Optimization of a computationally expensive simulator with quantitative and qualitative inputs

Research topic

Researchers from the CEA-LETI Optics and Photonics Department (DOPT) are developing photonic devices (sensors, imagers, photonic integrated circuits, etc.). The design of these high-tech objects involves many variables in terms of physical properties of materials and of geometry. As a result, numerical optimization is increasingly used. This allows to reach the objectives set out in the specifications more quickly. However the modeling of these micro-components is done through expensive numerical simulations (e.g. finite element method or finite differences in the time domain) which cannot be directly incorporated into the numerical optimization process as soon as the number of parameters exceeds a few units.

The use of metamodeling [1] allows in some instances to alleviate this difficulty: considering a reduced number of high-fidelity calculations (corresponding to a carefully selected parameter space sampling), the metamodel evaluates the system response for other parameter sets. Thus the metamodel can be used for optimization after a learning and building phase. It is much faster than the initial model while being accurate enough.

The methods currently developed in the laboratory help to identify the optimal values of quantitative parameters (width of a light guide, injected current, etc.). However they are not adapted to some commonly encountered problems in our field which also include qualitative variables (number of layers in a stack, material A or B in a part of the component, etc.).

The aim of this thesis is therefore to propose new metamodeling [2] and optimization methods valid for mixed problems, i.e. problems involving simultaneously qualitative and quantitative variables. In particular the study will focus on transposition of adaptive strategies [3] which progressively improve the metamodel during the search for the optimum.

In addition, two related issues of multifidelity and calibration will be addressed:

- the multifidelity approach is useful when the same physical phenomenon can be analyzed with several models more or less accurate and expensive. Usually a metamodel of the difference between the responses of the two simulators is built [4]. Instead, the integration of the different simulators within one unique qualitative variable with several levels will be investigated.

- during the calibration, it is crucial to identify the simulator parameters such that the output values approach at best the real experiments, taking into account their uncertainties. To the best of our knowledge, calibration in the context of qualitative variables has hardly been studied.

Context

This subject is proposed within the framework of a partnership between CEA-LETI and the OQUAIDO Chair in Applied Mathematics.

CEA-LETI is one of the Europe's leading research centers in microelectronics. The DOPT specializes in the design, manufacture and characterization of optical and optoelectronic components. DOPT researchers often use computationally expensive simulators to design these components. A metamodeling MATLAB toolbox, developed internally, allows multi-fidelity metamodeling and robust optimization.

The OQUAIDO Chair brings together, at the French national level, academic and technological research partners to solve problems related to the operation of numerical simulators, such as quantification of uncertainties, inversion and optimization.

Mines Saint-Etienne, which hosts the Chair, has carried on research at the cutting edge in these fields during the last ten years. Mixed problems are one of the scientific challenges identified by the Chair and studies have already been initiated [5].

CEA-DAM, a partner of the Chair, uses extensively numerical simulation. The laboratory of uncertainty analysis and quantification has developed an important expertise in metamodeling and calibration of expensive codes. The test case proposed to the Chair OQUAIDO by the CEA-DAM fits perfectly in the thesis' problematic and will also be one of the application.

Agenda

The work of the PhD student will initially consist of describing the state of the art in the field of metamodeling and the optimization of mixed problems. On this basis he/she will then have to conceptualize and implement the most efficient and the most suitable methods. The methods developed will be successively tested on toy cases, allowing to evaluate them objectively, then on problems representative of the laboratory needs and on the test case proposed by the CEA-DAM.

Developments can capitalize on the R packages produced by the OQUAIDO Chair, or other relevant software. They will have to be integrated into the MATLAB toolbox of metamodeling and optimization, which concentrate the expertise of the DOPT (for example by making calls from R to MATLAB).

References

[1] A. Forrester, D. A. Sobester, and A. Keane, *Engineering Design via Surrogate Modelling: A Practical Guide*. John Wiley & Sons, 2008.

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[3] D. R. Jones, M. Schonlau, and W. J. Welch, "Efficient Global Optimization of Expensive Black-Box Functions," *J. Glob. Optim.*, vol. 13, pp. 455–492, Dec. 1998.

[4] C. Durantin, J. Rouxel, J.-A. Désidéri, and A. Glière, "Multifidelity surrogate modeling based on radial basis functions," *Struct. Multidiscip. Optim.*, vol. 56, no. 5, pp. 1061–1075, Nov. 2017.

[5] O. Roustant, E. Padonou, Y. Deville, A. Clément, G. Perrin, J. Giorla and H. Wynn, "Group kernels for Gaussian process metamodels with categorical inputs," arXiv:1802.02368, 2018.

Required skills

The applicant should have in-depth knowledge in applied mathematics, especially in optimization and probabilistic modeling, and should be familiar with a scientific programming language such as R or Matlab. An interest for physics and its applications would be appreciated.

The position is based in Grenoble within the Optical Sensors Laboratory. The doctoral student will benefit from the software and calculation means available at the DOPT (simulators, computer cluster). He will also be able to spend research periods at Mines Saint-Etienne.

Keywords

Statistical Learning, Numerical Simulations, Computationally Expensive Simulation, Mixed Inputs, Multi-Physical Modeling

Contacts

Olivier Roustant (Prof., HDR) PhD supervisor Ecole des Mines de Saint-Etienne	Alain Glière (HDR) PhD deputy supervisor CEA - LETI DOPT/LCO
+33 (0)4 77 42 66 75 roustant@emse.fr	+33 (0)4 38 78 37 57 alain.gliere@cea.fr