its effectiveness in improving the patients prognosis, by applying the appropriate approach. Its contribution in the reduction of mortality was statistically proved by the FAME (Fractional Flow Reserve Versus Angiography for Multivessel Evaluation) study [128]. It is established that the FFR can be easily measured during coronary angiography by calculating the ratio of distal coronary pressure P_d to aortic pressure P_a. These pressures are measured simultaneously with a special guide-wire. FFR in a normal coronary artery equals to 1.0. FFR value of 0.80 or less identifies ischemia-causing coronary lesions with an accuracy of more than 90% [128].

Obviously, from an interventional point of view, the FFR is binding since it is invasive. It should also be noted that this technique induces additional costs, which are not covered by insurances in several countries. For these reasons, it is used only in less than 10% of the cases.

In this perspective, a new virtual version of the FFR, entitled VFFR, has emerged as an attractive and non-invasive alternative to standard FFR, see [145, 127]. VFFR is based on computational modeling, mainly fluid and fluid-structural dynamics. However, there are key scientific, logistic and commercial challenges that need to be overcome before VFFR can be translated into routine clinical practice.

While most of the studies related to VFFR use Navier-Stokes models, we focus on the non-newtonian case, starting with a generalized fluid flow approach. These models are more relevant for the coronary arteries, and we expect that the computation of the FFR should then be more accurate. We are also leading numerical studies to assess the impact (on the FFR) of the interaction of the physical devices (catheter, optical captors, spheroids) with the blood flow.

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.

- **Modeling cell dynamics.** Migration and proliferation of epithelial cell sheets are the two keystone aspects of the collective cell dynamics in most biological processes such as morphogenesis, embryogenesis, cancer and wound healing. It is then of utmost importance to understand their underlying mechanisms.

  Semilinear reaction-diffusion equations are widely used to give a phenomenological description of the temporal and spatial changes occurring within cell populations that undergo scattering (moving), spreading (expanding cell surface) and proliferation. We have followed the same methodology and contributed to assess the validity of such approaches in different settings (cell sheets [107], dorsal closure [46], actin organization [45]). However, epithelial cell-sheet movement is complex enough to undermine most of the mathematical approaches based on *locality*, that is mainly traveling wavefront-like partial differential equations. In [93] it is shown that Madin-Darby Canine Kidney (MDCK) cells extend cryptic lamellipodia to drive the migration, several rows behind the wound edge. In [133] MDCK monolayers are shown to exhibit similar non-local behavior (long range velocity fields, very active border-localized leader cells).

  Our aim is to start from a mesoscopic description of cell interaction: considering cells as independent anonymous agents, we plan to investigate the use of mathematical techniques adapted from the mean-field game theory. Otherwise, looking at them as interacting particles, we will use a multi-agent approach (at least for the actin dynamics). We intend also to consider approaches stemming from compartment-based simulation in the spirit of those developed in [90, 95, 97].

- **Game strategies for thermoelastography.** Thermoelastography is an innovative non-invasive control technology, which has numerous advantages over other techniques, notably in medical imaging [125]. 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 [106, 117], we have demonstrated that Nash game approaches are efficient to tackle ill-posedness. We intend to extend the results obtained for Laplace equations in [106], and the algorithms developed in Section 3.3.4 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. [136], 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 sub-spaces, 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, 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 dof's. 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 effciency, thus reducing energy consumption and pollutant emission.

From medical viewpoint, virtual fractional flow reserve vFFR is a promising technique to support clinicians in cardiostenting with cheap social costs compared to the analogic commercial solutions. Acumes has contributed to improve the involved computational apparatus (nonlinear fluid mechanics with ad hoc boundary conditions).

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 Highlights of the year

6.1 Awards

- M. Binois: 2020 Youden Award for best expository paper appearing in the 2019 issues of Technometrics (American Quality Association).
- M. Binois: Finalist for the 2020 Gordon Bell Special Prize for High Performance Computing-Based COVID-19 Research (ACM Gordon Bell prize).
- P. Goatin: ANR-3IA Côte d'Azur Senior Chair for the project *"Data driven traffic management"* (2020-2024).

7 New software and platforms

7.1 New software

7.1.1 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: `http://mgda.inria.fr`

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

Authors: Jean-Antoine Désidéri, Nicolas Niclausse, Thibaud Kloczko

Contacts: Jean-Antoine Désidéri, Thibaud Kloczko

Participant: Jean-Antoine Désidéri

7.1.2 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

7.1.3 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.

News of the Year: Demo movies are available from Youtube (see web site)

URL: http://youtu.be/MW_gIF8hUdk

Contact: Abderrahmane Habbal

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

8 New results

8.1 Macroscopic traffic flow models on networks

Participants Mickaël Binois, Paola Goatin, Alexandra Würth, Antonella Ferrara *(U Pavia, Italy)*, Giulia Piacentini *(U Pavia, Italy)*.

