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Activity Report 2016

Project-Team ACUMES

Analysis and Control of Unsteady Models for Engineering Sciences

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

RESEARCH CENTER
Sophia Antipolis - Méditerranée

THEME
Numerical schemes and simulations

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Project-Team ACUMES

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- 5.2.1. - Road vehicles
- 5.3. - Nanotechnology
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- 7.1.2. - Road traffic
- 8.1.1. - Energy for smart buildings

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2. Overall Objectives

2.1. 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.

3.1.1. 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 [95], or to the dynamics of turbulent flows for which large scale / small scale vortical structures interfere [123].

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 3.1.2.

3.1.1.1. 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 [64] for an existence result and [49], [63] 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 [55], [84] for some applications in traffic flow modelling, and [74], [79], [81] 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 [49], [63].

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.

3.1.1.2. 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 [56], [66] for the derivation of Lighthill-Whitham-Richards [107], [122] traffic flow model from Follow-the-Leader and [75] for results on crowd motion models (see also [97]). 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 [67], and extensively used since then to prove convergence of approximate solutions and deduce existence results, see for example [76] 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 [38], [78]. We refer, for example, to the notion of solution for non-hyperbolic systems [86], 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 [78].

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 [60]), and proved to be successful for studying emerging self-organised flow patterns [59]. The theoretical measure framework proves to be also relevant in addressing micro-macro limiting procedures of mean field type [87], 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* [130], [131]. Indeed, as observed in [114], 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 [106]). 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 [45], [46], [68], [105], 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 [118], 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 [62] 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, [36]) 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.

3.1.1.3. Non-local flows

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

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

where $u = u(t, \mathbf{x}) \in \mathbb{R}^N$, $N \geq 1$ is the vector of conserved quantities and the variable $W = W(t, x, u)$ 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 [33], sedimentation [40], supply chains [89], conveyor belts [90], biological applications like structured populations dynamics [113], or more general problems like gradient constrained equations [34]. Also, non-local in time terms arise in conservation laws with memory, starting from [61]. 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 [3], [6] [48], [52], [126]. 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 [3], [6] 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 [35] for scalar equations in one space dimension ($N = d = 1$), in [53] for scalar equations in several space dimensions ($N = 1$, $d \geq 1$) and in [29], [54], [58] for multi-dimensional systems of conservation laws. Besides, specific finite volume numerical methods have been developed recently in [29], [6] and [104].

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.

3.1.1.4. 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 [47]. In aerodynamics, inflow conditions like velocity modulus and direction, are subject to fluctuations [93], [112]. For some engineering problems, the geometry of the boundary can also be uncertain, due to structural deformation, mechanical wear or disregard of some details [70]. 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 [124], [129], 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 [125], [128], 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 [111]. 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 [93], [102], [108], [133] or an entropy closure method [65], or by discretizing the probability space and extending the numerical schemes to the stochastic components [28]. 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 [119], [129], [132].

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 [39]. Besides, we plan to extend previous works on sensitivity analysis [70], [109] 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 [41] (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 [129]. 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.

3.1.2. 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.

3.1.2.1. 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 [121] 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 [37], [88] for the backward time integration of the adjoint variables. The sensitivity equation method (SEM) offers a promising alternative [69], [98], 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 [70].
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) [123] , Detached-Eddy Simulation (DES) [127] or Organized-Eddy Simulation (OES) [43], 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 [100] or multiobjective optimization algorithm (see section below).

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

n 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 [71] [72]. 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 [73] 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 [116] 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 [135].

3.1.2.3. 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 [80]. Our proposal is designed to tackle derivative-free, expensive models, hence requiring very few model evaluations to converge to the solution.

3.1.2.4. 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 [30] 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 [134]. However, the lack of efficient and flexible numerical models, 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 an industrial context. In particular, the prediction of actuated flows requires the use of advanced turbulence closures, like Detached Eddy Simulation or Large Eddy Simulation [85]. They are intrinsically three-dimensional and unsteady, yielding a huge computational effort for each analysis, which makes their use tedious for optimization purpose. 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.
- *Hierarchical optimization of control devices.* The optimization of dozen of actuators, in terms of locations, frequencies, amplitudes, will be practically tractable only if a hierarchical approach is adopted, which mixes fine (DES) and coarse (URANS) simulations, and possibly experiments. We intend to develop such an optimization strategy on the basis of Gaussian Process models (*multi-fidelity kriging*).

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 [94]. Further improvements require more advanced models, keeping into better account interactions at the microscopic scale, and adapted control techniques, see [44] 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 [57], [83], 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 [99].
- *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 [96] 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 [50], [51]), 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 [64], [84] or via the Hamilton-Jacobi approach [50], [51] could allow to optimize the flow by controlling some specific vehicles corresponding to internal conditions.

4.3. Concurrent design for building systems

Building industry has to face more and more stringent requirements, including energy performance, structural safety and environmental impact. To this end, new materials and new technologies have emerged [103] to help the construction firms meet these requirements. At the same time, many different teams or firms interact, most of the interaction being of non-cooperative nature. The teams involved in construction have different goals, depending on which stage they operate. Indeed, the lifetime of a building goes through three stages: construction, use and destruction. To each of these phases correspond quality criteria related in particular to:

- Safety: structural, fire, evacuation, chemical spread, etc.
- Well-being of its occupants: thermal and acoustic comfort.
- Functionality of its intended use.
- Environmental impact.

These stages and criteria form a complex system, the so-called building system, whose overall quality (in an intuitive sense) is directly impacted by many heterogeneous factors, such as the geographical location or the shape or material composition of some of its components (windows, frames, thermal convectors positions, etc.) It is obvious that the optimization process of these settings must be performed at the "zero" stage of the project design. Moreover, the optimization process has to follow a global approach, taking into account all the concurrent criteria that intervene in the design of building systems.

The application of up-to-date concurrent optimization machinery (games, Pareto Fronts) for multiphysics systems involved in the building is an original approach. With our industrial partner, who wishes routine use of new high performance components in the construction of buildings, we expect that our approach will yield breakthrough performances (with respect to the above criteria) compared to the current standards.

