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► To cite this version:

Christophette Blanchet-Scalliet, Céline Helbert, Delphine Sinoquet, Miguel Munoz Munoz Zuniga, Rodolphe Le Riche, et al.. Activity report ciroquo research & industry consortium. Ecole Centrale de Lyon; Mines Saint-Etienne; Université Toulouse 3 (Paul Sabatier); Stellantis France; BRGM (Bureau de recherches géologiques et minières); CEA; IFP Energies Nouvelles; Institut de Radioprotection et de Sûreté Nucléaire; Storengy; INRIA; CNRS. 2024, pp.1-11. hal-04661116

HAL Id: hal-04661116

<https://hal.science/hal-04661116v1>

Submitted on 24 Jul 2024

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ACTIVITY REPORT

CIROQUO

RESEARCH & INDUSTRY

CONSORTIUM

(2021-2024)





ACTIVITY REPORT

CIROQUO Research & Industry consortium (2021-2024)

The aim of the CIROQUO Research & Industry Consortium - Consortium Industrie Recherche pour l'Optimisation et la QUantification d'incertitude pour les données Onéreuses - was to bring together academic and technological research partners to solve problems linked to the exploitation of numerical simulators, such as code transposition (how to go from small-scale to large-scale when only small-scale simulations are feasible), taking account of uncertainties affecting simulation results, validation and calibration (how to validate and calibrate a calculation code based on collected experimental data). This project arose from a simple observation: industries using large-scale calculation codes are often confronted with similar problems when using such codes, even if their fields of application are very varied. Despite the performance of today's computing servers, the increasing complexity of simulations means that calculation times are often on the order of an hour or a day. In practice, this limits the number of available runs. This is why the development of mathematical methods to exploit industrial simulators and the data they produce is a source of progress. ■

Consortium leader



Scientific coordinators



Academic partners



Technology research partners



Experts

Scientific expert: **Mathilde Mougeot** ■ Software experts: **Pascal Havé** and **Yves Deville**

The CIROQUO Research & Industry Consortium has benefited from the experience acquired over the last thirteen years through the DICE, ReDICE and OQUAIDO Chair projects.

This project emulated the major scientific challenges of the discipline, such as code transposition/calibration/validation, modeling of complex environments and stochastic codes. In each of these scientific fields, particular attention has been paid to large-scale problems. Real-life problems sometimes involve dozens or hundreds of inputs. Methodological advances have been proposed to take account of this additional difficulty. Developments in mathematical research are distinguished from the dominant work in machine learning by the exploration of costly numerical simulations, i.e., by the need to be thrifty in terms of the quantity of data available.

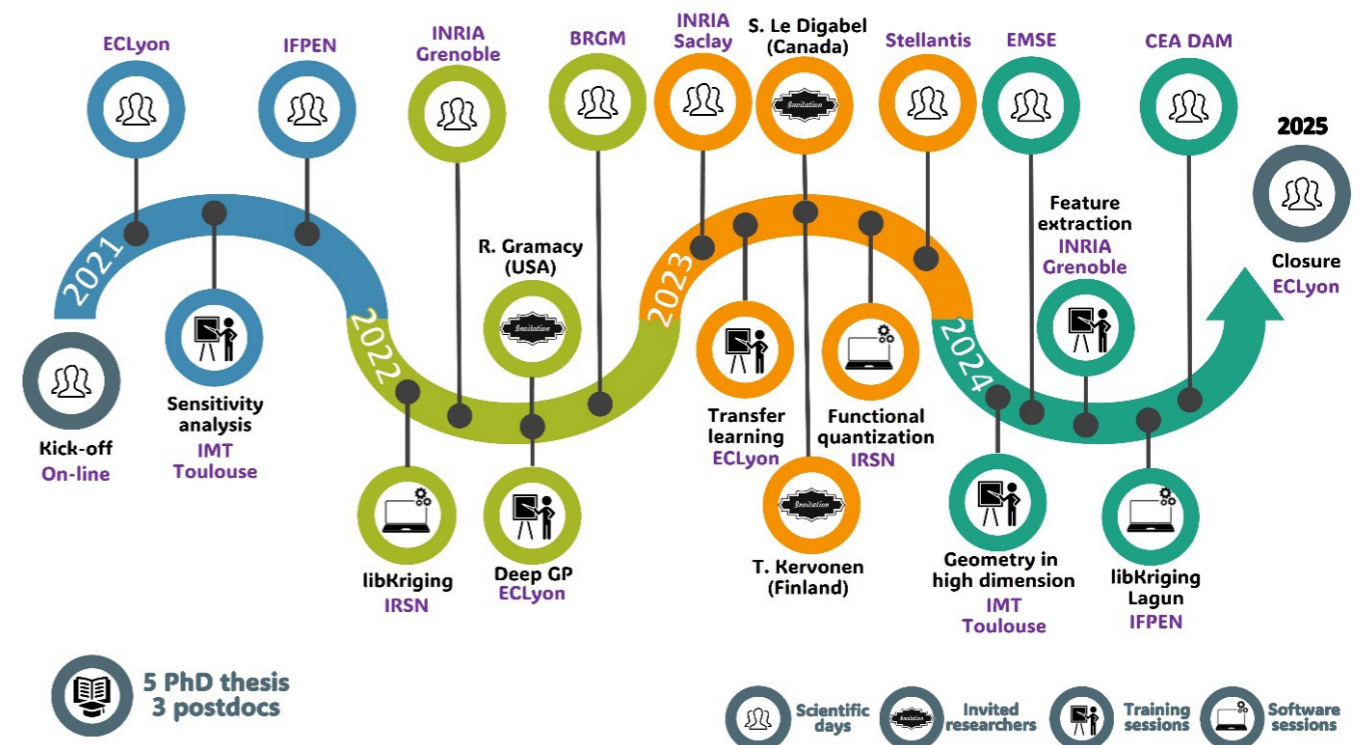
The consortium has been structured around a steering committee, whose role is to decide on the allocation of the Chair's resources, the acceptance of new members and the work planned. The committee is made up of representatives of the consortium's academic and technological research partners. ■

Website: <https://ciproquo.ec-lyon.fr/>



1 CONSORTIUM ACTIVITIES

The CIROQUO consortium organized various events throughout the project, as shown in the frieze below.



