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2021

ACTIVITY REPORT

Project-Team

PLATON

Uncertainty Quantification in Scientific Computing and Engineering

IN COLLABORATION WITH: Centre de Mathématiques Appliquées (CMAP)

DOMAIN

Applied Mathematics, Computation and Simulation

THEME

Numerical schemes and simulations

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Project-Team PLATON

Creation of the Project-Team: 2020 December 01

Keywords

Computer sciences and digital sciences

A3.4.1. – Supervised learning

A3.4.2. – Unsupervised learning

A3.4.5. – Bayesian methods

A3.4.7. – Kernel methods

A6. – Modeling, simulation and control

A6.1. – Methods in mathematical modeling

A6.1.1. – Continuous Modeling (PDE, ODE)

A6.1.2. – Stochastic Modeling

A6.1.5. – Multiphysics modeling

A6.2. – Scientific computing, Numerical Analysis & Optimization

A6.2.1. – Numerical analysis of PDE and ODE

A6.2.4. – Statistical methods

A6.2.6. – Optimization

A6.2.7. – High performance computing

A6.3. – Computation-data interaction

A6.3.1. – Inverse problems

A6.3.2. – Data assimilation

A6.3.3. – Data processing

A6.3.4. – Model reduction

A6.3.5. – Uncertainty Quantification

A6.5.2. – Fluid mechanics

Other research topics and application domains

B3. – Environment and planet

B3.3. – Geosciences

B4. – Energy

B4.3. – Renewable energy production

B5.2.1. – Road vehicles

B5.2.3. – Aviation

B5.2.4. – Aerospace

B5.5. – Materials

1 Team members, visitors, external collaborators

Research Scientists

- Pietro-Marco Congedo [Team leader, Inria, Senior Researcher, HDR]
- Olivier Le Maitre [CNRS, Senior Researcher]

Post-Doctoral Fellows

- Dinesh Kumar [Inria, until Nov 2021]
- Lalaina Rakotondrainibe [Inria]

PhD Students

- Michele Capriati [Institut Von Karman de dynamique des fluides - Belgique]
- Ana Isabel Del Val Benitez [Institut Von Karman de dynamique des fluides - Belgique, until Sep 2021]
- Nicolas Leoni [CEA]
- Paul Novello [CEA, until Nov 2021]
- Malo Pocheau [Bañuls Design]

Technical Staff

- Joao Miguel Felicio Dos Reis [Inria, Engineer, until Sep 2021]

Interns and Apprentices

- Florian Girault [Inria, from Mar 2021 until Aug 2021]

Administrative Assistant

- Hanadi Dib [Inria]

External Collaborator

- Giulio Gori [Politecnico di Milano]

2 Overall objectives

Computational approaches in science and engineering rely on numerical tools to produce effective, robust, and high fidelity predictions through the simulation of complex physical systems. The design and development of simulation tools encompass numerous aspects, ranging from the initial mathematical formulation of the problem to its actual numerical resolution, including the design of numerical algorithms suited to computational architectures of modern supercomputers, in particular massively parallel machines.

To fully achieve the promises of numerical simulations in sciences and engineering, it is essential to assess and improve their predictive capabilities continuously. Obvious improvements concern the modeling aspects (higher fidelity) and numerical efficiency (to enable higher resolution). However, as the computational capabilities are progressing, it is becoming more and more evident that accounting for the various uncertainties involved in the simulation process is critical. The reason is that the accurate simulation of a complex system has a practical utility if, and only if, one can prescribe with sufficient precision the system investigated. In other words, obtaining high fidelity predictions on a system different from the one targeted present limited interest. The problem here is that, except for purely academic situations, specifying precisely all the properties and forcing applied to a complex system is impossible. Whether the precise definition of the system is impossible because of inherent variabilities, lack of knowledge, or imprecise calibration procedures (experimental setups and measurements are inherently inexact), reducing totally uncertainty sources is not an option. As a result, the simulation should account for these uncertainties and quantify their impact on the predictions (similarly to the experimental error characterization) in order to assess objectively the truthfulness of the simulation and enable fully informed decision making. As a matter of fact, reliable numerical predictions require both sophisticated physical models and the systematic and comprehensive treatment of inherent uncertainties, including the calibration and validation procedures. Coarsely, the prediction errors result from physical simplifications in the mathematical model, numerical errors incurring from the discretization and numerical methods (solvers), and uncertainties in the definition of the model to be solved (input uncertainties).

Uncertainty management procedures are often tailored to the particular problem and application considered. In our experiences, it is hard to conceive a systematic a priori approach suitable for all problems. Most often, the UQ analysis consists in the gradual (re)definition and extension of its objectives , which can be somewhat vague initially. It is, therefore, crucial to have a *large portfolio of diverse numerical methods* to quickly propose and apply suitable treatments in response to the evolving understanding and needs as they emerge during the analysis.

The global objective of the research proposed within Platon is to develop advanced numerical methods and practices in simulations, integrating as much as possible the uncertainty management. Here, *uncertainty management* encompasses multiple uncertainty tasks: a) uncertainty characterization (the construction and identification of uncertainty models), b) uncertainty propagation (computation of the model-based prediction uncertainty), c) uncertainty reduction (by inference, data assimilation, conception of new experiments either physical or numerical,...) and d) uncertainty treatment in decision-making processes (sensitivity analysis, risk management, robust optimization,...). Note that one should not perceive these different uncertainty tasks as reflecting an ordered sequence of analysis steps. On the contrary, our vision and experience value a strong interaction between all these tasks which, ideally, must be visited in an order commanded by the initial information, the progress of the analysis and the resources available.

Progressing on all these tasks constitutes a significant challenge as the tasks involve a diversity of thematics and skills. This difficulty is prominent in the context of large scale simulations, where practitioners and researchers tend to be highly specialized in specific aspects (modeling, numerical schemes, parallel computing,...). Further, more massive simulations are often confused with better predictions and they overshadow the importance of uncertainties. At the same time, high simulation costs usually prevent applying straightforward uncertainty analyses as, for a fixed budget, one often prefers a simulation at the highest affordable resolution, rather than performing uncertainty analysis involving possibly less resolved simulations. However, this preference is most often not based on an objective assessment of the situation. In contrast, we believe that using complex models and exploiting fairly the predictions of large scale simulations need suitable uncertainty management procedures. Further, we are convinced of the importance of a research effort encompassing as much as possible all uncertainty tasks, to ensure the coherence and mutual relevance of the methods developed. Such an effort focusing on uncertainty management, rather than on a particular application, will be critical to improving the predictive capabilities of simulation tools and address industrial and societal needs.

Therefore, the main objectives of the team will be :

- Propose new methods and approaches for uncertainty management.
- Develop these methods into numerical tools applicable to large scale simulations.
- Apply and demonstrate the impact of uncertainty management in real applications with industrial and academic partners.

To achieve these objectives, we rely on the expertise and past researches of the permanent members, which cover most of the uncertainty tasks (propagation, inference, reduction, optimization,...), although not in a comprehensive way so far. The development of new predictive simulation tools also relies on collaborations, mainly within the international academic network that we have established over the past 15 years and within the Centre de Mathématiques Appliquées de l'École Polytechnique. The development of useful uncertainty management frameworks applicable to large scale simulations demand constant interactions with end-users (engineers, practitioners, researchers); we rely on our current network of industrial partners and EPICs[1] and extend it progressively.

3 Research program

The Team approach to research will be bottom-up: starting from new ideas and concepts to address both existing (known) and emerging (anticipated or not) problems. The later point, concerning the emerging problems, is particularly important in a quickly evolving research area with the constant improvement of the methodological and computational capabilities. The research thrust will be structured along two principal directions: a methodological axis and an applications axis.

3.1 UQ methodologies and tools

The Team will continuously work on developing original UQ representations and algorithms to deal with complex and large scale models, having high dimensional input parameters with complexes influences. We plan to organize our core research activities along different methodological UQ developments related to the challenges discussed above.

3.1.1 Surrogate modeling for UQ

Challenges. Surrogate models are crucial to enable the solution of both forward and backward UQ problems. Several alternative approaches, such as Polynomial Chaos, Gaussian Processes, and tensor format approximation, have been proposed and developed over the last decades. These approaches have been successfully applied to many different domains. Still, surrogates models for UQ management are facing many remaining limitations that require significant research works to handle large scale simulation-based studies and account for complex dependencies. These limitations concern multiple aspects, including the complexity related to the dimensionality of the input parameter, the definition of suitable basis representations, the complexity of the surrogate construction, and the control of the surrogate error.

Proposed actions. Platon will pursue long time efforts in the continuity of previous developments, such as the improvement of advanced sparse grid methods, sparsity promoting strategies and low-rank methods. Besides these generic developments, a first research axis will focus on the construction of surrogates for multi-physics problems (fluids, structures, chemistry,...) simulated by a system of coupled solvers. Classical surrogate methods consider the system of solvers as a single entity, and their construction requires the complete simulation with a high cost as a result. In contrast, we are proposing a *divide to simplify* strategy, using a surrogate of each constitutive solver, which reduces the input dimensionality of the local models, enables parallel construction and more flexible control of the computational effort. We will have to derive suitable error estimates of the contributions of the individual solver and procedures to decide the new computer experiments to reduce the error optimally. A second research axis on surrogate models will concern complexity reduction using transformation methods. Transformations can act on the input or output spaces of the model. In the first case, dimensionality reduction is achieved by finding low dimensional subspaces of the input space that convey most of the output variability. Platon will extend these methodologies to incorporate non-linear subspaces and alternative importance measures, in particular, to account for the surrogate's final usage (goal-oriented reduction). For the reduction of the output, we will consider generalizations of the preconditioning approach, which transforms the model output to a form admitting a much simpler surrogate and implicit enforcement of physical constraints. Here, the main challenges will be the automatic selection of the transformation among a dictionary and the design of computer experiments in this context (see below).