Traffic control by vehicle platooning.

In [33], a coupled PDE-ODE model describing the interaction between the bulk traffic flow and a platoon of connected vehicles is adopted to develop a control action aiming at reducing the fuel consumption of the overall traffic flow. The platoon is modeled as a capacity restriction acting on the surrounding traffic. The trajectory of the initial and final points of the platoon are optimized by means of a model predictive control strategy, acting on the speeds of the front-end and back-end of the platoon, thus resulting in controlling both the speed and the length of the platoon. The approach is assessed in simulations.
This work is part of G. Piacentini's PhD thesis.

Traffic flow model calibration by statistical approaches.

In the framework of A. Würth's internship, we have employed a Bayesian approach including a bias term to estimate first and second order model parameters, based on two traffic data sets: a set of loop detector data located on the A50 highway between Marseille and Aubagne provided by DIRMED, and publicy available data from the Minnesota Department of transportation (http://data.dot.state.mn.us/datatools/). The method proved to be effective and allowed to infer better performances of second order model, in particular regarding speed and density esimation.

8.2 Non-local conservation laws

Participants Paola Goatin, Raimund Bürger *(Universidad de Concepción, Chile)*, Daniel Inzunza *(Universidad de Concepción, Chile)*, Luis Miguel Villada *(U Bìo-Bìo, Chile)*.

In the framework of the Associated Team NOLOCO, we proposed a revised version often the non-local macroscopic pedestrian flow model proposed in [R. M. Colombo, M. Garavello, and M. Lécureux-Mercier. A class of nonlocal models for pedestrian traffic. *Math. Models Methods Appl. Sci.*, 22(4):1150023, 2012] to account for anisotropic interactions and the presence of walls or other obstacles in the walking domain. We proved the well-posedness of this extended model and we applied high-resolution numerical schemes to illustrate the model characteristics. In particular, numerical simulations highlight the role of different model parameters in the observed pattern formation. The results are published in [18].

8.3 Isogeometric Discontinuous Galerkin method for compressible flows

Participants Régis Duvigneau, Stefano Pezzano, Maxime Stauffert *(CEA Saclay)*.

The co-existence of different geometrical representations in the design loop (CAD-based and mesh-based) is a real bottleneck for the application of design optimization procedures in industry, yielding a major waste of human time to convert geometrical data. Isogeometric analysis methods, which consists in using CAD bases like NURBS in a Finite-Element framework, were proposed a decade ago to facilitate interactions between geometry and simulation domains.

We investigate the extension of such methods to Discontinuous Galerkin (DG) formulations, which are better suited to hyperbolic or convection-dominated problems. Specifically, we develop a DG method for compressible Euler and Navier-Stokes equations, based on rational parametric elements, that preserves exactly the geometry of boundaries defined by NURBS, while the same rational approximation space is adopted for the solution. The following research axes are considered in this context:

- **CAD-consistent adaptive refinement**
  Properties of NURBS functions are used to define an adaptive refinement strategy, which refines locally the discretization according to an error indicator, while describing exactly CAD geometries whatever the refinement level. The resulting approach exhibits an optimal convergence rate and capture efficiently local flow features, like shocks or vortices, avoiding refinement due to geometry approximation [24].

- **Arbitrary Eulerian-Lagrangian formulation for high-order meshes**
  To enable the simulation of flows around moving bodies, an Arbitrary Eulerian-Lagrangian (ALE) formulation is proposed in the context of the isogeometric DG method. It relies on a NURBS-based grid velocity field, integrated along time over moving NURBS elements. The gain of using exact-geometry representations is clearly quantified, in terms of accuracy and computational efficiency [31, 36].

- **Geometrically exact sliding interfaces**
  In the context of rotating machines (compressors, turbines, etc), computations are achieved using a rotating inner grid interfaced to an outer fixed grid. This coupling is combersome using classical piecewise-linear grids due to a lack of common geometrical interface. Thus, we develop a method based on a geometrically exact sliding interface using NURBS elements, ensuring a fully conservative scheme.

- **Isogeometric shape optimization**
  We develop an optimization procedure with shape sensitivity analysis, entirely based on NURBS representations [41]. The mesh, the shape to optimize, as well as the flow solutions are represented by NURBS, which avoids any geometrical conversion and allows to exploit NURBS properties regarding regularity or hierarchy.

8.4 Sensitivity analysis for compressible flows

Participants Régis Duvigneau, Maxime Stauffert *(CEA Saclay)*, Camilla Fiorini *(UVST)*, , Christophe Chalons *(UVST)*.