The dynamics of the project were made possible by the scientific days organized twice a year. A wide variety of exchanges have enabled ideas to be shared, and collaborations to be initiated that have opened up to related subjects. Once or twice a year, training days were organized on a specific theme, generally by the academic partners. The consortium also financed visits by foreign researchers to collaborate with project members. Each visit gave rise to a seminar open to all project members. ■



1.1 Scientific days

- **June 1, 2 and 3, 2021**, École Centrale de Lyon (Ecully)
- **November 18 and 19, 2021**, IFPEN (Rueil-Malmaison)
- **May 23, 24 and 25, 2022**, Inria Grenoble
- **November 16 and 17, 2022**, BRGM (Orléans)
- **May 23, 24 and 25, 2023**, Inria Saclay
- **November 23 and 24, 2023**, Stellantis (Poissy)
- **May 14, 15 and 16, 2024**, École des Mines de Saint-Étienne (France)
- **November 14 and 15, 2024**, CEA DAM (Bruyères-le-Châtel)
- **May 26, 27 and 28, 2025**, Ciroquo closing workshop, Valpré (Ecully)

1.2 Training sessions

- **July 1, 2021**, IMT (Toulouse), Sensitivity analysis by Agnès Lagnoux, Olivier Roustant and Clémentine Prieur
- **April 7, 2022**, IRSN, Libkriging by Yann Richet and Pascal Havé
- **June 21, 2022**, ICJ (Lyon), Deep GP by Robert Gramacy
- **June 20, 2023**, ICJ (Lyon), Transfert learning by Antoine De Mathelin and Mathilde Mougeot
- **September 21, 2023**, IRSN, Functional quantification by Charlie Sire
- **January 25-26, 2024**, IMT (Toulouse), High-dimensional geometry by Francesco Costantino and Fabrice Gamboa
- **July 3, 2024**, Inria Grenoble, Feature extraction by Olivier Zahm, Clémentine Prieur and Romain Verdière

1.3 Invited foreign researchers

- **June, 2022**, Inria Grenoble, Invitation of **Robert Gramacy** (Virginia Polytechnic and State University).
The visit of R. Gramacy was motivated by the training session on Deep Gaussian processes for CIROQUO members. At Inria Sophia Antipolis, the visit started a study on the problem of optimal training set size for local Gaussian processes. These are particularly suited when the function to model is non-stationary.
- **June, 2023**, CNRS Nice and IMT Toulouse, Invitation of **Toni Karvonen** (Department of Mathematics and Statistics at the University of Helsinki, Finland).

Toni Karvonen visited the I3S laboratory from May 28 to June 10, 2023. He gave a seminar at the laboratory entitled «Gaussian kernel: Convergence rates and implications for Gaussian process interpolation». His work at the laboratory, in collaboration with Luc Pronzato and Anatoly Zhigjvsky (Cardiff University, a visitor to the laboratory over the same period) focused on questions linked to the membership of polynomial functions to the RKHS or to the space of potentials associated with a given kernel.

Toni Karvonen continued his stay in France with a visit to IMT, with the authors of [12] on kernel quadrature in Sobolev spaces.

- **July, 2023**, Inria Saclay and IFPEN, Invitation of **Sébastien Le Digabel** (Polytechnique Montréal, Department of Mathematical and Industrial Engineering).

Sébastien Le Digabel (Polytechnique Montréal, GERAD lab) visited the Randopt team (Inria Saclay) from June 28 till June 30, 2023. During his stay, Sébastien worked with the group's team members on various topics in the context of blackbox (or derivative-free) optimization. He gave a talk entitled «Blackbox optimization: algorithms and applications» at Inria and Ecole Polytechnique. He also hosted a one-day training session on blackbox optimization methods and on NOMAD software at IFPEN.

- **October, 2024**, Ecole des Mines de Saint-Etienne, Invitation of **Enkeledj Harshrova** (Université de Lausanne, Suisse). E. Harshrova is a recognized expert in the extremes of multi-valued random fields.
- **October, 2024**, INRIA Grenoble, Invitation of **Matthieu Dolbeault** (RWTH Aachen, Germany). M. Dolbeault works on approximation of functions, random sampling, optimal recovery, reduced order modeling, high-dimensional approximation of PDEs and inverse problems.



2 SCIENTIFIC RESULTS

The CIROQUO consortium's scientific program focused on the following four areas:

- **work package 1:** Code calibration, validation and transposition
- **work package 2:** Metamodeling of codes in complex environments
- **work package 3:** Optimization and inversion in the presence of uncertainties
- **work package 4:** High dimensionality

In addition, part of the consortium's activity focused on software development and the link with machine learning.

The theses funded by the consortium are as follows:

- **Charlie Sire**, Sept. 2020-Nov 2023, supervised by **R. Le Riche** (EMSE), **D. Ruillière** (EMSE), **Y. Richet** (IRSN), **J. Rohmer** (BRGM), **L. Pheulpin** (IRSN). Title: Robust inversion under uncertainty for risk analysis - application to the failure of defences against flooding.
- **Noé Fellmann**, dec. 2021-, supervised by **C. Helbert** (ECL), **C. Blanchet-Scalliet** (ECL), **A. Spagnol** (IFPEN), **D. Sinoquet** (IFPEN). Title: Sensitivity analysis for optimization problems under uncertainties.
- **Adama Barry**, Jan. 2022-, supervised by **F. Bachoc** (IMT), **C. Prieur** (Inria Grenoble, UGA), **M. Munoz Zuniga** (IFPEN). Title: Design of experiments for calibration.
- **Mohamed Gharafi**, Jan. 2022-, supervised by **R. le Riche** (EMSE), **D. Brockhoff** (Inria Saclay), **F. Huguet** (Storengy). Title: Stochastic and surrogate-assisted multi-objective optimization.
- **Tanguy Appriou**, Jan. 2022-, supervised by **D. Rullière** (EMSE), **D. Gaudrie** (Stellantis). Title: Bayesian optimization in high dimension.