[1] EPIC: Industrial or Commercial Public Entity.

3.1.2 Uncertainty model, information theory and inference

Challenges. Uncertainty management in simulation can be considered in its infancy, and the control of the whole process, from the definition of the uncertainty model to the design of new simulations or experiments for uncertainty reduction, is still facing multiple challenges. Most past works on UQ have focused on forward-propagation and inverse problems when, in contrast, input uncertainty models and uncertainty reduction strategies, in general, have received much less attention.
Proposed actions. The uncertainty model directly affects the conclusion of UQ analyses (*e.g.*, sensitivity analyses, estimation of failure probabilities, rare events). Therefore, it is crucial to propose uncertainty models that consistently and objectively integrate all available information and expert knowledge(s). Platon will explore the application of maximum entropy principle, likelihood maximization and moment matching methods, for the construction of uncertainty models in engineering problems.
For the inverse problem, the Team will continue its efforts in Bayesian inference toward better treatment of the model error in the calibration procedure.
Concerning uncertainty reduction, a central question is the prediction of the improvement toward the specific objective brought by a new simulation (computer experiment). Platon will investigate different strategies of design of experiment (DoE) based on measures of the improvement, such as entropy reduction, besides the classical reduction of variance.
The DoE in inference consists in proposing new physical experiments to reduce the posterior uncertainty optimally. Optimizing information gain leads to expensive numerical procedures, and suitable model error and noise models are critical to ensure the robustness of these optimal DoE procedures when applied to real-life data. Platon will work on approximation and reduction methods for optimal DoE to enable applications in large-scale engineering problems; the extension of the optimization to uncertainty reduction in general model-prediction, not just the model parameter uncertainty.

3.1.3 Multi-fidelity, Multi-level and optimization under uncertainty

Challenges. Multi-fidelity and Multi-level (MF&L) methods have been proposed to reduce the cost of surrogate model construction or statistics estimations, by relying on simulators of different complexity (in the modeled physics, discretization, or both). Although these methods have proved to be effective, particularly in the context of expensive simulations, existing algorithms must be adapted to other tasks. MF&L strategies are also missing in Robust Optimization (RO) and Reliability-Based Optimization (RBO), where one has to evaluate the objective accurately, typically some statistics of the model output (moments, quantiles, ...).
Proposed action. The Team Platon will explore MF&L approaches and the design of computer experiments to obtain the best estimation at the lowest cost (or for a prescribed computational budget) for nontrivial goal, specifically optimization and reliability problems where the accuracy needed is not uniform, possibly unknown a priori and to be estimated as the construction proceeds.
In RO and RBO, our research will focus on the estimation of robustness and reliability measures with tunable fidelity to adapt the convergence of the statistics to the advancement of the optimization procedure. Platon will include MF&L in the so-called *bounding-box* approach to track the level of error in the statistical estimates. Another research axis will focus on alternative estimation methods, *e.g.* the *Quantile Bayesian regression*, to include MF&L features.

3.1.4 HPC and UQ problems

Challenges. Both intrusive and non-intrusive UQ methods are associated to large computational costs, ranging from several to millions of times the cost of a deterministic solution depending on the problem and task considered. This situation is a significant obstacle to the deployment of UQ analysis in large scale simulations, and computational aspects have been central for a long time. However, works concerning the exploitation of High-Performance Computing platforms with massive parallelism are still scarce, besides the trivial parallelism of some sampling methods (*e.g.*, Monte Carlo). Further, past efforts have concerned the formulation of the stochastic problem and relied on existing advanced solution methods (*e.g.* Domain Decomposition, linear algebra libraries, parallelism). However, few works have fully considered exploiting stochastic structures *and* HPC aspects to design novel computational strategies fully dedicated to UQ problems.

Proposed actions. Platon will continue to develop solvers for the resolution of multiple large systems resulting from the discretization of sampled stochastic problems. In particular, we shall focus on linear and non-linear (Newton-like) solvers, exchanging information (Krylov spaces) between successive solves to improve convergence rates of iterative methods. Besides the extension to non-linear problems, the work will focus on the implementation aspect and consider communication strategies when several instances of the random system are solved in parallel.
Platon will continue to develop specific domain decomposition methods for stochastic problems, and to propose effective stochastic preconditioners exploiting the independence of the local (uncertain) sub-problems. An additional but critical point concerns the association of adaptive mesh refinement (AMR, in space) with multiple resolution analysis (MRA, in the parameters) methods. Few works have solved UQ problems with deterministic AMR, and combining the two adaptive approaches within a parallel framework remains challenging; progress in this direction would enable efficient intrusive solvers for conservation laws.

4 Application domains

In this section, we provide some examples of UQ problems with industrial interests. We believe they are illustrative of how we envision interactions and knowledge transfer with industrial partners. These examples involve industrial and academic partnerships, with active projects and contracts.

4.1 Simulation of space objects

Challenges. The French Aerospace industry is facing enormous technological challenges in a highly competitive market. We focus on two relevant problems, *i.e.* the design of the booster of the Ariane6 launch vehicle and the atmospheric reentry of space vehicles or satellites. The launch vehicle's structure sustains severe mechanical and thermal stresses during the ignition stage, which are challenging to model accurately. Therefore, the design still relies heavily on experimental measurements and safety margins, when a better account of model uncertainty would help improve the design procedures. Concerning the atmospheric reentry, recent regulations impose the reentry of a human-made end-of-life space object with a rigorous assessment of the risk for human assets. The risk evaluation requires sequences of complex numerical simulations accounting for the multi-physics phenomena occurring during the reentry of a space object, e.g., fluid-structure interactions and heat transfer. Further, these simulations are inaccurate because they rely on overly simplified models (e.g., a reliable model of fragmentation is not available yet) and partial knowledge of the reentry conditions.

4.2 Predictive simulation of complex flows in nuclear reactors

Challenges. In the nuclear field, a systematic issue is that the calibration and validation of the mathematical model use experimental data measured on devices that are scaled versions of the actual design. One expects the scaled models to exhibit the same physics as the actual design, although the two operate in different conditions. Because of prohibitive computational cost, only parts of the reactor can be simulated with computational-fluid-dynamics (CFD) models. An open question is then how to accurately estimate the global prediction error associated with the resulting numerical model. The long-term objective in this field is to perform a so-called up-scaling approach, integrate simulations of different parts of the reactor and available experiments in scaled and actual designs, and improve the global predictive capability of the simulation and support the decision regarding new experiments.

4.3 Robust design of ORC turbines for renewable energy sources

Challenges. Organic Rankine Cycles (ORCs) are of key-importance in renewable energy systems. The thermodynamic properties of the organic fluids present technological advantages for low-grade heat sources, *e.g.* geothermal, solar, or industrial waste. The use of these systems in different physical locations worldwide and with different heat source conditions implies large variability in the turbine's operating conditions. For this reason, ORCs manufacturers are highly interested in evaluating the variability in the system efficiency and, eventually, in the robust designing of the turbines. Moreover, the molecular complexity of organic fluids requires sophisticated thermodynamic models. Nevertheless, the scarcity of experimental data makes hard the calibration of both thermodynamic models and parameters (among other critical properties, acentric factor), as well as the inference of a suitable turbulence model.

4.4 Uncertainty and inference in geosciences

Challenges. Uncertainty and inference are crucial in geosciences where all prediction is affected by lack of knowledge, imprecise calibration, and model error. It is essential to make the best use of the available information and objectively account for the actual state of knowledge. Besides, depending on the application, experimental observations can be very scarce or highly abundant, models can be crude or highly sophisticated, such that different methods are needed to adapt to the context. Further, these methods should ideally consider all sources of error (data error, calibration uncertainty, model error, numerical error) globally to balance them and ensure that resources are properly allocated to improve the prediction. For these reasons, Platon will continue to work on methodologies for applications in geosciences.

4.5 Research plan

Most of the actions proposed above are either initiated or planned to start shortly. They are organized and structured around Ph.D. and Post-Doc research activities and will not exceed the duration of the project. Apart from these actions, we will continuously conduct more exploratory research activities to improve, for instance, the treatment of (structural) model errors in uncertainty management, assess the potential application of machine learning algorithms to UQ, and advance toward holistic management of uncertainties.

5 Social and environmental responsibility

5.1 Impact of research results

Platon is involved in the development of advanced numerical tools to simulate Organic Rankine Cycles (ORCs), which are of key-importance in renewable energy systems. Specifically, we are working on the inference of thermodynamic models parameters for complex molecular compounds, using experimental data of the worldwide first facility at Politecnico di Milano. Secondly, we are developing a robust optimization framework for the shape design of ORC turbines. We hope to apply these methodologies to real-case scenarios in collaboration with manufacturers within the H2020-MSCA-ITN NICE (submitted this year).