The research project relies on the ADT BuildingSmart (see software development section) for the implementation of industrial standard software demonstrators.

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 [91], dorsal closure [32], actin organization [31]). 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 [77] it is shown that Madin-Darby Canine Kidney (MDCK) cells extend cryptic lamellipodia to drive the migration, several rows behind the wound edge. In [117] 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 [74], [79], [81].

- **Modeling cardio-stents.**

  Atherosclerosis or arterial calcification is a major vascular disease, caused by fatty deposits on the inner walls of arteries. Angioplasty techniques propose several solutions to remedy this pathology. We are interested in those which consist in introducing a metallic stent, to crush the lipid plaques, and ensure permanent enlargement of the damaged arterial wall. The implementation of such an element is accompanied by an immune reaction of the arterial walls, which is manifested by an accelerated proliferation of cells within the so called media, which highlights two major risks: restenosis, and thrombosis . One promising technique is to introduce a "Drug Eluting Stent", which is a metallic stent coated with a polymer layer containing an antiproliferative drug to slow the proliferation process, in order to improve the functioning of the stent. Our major objective in this part is to setup and develop the mathematical modeling and computational tools that lead to the effective estimation of the Fractional Flow Reserve [115], which is a promising new technique to help the cardiologists take decisions on stent implantation.

- **Game strategies for thermoelastography.** Thermoelastography is an innovative non-invasive control technology, which has numerous advantages over other techniques, notably in medical imaging [110]. 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 [92], [101], we have demonstrated that Nash game approaches are efficient to tackle ill-posedness. We intend to extend the results obtained for Laplace equations in [92], and the algorithms developed in Section 3.1.2.4 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. [120], 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. Highlights of the Year

5.1. Highlights of the Year

5.1.1. Awards

- P. Goatin got the *Trophée des Femmes en Or* for the “Smart City” category.

6. New Software and Platforms

6.1. BuildingSmart

BuildingSmart interactive visualization
KEYWORDS: Physical simulation - 3D rendering - 3D interaction

- Contact: Abderrahmane Habbal

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). The software is to be integrated in an immersive space (https://www.youtube.com/watch?v=wAm7faixBak) The project is hosted by the ACUMES project-team in collaboration with the SED service (Service d'Expérimentation et de Développement) and Experts from ArcelorMittal Construction. The project is financed by an Inria ADT which recruited an experienced engineer (starting in december 2015), whose main task is to study and develop solutions dedicated to interactive visualisation of building performances (heat, structural) in relation to the Building Information Modeling BIM framework.

7. New Results

7.1. Macroscopic traffic flow models on networks

Participants: Guillaume Costeseque, Paola Goatin, Bhargava Rama Chilukuri [Georgia Tech, USA], Maria Laura Delle Monache [U Rutgers - Camden], Aurélien Duret [IFSTTAR, France], Simone Göttlich [U Mannheim, Germany], Oliver Kolb [U Mannheim, Germany], Jorge A. Laval [Georgia Tech, USA], Benedetto Piccoli [U Rutgers - Camden], Armin Seyfried [Forschungszentrum Jülich, Germany], Antoine Tordeux [Forschungszentrum Jülich, Germany].

In collaboration with M.L. Delle Monache and B. Piccoli, and in the framework of the Associated Team ORESTE, we have introduced a new Riemann solver for traffic flow on networks. The Priority Riemann solver (PRS) provides a solution at junctions by taking into consideration priorities for the incoming roads and maximization of through flux. We prove existence of solutions for the solver for junctions with up to two incoming and two outgoing roads and show numerically the comparison with previous Riemann solvers. Additionally, we introduce a second version of the solver that considers the priorities as softer constraints and illustrate numerically the differences between the two solvers. See [24].

Still in collaboration with M.L. Delle Monache, we studied well-posedness of scalar conservation laws with moving flux constraints arising in the modeling of moving bottlenecks in traffic flow. In particular, we showed the Lipschitz continuous dependence of BV solutions with respect to the initial data and the constraint trajectory [23].

In collaboration with S. Göttlich and O. Kolb, we have investigated how second order traffic flow models, in our case the Aw-Rascle equations, can be used to reproduce empirical observations such as the capacity drop at merges and solve related optimal control problems. To this aim, we have proposed a model for on-ramp junctions and derive suitable coupling conditions. These are associated to the first order Godunov scheme to numerically study the well-known capacity drop effect, where the outflow of the system is significantly below the expected maximum. Control issues such as speed and ramp meter control have also been addressed in a first discretize-then optimize framework [25].

Together with J. A. Laval and B. R. Chilukuri, we have investigated the implications of source terms in the Hamilton-Jacobi formulation of macroscopic first order traffic flow models. Hamilton-Jacobi equations (without source terms) have been demonstrated to be very useful in traffic flow engineering since they provide explicit formula for initial and boundary-values problems. However, for sake of realism, additional source terms should be incorporated to account for continuous inflows or outflows on freeways for instance. We showed that explicit Lax-Hopf formula can still be obtained when the source term is exogenous, say the lateral inflow or outflow does not depend on the density on the main road. We also provide numerical methods based on Bellman's dynamic programming principle to deal with non-exogenous source terms in discrete time [7].

With A. Duret, we have designed a new traffic flow model for taking into account the multiclass and multilane features of real traffic. This model is based on a system of coupled Hamilton-Jacobi PDEs for an appropriate choice of framework that mixes spatial and Lagrangian coordinates. The coupling conditions emerge from the moving bottleneck theory that has been developed in the traffic flow literature several years ago but for which a real mathematical sound basis lacked. Very recently, there were some new results dealing with the existence of a solution under suitable assumptions [64]. However, these results were set for the hyperbolic conservation law in Eulerian coordinates and they are not straightforward to be extended to Hamilton-Jacobi equations in different coordinates. Despite that the well-posedness of the problem is still an open problem, a numerical method is developed by taking advantage of the classical representation formula available for HJ PDEs. This numerical scheme has been proved to provide good qualitative results [14].