The adjoint equation method, classically employed in design optimization to compute functional gradients, is not well suited to complex unsteady problems, because of the necessity to solve it backward in time. Therefore, we investigate the use of the sensitivity equation method, which is integrated forward in time, in the context of compressible flows. More specifically, the following research axes are considered:

- **Sensitivity analysis in presence of shocks**
  While the sensitivity equation method is a common approach for parabolic systems, its use for hyperbolic ones is still tedious, because of the generation of discontinuities in the state solution, yielding Dirac distributions in the sensitivity solution. To overcome this difficulty, we investigate a modified sensitivity equation, that includes an additional source term when the state solution exhibits discontinuities, to avoid the generation of delta-peaks in the sensitivity solution. We consider as typical example the 1D compressible Euler equations. Different approaches are tested to integrate the additional source term: a Roe solver, a Godunov method and a moving cells approach. Applications to uncertainty quantification in presence of shocks are demonstrated and compared to the classical Monte-Carlo method [26]. This study is achieved in collaboration with C. Chalons and C. Fiorini from University of Versailles.

- **Shape sensitivity analysis**
  When shape parameters are considered, the evaluation of flow sensitivities is more difficult, because equations include an additional term, involving flow gradient, due to the fact that the parameter affects the boundary condition location. To overcome this difficulty, we propose to solve sensitivity equations using an isogeometric Discontinuous Galerkin (DG) method, which allows to estimate accurately flow gradients at boundary and consider boundary control points as shape parameters. First results obtained for 2D compressible Euler equations exhibit a sub-optimal convergence rate, as expected, but a better accuracy with respect to a classical DG method [41].

8.5 Advanced Bayesian optimization

Participants Mickaël Binois, Régis Duvigneau, Abderrahmane Habbal, Mahmoud Elsawy *(Atlantis team)*, Frédéric Hauville *(Ecole Navale Brest)*, Olivier Lemaitre *(CNRS-LIMSI)*, Stéphane Lanteri *(Atlantis team)*, Victor Picheny *(Secondmind, UK)*, Matthieu Sacher *(ENSTA Bretagne)*.

Multi-fidelity Bayesian optimization

The objective of multi-fidelity optimization strategies is to account for a set of models of different accuracies and costs to accelerate the optimization procedure. In the context of Bayesian optimization, we develop such a multi-fidelity approach based on non-nested evaluations: each time a new evaluation is required, the algorithm selects a new design point associated to a fidelity level to maximize the expected improvement on the finest modeling level. The proposed approach is applied to the fluid-structure optimization of a sailing boat, which is described by five modeling levels. A significant acceleration of the optimization procedure is reported, without loss of accuracy [35].

The Kalai-Smorodinski solution for many-objective Bayesian optimization

Extending the short paper [16] on the use of the game-theoretic Kalai-Smorodinski solution in Bayesian optimization, we have refined the definition of solutions, discussed underlying assumptions, and shown empirically the improved performance of our proposed approach over naive heuristics. A realistic hyperparameter tuning problem with eight objectives as well as an expensive calibration problem with nine objectives have been considered as well.

In parallel, we have substantially improved the efficiency of the implementation, enabled specific treatment of calibration problems as well as handling noise in the `GPGame` package https://cran.r-project.org/web/packages/GPGame.

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 contexte 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.

First studies achieved using Bayesian optimization algorithms, demonstrate the potentiality of the proposed approach [25, 37].

8.6 Gaussian process based sequential design

Participants Mickaël Binois, Robert Gramacy *(Virginia Tech, USA)*, Michael Ludkovski *(UCSB, USA)*, Xiong Lyu *(UCSB, USA)*, Stefan Wild *(Argonne National Laboratory, USA)*, Nathan Wycoff *(Virginia Tech, USA)*.

Besides Bayesian optimization as above, Gaussian processes are useful for a variety of other related tasks. Here we first present a tutorial on the subject of modeling with input dependent noise with an implementation in the `hetGP R` package. Then the estimation of level-set in for noisy simulators with complex input noise is studied, before treating sequential design for efficient dimension reduction.

Heteroskedastic Gaussian process modeling and sequential design

An increasing number of time-consuming simulators exhibit a complex noise structure that depends on the inputs. For conducting studies with limited budgets of evaluations, new surrogate methods are required in order to simultaneously model the mean and variance fields. To this end, in [55] we present the `hetGP` package https://cran.r-project.org/web/packages/hetGP, implementing many recent advances in Gaussian process modeling with input-dependent noise. First, we describe a simple, yet efficient, joint modeling framework that relies on replication for both speed and accuracy. Then we tackle the issue of data acquisition leveraging replication and exploration in a sequential manner for various goals, such as for obtaining a globally accurate model, for optimization, or for contour finding. Reproducible illustrations are provided throughout.

