Multi-fidelity optimization with an adaptive high order finite element fullwave solver for nanophotonics

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The optimization of complex systems, based on numerical simulations, is currently growing strongly in many scientific and technological applications. The approach consists in implementing an optimization algorithm in order to seek for the optimal value of a set of parameters **x**, by controlling a simulator estimating the value of the cost function **J(x)** for each set of parameters proposed. A major difficulty lies in the computational time required for each simulation, which can amount to several hours when high-resolution numerical models are used. Optimization must therefore take into account a highly constrained computational budget and, in practice, limited to a few dozen simulations.

In this difficult context, Bayesian optimization methods [1] have recently demonstrated their ability to provide interesting results. The approach consists in building, on the basis of some observations of the cost function, a statistical model of Gaussian Process type, which is then enriched iteratively by determining the parameters maximizing the expected improvement [2] and by simulating the corresponding configurations. In the context of metasurface design, the Acumes and Atlantis project-teams at the Inria research center of Université Côte d'Azur have recently successfully applied this approach. In particular, this approach has proven to be very flexible, and capable of taking into account uncertainties (noisy observations) [3], performing simulations in parallel or taking into account several cost functions [4].

In the perspective of relying on expensive simulations, we are interested in the present study in extending this approach to multi-fidelity optimization. The idea is to mix several estimation levels of the cost function during the optimization, to progress more quickly. Indeed, assuming that there are different methods for the estimation of the cost function, hierarchical in terms of accuracy and computational cost, the algorithm can certainly sometimes rely on less accurate, but also less expensive, estimates, if these are sufficiently correlated with the fine estimates. The objective is then to converge towards the optimum, for the finest estimate, by using as much as possible coarser estimates. This multi-fidelity optimization strategy was mainly proposed by Le Gratiet [5]. An important point of the algorithm is the selection of the level(s) of fidelity to use for each new simulation. For this, one seeks to determine which level(s) is (are) the most relevant, in terms of information provided and computational cost. An expected result of the present study is the comparison of different formulations and the proposal of new approaches for this key step.

Most of the applications produced and published in the literature are concerned ith the use of different physical models to represent the estimation levels, i.e., different partial differential equations. In this internship, we want to explore the use of multi-fidelity algorithms on the basis of different numerical approximations of the solution. Thus, we will consider a single physical model, the Maxwell equations for electromagnetics, associated with different accuracy levels in the discretization in space and time. In this perspective, we will rely on a Discontinuous Galerkin method [6] for the resolution of the system of time-domain Maxwell equations [7], developed by the Atlantis team and allowing to refine the approximation arbitrarily, by increasing the number of elements in the mesh (type h-) or the degree of the elements (type p-). A second expected result is therefore a multi-fidelity optimization algorithm automatically selecting the h- and p-

refinement levels relevant to a given problem. The target application is the inverse design of optical metasurfaces.

The work will be based either on the DiceOptim[1] R software environment or the BoTorch[2] Python software, for the Bayesian optimization part, and on the Discontinuous Galerkin method implemented in the DIOGENeS[3] software suite, including a h- and p- refinement. Software contributions may give rise to the distribution of R or Python packages implementing the algorithms developed.

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[1] https://cran.r-project.org/web/packages/DiceOptim/

[2] https://botorch.org/

[3] https://diogenes.inria.fr