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News

Fundamental Research

Mathematics and IT

Numerical methods and optimization

In many IFPEN fields of application, there is a growing need for optimization and uncertainty treatment methods during the design and development phases of increasingly complex systems. The DOPING research project, led by the scientific division, has contributed to the development of appropriate cross-functional methods and their deployment via the internal ATOUT (Advanced Tools for Optimization and Uncertainty Treatment) platform.

## Optimization at the heart of system development

During the development process of complex systems, optimization mainly takes places at three levels:

- during the preliminary steps involving the setting up of simulators, for the calibration of numerical models on experimental data;
- during the design steps using these simulators;
- during the development of the systems' operation of systems.

In each of these steps, it is essential to accurately take into account all the inputs, with **their varied nature** (continuous and discrete variables, categorical, scalar and functional variables), and the often

**multiple and non-linear outputs.** It is also necessary to integrate uncertainties specific to the system under consideration, its production and its operating environment. An additional difficulty lies in the calculation time required to simulate these complex systems using existing numerical models. Their repeated use within optimization and statistical exploration processes then leads to the construction of substitute models, or meta-models, which are less time consuming.

## Three operational objectives

Attached to a fundamental research program, the DOPING project focused on scientific challenges affecting three operational objectives common to IFPEN's diverse fields of innovation ([Figure 1](#)) :

1. **Risk, uncertainty and sensitivity analysis** for understanding and controlling the operation of systems.
2. The **calibration of numerical models using experimental data** or **data assimilation** to predict the behavior of the system and reduce uncertainties associated with these predictions.
3. The optimal design of systems incorporating **reliability** and **robustness constraint**.

**Figure 1 : Operational objectives**

## The ATOUT platform

Capitalizing on research results is generally a crucial step with a view to potential future developments. Capitalization of the methods developed was conducted via an existing **internal platform** that was adapted and extended for multiple IFPEN applications in partnership with the Information Systems Division and Tech'Advantage, an IFPEN subsidiary. This platform, called ATOUT (Advanced Tools for Optimization and Uncertainty Treatment), is available to research and innovation divisions for their application needs and enables coupling with application-specific simulators ( [DeepLines™](#), [DeepLines](#), [FEMM](#), Abaqus®, [PlugIm!](#), [PumaFlow®](#), etc.).

## Main research topics

The research topics studied by the DOPING project lie at the crossroads of different mathematical fields: numerical optimization, statistical modeling, machine learning and uncertainty quantification ( [Figure 2](#)).

- **Experimental design** is a key step for constructing predictive response surfaces, from “black box” computationally expensive simulators. The choice of points to simulate is thus guided by the operational objective being pursued: global sensitivity or uncertainty analysis, probability estimation (of failure, for example [\[2\]](#), optimization or inversion [\[3\]](#). One of the recurrent difficulties is integration of the constraints on input variables, particularly constraints constructed from simulator outputs (“black box” constraints), or even instabilities or simulation failures (“hidden” constraints).

- The design of reliable technologies requires the development of appropriate **risk analysis and optimization tools**: (i) for the estimation, at reasonable simulation costs, of rare events, such as the failure of a one-shore wind turbine tower or of the anchoring system of a floating turbine [2], (ii) for inversion and optimization under probabilistic constraints [3] [4], such as constraints on failure probabilities.
- Some applications involve functional variables with spatial or time dependencies (for example in wind turbine applications: wind speed depends on time). A classic discretization approach with respect to these variables leads to vectors of a large size. The research conducted is aimed at preserving the functional nature of the variables, while reducing their dimension [3][4], prior to their integration in an optimization or inversion process.
- In the field of the optimal design of complex systems (design of mechanical systems or refining processes, oil field or wind farm optimization, etc.), the optimization problems to be solved may depend on discrete variables, in addition to continuous variables describing the dimensions or properties of the different components [1][5][6].

### What is a discrete variable ?

This could be, for example: a number of components (integer variables), different materials (categorical variables, generally unordered), the presence or not of certain components (binary variables).

Many of the results obtained in the DOPING project and validated on applications are now available in the ATOUT platform and have been used within the context of collaborative projects as well as the provision of services.

## Figure 2 : DOPING project research themes, theses and associated collaborations

### After DOPING comes DeTOCS

The research conducted in DOPING on these research topics is being continued into the DeTOCS (Design Tools for Optimization and Control of complex systems) project, with an extension of the scope of application and expertise to include **system control**. The DETOCS project is being conducted within the framework of several collaborative projects:

- ANR projects: the [SAMOURAI](#) project on optimization, uncertainty and reliability analysis based on simulations and meta-models and the [ALEKCIA](#) project aimed at developing innovative tools for the prediction and enhanced analysis of turbulent reactive flows in hydrogen IC engines;
- [CIROQUO](#), a “Consortium Industrie Recherche pour l’Optimisation et la Quantification d’incertitude pour les données Onéreuses” (industrial research consortium dedicated to the optimization and quantification of uncertainties for expensive data) bringing together 13 academic, technological research and industrial partners;

- a collaboration with Montreal Polytechnique's GERAD laboratory (via a Samuel de Champlain grant) focusing on the consideration of discrete variables in black box optimization;
- a collaborative project with Safran for the development of the [LAGUN](#) open-source simulation data optimization and exploration platform;
- as well as several PhD theses within the framework of the [INRIA/IFPEN](#) partnership: on robust inversion with functional inputs and control by learning methods with reinforcement.

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## Publications

- [1] Munoz Zuniga, M., and Sinoquet, D., Global Optimization for mixed categorical-continuous variables based on Gaussian process models with a randomized categorical space exploration step, 2020, INFOR: Information Systems and Operational Research, Taylor & Francis, 58, p.p.310-341, [DOI:10.1080/03155986.2020.1730677](#), [hal-02512185](#).
- [2] Murangira, A., Munoz Zuniga, M., Perdrizet, T., Structural reliability assessment through metamodel based importance sampling with dimension reduction, 2019, [DOI:10.1016/j.ress.2020.107289](#).
- [3] El Amri, M.R., Helbert, C., Lepreux, O., Munoz Zuniga, M., Prieur, C. and Sinoquet, D., Data driven stochastic inversion via functional quantization, Stat Comput, 2020, [DOI:10.1007/s11222-019-09888-8](#), [hal-0229176](#).
- [4] Van Ackooij, W., Aleksovskaja, I., Munoz Zuniga, M., (Sub-)Differentiability of Probability Functions with Elliptical Distributions, 2018, Set-Valued and Variational Analysis Volume 26, Issue 4, pp 887-910, [DOI:10.1007/s11228-017-0454-3](#), [hal-02013571](#)
- [5] Poirette Y., Guiton M., Huwart G., Sinoquet D. and Leroy J-M., An optimization method for the configuration of inter array cables for floating offshore wind farm, Proceedings of the International Conference on Offshore Mechanics and Arctic Engineering - OMAE 2017, [DOI:10.1115/OMAE2017-61655](#), [hal-02284402](#)
- [6] Psaltis A., Sinoquet D. and Pagot A., Systematic optimization methodology for heat exchanger network and simultaneous process design, 2016, Computers and Chemical Engineering, [DOI:10.1016/j.compchemeng.2016.09.013](#), [hal-0145282](#)

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