In collaboration with A. Tordeux, M. Herty and A. Seyfried, we studied the derivation of convection-diffusion macroscopic traffic flow models from a first order microscopic follow-the-leader model that takes into account a non-trivial time delay. The derivation is based on a change of variables from Lagrangian to Eulerian coordinates and makes use of Taylor expansions with respect to the time delay. The macroscopic diffusion term is due to the microscopic reaction time parameter and allows to reproduce the scatter of empirical flow-density data. Different numerical methods are proposed for computing the numerical flux and the linear stability of the homogeneous solutions obtained for each method is investigated. Interestingly, we recover some stability results for infinite systems of delayed ODEs [27].

7.2. Initial-boundary value problems for non-local scalar conservation laws

Participants: Cristiana de Filippis, Paola Goatin.

As a first step in this direction, we have proved global well-posedness results for weak entropy solutions of bounded variation (BV) of scalar conservation laws with non-local flux on bounded domains in one space dimension, under suitable regularity assumptions on the flux function. In particular, existence is obtained by proving the convergence of an adapted Lax-Friedrichs algorithm. Lipschitz continuos dependence from initial and boundary data is derived applying Kružhkov 's doubling of variable technique [22].

7.3. High order schemes for non-local conservation laws

Participants: Paola Goatin, Christophe Chalons [UVST], Luis Miguel Villada Osorio [U Bio-Bio].

We have designed Discontinuous Galerkin (DG) schemes and Finite Volume WENO (FV-WENO) schemes to obtain high-order approximations of the solutions of a class of non-local conservation laws in one space dimension. The DG schemes give the best numerical results but their CFL condition is very restrictive. On the contrary, FV-WENO schemes can be used with larger time steps. The evaluation of the convolution terms necessitates the use of quadratic polynomials reconstructions in each cell in order to obtain the high-order accuracy with the FV-WENO approach. See [21].

7.4. Isogeometric analysis for hyperbolic systems

Participants: Régis Duvigneau, Asma Azaouzi [ENIT], Maher Moakher [ENIT].

The use of high-order numerical schemes is necessary to reduce numerical diffusion/dispersion in simulations, maintain a reasonable computational time for 3D problems, estimate accurately uncertainties or sensitivities, etc. Moreover, the capability to handle exactly CAD data in physical solvers is desirable to foster design optimization or multidisciplinary couplings.

Consequently, we develop high-order isogeometric schemes for the applications targeted by the team, in particular for convection-dominated problems. Specifically, we investigate a Discontinuous Galerkin method for compressible Euler equations, based on an isogeometric formulation: the partial differential equations governing the flow are solved on rational parametric elements, that preserve exactly the geometry of boundaries defined by Non-Uniform Rational B-Splines (NURBS), while the same rational approximation space is adopted for the solution. This topic is partially studied in A. Azaouzi's PhD work.

7.5. Sensitivity equation method for hyperbolic systems

Participants: Régis Duvigneau, Camilla Fiorini [UVST], Christophe Chalons [UVST].

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 example the one-dimensional barotropic Euler equations. Different approaches are tested to integrate the additional source term: a Roe solver, a Godunov method and a moving cells approach. This study is achieved in collaboration with C. Chalons from University of Versailles, in the context of C. FIorini's PhD work.

7.6. Characterization of model uncertainty for turbulent flows

Participants: Régis Duvigneau, Jérémie Labroquère [THALES], Emmanuel Guilmineau [CNRS-ECN], Marianna Braza [CNRS-IMFT], Mathieu Szubert [CNRS-IMFT].

The uncertainty related to turbulence modeling is still a bottleneck in realistic flows simulation. Therefore, some studies have been conducted to quantify this uncertainty for two problems in which turbulence plays a critical role. Firstly, the impact of the model choice has been estimated in the case of a massively detached flow over a 2D backward facing step including an oscillatory active control device, whose parameters are optimized [5]. Secondly, the influence of the transition point location has been investigated, in the case of the 3D flow around a bluff-body, using models ranging from RANS to DES models [9], in collaboration with M. Braza from Institut de Mécanique des Fluides de Toulouse, in the context of the M. Szubert's PhD work.

7.7. Optimization accounting for experimental and numerical uncertainties

Participants: Régis Duvigneau, Matthieu Sacher [Ecole Navale], Frédéric Hauville [Ecole Navale], Olivier Le Maître [CNRS-LIMSI], Alban Leroyer [CNRS-ECN], Patrick Queutey [CNRS-ECN].

Optimization of real-life applications requires to account for the uncertainties arising during the performance evaluation procedure, that could be either experimental or numerical. A Gaussian-Process based optimization algorithm has been proposed to efficiently determine the global optimum in presence of noise, whose amplitude can be user-defined or inferred from observations. The method has been applied to two very different problems related to performance optimization in sport.

The first case corresponds to the optimization of the shape of a racing kayak, in the framework of SOKA project, in preparation to 2016 Olympic Games. The performance is estimated by coupling Newton's law with incompressible Navier-Stokes equations to compute the kayak velocity from the effort of the athlete, considered as input. The proposed method has been used here to filter the noise arising from the numerical simulation [18], [11]. This work is conducted in collaboration with Ecole Centrale de Nantes and National Kayak Federation.

The second case corresponds to the optimization of a sail trimming, whose performance can be estimated either experimentally in a wind tunnel, or numerically by solving a fluid-structure interaction problem. In the former case, uncertainty has been estimated according to measurements accuracy, while in the latter case the numerical noise has be inferred from a set of observations collected during the optimization[12]. This work is part of M. Sacher's PhD at Ecole Navale.

7.8. Modeling activated/inhibited cell-sheet wound dynamics

Participants: Abderrahmane Habbal, Hélène Barelli [Univ. Nice Sophia Antipolis, CNRS, IPMC], Grégoire Malandain [Inria, EPI Morpheme], Boutheina Yahyaoui [PhD, LAMSIN, Univ. Tunis Al Manar], Mekki Ayadi [LAMSIN, Univ. Tunis Al Manar].