6 Highlights of the year

6.1 Awards

- Lalaina has been awarded the "Prix de thèse Maths Entreprises 2021".

7 New software and platforms

7.1 New software

7.1.1 Stocholm

Name: Stocholm

Keyword: Uncertainty quantification

Functional Description: Stocholm is a numerical library permitting to respond to potential partners swiftly and draft UQ solutions addressing new questions. It includes Polynomial Chaos construction, manipulation, and algebra, adaptive sparse grid methods for integration, interpolation, and projection in high-dimension, stochastic multi-resolution analysis tools with error estimators, advanced regression methods with regularization techniques and Gaussian process modeling, sampling methods with LHS, QMC and Markov Chain Monte Carlo algorithms, Bayesian inference framework and fast density estimation methods, Bayesian optimization algorithms with robust and multi-objective strategies, ...

Release Contributions: We will continue integrating existing tools and new ones into the library StochOlm (C++), the most general one, to allow for maximum interoperability of the constitutive utilities. Having a unique library shared by the whole group also presents some interest for students and new researchers joining the Team, as they can benefit from the others' experience.

Contact: Pietro Marco Congedo

8 New results

8.1 Research axis 1: Uncertainty Quantification and Inference

Participants: P.M. Congedo, O. Le Maître, A. del Val, G. Gori, N. Leoni, M. Capriati, L. Rakotondrainibe, D. Kumar.

Project-team positioning

Many research groups are presently working on Uncertainty Quantification (UQ) and inference problems over the world and in France. For instance, the US has created and continues to expand large multi-disciplinary groups to address UQ challenges in energy and military domains through their national laboratories (SANDIA, Oak-Ridge, LLNL,...). These groups aim at providing generic methods and tools (mostly software) for the resolution of UQ problems (for example, the Dakota code from Sandia-Albuquerque) faced by other research groups from diverse application domains. Other countries are supporting smaller initiatives, including the CEA (civil and military) in France. Several large industrial groups, such as Bosch, EADS, or EdF, are also deploying UQ methodologies and tools (for example, the OpenTurns code from EADS/EDF) through dedicated RD units or services, responding to the demands of other services. These UQ activities have often emerged in well-established groups working in specific application domains (e.g., fluid dynamics, solid mechanics, electromagnetics, chemistry, material sciences, earth sciences, life sciences, ...), in response to some UQ aspects related to these particular domains. We cite G. Iaccarino (Uncertainty Quantification Lab within the Center for Turbulence Research, Stanford University), Y. Marzouk (Aerospace Computational Design Laboratory, MIT) and K. Wilcox (Institute for Computational Engineering and Sciences, University of Texas). The situation is globally similar in applied mathematics, where several groups develop advanced UQ methods within a broader research area (e.g., stochastic numerics, statistics, numerical analysis,...), sometimes with only a distant connection to engineering domains. For example, we can mention the research groups of M. Giles (Oxford), I. Bilionis (Purdue University), J. Garnier (Ecole Polytechnique), R. Abgrall (University of Zurich).

The objective of Platon is to team-up participants with the main interest in the development of UQ methodologies. While primarily targeting our current applications, our objective is to propose new applications through collaborations and progressive team development while maintaining the UQ as the project's identity. This strategy gives a somehow unique position of the Team within the national and international research landscapes. As far as computational mechanics and engineering are concerned, no group has been created with UQ management as the principal working area.

Then, the identity of Platon is to be contrasted with initiatives, including within Inria, which may have a UQ component, but within different methodological contexts and not as a central activity. For instance, some teams (*e.g.* SIERRA, TAO, SELECT, MODAL) develop statistical methods for data analysis, machine learning, and the treatment of large databases. Overall, the problems targeted in Platon are usually too costly, with high parametric dimension, and with few experimental data, so existing statistical methods can not be reused "as is", and require dedicated approaches.

On the application side, there are already Inria teams working on CFD applications, some even incorporating uncertainty quantification and sensitivity analysis activities. We mention here AIRSEA, which focuses on oceanic and atmospheric flows, CARDAMOM on free-surface hydraulics, and ACUMES on unsteady models in traffic flow and biology. In contrast to our project, all these efforts primarily address challenges in their respective application areas.

Scientific achievements

Our research activity features two main axes. The first is related to methodological developments, while the second is oriented to UQ problems with industrial interests. Three applications domains are concerned, *i.e.* Aerospace/Aeronautical, Energy, Geosciences. Achievements include relevant advancements in building efficient surrogate-based methods for different purposes, variance-reduction methods, and many contributions in various application domains.

In the following, we describe first the main contributions from a methodological point of view followed by more oriented-applications findings.

The first contribution concerns the estimation of a probability of failure, defined as the volume of the excursion set of a complex scalar performance function J below a given threshold, under a probability measure that can be recast as a multivariate standard gaussian law using an isoprobabilistic transformation. We proposed a method [44] able to deal with cases characterized by multiple failure regions, possibly very small failure probability (10^{-6}-10^{-9}), and when the number of evaluations of J is limited. A further extension of this work [45] targets the estimation of quantiles associated to very small levels of probability (up to $O(10^{-9})$).

The third contribution focused on constructing functional representations of quantities of interest (QoIs) of an uncertain system in high dimension [7]. A particular attention is focused on the ignition delay time of an iso-octane air mixture, using a detailed chemical mechanism with 3,811 elementary reactions. We assessed the possibility of constructing polynomial chaos (PC) representations in terms of the canonical random variables parametrizing the uncertain rates. Specifically, we explored two avenues, namely sparse regression (SR) using LASSO, and a coordinate transform (CT) approach, with also preconditioned variants of both approaches.

Another contribution concerns the estimation of the density function of the solution to a random nonautonomous second-order linear differential equation with analytic data processes [41]. We focused on computational aspects and propose several variance reduction methods to speed up the convergence.

Another contribution [8] deals with the problem of parameter calibration of a variable-diffusivity fractional diffusion model. A Karhunen-Loève (KL) decomposition of the random diffusivity field is used, leading to a stochastic problem defined in terms of a finite number of canonical random variables. Polynomial chaos (PC) techniques are used to express the dependence of the stochastic solution on these random variables. A non-intrusive methodology is used, and a deterministic finite-difference solver of the fractional diffusion model is utilized for this purpose. In the broad range of parameters addressed, the analysis shows that the uncertain parameters having a significant impact on the variance of the solution can be reliably inferred, even from limited observations.

Applications in Uncertainty Quantification and Inference

In the aerospace field, we worked on in-flight ice accretion under parametric uncertainty [12] by proposing for the first time in litterature a non-linear regression method to approximate the full icing model. Secondly, we worked on sensitivity analysis of structural turbulence uncertainty estimates to time and space resolution of numerical computations [13], which are obtained by means of the Eigenspace Perturbation Method (EPM). Third, we worked on the inference of catalytic recombination parameters from plasma wind tunnel experiments of von Karman Institute (VKI) [11]. We developed a dedicated

Bayesian framework, which is the first step in setting a digital twin of the VKI experiment. Fourth, we perform a Bayesian calibration of the freestream velocity and density starting from measurements of the pressure and heat flux at the stagnation point of a hypersonic high-enthalpy flow around a cylinder [35]. We demonstrate for the first time in literature the interest in using stagnation heat flux measurements to rebuild freestream conditions.

In the energy field, we worked on the first-ever accuracy assessment of a computational model for Non-Ideal Compressible-Fluid Dynamics (NICFD) flows [38]. The assessment relies on a comparison between numerical predictions, from the open-source suite SU2, and pressure and Mach number measurements of compressible fluid flows in the non-ideal regime. In [39], we explored the inference of the coefficients of fluid-dependent thermodynamic models, applicable to complex molecular compounds with non-ideal effects. The main objective was to numerically assess the potential of using experimental measurements of some expansion flows to infer the model parameters. Secondly, we investigated a tangent linear approximation [6, 14] to estimate the sensitivity of the ignition delay time with respect to individual rate parameters in a detailed chemical mechanism and to species enthalpies and entropies. Moreover, we worked on simplified chemistry models [9] in reactive computational fluid dynamics (CFD) simulations to alleviate the computational cost. This work propagates the uncertainties-arising in the calibration of a global chemistry model-through direct numerical simulations (DNS) of flame-vortex interactions.

In geosciences, the main contribution concerns an integrated data-driven regional coupled modeling system for the Red Sea [40], which is a vital resource for the Kingdom of Saudi Arabia. Resulting achievements include significant advancement in our understanding of the regional circulation and its connection to the global climate, development and validation of long-term Red Sea regional atmospheric-oceanic-wave reanalyses, and forecasting capacities. Secondly, we worked on the seismic wave propagation into an uncertain medium [48], where we focus on the peak ground motion at the free surface of the 3D domain. Third, we worked on inferring a spatially varying Manning's n field in a coastal ocean model [47]. The idea is to view the prior on the Manning's n field as a stochastic Gaussian field, expressed through a covariance function with uncertain hyper-parameters. Moreover, we worked on the computational load encountered in seismic imaging by Bayesian traveltime inversion [20]. We demonstrate the potential of the proposed approach using numerical experiments on the inference of two-dimensional domains with layered velocity models and different acquisition geometries (microseismic and seismic refraction contexts).

Collaborations

Since many years, we have three long-term partnerships with KAUST, von Karman Institute for Fluid-Dynamics (VKI) and Politecnico di Milano, respectively.

