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A solution process for simulation-based multiobjective design optimization with an application in the paper industry☆

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HIGHLIGHTS

- The challenges of simulation-based multiobjective design optimization are analyzed.
- A three-stage solution process is proposed, featuring interactive decision making.
- Demonstrated by a case study of multiobjective design optimization of a paper mill.
- Applicable to computationally intensive black-box formulations of real-life problems.

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ABSTRACT

In this paper, we address some computational challenges arising in complex simulation-based design optimization problems. High computational cost, black-box formulation and stochasticity are some of the challenges related to optimization of design problems involving the simulation of complex mathematical models. Solving becomes even more challenging in case of multiple conflicting objectives that must be optimized simultaneously. In such cases, application of multiobjective optimization methods is necessary in order to gain an understanding of which design offers the best possible trade-off. We apply a three-stage solution process to meet the challenges mentioned above. As our case study, we consider the integrated design and control problem in paper mill design where the aim is to decrease the investment cost and enhance the quality of paper on the design level and, at the same time, guarantee the smooth performance of the production system on the operational level. In the first stage of the three-stage solution process, a set of solutions involving different trade-offs is generated with a method suited for computationally expensive multiobjective optimization problems using parallel computing. Then, based on the generated solutions an approximation method is applied to create a computationally inexpensive surrogate problem for the design problem and the surrogate problem is solved in the second stage with an interactive multiobjective optimization method. This stage involves a decision maker and her/his preferences to find the most preferred solution to the surrogate problem. In the third stage, the solution best corresponding that of stage two is found for the original problem.

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1. Introduction

The widespread availability of powerful computers has made it possible to obtain detailed analyses of complex systems quickly and at a relatively low cost. Consequently, computer simulation has become a central tool in the design process across the industries. Computer simulation can be readily used to answer questions such as whether or not a system will meet specified requirements. To answer questions such as what is the maximum system performance and how the system should be designed to achieve the maximum performance, simulation must be combined with optimization. Solving an optimization problem that depends on the output of a simulation model is known as *simulation-based optimization*. In this paper, we consider computational challenges of simulation-based optimization encountered with real-life design optimization problems and relate them to a case study in the paper industry.

A computer simulation of a physical or some other system of interest typically consists of solving a system of algebraic and differential equations. From the optimization point of view, using a simulator as an external solver for a system of equations is equivalent to dividing the decision variables into two groups, the *dependent* and the *independent* variables, and substituting the dependent variables with functions of the independent ones. The choice between dependent and independent variables is often

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dictated by the simulator, which has to take the independent variables as input and provide the values of the dependent variables as output. Considering only the independent variables as decision variables reduces the dimensionality of the problem but, on the other hand, makes it a *black-box optimization* problem because the functional relationship between the independent and the dependent variables is known only implicitly. This prevents any algebraic manipulation and makes it very difficult to validate the assumptions of, for example, convexity and differentiability that many optimization methods rely on.

In a real-life design optimization problem, there is rarely a single performance measure fully appreciating the relative merits of each design. Instead, it is characteristic of a design optimization problem to have multiple, conflicting objectives. When optimization is applied, however, the optimization problem is commonly formulated with a single objective – often by considering a weighted sum of the design objectives or by treating all but one of them as constraints – because most of the optimization algorithms can handle only single-objective problems. A shortcoming of a simplistic single-objective problem formulation is that it provides little support for decision making, often requiring the parameters in the problem formulation to be adjusted by trial and error to achieve the desired outcome. The structure of a design optimization problem can often be reflected more closely by formulating it as a *multiobjective optimization* problem, in which all the objectives are to be optimized simultaneously. A multiobjective formulation comes with a cost, though, as it necessitates the involvement of a decision maker.

With an increasing complexity of design problems, finding an optimal design in real-life applications remains a challenging task [1–3]. The computational challenges in design optimization that we consider in this paper (and which we have found are the most pertinent ones) are the following.