In a previous paper [91], we have shown that the well-known Fisher-KPP equations are able to model the natural wound closure of cell-sheets. This family of equations, with constant coefficients, exhibit progressive fronts with constant speed and we have proved by confronting to experiments that F-KPP is remarkabely able to predict the dynamics of experimental wounds. However, this is no more the case when the cell-sheet is either inhibited or activated exogeneously. In this case, we used a F-KKP equation with time-dependent coefficients, and proved again that with this modification we were able to capture the wound dynamics [13]. To take into account further biological features in the mathematical model, we implemented a coupling between the mechanical behavior of the cell tissue and the evolution of the density, using classical linear visco-elastic models from the literature. Our present effort is on assessing the ability of the mechano-biological coupled system to render some of the cell-sheet dynamics that are missing from the Fisher-KPP equation alone.

7.9. A Nash game for the coupled problem of conductivity identification and data completion

Participants: Abderrahmane Habbal, Rabeb Chamekh [PhD, LAMSIN, Univ. Tunis Al Manar], Moez Kallel [LAMSIN, Univ. Tunis Al Manar], Nejib Zemzemi [Inria Bordeaux, EPI CARMEN].

In this work, we are interested in solving the electrocardiography inverse problem which could be reduced to the data completion problem for the Poisson equation. The difficulty comes from the fact that the conductivity values of the torso organs like lungs, bones, liver,...etc, are not known and could be patient dependent. Our goal is to construct a methodology allowing to solve both data completion and conductivity optimization problems at the same time.

In [92], [101] a Nash game approach was developed to tackle the data completion problem. Our algorithm turned out to be efficient and robust with respect to noisy data. In a first attempt, presented in [17], we formulated the identification-completion problem as a Stackelberg game. Some numerical experiments were successful in this joint identification, but some were not. Which led us to develop new formulations, with direct impact on the technological modus operandi in the theoretical tomography process. In few words, the new formulations are based on the remark that not all the over-specified data are necessary to ensure the existence and uniqueness for the Cauchy problem, since by Holmgren theorem, only a piece of these data (over a subset of the boundary with non zero superficial measure) is necessary and sufficient. Presently, we are investigating the ability of these new formulations to ensure identifiability of the conductivity coefficients, for Poisson and linear elasticity equations.

7.10. Bayesian Optimization approaches to find Nash equilibria

Participants: Mickael Binois [Univ. of Chicago], Victor Picheny [INRA, Toulouse], Abderrahmane Habbal.

Our aim here is to show that the Bayesian Optimization -BO- apparatus can be applied to the search of game equilibria, and in particular the classical Nash equilibrium (NE), known to be very costly the compute, notably when involved in the framework of large scale scientific computing areas.

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.

We have proposed in [26] a novel approach to solve Nash games with drastically limited budgets of evaluations based on GP regression, taking the form of a Bayesian optimization algorithm. Experiments on challenging benchmark problems demonstrate the potential of this approach compared to classical, derivative-based algorithms.

On the test problems, two acquisition functions performed similarly well. The first one, Stepwise Uncertainty Reduction -SUR- has recently emerged in the machine learning community. We introduced a new one, the Probability of Equilibrium P_E, which has the benefit of not relying on conditional simulation paths, which makes it simpler to implement and less computationally intensive in most cases. Still, the SUR approach has several decisive advantages; in particular, it does not actually require the new observations to belong to the grid (sampling of the , such that it could be optimized continuously. Moreover, it lays the groundwork for many extensions that may be pursued in future work.

First, SUR strategies are well-suited to allow selecting batches of points instead of only one, a key feature in distributed computer experiments. Second, other games and equilibria may be considered: the versatility of the SUR approach may allow its transposition to other frameworks, such as mixed-strategies or Bayesian games. In particular, our framework transposes directly to the case of noisy evaluations, as it can be directly modeled by the GPs without affecting the acquisition functions.

7.11. Crowd motion modeled by Fokker-Planck constrained Nash games

Participants: Alfio Borzí [Univ. Würzburg], Paola Goatin, Abderrahmane Habbal, Souvik Roy [Indian Statistical Institute, Kolkata].

Fokker-Planck-Kolmogorov (FPK) equations are PDEs which govern the dynamics of the probability density function (PDF) of continuous-time stochastic processes (e.g. Ito processes). In [36] a FPK-constrained control framework, where the drift was considered as control variable is developed and applied to crowd motion.

We consider in [42] the extension of the latter framework to the case where two crowds (or pedestrian teams) are competing through a Nash game. The players strategies are the drifts, which yield two uncoupled FPK equations for the corresponding PDFs. The interaction is done through cost functions : each player would prefer to avoid overcrowding (w.r.t. the other one, hence the coupling) additionally to have her own preferred trajectory and obstacle avoidance. In this particular setting, we prove the existence and uniqueness of the Nash equilibrium (NE). The NE is computed by means of a fixed point algorithm and adjoint-state method is used to compute the pseudo-gradients. We finally present some numerical experiments to illustrate which dynamics may arise from such equilibria.

7.12. Concurrent Aerodynamic Optimization of Rotor Blades Using a Nash Game Method

Participants: Enric Roca León [ONERA DAAP Meudon, doctoral student], Arnaud Le Pape [ONERA DAAP Meudon, research engineer], Michel Costes [ONERA DAAP Meudon, research engineer], Jean-Antoine Désidéri, David Alfano [Airbus Helicopters].

A multiobjective strategy adapted to the aerodynamic concurrent optimization of helicopter rotor blades is developed. The present strategy is based on Nash games from game theory, where the objective functions are minimized by virtual players involved in a noncooperative concurrent game. A method is presented to split the design vector into two subspaces, defined to be the strategies of the players in charge of the minimization of the primary and the secondary objective functions, respectively. This split of territory allows the optimization of the secondary function while causing the least possible degradation of the first one. This methodology is applied to the model rotor ERATO, seeking to maximize the figure of merit in hover while minimizing the required rotor power in forward flight, assuming frozen structural properties. An initial constrained optimization in hover is conducted using a previously developed adjoint-based technique using the three-dimensional Navier–Stokes solver elsA along with the gradient-based CONMIN algorithm. The chord, twist, and sweep distributions of the baseline blade are parameterized using Bézier and cubic splines for a total of 16 design variables. The obtained optimized rotor is then used as a starting point to launch constrained and unconstrained Nash games. The comprehensive rotor code Eurocopter's Helicopter Overall Simulation Tool (HOST) is used to evaluate forward flight performance, and a surrogate model is built to obtain the hover performance at low computational cost. Twist and sweep distribution laws are optimized independently at first, and then a final joint optimization involving twist, sweep, and chord is performed. The results demonstrate the potential of this technique to obtain helicopter rotor designs realizing interesting trade-offs between strongly antagonistic objectives [8].