With KAUST, we are working on new stochastic particle tracking methods to identify and track oil spills in open waters, combining satellite images and uncertainties in predicted currents. We also develop new assimilation schemes, inference methods for fractional diffusion models, and the selection and reduction of observations. There are several joint publications (7 journal papers) and exchanges of students.

With VKI, we work on UQ methods and inverse problems for atmospheric re-entry and ablation problems. We were involved in the MSCA ITN UTOPIAE project and are currently involved in a joint project with European Space Agency (TRP-ESA). In terms of production, there are several joint publications (6 journal papers) and three joint PhDs (A. Cortesi, A. Del Val, M. Capriati).

With Politecnico di Milano, we have several activities in the Aeronautical and Energy fields. We work on the characterization of the thermodynamic model with Bayesian approaches, uncertainty on the turbulence model for RANS aerodynamic simulation, multi-fidelity approaches. We were involved in the MSCA ITN UTOPIAE project and are currently involved in the EU CS2 MONNALISA project. We had two joint PhD (F. Fusi, G. Gori) and several joint publications (5 Journal papers).

Concerning the activities with the BRGM, we worked on subsurface flows with the development of a stochastic level set approach to handle uncertainties in steep saturation profiles and the application of Polynomial Chaos expansions to the Biot problem with uncertain soil properties. Note that the contact at BRGM was Pierre Sochala, who has now moved to CEA DAM. Collaboration with him will undoubtedly continue in the coming years.

During these two years, we have also collaborated with Universitat Politècnica de València (via an exchange student, *i.e.* Marc Journet) and CWI (via several visits of Nassim Razaaly). These collaborations lead to two and one journal papers, respectively.

External support

- Horizon2020 MSCA-ITN UTOPIAE Project (2017-2021)
- CleanSky2 MONNALISA Project (2020-2022)

Self assessment

We have proposed innovative methods that represent the state of the art. In addition to developing methods-oriented research, we proposed UQ methods tailored to specific applications in collaboration with other academic and industrial partners. This action has allowed us to position ourselves with high-impact papers in many application areas.

A weakness may be finding a balance between two different axes. The first axis concerns the development of high-level research from a methodological point of view, while the second one involves collaborations with industrial partners within research contracts and European projects. We think that the team's current size does not fit very well in the long term with this double effort. For this reason, the recruitment of new forces seems mandatory to keep sustaining a good balance between these two main axes of research.

8.2 Research axis 2: Solvers, Numerical Schemes and HPC

Personnel

Participants: P.M. Congedo, O. Le Maître, J. Reis.

Project-team positioning

Research on solvers, numerical schemes, and HPC algorithms specifically dedicated to UQ problems is scarce. Indeed, advanced sampling and stochastic estimation procedures, the subject of intensive outgoing research, rely on state-of-the-art deterministic solvers to generate the solution samples. To our knowledge, there is no research group (within or outside Inria) focusing entirely on the computational aspects of UQ problems. Groups producing computational utilities for UQ (e.g., Sandia's Dakota, OpenTurns) focus on the sampling part (statistical treatment), and the efficient generation of the samples is left to the user. In recent years, few works have concerned Galerkin solvers, their preconditioning, and the adaptation of domain decomposition methods (DDM) for (usually elliptic) stochastic PDEs. We can mention some activities in Manchester (preconditioning), Munich and Lausanne (DDM), and Bath (solvers for multi-level methods). In Platon, we are trying to exploit the structure of the stochastic problems to propose new strategies for their resolution (Galerkin method) or the generation of solution samples. These strategies can consist of adapting deterministic solvers to factorize the computational effort over multiple samples or, on the contrary, the definition of entirely new solution procedures to exploit parallel methods in stochastic problems better, beyond the independent resolution of independent samples. Our objective is to produce parallel and scalable methods for large-scale stochastic problems. We have teamed up with Paul Mycek (Cerfacs, Parallel Algorithms) and Luc Giraud (Inria, HiePACS) to work on scalable methods for sampling stochastic elliptic problems. In Joao Reis' thesis (Inria), we have focused on a new class of stochastic preconditioners that rely on low dimensional local parametrizations of the stochastic coefficient to precompute and assemble sample-dependent preconditioners efficiently. In Nicolas Venkovic's thesis (Cerfacs), we relied upon Krylov recycling methods to accelerate the resolution of a sequence of sampled elliptic problems, exploiting their spectral similarities.

It becomes more and more critical to devise solution methods tailored to the stochastic problem when the numerical complexity of the underlying deterministic problem increases. For elliptic problems, highly efficient deterministic solvers' availability has somehow limited the research on stochastic solvers. The situation is different for models based on fractional diffusion operators (in space or time), where the numerical difficulties to solve these operators have virtually prevented any work on problems with stochastic fractional and diffusion coefficients. A few years ago, KAUST (Omar Knio) and KFUPM (Kassem Mustapha) initiated a research program on fractional diffusion models. Platon is involved in this program to deal with the stochastic extensions. Several new numerical schemes and algorithms to solve deterministic fractional diffusion equations have been designed. These schemes are suitable for an extension to stochastic problems (e.g., allowing for spatially variable coefficients and achieving efficient -scalability- enabling sampling methods and inverse problems). These efforts lead to the first work on UQ and inverse problems in fractional diffusion models [8], and we are proud to announce the first-ever Galerkin solution of the time-fractional diffusion equation (Fokker-Planck), with stochastic fractional coefficient and diffusivity field.

Scientific achievements

The first achievement [25, 16] concerns the adaptation of some classical Domain Decomposition (DD) Methods to the sampling of stochastic problems. Specifically, we worked on a new numerical method to efficiently generate samples of the solution of stochastic elliptical equations with random coefficients. Particular emphasis is placed on coefficients with high variance and short correlation length. Classical deterministic DD methods are based on iterative approaches which require preconditioning strategies capable of maintaining a high rate of convergence when the number of subdomains increases. In our stochastic context, determining a classical preconditioner suitable for each sample can be expensive, and alternative strategies can be more efficient. Each sample amounts to solving a reduced linear system for the values of the solution at the interfaces of the subdomains, according to a finite element discretization. This reduced system is then solved by an iterative method.

We proposed three main contributions to efficient preconditioning, by introducing surrogates of 1) the reduced global operator, 2) the contribution of each subdomain to the reduced global operator, and 3) local preconditioners (multi-preconditioning). The first contribution focuses on the iterative Schwarz method and introduces a stochastic preconditioner consisting of a surrogate of the Schwarz system for the unknown values on the interface of the subdomains. The second contribution extends the previous idea to nonoverlapping DD methods by building surrogates of the local components of the Schur complement. Finally, the third contribution concerns a totally local preconditioner: the two-level Neumann-Neumann preconditioner. Throughout each contribution, a large number of numerical experiments show the effectiveness of surrogate-based preconditioning.

The second achievement concerns several contributions on the space-fractional diffusion equations, which can model accurately anomalous diffusion phenomena. Main contributions are the following ones:

- The first concerns hierarchical matrix approximations for space-fractional diffusion equations [34]. Space fractional diffusion models generally lead to dense discrete matrix operators, which lead to substantial computational challenges when the system size becomes large. For a state of size N , full representation of a fractional diffusion matrix would require $O(N^2)$ memory storage requirement, with a similar estimate for matrix-vector products. We present H^2 matrix representation and algorithms that are amenable to efficient implementation on GPUs, and that can reduce the cost of storing these operators to O(N) asymptotically. Attention is focused on smooth particle approximation of the governing equations, which lead to discrete operators involving explicit radial kernels. The algorithms are first tested using the fundamental solution of the unforced space fractional diffusion equation in an unbounded domain, and then for the steady, forced, fractional diffusion equation in a bounded domain. Our experiments show that the construction of the fractional diffusion matrix, the matrix-vector multiplication, and the generation of an approximate inverse pre-conditioner all perform very well on a single GPU on 2D problems with N in the range $10^5 – 10^6$. Overall, the present experiences showed that the H^2 matrix framework promises to provide practical means to handle large-scale space fractional diffusion models in several space dimensions, at a computational cost that is asymptotically similar to the cost of handling classical diffusion equations.

- The secont contribution [42] explores different particle-based approaches for the simulation of space–fractional diffusion equations in unbounded domains. We rely on smooth particle approximations and consider five different methods for estimating the fractional diffusion term. The first method is based on a direct differentiation of the particle representation, following the Riesz definition of the fractional derivative, and results in a non-conservative scheme. Three methods follow the particle strength exchange (PSE) methodology and are by construction conservative, meaning that the total particle strength is time-invariant. The first PSE algorithm estimates the fractional diffusion flux using direct differentiation and uses an integral representation of the divergence operator. The second one relies on the integral representation of the fractional Laplacian to derive a suitable particle strength exchange formula for the diffusion term. The third PSE construction employs the Green's function of the fractional diffusion equation. A fifth method is developed based on the diffusion velocity approach, where the diffusion term is transformed into a transport term. The performance of all five methods is assessed, for which analytical solutions are known. Computational experiments are used to gain insight into the generalization of the present constructions, such as applications in bounded domains or variable diffusivity.