Sequential learning of active subspace

Continuing a work started at Argonne National Laboratory, in [150] we consider the combination of Gaussian process regression modeling with the active subspace methods (ASMs), which have become a popular means of performing subspace sensitivity analysis on black-box functions. Naively applied, however, ASMs require gradient evaluations of the target function. In the event of noisy, expensive, or stochastic simulators, evaluating gradients via finite differencing may be infeasible. In such cases, often a surrogate model is employed, on which finite differencing is performed. When the surrogate model is a Gaussian process, we show that the ASM estimator is available in closed form, rendering the finite-difference approximation unnecessary. We use our closed-form solution to develop acquisition functions focused on sequential learning tailored to sensitivity analysis on top of ASMs. We also show that the traditional ASM estimator may be viewed as a method of moments estimator for a certain class of Gaussian processes. We demonstrate how uncertainty on Gaussian process hyperparameters may be propagated to uncertainty on the sensitivity analysis, allowing model-based confidence intervals on the active subspace. Our methodological developments are illustrated on several examples.

Evaluating Gaussian Process Metamodels and Sequential Designs for Noisy Level Set Estimation

We consider the problem of learning the level set for which a noisy black-box function exceeds a given threshold. To efficiently reconstruct the level set, we investigate Gaussian process (GP) metamodels. Our focus in [40] is on strongly stochastic samplers, in particular with heavy-tailed simulation noise and low signal-to-noise ratio. To guard against noise misspecification, we assess the performance of three variants: (i) GPs with Student-t observations; (ii) Student-t processes (TPs); and (iii) classification GPs modeling the sign of the response. In conjunction with these metamodels, we analyze several acquisition functions for guiding the sequential experimental designs, extending existing stepwise uncertainty reduction criteria to the stochastic contour-finding context. This also motivates our development of (approximate) updating formulas to efficiently compute such acquisition functions. Our schemes are benchmarked by using a variety of synthetic experiments in 1–6 dimensions. We also consider an application of level set estimation for determining the optimal exercise policy of Bermudan options in finance.

8.7 Prioritized multi-objective optimization of a sandwich panel

Participants Jean-Antoine Désidéri, Pierre Leite *(Essilor, Créteil)*, Quentin Mercier *(formerly at ONERA Châtillon)*.

The potential of the prioritized multi-objective optimization approach has been demonstrated by applying it to the sizing of a sandwich panel with respect to mechanical criteria: mass, critical failure forces under bending load (1st and 2nd modes), and blast mitigation measured by the core energy absorption, deflection, or both. Several objective functions are defined by analytical models. Four numerical test-cases were documented.

In each test-case, in a first phase of optimization, the Primary Pareto Front associated with two criteria only, considered preponderant, was first established. Mass was always retained in these primary objective functions. In a second phase, a starting point on the Primary Pareto Front is selected and the corresponding design is improved with respect to secondary criteria by the construction of a continuum of Nash equilibria tangent to the front in function space at the starting point, thus only marginally degrading the primary criteria.

The second phase of optimization can be viewed as a form of adaptation of the optimization process. Here it permits to account for four criteria, at a more economical and simpler strategy than it would be to evaluate and analyze a complete Pareto front in a four-dimensional function space. [39]

(All the numerical experiments were realized using the software platform `http://mgda.inria.fr`.)

8.8 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 [108] 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 two first 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.

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 such an approach is applied to solve Inverse problems for nonlinear systems.

8.9 Virtual FFR quantified with a generalized flow model using Windkessel boundary conditions ; Application to a patient-specific coronary tree

Participants Abderrahmane Habbal, Keltoum Chahour *(PhD, ACUMES and EMI, Univ. Mohammed V)*, Rajae Aboulaich *(EMI, Univ. Mohammed V)*, Nejib Zemzemi *(Inria Bordeaux, EPI CARMEN)*, Mickaël Binois.

Fractional flow reserve (FFR) has proved its efficiency in improving patients diagnosis. From both economical and clinical viewpoints, a realistic simulation of vascular blood flow inside the coronary arteries could be a better alternative to the invasive FFR. In this view, we consider a 2D reconstructed left coronary tree with two artificial lesions of different degrees. We use a generalized fluid model with a Carreau law and use a coupled multidomain method to implement Windkessel boundary conditions at the outlets. We introduce our methodology to quantify the virtual FFR, and lead several numerical experiments. We compare FFR results from Navier Stokes versus generalized flow model, and for Windkessel versus traction free outlets boundary conditions or mixed outlets boundary conditions. We also investigate some sources of uncertainty that the FFR index might encounter during the invasive procedure, in particular the arbitrary position of the distal sensor. The computational FFR results show that the degree of stenosis is not enough to classify a lesion, while there is a good agreement between Navier Stokes and the non Newtonian flow model adopted in classifying coronary lesions. Furthermore, we highlight that the lack of standardization while making FFR measurement might be misleading regarding the significance of stenosis [19].

9 Bilateral contracts and grants with industry

9.1 Bilateral contracts with industry

- **Etic Data** (2019-2020): Acumes has set up a 12 months research and development contract with the company Etic Data on "Predictive modeling and proactive driving of customers behaviour in massive data BtoC context".
- **Mycophyto** (2020-...): this research contract involving Université Côte d'Azur is financing the post-doctoral contract of Khadija Musayeva.