7.13. Parametric optimization of pulsating jets in unsteady flow by Multiple-Gradient Descent Algorithm (MGDA)

Participants: Jean-Antoine Désidéri, Régis Duvigneau.

Two numerical methodologies are combined to optimize six design characteristics of a system of pulsating jets acting on a laminar boundary layer governed by the compressible Navier-Stokes equations in a time-periodic regime. The flow is simulated by second-order in time and space finite-volumes, and the simulation provides the drag as a function of time. Simultaneously, the sensitivity equations, obtained by differentiating the governing equations w.r.t. the six parameters are also marched in time, and this provides the six-component parametric gradient of drag. When the periodic regime is reached numerically, one thus disposes of an objective-function, drag, to be minimized, and its parametric gradient, at all times of a period. Second, the parametric optimization is conducted as a multi-point problem by the Multiple-Gradient Descent Algorithm (MGDA) which permits to reduce the objective-function at all times simultaneously, and not simply in the sense of a weighted average [19].

7.14. Stochastic Multiple Gradient Descent Algorithm

Participants: Jean-Antoine Désidéri, Quentin Mercier [ONERA DADS Châtillon, doctoral student], Fabrice Poirion [ONERA DADS Châtillon, research engineer].

We have proposed a new method for multiobjective optimization problems in which the objective functions are expressed as expectations of random functions. This method is based on an extension of the classical stochastic gradient algorithm and a deterministic multiobjective algorithm, the Multiple-Gradient Descent Algorithm (MGDA). In MGDA a descent direction common to all specified objective functions is identified through a result of convex geometry. The use of this common descent vector and the Pareto stationarity definition into the stochastic gradient algorithm makes the algorithm able to solve multiobjective problems. The mean square and almost sure convergence of this new algorithm are proven considering the classical stochastic gradient algorithm hypothesis. The algorithm efficiency is illustrated on two academic examples and its performance is compared to the deterministic MGDA algorithm coupled with a Monte-Carlo expectation estimator. A third example is treated, considering the optimization of a sandwich material under constitutive material uncertainties.

7.15. Finite-volume goal-oriented mesh adaptation for aerodynamics using functional derivative with respect to nodal coordinates

Participants: Giovanni Todarello [ONERA DMFN Châtillon, intern], Floris Vonck [ONERA DMFN Châtillon, intern], Sébastien Bourasseau [ONERA, doctoral student], Jacques Peter [ONERA DMFN Châtillon, research engineer], Jean-Antoine Désidéri.

A new goal-oriented mesh adaptation method for finite volume/finite difference schemes is extended from the structured mesh framework to a more suitable setting for adaptation of unstructured meshes. The method is based on the total derivative of the goal with respect to volume mesh nodes that is computable after the solution of the goal discrete adjoint equation. The asymptotic behaviour of this derivative is assessed on regularly refined unstructured meshes. A local refinement criterion is derived from the requirement of limiting the first order change in the goal that an admissible node displacement may cause. Mesh adaptations are then carried out for classical test cases of 2D Euler flows. Efficiency and local density of the adapted meshes are presented. They are compared with those obtained with a more classical mesh adaptation method in the framework of finite volume/finite difference schemes [46]. Results are very close although the present method only makes usage of the current grid [10].

7.16. Quasi-Riemannian approach to constrained optimization

Participants: Didier Bailly [Research Engineer, ONERA Department of Applied Aerodynamics, Meudon], Jean-Antoine Désidéri.

In differentiable optimization, the Broyden-Fletcher-Goldfarb-Shanno (BFGS) method is one of the most efficient methods for unconstrained problems. Besides function values, it only requires the specification of the gradient. An approximate Hessian is calculated by successive approximations as part of the iteration, using rank-1 correction matrices. As a result, the iteration has superlinear convergence : when minimizing a quadratic function in n variables, if the one-dimensional minimizations in the calculated directions of search are done exactly, the Hessian matrix approximation is exact after n iterations, and from this, the iteration identifies to Newton's iteration, and produces the exact local optimum in only one additional iteration ($n+1$ in total).

However the BFGS method does extend to constrained problems very simply. Following Gabay [82] and other authors, Chunhong Qi *et al* [120] have proposed a "Riemannian" variant, RBFGS that indeed incorporates equality constraints in the formulation and actually demonstrates superior convergence rates for problems with a large number of variables. However these Riemannian formulations are non trivial to implement since they require procedures implementing non-trivial differential-geometry operators ('retraction' and 'metric transport') to be developed. In their paper, they assume a formal expression of the constraint to be known. But, in PDE-constrained optimization, many constraints are functional, and it is not clear how can the metric transport operator in particular can be defined.

We are investigating how can a quasi-Riemannian method can be defined based on the sole definition of evaluation procedures for the gradients. By condensing all the equality constraints in one, a purely-explicit approximate retraction operator has been defined that yields a point whose distance to the contraint surface is fourth-order at least. The associated transport operator is currently being examined formally. These techniques will be experimented in the context of constrained optimum-shape design in aerodynamics [20]

7.17. Multifidelity surrogate modeling based on Radial Basis Functions

Participants: Jean-Antoine Désidéri, Cédric Durantin [CEA LETI Grenoble, doctoral student], Alain Glière [CEA LETI Grenoble, research engineer], Justin Rouxel [CEA LETI Grenoble, doctoral student].