Three post-doctoral contracts have also been funded by the project:

- **Valentin BREAZ** (Inria Grenoble), Jan. 2023-April 2024, Dimension reduction for wind turbine reliability analysis.
- **Chifaa DAHIK** (IMT Toulouse), Oct. 2022-Sept 2023, Metamodeling on non-Euclidean spaces.
- **Charlie Sire** (INRIA Saclay), Dec. 2023-Nov 2024, Calibration and transposition.



PhD: design of experiments for code calibration

Context

Numerical simulators play a key role in the study and understanding of physical phenomena or systems. They generally depend on parameters that need to be calibrated using physical observations and numerical evaluations before they can play their role. This calibration procedure thus requires the selection of a certain number of physical and numerical experimental design points.

The aim of Adama Barry's thesis is to propose a statistical methodology for the selection of physical and numerical experimental designs dedicated to the calibration of expensive computational codes.

Results

- Introduction of a hybrid methodology including three new criteria for the selection of optimal physical experimental designs, and three new criteria for the sequential selection of numerical experimental designs.
- Development of an optimization algorithm combining simulated annealing and a greedy algorithm.
- Comparison results with state of art.

Publications

- **A. Barry, F. Bachoc, S. Bouquet, M. Munoz Zuniga and C. Prieur (2024)**, Optimal Design of Physical and Numerical Experiments for Computer Code Calibration, in submission <https://inria.hal.science/hal-04615127>

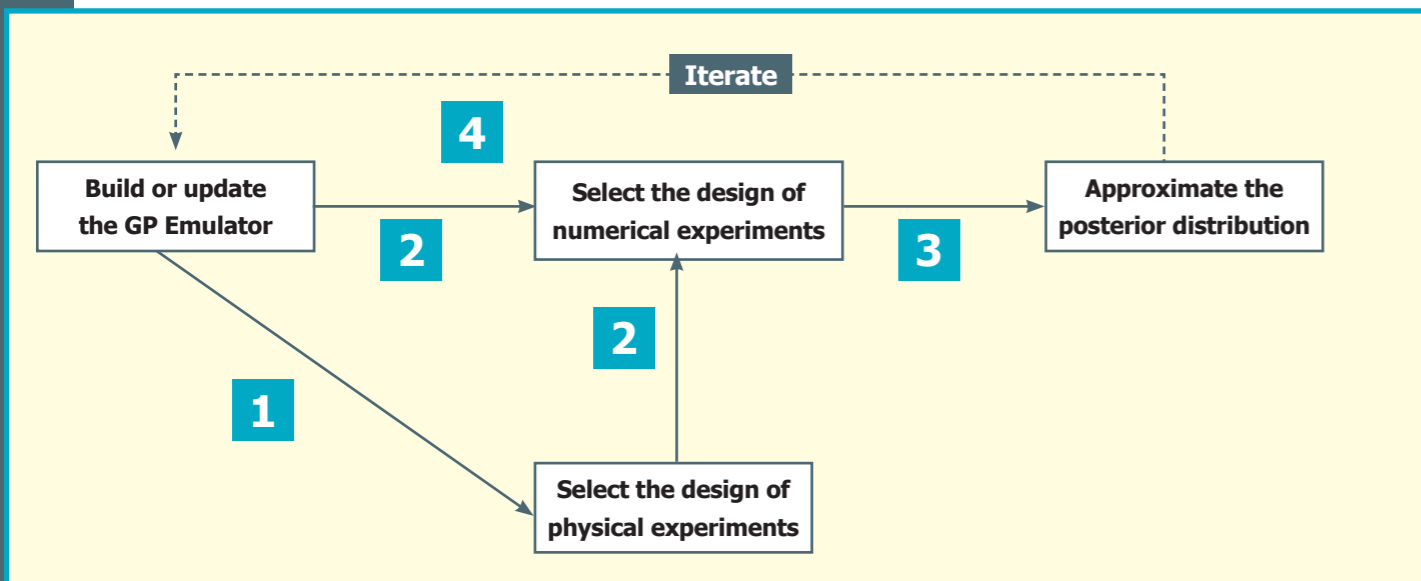


Figure: schematic representation of the proposed hybrid approach for calibration. The process begins by building an initial emulator from a first batch of numerical experiments. After the physical experiments have been selected, they are used in combination with the emulator to enrich the design numerical experiments. The updated version of the emulator is then used to approximate the posterior distribution and estimate calibration parameters. These steps can also be carried out sequentially.



Post-doc: calibration and transposition

Context

Industrial studies often rely on numerical simulation codes, that can be seen as black boxes to model complex phenomena. These codes, generally very costly, depend on parameters that must be calibrated to best match the physical measurements. This calibration is complex, especially when a model error must be considered to correspond to physical reality. The structure of the model error is a major question, and strategies like the one proposed by Kennedy and A. O'Hagan (2001) cannot be directly applied in transposition contexts. Transposition can correspond, for example, to a situation of unmeasured output. More precisely:

- The variable of interest is $y(x) = (y_t(x))_{t=1}^2$
- The numerical code is $f(x, \lambda) = (f_t(x, \lambda))_{t=1}^2$ with $\lambda = (\lambda_i)_{i=1}^p$ the variables to calibrate.
- We get measures at $(x_j)_{j=1}^n : y_{1,obs} = (y_1(x_j) + \varepsilon_j)_{j=1}^n$, with ε_j the measurement error.
- We want to predict $y_2(x_0)$ at x_0 .