- The third contribution [43] proposes and analyzes the first finite difference method for solving variable-coefficient one-dimensional (steady state) fractional DEs, with two-sided fractional derivatives (FDs). The nonlocal nature of the fractional diffusion operators makes substantially more difficult the mathematical analysis of these models and the establishment of suitable numerical schemes. The proposed scheme combines first-order forward and backward Euler methods for approximating the left-sided FD when the right-sided FD is approximated by two consecutive applications of the first-order backward Euler method. Our scheme reduces to the standard second-order central difference in the absence of FDs. The existence and uniqueness of the numerical solution are proved, and truncation errors of order h are demonstrated (h denotes the maximum space step size). The numerical tests illustrate the global O(h) accuracy, except for nonsmooth cases which, as expected, have deteriorated convergence rates.

Collaborations

CERFACS: We worked with Paul Mycek on the stochastic preconditioning of domain decomposition methods (Joao Reis' thesis). The resulting parallel stochastic elliptic solver heavily rely on the library `StochOlm` for stochastic quadrature and PC expansions of the local contributions to the preconditioner [16, 33].
KAUST: We worked with Omar Knio on numerical schemes for fractional diffusion equation and their extension to the stochastic case [42, 43, 34].

External support

- The activities of Joao Reis have been funded from the ITN-MSCA UTOPIAE.

- The KAUST and KFUPM initiative funded a 2 week research stay (Jan 2020, O. Le Maître) in Saudi Arabia.

Self assessment

The current activity on the solvers with CERFACS will end with the defence of Nicolas Venkovic's thesis. After the local preconditioning methods of Joao Reis' thesis, it is unclear what should be proposed to continue stochastic Domain Decomposition methods. We are currently discussing with Paul Mycek to assess the possible continuation of our collaboration on stochastic solvers and potential funding of a PhD student (at Inria).

Concerning the fractional diffusion models, we are already engaged in the extension of the hierarchical matrix method [34] to solve the spatial stochastic fractional diffusion equation with a Galerkin method and to develop sparse storage strategies to reduce the complexity of the stochastic time-fractional problem. These are promising and very original researches. We (Platon) are dependent on the collaboration to access some of the numerical utilities (H-matrices).

8.3 Research axis 3: Optimization under uncertainty

Personnel

Participants: P.M. Congedo, O. Le Maître, M. Pocheau, M. Rivier, L. Rakotondrainibe
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Project-team positioning

Optimization Under Uncertainty is an important axis of research, due to both the evergrowing computational power available and the need for efficiency, reliability and cost optimality. The presence of uncertainty could make the solution of a deterministic optimization problem suboptimal or even infeasible. Since this behavior could impact strongly the design performances, both academia and industry focused their effort to developing optimization under uncertanty methodologies. Optimization under uncertainty is a broad domain including several modeling paradigms, such as for example stochastic programming, Reliability-Based Design Optimization (RBDO, that deals with probabilistic and worst-case feasibility constraints), and Robust Design Optimization (RDO, where the deterministic objectives are replaced with averaged or worst-case ones, possibly in a multi-objective context such as the classical Taguchi optimization).

Note that most of the groups active in optimization under uncertainty also have strong activities in uncertainty quantification. Thus there is an overlap with the state of the art presented in Section 8.1. The Optimization & Uncertainty Quantification Group of Sandia-Albuquerque aim at providing advanced methods for the resolution of optimization under uncertainty problems. We mention as well optimization under uncertainties activities emerged in well-established groups working in specific application domains. We cite the Aerospace Computational Design Laboratory from MIT and the Institute for Computational Engineering and Sciences from University of Texas. In France, we can mention the OQUAIDO Chair (Optimization and QUAntification of Uncertainties), hosted by the École des Mines de Saint-Étienne from 2016 to 2021, aiming to bring together academic and industrial partners to solve problems related to uncertainty quantification, inversion and optimization.

In the context of the Optimization under Uncertainty, Platon is devoted to developing novel methods to tackle constrained multi-objective optimization, with specific attention on cost-efficient and mainly derivative-free strategies. Specifically, we look for an optimal trade-off between computational cost and accuracy in the case of problems involving complex and expensive numerical solvers. Platon is exploring also dedicated representation and the design of computer experiments to obtain the best estimation at the lowest cost (or for a prescribed computational budget) for nontrivial goal, specifically optimization and reliability problems where the accuracy needed is not uniform, possibly unknown a priori and to be estimated as the construction proceeds. More recently, we have worked also on sample average approximation methods using a risk-averse stochastic programming formulations.

Several Inria Teams have the optimization problem as core activity, such as for example BONUS, EDGE, INOCS, POLARIS, RANDOPT. Main difference is that we are not interested in working on generic optimization algorithms, as mentioned before. In our past and current works, we use standard optimization algorithms, mainly for continuous optimization. We focus our attention on dedicated representations to efficiently estimate uncertainty-based metrics within an optimization problem. The Inria teams POLARIS and INOCS work on innovative methods for stochastic optimization that are quite different from those proposed by Platon.

Scientific achievements

The first achievement concerns a novel methodology [17] to deal with constrained multiobjective optimization where fitness functions are uncertainty-driven metrics. This method relies on two main ideas. First, the accuracy for approximating the objectives and constraints at a given design should be driven by the probability for this design of being non-dominated. This choice permits to reduce the effort for evaluating designs which are unlikely to be optimal. Secondly, these approximated evaluations and their associated errors can be used to construct a predictive representation of the objectives and constraints over the whole design space to accelerate the optimization process. This method is novel since it permits to handle multi-objective problems with several metrics formulations (both RBDO and RDO) and features a very parsimonious behavior. Note that this algorithm is applicable with generic optimization methods.

The second achievement [18] focuses on the minimization of the quantile and the direct construction of a quantile regression model over the design space, from a limited number of training samples. Robust optimization strategies typically aim at minimizing some statistics of the uncertain objective function and can be expensive to solve when the statistic is costly to estimate at each design point. Surrogate models of the uncertain objective function can be used to reduce this computational cost. However, such surrogate approaches classically require a low-dimensional parametrization of the uncertainties, limiting their applicability. A Bayesian quantile regression procedure is proposed to construct the full posterior distribution of the quantile model. Sampling this distribution, we can assess the estimation error and adjust the complexity of the regression model to the available data. The Bayesian regression is embedded in a Bayesian optimization procedure, which generates sequentially new samples to improve the determination of the minimum of the quantile. The method proposed here targets problems that are not amenable to low dimensional parametrizations of the uncertainties, with an efficiency which is independent with respect to the number of uncertainties.

The third achievement deals with multi-fidelity approaches combining evaluations of the quantity of interest at different fidelity levels. The use of multi-fidelity approaches in the context of Efficient Global Optimization (EGO) is still a research topic, even if EGO has become a standard approach for the global optimization of complex systems with high computational costs. We propose [19] a new effective infilling strategy for multi-fidelity EGO. Our infilling strategy has the particularity of relying on non-nested training sets, a characteristic that comes with several computational benefits. The resulting EGO procedure achieves a significantly reduced computational cost, avoiding computations at useless fidelity levels whenever possible, but it is also more robust to low correlations between levels and noisy estimations.

Finally, we worked on a decision-making problem using a risk-neutral and two risk-averse two-stage stochastic programming formulations, where the conditional value at risk is used to represent risk [15]. A sample average approximation methodology is integrated with an adapted L-Shaped solution method, which can solve risk-neutral and specific risk-averse problems. This methodology provides a framework to understand and quantify the impact of the sample size on the variability of the results. This method has been applied to a virtual power plant (VPP) involving a self-scheduling and market involvement problem under uncertainty in the wind speed and electricity prices. Following this paper, a detailed investigation of the numerical efficiency of several sampling schemes has been performed for the two-stages optimization problem, and resulted in a work to be published in 2022.

Applications of Robust Optimization

The team has a second research component which consists in tailoring some methodologies for robust optimization to specific applications in different fields of engineering.

In the aerospace field, we worked [37] to improve the aerodynamic design of helicopter airfoils under an uncertainty quantification perspective. The robust approach shows the capability to reach the same mean performance of the deterministic one, but with a lower degradation of performances in off-design situations considered through the uncertainty.

In the energy field, we worked on an original and fast robust shape optimization [46] approach to overcome the limitation of a deterministic optimization that neglects operating conditions variability, applied to a well-known supersonic turbine nozzle for ORC applications. We propose here a mono-objective formulation which consists in minimizing the α-quantile of the targeted Quantity of Interest (QoI) under a probabilistic constraint, at a low computational cost. This problem is solved by using an efficient robust optimization approach, coupling a state-of-the-art quantile estimation and a classical Bayesian optimization method. Secondly, we worked on the desing of centrifugal pumps [36]. We apply some advanced optimization techniques to the blade optimization of an ERCOFTAC-like pump, and we assess the robustness of the optimal profiles through an uncertainty propagation study.

Collaborations

During the EU MSCA-ITN Utopiae project, we had the opportunity to host a PhD student from DLR (German Aerospace Center) working on quantile regression [18]. This fruitful collaboration lead us to submit a joint contribution with DLR to the new project funding of Horizon Europe. This project, called NEXTAIR (detailed in the following section), has been accepted and will start in a few months. It will allow the collaboration to continue through a joint PhD thesis working specifically on using gradients for robust optimization.