Multiple models of a physical phenomenon are sometimes available with different levels of approximation. The high fidelity model is more computation-ally demanding than the coarse approximation. In this context, including information from the lower fidelity model to build a surrogate model is desirable. Here, the study focuses on the design of a miniaturized photoacoustic gas sensor which involves two numerical mod- els. First, a multifidelity metamodeling method based on Radial Basis Function, the co-RBF, is proposed. This surrogate model is compared with the classical co-kriging method on two analytical benchmarks and on the photoacoustic gas sensor. Then an extension to the multifidelity framework of an already existing RBF- based optimization algorithm is applied to optimize the sensor efficiency. The co-RBF method brings promising results on a problem in larger dimension and can be considered as an alternative to co-kriging for multifidelity metamodeling.

8. Partnerships and Cooperations

8.1. National Initiatives

8.1.1. Project BOUM

G. Costeseque holds a BOUM (SMAI) project on *"Mathematical homogenization techniques for traffic flow models"* with W. Salazar and M. Zaydan (LMI, INSA Rouen) and J.A. Firozaly (CERMICS, Ecole des Ponts ParisTech and LAMA, Université Paris-Est Créteil).

8.2. European Initiatives

8.2.1. FP7 & H2020 Projects

8.2.1.1. TraM3

Type: FP7

Defi: NC

Instrument: ERC Starting Grant

Objectif: NC

Duration: October 2010 - March 2016

Coordinator: Inria

Inria contact: Paola Goatin

Abstract: The project intends to investigate traffic phenomena from the macroscopic point of view, using models derived from fluid-dynamics consisting in hyperbolic conservation laws. The scope is to develop a rigorous analytical framework and fast and efficient numerical tools for solving optimization and control problems, such as queues lengths control or buildings exits design. See also: http://www-sop.inria.fr/members/Paola.Goatin/tram3.html

8.3. International Initiatives

8.3.1. Inria International Labs

Inria@SiliconValley

Associate Team involved in the International Lab:

8.3.1.1. ORESTE

Title: Optimal REroute Strategies for Traffic managEment

International Partner (Institution - Laboratory - Researcher):

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

Start year: 2015

See also: http://www-sop.inria.fr/members/Paola.Goatin/ORESTE/index.html

This project focuses on traffic flow modeling and optimal management on road networks. Based on the results obtained during the first three years, we aim at further develop a unified macroscopic approach for traffic monitoring, prediction and control. In particular, we aim at investigating user equilibrium inference and Lagrangian controls actuations using macroscopic models consisting of conservation laws or Hamilton-Jacobi equations.

8.4. International Research Visitors

8.4.1. Visits of International Scientists

- L.M. Villada-Osorio (February-July 2016, University of Bio-Bio, Chile): high order Discontinuous Galerkin and WENO finite volume schemes for non-local scalar conservation laws in one space-dimension.
- A. Borzí (June and October 2016, University of Wuerzburg): Stochastic differential games and Fokker-Planck equations.
- A. Keimer (November 2016, UC Berkeley): modeling and well-posedness study for Dynamic Traffic Assignement.

8.4.1.1. Internships

- C. De Filippis (April-August 2016, University of Milan - Bicohcca): well-posedness of initial-boundary value problems for non-local scalar conservation laws in one space-dimension.

9. Dissemination

9.1. Promoting Scientific Activities

9.1.1. Scientific Events Organisation

9.1.1.1. General Chair, Scientific Chair

- P. Goatin was member of the scientific committee of *"PED2016 - Conference on Pedestrian and Evacuation Dynamics"*, Hefei (China), October 2016.
- P. Goatin is member of the the scientific committee of the annual seminar CEA-GAMNI *"Numerical fluid-mechanics"*.
- A. Habbal was member of the scientific committee of the *CARI 2016 Colloque Africain sur la Recherche en Informatique et Mathematiques Appliquees*, Tunis (Tunisia) 10-14 October 2016.

9.1.1.2. Member of the Organizing Committees

- P. Goatin organized the Workshop *"TRAM3 Terminus"*, Sophia Antipolis (France), January 2016.
- R. Duvigneau was co-organizer of the mini-symposium "Surrogate Models for Efficient Robust Optimization and Data Assimilation in Computational Mechanics", part of SIAM Conference on Uncertainty Quantification, Lausanne, April 2016.

9.1.2. Journal

9.1.2.1. Reviewer - Reviewing Activities

- J.-A. Désidéri has made reviews for the *International Journal of Information Technology & Decision Making*, and *Comptes Rendus de l'Académie des Sciences*,
- R. Duvigneau is a reviewer for the following international journals : Computers & Fluids, International Journal for Numerical Methods in Fluids, Computer Methods for Applied Mechanical Engineering, Computer Aided Geometric Design, Applied Mathematics & Mechanics, Engineering Optimization.
- P. Goatin is reviewers for the following international journals: Acta Applicandæ Mathematicæ ; African Journal of Mathematics and Computer Science Research; Algorithms; Annales de l'Institut Henri Poincaré (C) Analyse Non Linéaire; Applied Mathematics and Computation; Computer-aided Civil and Infrastructure Engineering; Discrete and Continuous Dynamical Systems; European Journal of Operational Research; IEEE Transactions on Automatic Control; IEEE Transactions on Intelligent Transportation Systems; International Journal of Dynamical Systems and Differential Equations; Journal of Computational Physics; Journal of Flow, Turbulence and Combustion; Mathematical Models and Methods in Applied Sciences; Mathematics of Computation; Networks and Heterogeneous Media; New Journal of Physics; Nonlinear Analysis Ser. B: Real World Applications; SIAM Journal of Mathematical Analysis; SIAM Journal of Applied Mathematics; SIAM Journal of Numerical Analysis; SIAM Journal on Scientific Computing.
- A. Habbal is reviewer for the following international journals: Applied Mathematics (AM), Scientific Research Publishing ; Journal of Structural and Multidisciplinary Optimization ; Journal of Math. Model. Nat. Phenom. ; International Journal of Mechanical Sciences ; Modern Applied Science ; Asian Journal of Control ; Applied Mathematics and Computation ; Computer Methods in Applied Mechanics and Engineering ; Bulletin of Mathematical Biology ; Journal of Pure and Applied Functional Analysis ; AMS reviews.