Here, the transposition comes from the fact that the output y_2 is not the one measured. The objective is therefore to carry out a Bayesian approach with model error.

Method

In our study, we consider a model error embedded in the parameters to calibrate. Here, this embedding is considered by integrating additional parameters $(\lambda_i)_{i=p+1}^q$ to the code, with a hierarchical description of the prior distribution of Λ with hyperparameters α , especially for $(\lambda_i)_{i=p+1}^q$. Then we have $y_t(x) = f_t(x, \Lambda)$ with Λ a random vector in \mathbb{R}^q , with density $p_\Lambda(\Lambda | \alpha)$ with hyperparameters α in \mathbb{R}^r .

The test case, provided by CEA DAM and developed by Rémi Chauvin, models the impact of a cylinder with length l_0 , radius r_0 launched at velocity v_0 against a rigid wall. The code has 3 outputs: the length difference $l_f - l_0$, the final radius r_f and the deformation ε_{max} .

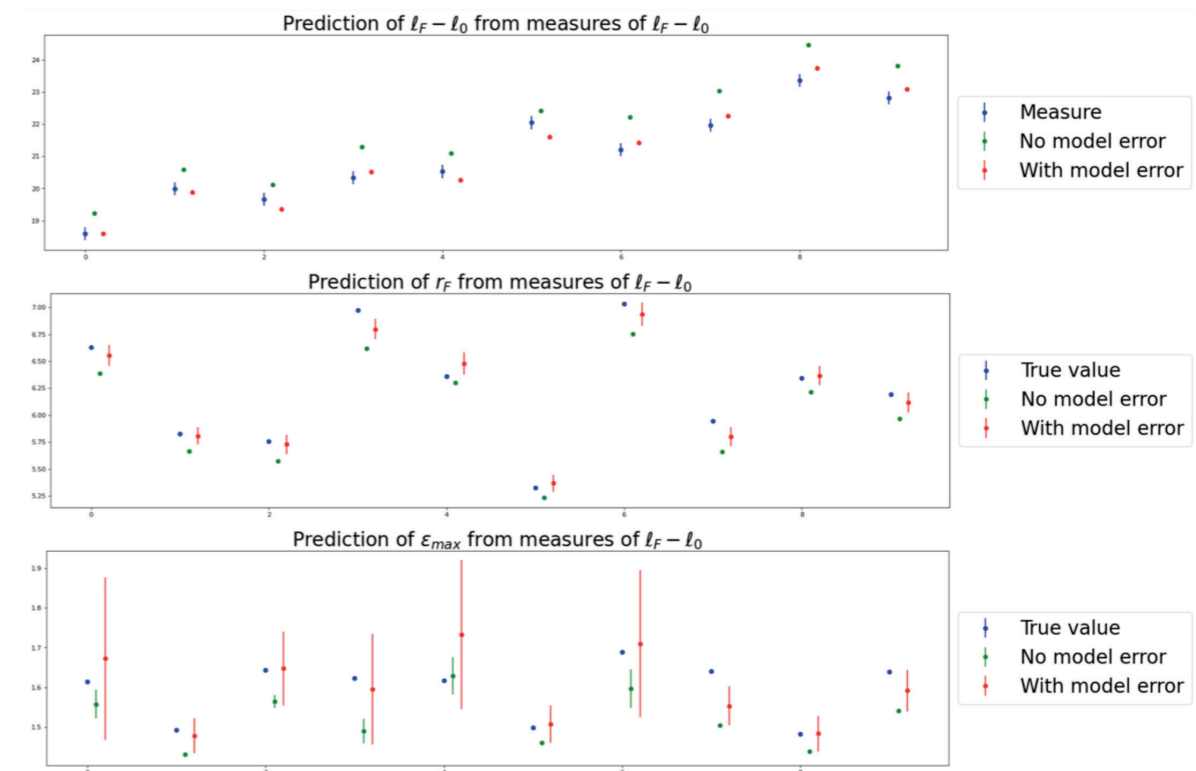


Figure 1: calibration and transposition with and without model error.



WORK PACKAGE 2

Post-doc: dimension reduction for wind turbine reliability analysis

Context

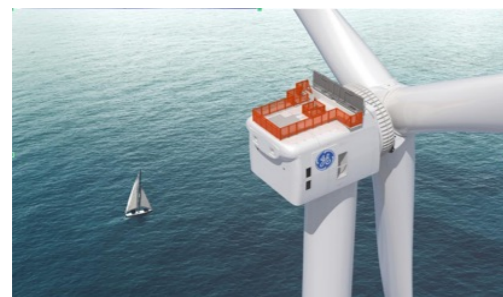
This project aims to assess the reliability of a wind turbine (WT) subject to extreme environmental conditions within a year, focusing on estimating its failure probability. Utilizing a 3D wind generator and WT numerical model, it addresses industrial challenges linked to the H2020-HIPERWIND project, which seeks to develop an efficient reliability computation framework. The objective is to improve state-of-the-art methods for rare event probability estimation in high-dimensions by (1) reducing the simulation costs through (local) metamodels based on Gaussian Processes (Kriging), and (2) by exploring innovative dimension reduction techniques to meet the computational constraints while ensuring precise reliability estimates.

Results

- **Theory:** certified high-dimensional reliability estimation via a goal-oriented version of active subspace dimension reduction method.
- **Methodology:** new gradient-free dimension reduction method, which we further adapt for reliability estimation. We obtain state of the art results on competitive benchmarks.
- **Algorithm:** iterative algorithm to gradually improve both high-dimensional Kriging and gradient-free dimension reduction for reliability. Our algorithm is motivated by practical considerations and computational constraints (expensive black-box model).
- **Application:** extensive tests for reliability analysis on different realistic toy cases (WT surrogate model mNARX, 2D truss model) and on the industrial simulator OpenFAST.