10 Partnerships and cooperations

10.1 International initiatives

10.1.1 Inria International Labs

Acronym: NOLOCO (Inria Chile)

Title: Efficient numerical schemes for non-local transport phenomena

Duration: 2018 - 2020

Coordinator: Paola Goatin

Partners:

- Department of Mathematics, Universidad del Bio-Bio (Chile): Prof. Luis Miguel Villada Osorio
- Center for Research in Mathematical Engineering (CI2MA), Universidad de Concepcion (Chile): Prof. Raimund Burger
- Laboratoire de Mathématiques Université de Versailles St. Quentin (France): Prof. Christophe Chalons

Inria contact: Paola Goatin

Summary: This project tackles theoretical and numerical issues arising in the mathematical study of conservation laws with non-local flux functions. These equations include in a variety of applications, ranging from traffic flows to industrial processes and biology, and are intended to model macroscopically the action of non-local interactions occurring at the microscopic level.

The team, bi-located in France and Chile, has complementary skills covering the analysis, numerical approximation and optimization of non-linear hyperbolic systems of conservation laws, and their application to the modeling of vehicular and pedestrian traffic flows, sedimentation and other industrial problems.

Based on the members' expertise and on the preliminary results obtained by the team, the project will focus on the following aspects: - The development of efficient, high-order finite volume numerical schemes for the computation of approximate solutions of non-local equations. - The sensitivity analysis of the solutions on model parameters or initial conditions

The impact of the project is therefore twofold: while addressing major mathematical advances in the theory and numerical approximation of highly non-standard problems, it puts the basis for innovative tools to handle modern applications in engineering sciences.
See also: https://team.inria.fr/acumes/assoc-team/noloco/

10.1.2 Inria international partners

Declared Inria international partners

Acronym: ORESTE

Title: Optimal REroute Strategies for Traffic managEment

Duration: 2018 - 2022

Coordinator: Paola Goatin

Partners:

- University of California Berkeley (United States) - Electrical Engineering and Computer Science (EECS) (EECS) - Prof. Alexandre M. Bayen

Inria contact: Paola Goatin

Summary: The rapidly changing transportation ecosystem opens new challenges in traffic modeling and optimization approaches. We will focus in particular on the two following aspects:

Route choice apps impact. The vast use of personal route choice systems through phone applications or other devices is modifying the traditional flow of networks, requiring new models for accounting of the guidance impact. Indeed, routing apps have changed traffic patterns in the US and Europe, leading to new congestion patterns where previously no traffic was observed. Over the last decade, GPS enabled smart phones and connected personal navigation devices have disrupted the mobility landscape. Initially, the availability of traffic information led to better guidance of a small portion of motorists in the system. But as the majority of the driving public started to use apps, the systematic broadcasting of “selfish” best routes led to the worsening of traffic in numerous places, ultimately leading to the first lawsuit against one specific company in particular (Waze) accused to be the cause of these problems. This is just the beginning of an evolution, which, if not controlled and regulated, will progressively asphyxiate urban landscapes (already nearly hundreds of occurrences of this phenomenon are noticed by the popular media, which indicates the presence of probably thousands of such issues in the US alone). Traffic managers are typically not equipped to fix these problems, and typically do not fund this research, as in order to be able to regulate and fix the problem, fundamental science needs to be advanced, modeling and game theory in particular, so remediation can happen (for which the traffic managers are equipped). In this project, we will mainly focus on the development and study of new macroscopic dynamical models to describe the aforementioned phenomena, and we will explore control strategies to mitigate their impact.

Autonomous vehicles. Besides, the foreseen deployment of connected and autonomous vehicles (CAVs) opens new perspectives both in traffic modeling and control. Indeed, CAVs are expected to modify the classical macroscopic traffic dynamics due to their peculiar motion laws, which are more uniform than human drivers' and follow different rules. Besides, due to their extended information on neighboring traffic conditions, the resulting dynamics would have a non-local character, justifying the use of rapidly developing non-local models. In any case, the different behavior of autonomous vehicles requires the design of new multi-class models capable of accounting for different vehicle classes characteristics and mutual interactions. Moreover, CAVs could be used as endogenous variable speed limiters, thus providing new action points to control traffic flow. Preliminary results show that the presence of few controlled vehicles can positively affect traffic conditions. In this setting, the interaction of AVs with the surrounding traffic can be described by strongly coupled PDE-ODE systems, which have been largely studied by the ACUMES team. Yet, the study of CAVs impact in realistic situations requires further research, in particular towards model validation, for which the Berkeley team will provide the necessary data.
See also: https://team.inria.fr/acumes/assoc-team/oreste