9.1.3. Invited Talks

- J.-A. Désidéri: ONERA Palaison, April 2016.
  Invited talk: *“Multiple Gradient Descent Algorithm for Multiobjective Optimization”*,
- R. Duvigneau: Ecole Navale, Brest, January 2016.
  Invited talk: *"The Sensitivity Equation Method for optimization, fast estimation of neighboring solutions and uncertainty propagation"*.
- R. Duvigneau: Ecole des Mines Paris-Tech, Sophia-Antipolis, June 2016.
  Invited talk: *"Optimization of complex fluid systems using a statistical learning strategy"*.
- P. Goatin: EU-US Frontiers of Engineering Symposium, Helsinki (Finland), October 2016.
  Session: “The road to future urban mobility”.
  Invited talk: *“Traffic management by macroscopic models”*.
- P. Goatin: SIMAI 2016 - XIII Congress of the Italian Society of Industrial and Applied Mathematics, Milano (Italy), September 2016.
  Mini-symposium: “Analysis and numerics for the modeling through conservation laws”.
  Invited talk: *“A Riemann Solver at junctions preserving priorities”*.
  Mini-symposium: “Mean-field models in pedestrian dynamics”.
  Invited talk: *“Non-local macroscopic models of traffic flow”*.
- P. Goatin: 11th Meeting on Nonlinear Hyperbolic PDEs and Applications, Trieste (Italy), June 2016.
  Invited talk: *“Conservation laws with local constraints arising in traffic modeling”*.
- P. Goatin: SIAM Conference on Uncertainty Quantification, Lausanne (Switzerland), April 2016.
  Mini-symposium: “Data-driven methods for uncertainty quantification”.
  Invited talk: *“Parametric uncertainty in macroscopic traffic flow models calibration from GPS data”*.
- P. Goatin: Workshop “Analysis and control on networks: trends and perspectives”, Padova (Italy), March 2016.
  Invited talk: *“Optimization based control of networks of discretized PDEs: Application to road traffic management”*.
- P. Goatin: ANR HJNet 5th Meeting, Tours (France), January 2016.
  Invited talk: *“Conservation laws with local and unilateral flux constraints”*.
- A. Habbal: IX NPU-UTC Sino-French Seminar on Virtual Prototyping for Design and Fabrication, 11-15 April 2016.
  Invited talk: *“Pareto optimality and game equilibria, two approaches to solve multiobjective optimization”*.
- A. Habbal: Lorentz Center workshop SAMCO: Surrogate-Assisted Multi-Criteria Optimization, February 29 - March 4, 2016.
  Invited senior participant: *"Many objectives and selection algorithms"*.

9.1.4. Scientific Expertise

J.-A. Désidéri has been a consultant for ONERA (since 2007) at DMFN-Châtillon (Dept. of Numerical Fluid Mechanics) and DAAP-Meudon (Dept. of Applied Aerodynamics), and also directs a thesis at DADS-Châtillon (Dept. of Aeroelasticity and Structural Dynamics).

9.1.5. Research Administration

- P. Goatin is member of BCP ("Bureau du Comité des Projets") at Inria Sophia Antipolis Méditerranée.

9.2. Teaching - Supervision - Juries

9.2.1. Teaching

Master: Advanced Optimization, 40.5 hrs, M2, Ecole Polytechnique Universitaire (EPU), Nice Sophia Antipolis (J.-A. Désidéri, R. Duvigneau).

Master: Conservation laws and finite volume scheme, 30 hrs, M2, Ecole Polytechnique Universitaire (EPU), Nice Sophia Antipolis (P. Goatin).

Master: Multidisciplinary Optimization, 22.5 hrs, joint *Institut Supérieur de l'Aéronautique et de l'Espace* (ISAE Supaéro, "Complex Systems") and M2 (Mathematics), Toulouse (J.-A. Désidéri, R. Duvigneau).

Licence: Summer Project in Mathematical Modeling, 36 hrs, L3, Ecole Polytechnique Universitaire (EPU), Nice Sophia Antipolis (A. Habbal).

Master: Numerical Methods for Partial Differential Equations, 66 hrs, M1, Ecole Polytechnique Universitaire (EPU), Nice Sophia Antipolis (A. Habbal and R. Duvigneau).

Master: Concurrent design in building structures, M2 Students Project, Ecole Polytechnique Universitaire (EPU), Nice Sophia Antipolis (A. Habbal).

9.2.2. Supervision

PhD in progress : Cédric Durantin, *Meta-modelling for the optimization of nanophotonic devices*, October 2014. Supervisors : J.-A. Désidéri and A. Glière (CEA LETI).

PhD in progress : Quentin Mercier, *Multicriterion optimization under uncertainties : the stochastic multiple gradient approach. Application to aerelasticity*, October 2015. Supervisors : J.-A. Désidéri and F. Poirion.

PhD in progress : Maroua Mokni, *Development, analysis and numerical evaluation of MGDA*, October 2013. Supervisors : J.-A. Désidéri and M. Ayadi (LAMSIN-ENIT, Tunisia).

PhD in progress : Sosina Mengistu-Gashaw (EURECOM), *Mobility and connectivity modelling of 2-wheels traffic for ITS applications* , March 2015. Supervisors: P. Goatin and J. Härri (EURECOM).

PhD in progress: Boutheina Yahyaoui, *Validation of mecano-chemo-biological models for cell sheet wound closure*, Jan 2013, Supervisors: A. Habbal, Mekki Ayadi (LAMSIN, ENIT, Tunis)

PhD in progress: Rabeb Chamekh, *Game strategies for thermo-elasticity*, Jan 2015, Supervisors: A. Habbal, Moez Kallel (LAMSIN, ENIT, Tunis)

PhD in progress: Kelthoum Chahour, *Modeling and optimal design of coronary angioplastic stents*, Nov 2015, Supervisors: A. Habbal, Rajae Aboulaich (LERMA, EMI, Rabat)

PhD in progress: A. Azaouzi, *isogeometric analysis methods for hyperbolic systems*, ENIT (Tunisia) / University of Nice - Sophia Antipolis, Oct. 2013, supervisors: R. Duvigneau and M. Moakher (ENIT).