The collaboration with ArianeGroup has been ongoing for eight years and was initiated by P.M. Congedo in the Bacchus team. Concerning Platon, works on robust optimization are essentially associated with Mickael Rivier's CIFRE thesis (2017-2020). After his PhD defense in 2020, Mickael Rivier was hired in a permanent position by ArianeGroup and became one of ArianeGroup's contact persons in uncertainty quantification and optimization. A contract with ArianeGroup (which served to fund a post-doc for Platon) is ongoing on optimization for non-stationary problems.

The collaboration with KAUST, and in particular Ricardo Lima, has brought specific stochastic optimization problems with structures that considerably differ from our other researches (e.g. two-stages optimization, introduction of recourse, discrete optimization, ...). These problems also involve different risk mitigation approaches. Working on these problems we have learn alternative formulations and uncertainty treatments that we plan to apply to engineering applications. Similarly, we have contributed with sampling and uncertainty modelling strategies that are original for this types of problems.

External support

- "Contract d'accompagnement" with ArianeGroup 2017-2020.
- Research Contract with ArianeGroup, 2020-2022.
- Horizon2020 MSCA-ITN UTOPIAE Project (2017-2021).

Self assessment

Concerning the strong point, we proposed advanced state-of-the-art methods in different aspects of optimization under uncertainty, which are topics of great interest in academia. At the same time, we consolidated industrial collaborations that have allowed us to develop high-impact projects with a relevant societal impact.

Concerning a potential weakness, we think it is particularly challenging, given the size of the team, to keep proposing innovative methods and, at the same time, to contribute to projects at the industrial and European scale. New recruitments seem necessary to ensure this twofold effort.

9 Bilateral contracts and grants with industry

Participants: P.M. Congedo, O. Le Maitre, M. Rivier, M. Pocheau, L. Rakotondrainibe.

9.1 Bilateral contracts with industry

9.1.1 CEA CESTA

Since 2019, P.M. Congedo and O. Le Maître are leading a project with CEA-CESTA, (called Standard in Simulation in Section 9), about the introduction of Uncertainty Quantification tools in the "standard simulation" protocol used at CEA-CESTA. Five people are working on this project (4 Research Engineers from CEA-CESTA and two researchers from Platon). The amount of the grant is of 70 K euros.

9.1.2 ArianeGroup

The project concerns the optimization of the ignition device, taking into account the effects induced by the ignition transient. The simulation of the ignition device is carried out by ArianeGroup via a numerical chain made up of a CFD fluid code and a structural code which predicts the dynamic forces. We are testing several techniques, which are tailored to the problem of interest. The amount of the grant is of 150 K euros.

9.1.3 ArianeGroup

Until 2020, the team benefitted from a "contrat d'accompagnement" for the Cifre thesis of Mickael Rivier, on optimization under uncertainty. The amount of the grant was 30 K euros.

9.1.4 Bañulsdesign

Since 2019, the team benefits from a "contrat d'accompagnement" for the Cifre thesis of Malo Pocheau, on the modelling of foilers. The amount of the grant is 30 K euros.

10 Partnerships and cooperations

Participants: P.M. Congedo, O. Le Maitre, Dinesh Kumar, Joao Reis, Anabel del Val.

10.1 European initiatives

10.1.1 Horizon Europe

- MONNALISA: The CleanSky2 MONNALISA Project (2020-2022) (see for additional details) includes three institutions with Politecnico di Milano as coordinator. The funding for Inria is of 150 K euros. In this project, we aim at developing and validating an innovative, physics-based low-order method to predict the non-linear aerodynamic characteristics of lifting surfaces with controls whose geometry could significantly differ from the usual ones.

- NEXTAIR: The NEXAIRT HORIZON-CL5-2021-D5-01 (2021-2025) includes 15 institutions (Onera is the coordinator). The funding for Inria is of 300 K euros. NEXTAIR will develop and demonstrate innovative design methodologies, data fusion techniques enabling digital transformation of aircraft design, manufacturing and maintenance. It will increase high-fidelity modeling and simulation capabilities to accelerate and reduce the risk of disruptive new configurations and breakthrough technology designs. Moreover, NEXTAIR will also improve the effectiveness of uncertainty quantification and robust optimization technique to effectively account for manufacturing uncertainty and operational variability in the industrial multi-discipline design of aircraft and engine components.

10.1.2 FP7 & H2020 projects

- UTOPIAE: The Horizon2020 MSCA-ITN UTOPIAE Project (2017-2021) (see for additional details) includes 11 Institutions (University of Strathclyde (coordinator) with 15 Early Stage Researcher (ESR) recruited (two PhDs in Platon Team, G. Gori and J. Reis). The funding for Inria is of 520 K euros. UTOPIAE is a European research and training network looking at cutting edge methods bridging optimisation and uncertainty quantification applied to aerospace systems. The network is funded by the European Commission through the Marie Skłodowska-Curie Actions of H2020. The network is made up of 15 partners across 6 European countries, including the UK, and one international partner in the USA, collecting mathematicians, engineers and computer scientists from academia, industry, public and private sectors.

10.1.3 Other european programs/initiatives

- ReChar-TPS: Call for tenders from the European Space Agency (ESA), ReChar-TPS with von Karman Institute for Fluid Dynamics and ArianeGroup (ESA contract 4000131694/20/NL/AR/idb). This project deals with the reliable characterization of ablative materials for Thermal Protection Systems. Our contributions concern the development and application of Uncertainty Quantification methodologies to learn macroscopic material properties from microstructure simulations. The funding for Inria is of 10 K euros.

11 Dissemination

11.1 Promoting scientific activities

11.1.1 Scientific events: organisation

General chair, scientific chair:

- Pietro Marco Congedo has been the Scientific Chair of the CWI-Inria Workshop 2021, held online on 5-6 July 2021.

Member of the organizing committees:

- Pietro Marco Congedo has been a member of the Organization committee of the seminar HyFAR-ARA about "Laminar-turbulent transition in hypersonic regimes", held online on 25-17 May 2021.

11.1.2 Scientific events: selection

Member of the conference program committees

- Olivier Le Maître has served in the scientific committee of the Congrès Français de Mécanique (2021, rescheduled to 2022)

- Olivier Le Maître has served in the scientific committee of the 4th International Conference on Uncertainty Quantification in Computational Sciences and Engineering (2021)

11.1.3 Journal

Member of the editorial boards

- Olivier Le Maître is member of the editorial board of the International Journal for Uncertainty Quantification.

- Pietro Marco Congedo is Editor of the Journal "Mathematics and Computer in Simulation (MATCOM)" from Elsevier.

11.1.4 Invited talks

Pietro Marco Congedo has given a seminar at the ESA AITTAO 10666 Progress Meeting, the 30th of Avril 2021.

Pietro Marco Congedo has given a seminar at the "Séminaire de Machine learning", organized at the LMFA of the Ecole Centrale Lyon, 8 Décembre 2021.

11.1.5 Scientific expertise

Since 2019, Pietro Marco Congedo and Olivier Le Maître have provided a consulting activity to CEA CESTA. The consulting deals with integrating Uncertainty Quantification strategies within CESTA's "simulations standard," which covers the simulation processes and the certification of the numerical predictions.

11.1.6 Research administration

Pietro Marco Congedo is the Scientific Director of the Inria International Lab CWI-Inria.

11.2 Teaching - Supervision - Juries

Teaching at University

- PM Congedo, 2021: ENSTA ParisTech, Palaiseau, Graduate level (20h/y), Numerical methods in Fluid Mechanics.
- OP Le Maître, 2021: Université Paris Saclay, Doctoral School SMEMAG (22h/y), Uncertainty Quantification Methods.

11.2.1 Supervision

- Pietro Marco Congedo is the co-advisor of the thesis of Michele Capriati in collaboration with von Karman Institute for Fluid-dynamics (Belgium).
- Pietro Marco Congedo and Olivier Le Maître have been co-advisors of the thesis of Ana Isabel Del Val Benitez, who defended her thesis the 19th of November 2021 from "Institut Polytechnique de Paris".
- Pietro Marco Congedo and Olivier Le Maître are the co-advisors of the thesis of Nicolas Leoni in collaboration with CEA Saclay.
- Pietro Marco Congedo is the co-advisor of the thesis of Paul Novello in collaboration with CEA CESTA.
- Olivier Le Maître is the advisor of the thesis of Malo Pocheau in collaboration with Bañuls Design.
- Olivier Le Maître is the advisor of the thesis of Marius Duvillard in collaboration with CEA Cadarache.
- Pietro Marco Congedo and Olivier Le Maître have been co-advisors of the thesis of Joao Miguel Felicio Dos, who defended his thesis the 4th of October 2021 from "Institut Polytechnique de Paris".

11.2.2 Juries

- Pietro Marco Congedo has been reviewer for the HDR of Pierre Sochala (12 Janvier 2021) from Ecole Polytechnique, IPP.
- Pietro Marco Congedo has been reviewer for the PhD thesis of Martin BUISSON (5 Février 2021) from Ecole Centrale Lyon.
- Pietro Marco Congedo has been reviewer for the PhD thesis of Victor Trappler (31 Mai 2021) from Université Grenoble Alpes.
- Pietro Marco Congedo has been reviewer for the PhD thesis of Marc Schouler (7 Décembre 2021) from Université de Toulouse.
- Olivier Le Maître was Research Director for the HdR of Pierre Sochala (12 Janvier 2021) from IPP.
- Olivier Le Maître has served as reviewer in the PHD of Sofia Rem Mouradi (16 Mars 2021) from INP Toulouse.
- Olivier Le Maître has served as chairperson in the PhD committee of Luc Bonnet (13 Décembre 2021) from Université Paris Saclay.