Informal international partners

- University of Milano Bicocca, Mathematics and Applications (M. Garavello: https://sites.google.com/site/maurogaravello/)
- University of Rutgers - Camden, Department of Mathematical Science (B. Piccoli: https://piccoli.camden.rutgers.edu/)
- University of Texas Arlington (S. Roy, https://mentis.uta.edu/explore/profile/souvik-roy)

10.1.3 Participation in other international programs

PHC Procope

Program: Program Hubert Curien Procope (Germany)

Title: Non-local conservation laws for engineering applications

Duration: January 2019 - December 2020

Coordinator: P. Goatin and S. Göttlich (Univ. Mannheim)

Partners:

- University of Mannheim (Germany)

Inria contact: Paola Goatin

Summary: This project tackles theoretical and numerical issues arising in the mathematical study of conservation laws with non-local flux functions. These equations appear in a variety of applications, ranging from traffic flows to industrial processes and biology, and are intended to model macroscopically the action of non-local interactions occurring at the microscopic level. The team, bi-located in France and Germany, has complementary skills covering the analysis, numerical approximation and optimization of non-linear hyperbolic systems of conservation laws, and their application to the modeling of vehicular and pedestrian traffic flows, manufacturing systems and other industrial problems. Based on the members expertise and on the preliminary results obtained by both teams, the project will focus on the following interconnected aspects: The treatment of boundary conditions, both from the analytical and the numerical point of views, in order to provide a sound basis to address specific problems arising in the applications. The development of efficient, high-order finite volume numerical schemes for the computation of approximate solutions of non-local equations. The investigation of optimal control problems with corresponding optimality systems and the design of appropriate and adaptive optimization algorithms. Targeted applications include vehicular traffic (mainly in connection with vehicle-to-vehicle communication and consumption/pollution estimation), crowd motion (in connection with safe building evacuation procedures), and manufacturing systems (intelligent production). The impact of the project is therefore twofold: while addressing major mathematical advances in the theory and numerical approximation of highly non-standard problems, it puts the basis for innovative tools to handle modern applications in engineering sciences.

PHC Utique

Program: Program Hubert Curien PHC Utique (Tunisia)

Project acronym: NAMReD

Project title: Novel Algorithms and Models for Data Reconstruction

Duration: January 2018 - December 2020

Coordinator: A. Habbal and M. Kallel (Univ. Tunis al Manar)

Summary: The project goal is the design of new and efficient algorithms tailored for data reconstruction involving ill-posed problems. We rely on an original use of game theory and p-Kirchhoff methods. We apply these approaches for missing data recovery and image restoration.

10.2 European initiatives

10.2.1 Collaborations in European programs, except FP7 and H2020

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 https://www.cost.eu/actions/CA18232/#tabs|Name:parties

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 modelling and analysing 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.

10.3 National initiatives

10.3.1 ANR

- **Project OPERA** (2019-2021): Adaptive planar optics
  This project is composed of Inria teams ATLANTIS, ACUMES and HIEPACS, CNRS CRHEA lab. and company NAPA. Its objective is the characterization and design of new meta-surfaces for optics (opera web site).

11 Dissemination

11.1 Promoting scientific activities

11.1.1 Scientific events: organisation

General chair, scientific chair

- P. Goatin is member of the scientific committee of the annual seminar CEA-GAMNI *"Numerical fluid-mechanics"*.

- A. Habbal was member of the scientific committee of the CARI 2020 Colloque Africain sur la Recherche en Informatique et Mathématiques Appliquées Thies, Senegal, October 2020.

Member of the organizing committees

- P. Goatin was member of the organizing committee of the IPAM (UCLA) long program on *"Mathematical Challenges and Opportunities for Autonomous Vehicles"*, Los Angeles (USA), fall 2020

- P. Goatin was member of the organizing committee of the International on-line program *"Fifty Years of Kruzhkov Entropy Solutions, and Beyond"*, fall 2020.

11.1.2 Scientific events: selection

Reviewer

- M. Binois reviewed for the following conferences: AISTATS 2020, ICLR 2021, ICML 2020, IJCAI-PRICAI 2020 and NeurIPS 2020.

- R. Duvigneau reviewed for the AIAA Aviation Forum 2021.

- P. Goatin was Associate Editor for the 23rd Intelligent Transportation Systems Conference (IEEE ITSC 2020).

- A. Habbal reviewed for the CARI 2020 conference

11.1.3 Journal

Member of the editorial boards

- P. Goatin is Managing Editor of *Networks and Heterogeneous Media.*

- P. Goatin is Associate Editor of *SIAM Journal on Applied Mathematics.*

Reviewer - reviewing activities

- M. Binois is a reviewer for the following international journals: Annals of Applied Statistics, Journal of Applied Statistics, Computers & Operations Research, Information and Inference, Journal of Mechanical Engineering Science (Part. C), Journal of Uncertainty Quantification, Mathematical Programming, Optimization and Engineering, Structural and Multidisciplinary Optimization, and Technometrics.