Publications

- **V. Breaz, M. Munoz Zuniga, O. Zahm.** Literature review on rare event probability estimation in high dimension <hal-04564739>
- **V. Breaz, M. Munoz Zuniga, O. Zahm.** Rare event probability estimation and dimension reduction via sequential surrogate-assisted active subspaces (submitted soon)



Rare event estimation for the 2D truss model				
Method	Cost	Rel. bias	CoV	RMSE
CE+seqSAAS	1760 [±] 675	0.008	0.14	0.14
SIS	25000 [±] 1000	0.030	1.10	1.05
ASSIS	400[±]50	0.300	0.15	0.20

Left: offshore wind turbine;

Right: our proposed reliability method (Cross-entropy plus sequential surrogate-assisted active subspaces / CE+seqSAAS) outperforms in terms of accuracy two state of the art reliability methods in high-dimensions (Sequential Importance Sampling / SIS, and Active Subspace SIS / ASSIS) on a benchmark 10D reliability problem (2D truss structure with 23 bars).

Post-doc: metamodeling on non-Euclidean spaces

Context

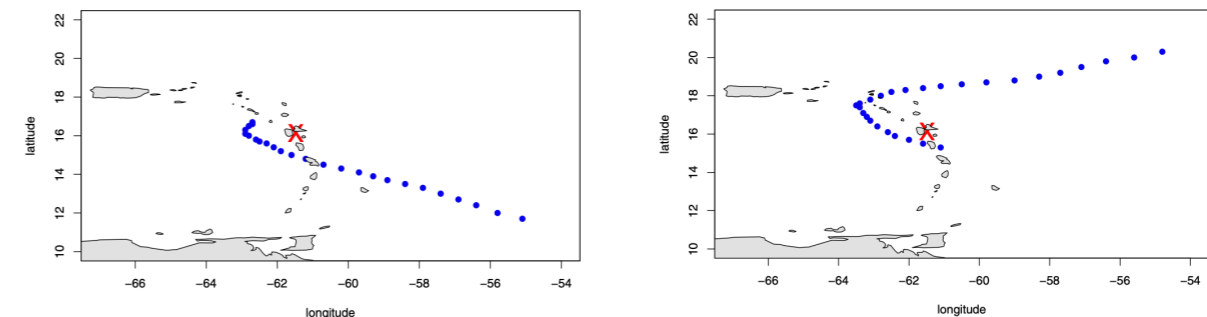
The analysis of large numerical simulators requires the construction of a simplified model, called a metamodel. In this post-doc, we wish to extend the application of Gaussian process type metamodels, often used in this context, to the case where the simulator inputs are graphs. An application example is provided by the BRGM, where the aim is to predict marine submersion caused by a cyclone based on physical features and the shape of the trajectory. This last variable can be modeled by a graph, whose vertices are the points of the trajectory, and the edges and weights are defined from the neighbors and the features of the cyclone.

Results

- Construction of a new class of kernels on graphs, carried out from the Laplacian of graphs, physical features and kernels on positive semi-definite matrices.
- Implementation on the "cyclones" test case. The use of a non-Euclidean metamodel here improves the robustness of the prediction with respect to the choice of the design of experiments.
- Implementation on a molecule classification problem. The new kernel is competitive with other approaches in the literature, with lower computational cost.

Deliverables

- A technical report and oral presentation materials.
- Software implementations (R and Python) allowing to reproduce the results.



Examples of cyclone trajectories around the Guadeloupe island, measured every 3 hours (blue dots). At each time step, the location and physical features (wind speed, radius from the eye of the cyclone) are available. The aim is to predict the water height at the location indicated by the red cross.



PhD: robust inversion under uncertainty for risk analysis - application to coastal flood risk

Context

Probabilistic studies of flood risk are essential for assessing the potential impact on vulnerable areas, particularly in the presence of industrial facilities, and especially nuclear ones. These studies are complex, requiring numerous iterations with computationally time-consuming hydraulic simulators, while managing low probabilities of occurrence. Communicating probabilistic results to a non-specialist audience is also a challenge. This work proposes quantification methods to represent the continuous probability distributions involved, with the aim of facilitating the estimation of flood risk and its causes.

Results

First, a visualization method is proposed. It relies on functional quantization and spatial output metamodeling methods to identify a restricted set of prototype flood maps. The R package FunQuant has been developed in parallel to facilitate the reproduction of this work on other applications.