11.3 Popularization

11.3.1 Internal or external Inria responsibilities

- Pietro Marco Congedo is the Deputy Coordinator of "Maths/Engineering" Program of the Labex Mathématiques Hadamard (IPP and Paris-Saclay University), since 2018.
- Pietro Marco Congedo is member of the Conseil du Laboratoire du CMAP (Ecole Polytechnique IPP).
- Olivier Le Maître is the corresponding member of the Inria SIF center with the French Agency for Math and Industry (AMIES), since 2019.

11.3.2 Interventions

Anabel del Val, Joao Reis and Giulio Gori participated in several outreach activities in the EU MSCA ITN UTOPIAE project. For example, they had the opportunity to showcase some aspects of their research in the Glasgow Science Centre.

12 Scientific production

12.1 Major publications

[1] G. Gori, O. P. Le Maître and P. M. Congedo. 'On the sensitivity of structural turbulence uncertainty estimates to time and space resolution'. In: *Computers and Fluids* (2021). DOI: 10.1016/j.compfluid.2021.105081. URL: https://hal.archives-ouvertes.fr/hal-03299149.

[2] N. Razaaly and P. M. Congedo. 'Extension of AK-MCS for the efficient computation of very small failure probabilities'. In: *Reliability Engineering and System Safety* 203 (Nov. 2020), p. 107084. DOI: 10.1016/j.ress.2020.107084. URL: https://hal.inria.fr/hal-03047283.

[3] J. F. d. REIS, O. P. Le Maître, P. M. Congedo and P. Mycek. 'Stochastic Preconditioning of Domain Decomposition Methods for Elliptic Equations with Random Coefficients'. In: *Computer Methods in Applied Mechanics and Engineering* (2021). URL: https://hal.inria.fr/hal-03201297.

[4] C. Sabater, O. Le Maitre, P. M. Congedo and S. Görtz. 'A Bayesian Approach for Quantile Optimization Problems with High-Dimensional Uncertainty Sources'. In: *Computer Methods in Applied Mechanics and Engineering* 376 (2021), p. 113632. URL: https://hal.archives-ouvertes.fr/hal-03086453.

[5] P. Sochala, F. De Martin and O. Le Maitre. 'Model Reduction for Large-Scale Earthquake Simulation in an Uncertain 3D Medium'. In: *International Journal for Uncertainty Quantification* 10.2 (2020), pp. 101–127. DOI: 10.1615/Int.J.UncertaintyQuantification.2020031165. URL: https://hal.archives-ouvertes.fr/hal-02570132.

12.2 Publications of the year

International journals

[6] S. Almohammadi, M. Hantouche, O. Le Maitre and O. M. Knio. 'A tangent linear approximation of the ignition delay time. I: Sensitivity to rate parameters'. In: *Combustion and Flame* 230 (Aug. 2021), p. 111426. DOI: 10.1016/j.combustflame.2021.111426. URL: https://hal.archives-ouvertes.fr/hal-03190168.

[7] S. M. Almohammadi, O. Le Maitre and O. M. Knio. 'Computational Challenges in Sampling and Representation of Uncertain Reaction Kinetics in Large Dimensions'. In: *International Journal for Uncertainty Quantification* 12.1 (2022), pp. 1–24. DOI: 10.1615/Int.J.UncertaintyQuantification.2021035691. URL: https://hal.archives-ouvertes.fr/hal-03282657.

[8] H. H. Alzahrani, M. Lucchesi, K. Mustapha, O. Le Maitre and O. M. Knio. 'Bayesian calibration of order and diffusivity parameters in a fractional diffusion equation'. In: *Journal of Physics Communications* 5.8 (24th Aug. 2021), p. 085014. DOI: 10.1088/2399-6528/ac1507. URL: https://hal.archives-ouvertes.fr/hal-03384280.

[9] J. M. Armengol, O. Le Maitre and R. Vicquelin. 'Bayesian calibration of a methane-air global scheme and uncertainty propagation to flame-vortex interactions'. In: *Combustion and Flame* 234 (Dec. 2021), p. 111642. DOI: 10.1016/J.COMBUSTFLAME.2021.111642. URL: https://hal.archives-ouvertes.fr/hal-03318385.

[10] P. Bacigaluppi, J. Carlier, M. Pelanti, P. M. Congedo and R. Abgrall. 'Assessment of a non-conservative Residual Distribution scheme for solving a four-equation two-phase system with phase transition'. In: *Journal of Scientific Computing* 90.1 (Jan. 2022). DOI: 10.1007/s10915-021-01706-6. URL: https://hal.inria.fr/hal-03495885.

[11] A. Del Val, O. LE MAÎTRE, T. E. Magin, O. Chazot and P. M. Congedo. 'A surrogate-based optimal likelihood function for the Bayesian calibration of catalytic recombination in atmospheric entry protection materials'. In: *Applied Mathematical Modelling* 101 (20th Dec. 2021), pp. 791–810. DOI: 10.1016/j.apm.2021.07.019. URL: https://hal.inria.fr/hal-03495878.

[12] G. Gori, P. M. Congedo, O. LE MAÎTRE, T. Bellosta and A. Guardone. 'Modeling In-Flight Ice Accretion Under Uncertain Conditions'. In: *Journal of Aircraft* (1st Dec. 2021), pp. 1–15. DOI: 10.2514/1.C036545. URL: https://hal.inria.fr/hal-03495860.

[13] G. Gori, O. P. Le Maître and P. M. Congedo. 'On the sensitivity of structural turbulence uncertainty estimates to time and space resolution'. In: *Computers and Fluids* (2021). DOI: 10.1016/j.compfluid.2021.105081. URL: https://hal.archives-ouvertes.fr/hal-03299149.

[14] M. Hantouche, S. Almohammadi, O. Le Maitre and O. M. Knio. 'A tangent linear approximation of the ignition delay time. II: Sensitivity to thermochemical parameters'. In: *Combustion and Flame* (Sept. 2021), p. 111677. DOI: 10.1016/j.combustflame.2021.111677. URL: https://hal.archives-ouvertes.fr/hal-03384214.

[15] R. M. Lima, A. J. Conejo, L. Giraldi, O. Le Maitre, I. Hoteit and O. M. Knio. 'Sample average approximation for risk-averse problems: A virtual power plant scheduling application'. In: *EURO Journal on Computational Optimization* 9 (Mar. 2021). URL: https://hal.archives-ouvertes.fr/hal-03188611.

[16] J. F. d. REIS, O. P. Le Maître, P. M. Congedo and P. Mycek. 'Stochastic Preconditioning of Domain Decomposition Methods for Elliptic Equations with Random Coefficients'. In: *Computer Methods in Applied Mechanics and Engineering* (2021). URL: https://hal.inria.fr/hal-03201297.

[17] M. Rivier and P. M. Congedo. 'Surrogate-Assisted Bounding-Box approach applied to constrained multi-objective optimisation under uncertainty'. In: *Reliability Engineering and System Safety* 217 (Jan. 2022), p. 108039. DOI: 10.1016/j.ress.2021.108039. URL: https://hal.inria.fr/hal-03495871.

[18] C. Sabater, O. Le Maitre, P. M. Congedo and S. Görtz. 'A Bayesian Approach for Quantile Optimization Problems with High-Dimensional Uncertainty Sources'. In: *Computer Methods in Applied Mechanics and Engineering* 376 (2021), p. 113632. URL: https://hal.archives-ouvertes.fr/hal-03086453.

[19] M. Sacher, O. Le Maitre, R. Duvigneau, F. Hauville, M. Durand and C. Lothode. 'A Non-Nested Infilling Strategy for Multi-Fidelity based Efficient Global Optimization'. In: *International Journal for Uncertainty Quantification* 11.1 (Jan. 2021), pp. 1–30. URL: https://hal.inria.fr/hal-02901774.

[20] P. Sochala, A. Gesret and O. Le Maitre. 'Polynomial surrogates for Bayesian traveltime tomography'. In: *GEM - International Journal on Geomathematics* 12.1 (Dec. 2021). DOI: 10.1007/s13137-021-00184-0. URL: https://hal.archives-ouvertes.fr/hal-03384145.

International peer-reviewed conferences

[21] G. Gori, T. Bellosta, A. Guardone, P. Congedo and O. Le Maitre. 'Uncertainty quantification for in-flight ice accretion under Appendix-C and Appendix-O conditions'. In: AIAA AVIATION 2021 FORUM. VIRTUAL EVENT, United States: American Institute of Aeronautics and Astronautics, 28th July 2021. DOI: 10.2514/6.2021-2645. URL: https://hal.inria.fr/hal-03498436.

[22] E. Solai, H. Beaugendre, U. Bieder and P. M. Congedo. 'Accuracy Assessment of Li-ion Batteries Internal Resistance Model Through CFD Simulations, Experimental Measurements And Uncertainties'. In: HEFAT 2021 - 15th International Conference on Heat Transfer, Fluid Mechanics and Thermodynamics. Virtual conference, Netherlands, 25th July 2021. URL: https://hal.inria.fr/hal-03417087.