- R. Duvigneau is reviewer for the following international journals: Computers and Fluids, International Journal for Numerical Methods in Fluids, Journal of Fluid and Structures, Computer Methods for Applied Mechanics Engineering, Computer Aided Geometric Design, Applied Mathematics and Mechanics, Engineering Optimization, Ocean Engineering.

- P. Goatin reviewed for the following international journals: Annales de l'Institut Henri Poincaré / Analyse non lineaire, IEEE Transactions on Automatic Control, Vietnam Journal of Mathematics.

- A. Habbal was reviewer for the following international journals : Journal of Scientific Computing, Journal of Dynamical and Control Systems, Revue Africaine de la Recherche en Informatique et Mathématiques Appliquées, Systems and Control Letters, AMS Mathematical Reviews, Numerische Mathematics

11.1.4 Invited talks

- M. Binois: Université Mohammed VI Polytechnique, Ben Guérir (Morocco), January 2020. Invited talk: *Scaling up multi-objective Bayesian optimization.*

- M. Binois: Dagstuhl Seminar 20031 - Scalability in Multiobjective Optimization, Dagstuhl (Germany), January 2020. Talk: *Scaling up multi-objective Bayesian optimization.*

- P. Goatin: IPAM (UCLA) long program on *"Mathematical Challenges and Opportunities for Autonomous Vehicles"* (November 2020, on-line)
  Workshop "Large Scale Autonomy: Connectivity and Mobility Networks".
  Talk: *A multi-population traffic flow model on networks accounting for vehicle automation.*

- P. Goatin: SophI.A Summit (November 2020, on-line)
  Invited talk: *"Data driven traffic management".*

- P. Goatin: Thematic trimester *"Fifty Years of Kruzhkov Entropy Solutions, and Beyond"* (November 2020, on-line)
  Talk: *Entropy conditions in traffic flow applications.*

- P. Goatin: IPAM (UCLA) long program on *"Mathematical Challenges and Opportunities for Autonomous Vehicles"* (September 2020, on-line)
  Tutorial lecture: *Macroscopic models for Autonomous Vehicles.*

11.1.5 Scientific expertise

- P. Goatin is member of the advisory board of DISMA Excellence Project of Politecnico di Torino (2018-2022).

- P. Goatin was proposal reviewer for FONDECYT (Chile).

- A. Habbal is member of and reviewer for the CNRS MODCOV Project `https://modcov19.math.cnrs.fr/`

11.1.6 Research administration

- R. Duvigneau is head of the Scientific Committee of Platforms (cluster and immersive space) at Inria Sophia Antipolis Méditerranée.
- R. Duvigneau is member of the Scientific Committee of OPAL computing Platform at Université Côte d'Azur.
- P. Goatin is member of the board of the Doctoral School of Fundamental and Applied Sciences (ED SFA) of Université Côte D'Azur.
- P. Goatin is member of the GAMNI-SMAI committee.
- P. Goatin was member of the Full Professor hiring committee of Université de Franche-Comté in Applied Mathematics (PR).
- A. Habbal is founding member of the African scholarly Society on Digital Sciences (ASDS)

11.2 Teaching - Supervision - Juries

11.2.1 Teaching

- Master: M. Binois, Optimisation bayésienne, 6 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: R. Duvigneau, Advanced Optimization, 28 hrs, M2, Polytech Nice Sophia - Université Côte d'Azur.
- Master: A. Habbal, Numerical Methods for Partial Differential Equations, 66 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, 66 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, Combinatorial optimization, 15 hrs, M1, Mohammed VI Polytechnic University, Morocco.
- Licence (L3): A. Habbal, Implement and Experiment PSO, 48 hrs, L3 Semester Project, Polytech Nice Sophia - Université Côte d'Azur.

11.2.2 Supervision

- PhD in progress: S. Pezzano, *Isogeometric analysis with moving grids*, Univ. Côte d'Azur. Supervisor: R. Duvigneau.
- PhD in progress: S. Chabbar, *Modeling and simulation of tumor growth ; the case of prostate cancer*, Jan 2019, Supervisors: A. Habbal, Rajae Aboulaich (LERMA, EMI, Rabat), A. Ratnani (UM6P, Benguerir, Morocco).
- PhD in progress: Marwa Ouni, *Solving inverses problems in fluid mechanics with game strategies*, October 2016, Supervisors: A. Habbal, Moez Kallel (LAMSIN, ENIT, Tunis).