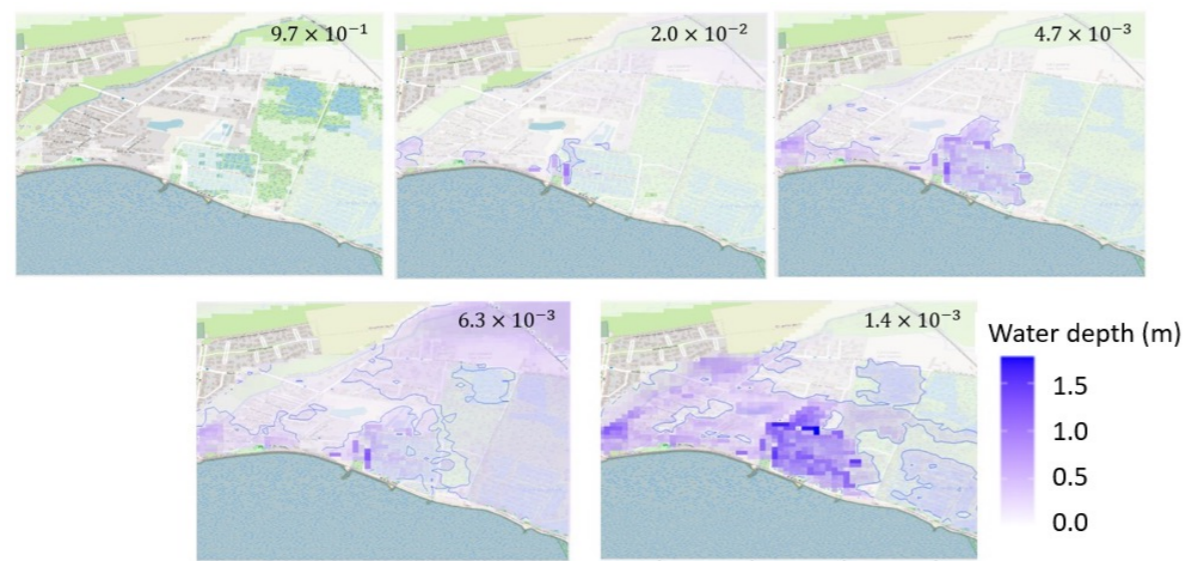


Figure 1: Prototype maps and their probabilities for the Boucholeurs case

Next, the Augmented Quantization method is presented, in order to propose mixture models that can integrate various distributions, including Dirac or uniform measurements. This approach, based on a reformulation of the classical quantization problem using the Wasserstein distance, is applied in particular to the study of the influence of input variables on a specific flood regime. Two application cases are considered: a river case involving the Loire, and a coastal case involving the Boucholeurs, located on the French Atlantic coast.

Publications

- **Charlie Sire, Rodolphe Le Riche, Didier Rullière, Jérémy Rohmer, Lucie Pheulpin and Yann Richet.** Quantizing rare random maps: application to flooding visualization, 2023. Journal of Computation and Graphical Statistics. <https://doi.org/10.1080/10618600.2023.2203764>
- **Jérémy Rohmer, Charlie Sire, Sophie Lecacheux, Deborah Idier and Rodrigo Pedreras.** Improved metamodels for predicting high-dimensional outputs by accounting for the dependence structure of the latent variables: application to marine flooding. Stoch Environ Res Risk Assess 37, 2919–2941 (2023). <https://doi.org/10.1007/s00477-023-02426-z>

PhD: sensitivity analysis for optimization problems under uncertainty

Context

The design of a complex system is frequently obtained as the solution of a constrained optimization problem. This can prove non-trivial in the presence of many design parameters and when the system response and the set of admissible solutions are affected by numerous uncertainties (such as meteorological variables, wind speed or direction to be considered for an offshore wind turbine, for example).

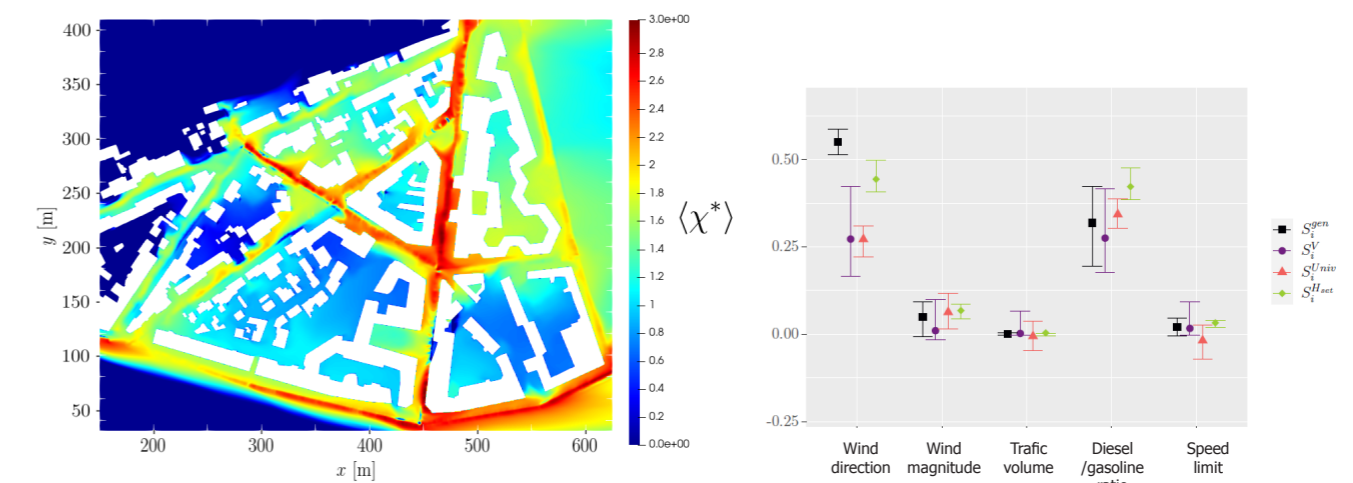
Noé Fellmann’s PhD thesis (“Goal-oriented sensitivity analysis for optimization problems under uncertainty”) aims to propose methods for characterizing the influence of uncertain variables in order to reduce the dimension of the optimization problem.

Results

- Development of three sensitivity analysis methods for models whose outputs are sets. Application to the quantification of uncertainties on sets of feasible solutions of type $\Gamma_U = \{x \in \mathcal{X}, g(x, U) \leq 0\}$ with x design parameters and U uncertain variables.
- Development of a constrained Bayesian optimization methodology, exploiting previous dimension reduction techniques, and parsimonious in the number of calls to the numerical model.

Publications

- **N. Fellmann, C. Blanchet-Scalliet, C. Helbert, A. Spagnol and D. Sinoquet.** Kernel-based sensitivity analysis for (excursion) sets, accepted for publication in Technometrics, 2024 (hal-04094561v3)
- **N. Fellmann, M. Pasquier, C. Blanchet-Scalliet, C. Helbert, A. Spagnol and D. Sinoquet.** Sensitivity analysis for sets: application to pollutant concentration maps. 2023 (hal-04312097)



Application of global sensitivity analysis to pollutant concentration maps. Left: example of a pollutant concentration map. Right: sensitivity indices obtained for 5 uncertain variables related to vehicle traffic and wind conditions (Black: aggregated Sobol indices, other colors: 3 proposed indices).



