Editorial: Simulation-based optimisation techniques for computationally expensive engineering design problems

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The use of computer simulations is ubiquitous in contemporary engineering design. In numerous fields, including mechanical engineering, civil engineering, electrical engineering, structural and aerospace engineering, automotive industry, oil industry, to name just a few, simulation plays a critical role not only for verification purposes, but, more importantly in the design process itself. The complexity of structures and systems have long exceeded the point where carrying out the design optimisation, such as the adjustment of the geometry and/or material parameters so that the system meets given performance requirements, was possible using explicit analytical descriptions and simple theoretical models. In most cases, it is not just the isolated device that needs to be considered but also its – sometimes complex – interactions with the environment that affect the device's performance. On the other hand, using accurate, realistic simulations allows the engineers to avoid costly prototyping and to realise the design closure with numerical models rather than through physical system measurements and prototype re-building.

High-fidelity numerical models can be very accurate but, at the same time, they are computationally expensive. Simulation times of several hours, days, or weeks are not uncommon. Even creating the model that accounts for all relevant system components may be a challenging task. One of the consequences is that a direct use of high-fidelity simulations in the optimisation loop may be prohibitive. The presence of massive computing resources is not always translated in computational speedup, which is due to a growing demand for simulation accuracy, both by including multi-physics and second-order effects, and by using finer discretisation of the structure under consideration. As conventional optimisation algorithms (e.g., gradient-based schemes with numerical derivatives) require tens, hundreds or even thousands of objective function calls per run (that depends on the number of design variables), the computational cost of the whole optimisation process may not be acceptable.

Another problem is that objective functions coming from computer simulations are often analytically intractable (i.e., discontinuous, non-differentiable, and inherently noisy). Moreover, sensitivity information is frequently unavailable, or too expensive to compute. While in some cases it is possible to obtain derivative information inexpensively through adjoint sensitivities, numerical noise is an important issue that can complicate simulation-driven design. We should also mention that adjoint-based sensitivities require detailed knowledge of and access to the simulator source code and this is something that cannot be assumed to be generally available.

In many situations, one has to deal with the presence of uncertainties. In particular, material properties and geometry of the manufactured device may differ from their nominal values as a result fabrication tolerances. Therefore, the optimisation process may seek for the robust design which ensures the highest probability of satisfying the performance requirements under the presence of uncertainties rather than just for the optimal design.

All of the aforementioned difficulties make it necessary to seek for optimisation techniques that are computationally efficient (i.e., reduce the number of CPU-intensive simulations during the optimisation run as much as possible), robust (e.g., are able to handle noisy and discontinuous objective functions), and reliable (in particular, have good convergence properties), but also simple to implement so that they can be easily acquired by engineers and designers, especially those who want to interface them with commercial simulation software.

There has been substantial research effort towards the development of techniques that are efficient in the sense explained in the previous paragraph. One example include surrogate-based optimisation (SBO) methodologies, where the direct optimisation of the computationally expensive model is replaced by an iterative process that involves the creation, optimisation and updating of a fast and analytically tractable surrogate model, both function-approximation- and physically-based. Other approaches include various derivative-free optimisation techniques, e.g., different variants of pattern search algorithm, filtering methods or meta-heuristics (e.g., genetic algorithms and particle swarm optimisers). Meta-modelling techniques are another large area of research that aim at constructing local or quasi-global response surfaces surrogate of nice properties (in particular, fast and smooth) using the sampled data from the original, high-fidelity model. A number of meta-modelling techniques have been developed including radial basis function interpolation, kriging, moving least-squares, artificial neural networks, and support vector regression. Substantial progress has been observed in the use of adjoint sensitivities, which are now more and more commonly used in various fields of engineering and science, as well as available through a growing number of commercial simulation software packages.

Despite of the progress in the development of techniques for computationally expensive engineering design problems, a number of issues remain open. This special issue of *International Journal of Mathematical Modelling and Numerical Optimisation* includes several papers covering various aspects of the field, including new algorithms, design automation, simulation-driven optimisation and modelling techniques, as well as applications in various areas of science and engineering.

The special issue opens with the paper by S. Dominique et al. which introduces a novel genetic algorithm called genetic algorithm with territorial core evolution (GATE). The algorithm is specifically designed to lessen the computational cost, i.e., reducing the number function calls, of expensive engineering design problems. The authors present the theory and details of the algorithm and apply it to a variety of test problems from the literature.

In the second paper, S. Pannier and W. Graf address the problem of fuzzy reliability-based optimisation, which is, normally, numerically expensive and involves highly non-linear responses, by using simulation-driven sequential metamodels. The authors elaborate two different approaches, namely, by reducing the dimensionality the objective function, and by adapting local metamodels. The approaches introduced can be applied for arbitrary (derivative-free) simulation techniques. The authors utilise the approaches for fuzzy reliability-based optimisation of an industry-relevant deep drawing process.

The following paper, S.A. Kyriacou et al. proposes a technique to reduce the computational cost of metamodel-assisted evolutionary algorithms (MAEAs). The technique utilises the principal-component analysis (PCA) of the non-dominated individual within each generation to efficiently drive the evolution operators. The technique is applied to the problem of multi-objective design optimisation of a matrix hydraulic turbine, where each function evaluation is based on a three-dimensional computational fluid dynamic (CFD) analysis.

The next paper, S. Koziel et al. discusses computationally efficient simulation-driven design optimisation of microwave structures. The authors consider two techniques that exploit coarse-discretisation electromagnetic models. By proper management of these models, the optimised design can be obtained as a low cost corresponding to a few evaluations of the high-fidelity model of the device of interest. In the first approach, variable-fidelity optimisation – a sequence of models of increasing resolution is utilised with the (approximate) optimum design of the coarser one being the initial guess for the finer one. The design is further refined using a suitably constructed response surface approximation model. The second technique accounts for the discrepancy between the low- and high-fidelity models by proper adjustment of the design specifications.

A metamodelling approach using direct and inverse multiquadrics radial basis functions is presented in the paper by E.R. da Silva et al. The proposed technique is based on the iterative construction of response surfaces with radial basis functions using the design points evaluated during the optimisation process, which is carried out by means of a controlled random search algorithm. The authors apply their technique on several test functions before they use it to optimise a turbomachinery blade cascade using CFD analysis.

In the following paper by M. Prieß and T. Slawig, parameter optimisation of marine ecosystem models is discussed. The optimisation process can be very expensive in terms of model and gradient evaluations, especially for complex three-dimensional models. The authors apply the aggressive space mapping algorithm to minimise the misfit between one-dimensional model output and observational data. They show that a very reasonable solution can be obtained while yielding a significant reduction in the total optimisation cost when compared to the direct model optimisation.

In the last paper, S. Hosder gives an overview of computationally efficient stochastic response surface techniques based on non-intrusive polynomial chaos (NIPC) for uncertainty quantification in numerical models. The NIPC methods have been increasingly used for uncertainty propagation in high-fidelity CFD simulations due to their non-intrusive nature and strong potential for addressing the computational efficiency and accuracy requirements associated with large-scale complex stochastic simulations. The theory and descriptions of various NIPC methods used for non-deterministic CFD simulations are presented. Several stochastic fluid dynamics examples are given to demonstrate the application and effectiveness of NIPC methods for uncertainty quantification in fluid dynamics.

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