11.2.3 Juries

- J.-A. Désidéri was reviewer of O. Montonen's Ph.D. thesis "On Multi-objective Optimization from the Nonsmooth Perspective", University of Turku (Finland).
- J.-A. Désidéri was reviewer of N. Garland's Ph.D. thesis "Introspective meta-modelling for the analysis of simulated physical phenomena", École Nationale Supérieure des Mines (Saint-Étienne).
- R. Duvigneau was reviewer of Mickaël Rivier's PhD thesis *"Low-cost methods for constrained multi-objective optimization under uncertainty"*, Ecole Polytechnique, September 30th, 2020.
- P. Goatin was member of the committee of S. Mollier's PhD thesis *"Two-dimensional models for large-scale traffic networks"*, Université de Grenoble, February 13th, 2020.
- P. Goatin was referee of M. Menci's PhD thesis *"Analytical foundations of a class of hybrid models with applications to collective dynamics"*, Università Campo Bio-Medico di Roma, March 2020.
- P. Goatin was external member of the committee of N. Salehi's PhD thesis *"Realistic on-ramp coupling conditions for macroscopic highway network models"*, Temple University, May 28th, 2020.
- P. Goatin was president of the committee of B. Guelmame's PhD thesis *"On a Hamiltonian regularization and regularity of entropy solutions of some nonlinear hyperbolic equations"*, Univ. Côte d'Azur, September 23rd, 2020.

11.3 Popularization

11.3.1 Articles and contents

- M.L. Delle Monache and P. Goatin, *Traffic management via Autonomous Vehicles*, ECCOMAS Newsletter, July 2020, 10-15.

12 Scientific production

12.1 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] 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.

[8] 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.

[9] 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.

[10] 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).

[11] 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.

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

[13] 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).

[14] 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.

12.2 Publications of the year

International journals

[15] E. Bertino, R. Duvigneau and P. Goatin. 'Uncertainty quantification in a macroscopic traffic flow model calibrated on GPS data'. In: *Mathematical Biosciences and Engineering* 17.2 (2020), pp. 1511–1533. URL: https://hal.archives-ouvertes.fr/hal-02379540.

[16] M. Binois, V. Picheny, P. Taillandier and A. Habbal. 'The Kalai-Smorodinski solution for many-objective Bayesian optimization'. In: *Journal of Machine Learning Research* 21.150 (2020), pp. 1–42. URL: https://hal.inria.fr/hal-01656393.

[17] C. Bonnet, K. Chahour, F. Clément, M. Postel and R. Yvinec. 'Multiscale population dynamics in reproductive biology: singular perturbation reduction in deterministic and stochastic models'. In: *ESAIM: Proceedings and Surveys* 67 (2020), pp. 72–99. DOI: 10.1051/proc/202067006. URL: https://hal.inria.fr/hal-03047923.

[18] R. Bürger, P. Goatin, D. Inzunza and L. M. Villada. 'A non-local pedestrian flow model accounting for anisotropic interactions and domain boundaries'. In: *Mathematical Biosciences and Engineering* 17.5 (2020), pp. 5883–5906. URL: https://hal.archives-ouvertes.fr/hal-02720191.

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[21] F. A. Chiarello, P. Goatin and L. M. Villada. 'Lagrangian-Antidiffusive Remap schemes for non-local multi-class traffic flow models'. In: *Computational and Applied Mathematics* 39.60 (2020). URL: https://hal.archives-ouvertes.fr/hal-01952378.

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[23] M. L. Delle Monache, K. Chi, Y. Chen, P. Goatin, K. Han, J.-M. Qiu and B. Piccoli. 'A three-phase fundamental diagram from three-dimensional traffic data'. In: *Axioms* 10.1 (2021). DOI: 10.3390/axioms10010017. URL: https://hal.inria.fr/hal-01864628.

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[27] M. Garavello, P. Goatin, T. Liard and B. Piccoli. 'A multiscale model for traffic regulation via autonomous vehicles'. In: *Journal of Differential Equations* 269.7 (2020), pp. 6088–6124. URL: https://hal.archives-ouvertes.fr/hal-02308788.

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[36] S. Pezzano and R. Duvigneau. 'A NURBS-based Discontinuous Galerkin Framework for Compressible Aerodynamics'. In: AIAA Aviation 2020 Forum. Proceedings of AIAA Aviation 2020 Forum. Reno, United States, June 2020. URL: https://hal.inria.fr/hal-02887354.

Conferences without proceedings

[37] M. M. R. Elsawy, S. Lanteri, R. Duvigneau and P. Genevet. 'Statistical Learning Optimization for Highly Efficient Metasurface Designs'. In: SIAM Conference on Computational Science and Engineering 2021. Texas, United States, 1st Mar. 2021. URL: https://www.hal.inserm.fr/inserm-03070707.

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Reports & preprints

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[40] X. Lyu, M. Binois and M. Ludkovski. *Evaluating Gaussian Process Metamodels and Sequential Designs for Noisy Level Set Estimation*. Mar. 2020. URL: https://hal.inria.fr/hal-03124928.

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[53] E. Bertino, R. Duvigneau and P. Goatin. 'Uncertainties in traffic flow and model validation on GPS data'. 2015.

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