PhD: stochastic and metamodeling-assisted multi-objective optimization

Context

Storengy offers gas storage services in underground facilities such as salt caverns, aquifers, and depleted fields. To ensure safe and efficient operation, the company has developed models and simulators. However, to guarantee the reliability of these models, they must be calibrated through multi-objective optimization, aiming to minimize the error between predicted and actual data. This task is complex due to the black-box nature of the models and the high cost of solution evaluations.

Following a previous thesis, a multi-objective optimization framework called Sofomore was proposed. It uses several single-objective algorithms to optimize a scalar function named «uncrowded hypervolume improvement» (UHVI). This approach allows for the dynamic management of trade-offs between different objectives, thus obtaining an approximation of p-points uniformly distributed on the Pareto front. COMO-CMA-ES, an instance of this framework, uses the single-objective CMA-ES algorithm.

The objective of Mohamed Gharafi's thesis is to extend this algorithm to expensive problems by substituting some of the costly function evaluations with less expensive evaluations on a surrogate model.

Results

We developed a variant of COMO-CMA-ES assisted by a linear-quadratic model. A comparative study on the COCO platform shows that this new approach accelerates convergence by 25% to 300% compared to the basic version of COMO-CMA-ES.

We also developed a surrogate assisted variant of CMA-ES, which preserves invariance with respect to a monotonic transformation of the objective function. This variant uses a linear-quadratic model to learn the ranks of solutions rather than their values. The proposed method is not limited to the linear-quadratic model and offers significant potential for improvement through the learning of a rank transformation adapted to the surrogate method used.

Publications

- Benchmarking of Two Implementations of CMA-ES with Diagonal De-coding on the bboB Test Suite, GECCO 2022 Companion - The Genetic and Evolutionary Computation Conference, Boston, United States (hal-03671431)
- Multiobjective optimization with a quadratic surrogate-assisted CMA-ES, GECCO 2023 - Genetic and Evolutionary Computation Conference, Lisbon, Portugal (hal-04078483)



PhD: bayesian optimization in high dimension

Context

Many engineering systems depend on parameters whose optimization can improve the performances. However, in practice, the number of design parameters, or dimension of the problem, is often large making their simultaneous optimization difficult. Moreover, the performances of such systems being obtained through costly numerical simulations, it is necessary to use surrogate models whose construction and optimization is also particularly difficult in high dimension.

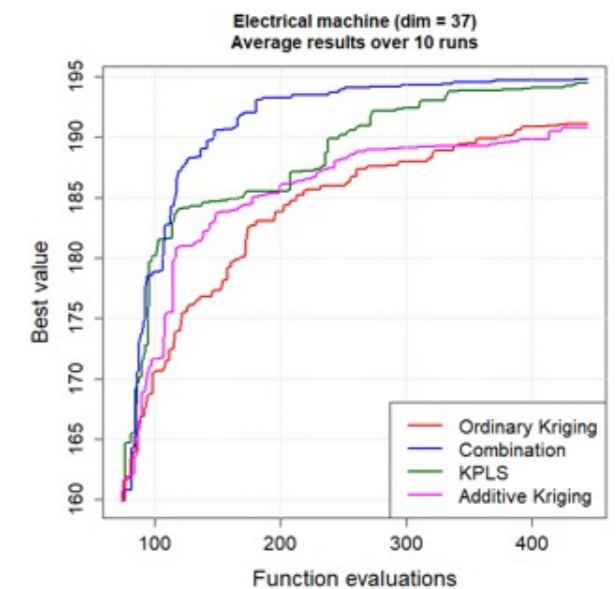
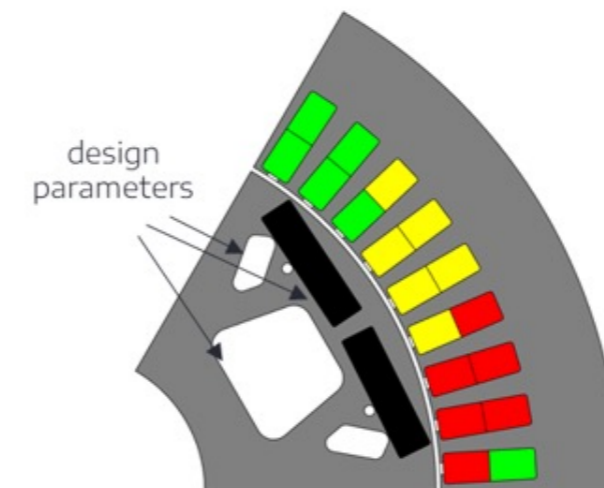
Tanguy Appriou's PhD thesis ("Optimization methods for dimensioning highly parametrized systems") aims at proposing surrogate-based optimization methods adapted to high-dimensional problems.

Results

- Development of a method adapted to high dimensions to construct surrogate models with a limited number of training samples. Comparison of the performances in terms of prediction quality and in terms of precision of the confidence intervals compared to standard methods, on artificial and real-world test problems.
- Implementation of the models developed inside a Bayesian optimization procedure for high-dimensional problems, where the number of calls to the numerical model is limited. Comparison of the performances on a benchmark.
- Industrial application: design optimization of an e-machine. The developed algorithm found better performing solutions while reducing the lead time.