Conferences without proceedings

[23] N. Leoni, P. M. Congedo, O. Le Maitre and M.-G. Rodio. 'Bayesian Inference of Model Error in Imprecise Models'. In: WCCM-ECCOMAS 2021 - 14th World Congress on Computational Mechanics. Paris / Virtual, France, 11th Jan. 2021. URL: https://hal.archives-ouvertes.fr/hal-03119715.

Scientific book chapters

[24] G. Gori, J. Reis, P. Congedo and O. L. Maître. 'Introduction to Spectral Methods for Uncertainty Quantification'. In: *Optimization Under Uncertainty with Applications to Aerospace Engineering*. Springer International Publishing, 10th Sept. 2021, pp. 1–34. DOI: 10.1007/978-3-030-60166-9_1. URL: https://hal.inria.fr/hal-03498457.

Doctoral dissertations and habilitation theses

[25] J. F. d. REIS. 'Preconditioning of Domain Decomposition Methods for Stochastic Elliptic Equations'. Institut Polytechnique de Paris, 4th Oct. 2021. URL: https://hal.inria.fr/tel-03498777.

[26] A. del Val. 'Bayesian calibration and assessment of gas-surface interaction models and experiments in atmospheric entry plasmas'. Institut polytechnique de Paris; Ecole Polytechnique (Palaiseau, France); Centre de Mathématiques Appliquées, École Polytechnique, France, 19th Nov. 2021. URL: https://hal.inria.fr/tel-03504757.

Reports & preprints

[27] B. Arizmendi, T. Bellosta, A. Del Val, G. Gori, J. Reis and M. Prazeres. *On Real-time Management of On-board Ice Protection Systems by means of Machine Learning*. 14th Apr. 2021. URL: https://hal.inria.fr/hal-03197683.

[28] J. M. Armengol, O. Le Maitre and R. Vicquelin. *Bayesian inference and uncertainty quantification of reduced chemical schemes*. 12th Mar. 2021. URL: https://hal.archives-ouvertes.fr/hal-03167494.

[29] F. Girault and P. M. Congedo. *Uncertainty Characterization of ablative materials for atmospheric reentry of spacecrafts using PuMA*. RR-9417. Inria Saclay -Île de France, 24th Sept. 2021. URL: https://hal.inria.fr/hal-03384925.

[30] P. Novello, G. Poëtte, D. Lugato and P. M. Congedo. *Goal-oriented sensitivity analysis of hyperparameters in deep learning*. 13th Dec. 2021. URL: https://hal.archives-ouvertes.fr/hal-03128298.

[31] P. Novello, G. Poëtte, D. Lugato and P. M. Congedo. *Variance Based Samples Weighting for Supervised Deep Learning*. 28th Jan. 2021. URL: https://hal.inria.fr/hal-02885827.

[32] A. del Val, D. Luís and O. Chazot. *Experimental methodology for the accurate stochastic calibration of catalytic recombination affecting reusable spacecraft thermal protection systems*. 29th Dec. 2021. URL: https://hal.inria.fr/hal-03504760.

[33] N. Venkovic, P. Mycek, L. Giraud and O. Le Maitre. *Recycling Krylov subspace strategies for sequences of sampled stochastic elliptic equations*. RR-9425. Inria Bordeaux - Sud Ouest, 5th Oct. 2021. URL: https://hal.archives-ouvertes.fr/hal-03366966.

12.3 Cited publications

[34] W. Boukaram, M. Lucchesi, G. Turkiyyah, O. Le Maitre, O. Knio and D. Keyes. 'Hierarchical matrix approximations for space-fractional diffusion equations'. In: *Computer Methods in Applied Mechanics and Engineering* 369 (Sept. 2020), p. 113191. DOI: 10.1016/j.cma.2020.113191. URL: https://hal.archives-ouvertes.fr/hal-02864782.

[35] A. F. Cortesi, P. G. Constantine, T. Magin and P. M. Congedo. 'Forward and backward uncertainty quantification with active subspaces: application to hypersonic flows around a cylinder'. In: *Journal of Computational Physics* 407 (Apr. 2020), p. 109079. DOI: 10.1016/j.jcp.2019.109079. URL: https://hal.inria.fr/hal-03052824.

[36] A. Fracassi, R. De Donno, A. Ghidoni and P. M. Congedo. 'Surrogate based shape optimization and uncertainty assessment of a ERCOFTAC pump'. In: *Engineering Optimization* (Apr. 2020), pp. 1–18. DOI: 10.1080/0305215X.2020.1858075. URL: https://hal.inria.fr/hal-03495850.

[37] F. Fusi, P. M. Congedo, A. Guardone and G. Quaranta. 'Assessment of robust optimization for design of rotorcraft airfoils in forward flight'. In: *Aerospace Science and Technology* 107 (June 2020), p. 106355. DOI: 10.1016/j.ast.2020.106355. URL: https://hal.inria.fr/hal-03045531.

[38] G. Gori, M. Zocca, G. Cammi, A. Spinelli, P. M. Congedo and A. Guardone. 'Accuracy assessment of the Non-Ideal Computational Fluid Dynamics model for siloxane MDM from the open-source SU2 suite'. In: *European Journal of Mechanics - B/Fluids* 79 (Jan. 2020), pp. 109–120. DOI: 10.1016/j.euromechflu.2019.08.014. URL: https://hal.archives-ouvertes.fr/hal-02389668.

[39] G. Gori, M. Zocca, A. Guardone, O. Le Maitre and P. M. Congedo. 'Bayesian inference of thermodynamic models from vapor flow experiments'. In: *Computers and Fluids* 205 (June 2020), p. 104550. DOI: 10.1016/j.compfluid.2020.104550. URL: https://hal.archives-ouvertes.fr/hal-03010091.

[40] I. Hoteit, Y. Abualnaja, S. Afsal, B. Ait El Fquih, T. Akylas, C. Antony, C. Dawson, K. Asfahani, R. J. W. Brewin, L. Cavaleri et al. 'Towards an End-to-End Analysis and Prediction System for Weather, Climate, and Marine Applications in the Red Sea'. In: *Bulletin of the American Meteorological Society* (Sept. 2020), pp. 1–61. DOI: 10.1175/BAMS-D-19-0005.1. URL: https://hal.archives-ouvertes.fr/hal-03010422.

[41] M. Jornet, J. Calatayud, O. Le Maitre and J. C. Cortés. 'Variance Reduction Methods and Multilevel Monte Carlo Strategy for Estimating Densities of Solutions to Random Second-Order Linear Differential Equations'. In: *International Journal for Uncertainty Quantification* 10.5 (2020), pp. 467–497. URL: https://hal.archives-ouvertes.fr/hal-03021795.

[42] M. Lucchesi, S. Allouch, O. Le Maitre, K. Mustapha and O. Knio. 'Particle simulation of space–fractional diffusion equations'. In: *Computational Particle Mechanics* 7.3 (May 2020), pp. 491–507. DOI: 10.1007/s40571-019-00275-8. URL: https://hal.archives-ouvertes.fr/hal-02327700.

[43] K. Mustapha, K. Furati, O. Knio and O. Le Maitre. 'A Finite Difference Method for Space Fractional Differential Equations with Variable Diffusivity Coefficient'. In: *Communications on Applied Mathematics and Computation* 2.4 (Dec. 2020), pp. 671–688. DOI: 10.1007/s42967-020-00066-6. URL: https://hal.archives-ouvertes.fr/hal-03010233.

[44] N. Razaaly and P. M. Congedo. 'Extension of AK-MCS for the efficient computation of very small failure probabilities'. In: *Reliability Engineering and System Safety* 203 (Nov. 2020), p. 107084. DOI: 10.1016/j.ress.2020.107084. URL: https://hal.inria.fr/hal-03047283.

[45] N. Razaaly, D. Crommelin and P. M. Congedo. 'Efficient Estimation of Extreme Quantiles using Adaptive Kriging and Importance Sampling'. In: *International Journal for Numerical Methods in Engineering* 121.9 (May 2020), pp. 2086–2105. DOI: 10.1002/nme.6300. URL: https://hal.inria.fr/hal-02436230.

[46] N. Razaaly, G. Persico, G. Gori and P. M. Congedo. 'Quantile-based robust optimization of a supersonic nozzle for organic rankine cycle turbines'. In: *Applied Mathematical Modelling* 82 (June 2020), pp. 802–824. DOI: 10.1016/j.apm.2020.01.048. URL: https://hal.inria.fr/hal-03047877.

[47] A. Siripatana, O. Le Maitre, O. Knio, C. Dawson and I. Hoteit. 'Bayesian inference of spatially varying Manning's n coefficients in an idealized coastal ocean model using a generalized Karhunen-Loève expansion and polynomial chaos'. In: *Ocean Dynamics* 70.8 (Aug. 2020), pp. 1103–1127. DOI: 10.1007/s10236-020-01382-4. URL: https://hal.archives-ouvertes.fr/hal-03010151.

[48] P. Sochala, F. De Martin and O. Le Maitre. 'Model Reduction for Large-Scale Earthquake Simulation in an Uncertain 3D Medium'. In: *International Journal for Uncertainty Quantification* 10.2 (2020), pp. 101–127. DOI: 10.1615/Int.J.UncertaintyQuantification.2020031165. URL: https://hal.archives-ouvertes.fr/hal-02570132.