Computational cost In simulation-based optimization, the objective and constraint functions depend on the decision variables not only directly, but also indirectly through the simulation model. Therefore, to calculate the values of those functions, a simulation must be carried out, which may well take from few minutes to several days. Moreover, the simulation must be repeated every time an optimization method needs to evaluate the objective and constraint functions. Thus, the time required for one simulation run on average, or the computational cost of the simulation, is a major factor limiting the practicability of simulation-based optimization.

Conflicting objectives Multiple, conflicting objectives give rise to a set of solutions, called the Pareto optimal set, that correspond to different trade-offs among the objectives and are not self-evidently comparable. This is in contrast to single-objective optimization, in which an optimum, if it exists, is uniquely defined. With multiple objectives, the identification of the preferred solution requires the involvement of a decision maker and sufficient methodological support to explore the alternative solutions. It is, however, challenging to implement a system that can provide a fast enough response for successful decision making when applied to computationally expensive simulation-based optimization.

Black-box models The lack of closed form expressions for the objective and constraint functions effectively requires a design optimization problem to be treated as a global optimization problem. The necessity of global optimization increases the computational cost of design optimization and limits the size of the design optimization problems that can be solved. Fortunately, it is rarely necessary to guarantee global optimality, but instead, a sufficient improvement over an existing design is acceptable.

Stochasticity In many real-life design optimization problems, the system of interest is best modeled by a stochastic process. In that case, the model output is a random vector, often with an unknown probability distribution. The model output can be sampled by a computer simulation, although the computational cost of simulating the output increases with the sample size. Moreover, unless the sample size is sufficiently large, sampling error introduces noise to the values of the objective and constraint functions that depend on some statistic of the model output.

The above challenges are intertwined in the sense that the presence of each one of them makes the others more difficult to address. For example, global optimization quickly becomes impractical if the computational cost of the design optimization problem increases. Likewise, stochasticity and conflicting objectives both aggravate the difficulties caused by a high computational cost because more computation is required to sample the model output and to assess the trade-offs, respectively.

An overview of optimization methods applied to solving multiobjective engineering problems is given in [4]. Metamodeling techniques have been found to be beneficial tools in supporting design optimization [5,6]. In multiobjective design optimization, most of the efforts have been devoted to finding a number of Pareto optimal solutions (see, e.g., [7–10]) without considering support for a decision maker. Only few applications of interactive multiobjective optimization methods to design optimization problems can be found, e.g., in [11–16]. For example, Tappeta et al. [11] have proposed an approach which differs from ours in three aspects. First, it requires constructing individual metamodels for all objective and constraint functions. Second, a local approximation of the Pareto optimal set is considered. Finally, there is no clear distinction between interaction with a decision maker and the demanding computations which would imply long waiting times in case a decision maker wishes to explore different (other than local) Pareto optimal solutions. To our knowledge, there is no off-the-shelf interactive method which could be directly applied to computationally expensive simulation-based multiobjective optimization problems without creating waiting times for a decision maker.

We present in this paper a three-stage solution process that is designed to address the challenges of computationally expensive multiobjective design optimization. A wide range of optimization algorithms can be integrated with the solution process, which makes it applicable to many real-life design optimization problems. In the first stage, termed the *pre-decision making* stage, sufficient information is gathered about the alternative solutions to the multiobjective design optimization problem. In the second stage, termed the *decision making* stage, a human decision maker is involved by using an interactive method to solve a computationally inexpensive surrogate problem constructed on the basis of the information gathered in the first stage. In the third stage, termed the *post-decision making* stage, the original design optimization problem is solved with the purpose of finding a solution that best matches the preferred solution to the surrogate problem identified in the second stage.

The three-stage solution process has the benefit that it separates the time-consuming simulation-based optimization from the decision making stage. This allows fluent interaction with the decision maker regardless of the computational intensiveness of the simulation model. The solution process is motivated by the PAINT method [17], which can be used to create a surrogate problem for decision making, as well as by the availability of multiobjective optimization methods such as ParEGO [18] and SMS-EGO [19] that provide a finite approximation to the Pareto optimal set of a multiobjective optimization problem.

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