Publications

- Appriou, T., Rullière, D. and Gaudrie, D., 2023. Combination of optimization-free kriging models for high-dimensional problems. Computational Statistics, pp.1-23. (hal-03812073)
- Appriou, T., Rullière, D. and Gaudrie, D., 2024. High-dimensional Bayesian Optimization with a Combination of Kriging models. (hal-04477236)



SOFTWARE

All the software developed in the context of the CIROQUO project is open-source and available online (<https://github.com/CIROQUO>), distributed under OSS licenses, which allows free use, modification and distribution, provided that the original copyright notice and disclaimer are included.

libKriging: C++ library for Gaussian Process Regression

From the early 2000s, some kriging/GPR libraries were developed in R language, to support applications in the field of computer experiments covered by previous CIROQUO instances: Dice, ReDice and OQUAIDO projects. The most famous DiceKriging and DiceOptim package, are still often used and referenced by researchers ("DiceKriging, DiceOptim: Two R Packages for the Analysis of Computer Experiments [...]” *Journal of Statistical Software*, 51(1), 1–55. <https://doi.org/10.18637/jss.v051.i01>).

However, these packages do not match newer technological challenges and lack flexibility to address some scientific targets. The libKriging library was designed to fulfill these needs, with a language-agnostic approach, and a focus on performance and documentation:

- a C++ core library, wrapped in R (<https://cran.r-project.org/package=rilibkriging>), Python (<https://pypi.org/project/pylibkriging/>) and Matlab/Octave languages, that covers the main functionalities of DiceKriging,
- a focus on performance, with parallel and fine-tuning linear algebra and optimization,
- an extensive documentation (<https://libkriging.readthedocs.io>), with a consistency between mathematical formulation and code implementation (Armadillo readable syntax).

The libKriging library is available on GitHub (<https://github.com/libKriging/libKriging>) and may be tested online in [R notebook](#) or [Python notebook](#).

[JSS2012] Roustant, O., Ginsbourger, D., & Deville, Y. (2012). DiceKriging, DiceOptim: Two R Packages for the Analysis of Computer Experiments by Kriging-Based Metamodeling and Optimization. *Journal of Statistical Software*, 51(1), 1–55. <https://doi.org/10.18637/jss.v051.i01>

Dolka: transitional R package for DiceKriging/DicOptim/KrigInv

[dolka](#) is a transitional R package aimed at helping to use rilibkriging as an alternative to DiceKriging when doing Bayesian optimization with DiceOptim or when performing kriging inversion with KrigInv. It provides a compatibility layer to use rilibkriging as a drop-in replacement for DiceKriging, DiceOptim and KrigInv for R users.

FunQuant: R package to perform quantization in the context of rare events and time-consuming simulations

FunQuant is a R package that has been specifically developed for carrying out quantization in the context of rare events. While several packages facilitate straightforward implementations of the Lloyd’s algorithm, they lack the specific specification of any probabilistic factors, treating all data points equally in terms of weighting. Conversely, FunQuant considers probabilistic weights based on the Importance Sampling formulation to handle the problem of rare event (<https://github.com/charliesire/FunQuant>). A straightforward online demo is available at https://colab.research.google.com/github/charliesire/FunQuant/blob/main/short_example_1D.ipynb.

3 PUBLICATIONS

- A. F. López-Lopera, F. Bachoc, and O. Roustant.** High-dimensional Additive Gaussian Processes under Monotonicity Constraints. In A. H. Oh, A. Agarwal, D. Belgrave, and K. Cho, editors, *Advances in Neural Information Processing Systems*, 2022. [[http](#)]
- M. Gharafi, N. Hansen, D. Brockhoff, and R. Le Riche.** Benchmarking of Two Implementations of CMA-ES with Diagonal Decoding on the bboB Test Suite. In *GECCO 2022 Companion - The Genetic and Evolutionary Computation Conference*, Boston, United States, July 2022. GECCO. [[DOI](#) | [http](#)]
- C. Sire, R. L. Riche, D. Rullière, J. Rohmer, L. Pheulpin, and Y. Richet.** Quantizing rare random maps: application to flooding visualization. *Journal of Computational and Graphical Statistics*, 0(ja):1–31, 2023. [[DOI](#) | [arXiv](#) | [http](#)]
- M. Gharafi, N. Hansen, D. Brockhoff, and R. Le Riche.** Multiobjective Optimization with a Quadratic Surrogate-Assisted CMA-ES. In *Proceedings of the Genetic and Evolutionary Computation Conference, GECCO '23*, page 652–660, New York, NY, USA, 2023. Association for *Computing Machinery*. [[DOI](#) | [http](#)]
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- M. Gharafi, N. Hansen, D. Brockhoff, and R. Le Riche.** Multiobjective optimization with a quadratic surrogate-assisted CMA-ES. In *GECCO 2023 - Genetic and Evolutionary Computation Conference*, Lisbon, Portugal, July 2023. GECCO. [[DOI](#) | [http](#) | [.pdf](#)]
- J. Rohmer, C. Sire, S. Lecacheux, D. Idier, and R. Pedreros.** Improved metamodels for predicting high-dimensional outputs by accounting for the dependence structure of the latent variables: application to marine flooding. *Stochastic Environmental Research and Risk Assessment*, 37(8):2919–2941, Aug. 2023. [[DOI](#) | [http](#)]
- C. Sire, Y. Richet, R. Le Riche, D. Rullière, J. Rohmer, and L. Pheulpin.** FunQuant: A R package to perform quantization in the context of rare events and time-consuming simulations. 7 pages, 4 figures. Submitted to *Journal Of Open Source Software*, Aug. 2023. [[http](#)]
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- O. Roustant, N. Lüthen, and F. Gamboa.** Spectral decomposition of $H_1(\mu)$ and Poincaré inequality on a compact interval — Application to kernel quadrature. *Journal of Approximation Theory*, 301:106041, 2024. [[DOI](#) | [http](#)]
- N. Fellmann, C. Blanchet-Scalliet, C. Helbert, A. Spagnol, and D. Sinoquet.** Kernel-based Sensitivity Analysis for (excursion) sets. *Technometrics*, 0(ja):1–21, 2024. [[DOI](#) | [http](#)]
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