PhD in progress: M. Sacher, *advanced methods for numerical optimization of yacht performance*, Ecole Navale , Oct. 2014, supervisors: R. Duvigneau, O. Le Maitre (LIMSI), F. Hauville and J.-A. Astolfi (Ecole Navale).

PhD in progress: C. Fiorini, *Sensitivity equation method for hyperbolic systems*, Univ. Versailles, Oct. 2014, supervisors: R. Duvigneau, C. Chalons (Univ. Versailles).

PhD in progress : Nicolas Laurent-Brouty (ENPC), *Macroscopic traffic flow models for pollution estimation and control*, September 2016. Supervisor: P. Goatin.

PhD in progress : Emanuele Marrone (Université de Nice Sophia Antipolis), *Conservation laws with non- local flux*, October 2016. Supervisor: P. Goatin .

PhD in progress : Nikodem Dymski (Maria Curie Sklodowska University & Université de Nice Sophia Antipolis), *Conservation laws in the modeling of collective phenomena*, October 2016. Supervisors: P. Goatin and M.D. Rosini (UMCS).

9.2.3. Juries

- P. Goatin was member of the committee of C. Perrin's PhD thesis *"Modèles hétérogènes en mécanique des fluides : phénomènes de congestion, écoulements granulaires et mouvement collectif"*, Université de Grenoble, July 8th, 2016.
- P. Goatin was referee of R. Sainct's PhD thesis *"Etude des instabilités dans les modèles de trafic"*, Université Paris-Est, September 22th, 2016.
- P. Goatin was member of the committee of M. Campanella's PhD thesis *"Microscopic modelling of walking behaviour"*, Delft University of Technology, November 21st, 2016.
- R. Duvigneau was member of the committee of Kevin Kasper's PhD thesis *"Apprentissage d'estimateurs sans modèle avec peu de mesures - Application à la mécanique des fluides"*, ENS Cachan, October 12th, 2016.

10. Bibliography

Publications of the year

Articles in International Peer-Reviewed Journals

[1] A. AGGARWAL, P. GOATIN. *Crowd Dynamics through Non-Local Conservation Laws*, in "Boletim da Sociedade Brasileira de Matemática / Bulletin of the Brazilian Mathematical Society", 2016, vol. 47, pp. 37 - 50 [*DOI :* 10.1007/S00574-016-0120-7], https://hal.inria.fr/hal-01402613

[2] A. BENKI, A. HABBAL, G. MATHIS. *Computational design of an automotive twist beam*, in "journal of computational design and engineering", 2016, vol. 3, pp. 215 - 225 [*DOI :* 10.1016/J.JCDE.2016.01.003], https://hal.inria.fr/hal-01405109

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[5] R. DUVIGNEAU, J. LABROQUÈRE, E. GUILMINEAU. *Comparison of turbulence closures for optimized active control*, in "Computers and Fluids", January 2016, n^o^ 124 [*DOI :* 10.1016/J.COMPFLUID.2015.10.011], https://hal.inria.fr/hal-01251823

[6] P. GOATIN, S. SCIALANGA. *Well-posedness and finite volume approximations of the LWR traffic flow model with non-local velocity*, in "Networks and Hetereogeneous Media", January 2016, vol. 11, n^o^ 1, pp. 107-121, https://hal.archives-ouvertes.fr/hal-01234584

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[10] G. TODARELLO, F. VONCK, S. BOURASSEAU, J. PETER, J.-A. DESIDERI. *Finite-volume goal-oriented mesh adaptation for aerodynamics using functional derivative with respect to nodal coordinates*, in "Journal of Computational Physics", May 2016, vol. 313, 21 p. [*DOI :* 10.1016/J.JCP.2016.02.063], https://hal.inria.fr/hal-01410153

International Conferences with Proceedings

[11] A. LEROYER, P. QUEUTEY, R. DUVIGNEAU. *Towards performance optimisation in kayak using CFD*, in "15ème Journées de l'Hydrodynamique", Brest, France, November 2016, https://hal.inria.fr/hal-01387792

[12] M. SACHER, F. HAUVILLE, R. DUVIGNEAU, O. LE MAÎTRE, N. AUBIN. *Experimental and numerical optimizations of an upwind mainsail trimming*, in "The 22nd Chesapeake Sailing Yacht Symposium", Chesapeake, United Kingdom, March 2016, https://hal.inria.fr/hal-01387783

Conferences without Proceedings

[13] M. AYADI, A. HABBAL, B. YAHYAOUI. *Modeling the dynamics of cell-sheet : From Fisher-KPP equation to bio-mechano-chemical systems: Fisher-KPP equation to study some predictions on the injured cell sheet*, in "13th African Conference on Research in Computer Science and Applied Mathematics", Autrans, Tunisia, October 2016, https://hal.inria.fr/hal-01405266

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Scientific Books (or Scientific Book chapters)

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Research Reports

[20] J.-A. DÉSIDÉRI. *A quasi-Riemannian approach to constrained optimization*, Inria Sophia Antipolis, December 2016, n° RR-9007, https://hal.inria.fr/hal-01417428

Other Publications

[21] C. CHALONS, P. GOATIN, L. M. VILLADA. *High order numerical schemes for one-dimension non-local conservation laws*, December 2016, working paper or preprint, https://hal.inria.fr/hal-01418749

[22] C. DE FILIPPIS, P. GOATIN. *The initial-boundary value problem for general non-local scalar conservation laws in one space dimension*, September 2016, working paper or preprint, https://hal.inria.fr/hal-01362504

[23] M. L. DELLE MONACHE, P. GOATIN. *Stability estimates for scalar conservation laws with moving flux constraints*, October 2016, working paper or preprint [*DOI :* 10.3934/XX.XX.XX.XX], https://hal.inria.fr/hal-01380368

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