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Procedia Computer Science 18 (2013) 855 – 860

Procedia Computer Science

International Conference on Computational Science, ICCS 2013

Computational Optimization, Modelling and Simulation: Recent Trends and Challenges

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Abstract

Modelling, simulation and optimization form an integrated part of modern design practice in engineering and industry. Tremendous progress has been observed for all three components over the last few decades. However, many challenging issues remain unresolved, and the current trends tend to use nature-inspired algorithms and surrogate-based techniques for modelling and optimization. This 4th workshop on Computational Optimization, Modelling and Simulation (COMS 2013) at ICCS 2013 will further summarize the latest developments of optimization and modelling and their applications in science, engineering and industry. In this review paper, we will analyse the recent trends in modelling and optimization, and their associated challenges. We will discuss important topics for further research, including parameter-tuning, large-scale problems, and the gaps between theory and applications.

Keywords: algorithm; black-box modelling; computational optimization; optimization algorithm; modelling; metaheursitics; nonlinear optimization; stochastic optimization; surragate-based optimization; simulation;

1. Introduction

For any design and modelling purpose, the ultimate aim is to gain sufficient insight into the system of interest so as to provide more accurate predictions and better designs. Therefore, computational optimization, modelling and simulation forms an integrated part of the modern design practice in engineering and industry. As resources are limited, to minimize the cost and energy consumption, and to maximize the performance, profits and efficiency can be crucially important in all designs [1-6]. The stringent requirements of minimizing environmental impact and carbon footprint require a paradigm shift in scientific thinking and design practice. However, real-world problems are usually far more complex than models can capture and far more nonlinear than optimization tools can handle; consequently, approximations are necessity as well as a practical possibility.

Most design optimization typically involves uncertainty in material properties and parameters. In this case, optimal design does not necessarily mean robust. In fact, we often have to settle for the robust, suboptimal design

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Selection and peer review under responsibility of the organizers of the 2013 International Conference on Computational Science
doi:10.1016/j.procs.2013.05.250

options. After all, we wish to solve our design and modelling problems with sufficiently good accuracy assuming reasonable time expenditures [1,5].

Despite the significant progress made in the last few decades, many challenging issues still remain unresolved. Challenges may be related to various aspects and depend on many intertwined factors. In the current context, such challenges are related to nonlinearity, scale of the problem, time constraint and the complexity of the system. First, many problems are highly nonlinear, and thus their objective landscapes are multimodal. Consequently, multiple optima may be present. Many traditional algorithms do not cope well with such high multimodality. This necessitates new techniques to be developed. Second, many real-world problems may be very large-scale, though most optimization methods are tested over small-scale problems. Third, by far the most important factor concerning the solution process is the time constraint. Solutions have to be obtained within a reasonably time, ideally instantaneously in many applications, which poses additional challenges. Finally, the systems we try to model are usually very complex; however, we often use over-simplified models to approximate the true systems, which can introduce many unknown factors that affect the results and validation of the models [5,6].

The fourth workshop on Computational Optimization, Modelling and Simulations (COMS 2013) at the ICCS 2013 strives to provide an opportunity to foster discussion on the latest developments in optimization and modelling with a focus on applications in science, engineering and industry. In the remaining sections of this summary paper, we briefly review the recent trends, major challenges and discuss important topics for further research. We will also briefly introduce the topics and papers in this workshop.

2. Trends and Challenges in Computational Optimization

For proper formulation of optimization problems, the design objectives and behaviors of a system have to be re-formulated in mathematical terms to define an objective function (or functions) so that the formal relationship between the values of the designable parameters and the system performance can be established. In some cases, this relationship can be represented in a form of a scalar function that can be minimized, while in many other cases, a set of competing objectives can be only formulated, leading to a complex, multi-objective optimization problem. Even if the solution sets to a multi-objective problem can be found, it can result in a decision-making process to select the best combination out of a feasible set of, usually non-commensurable, objective sets. Such selection is not trivial, depending on the utility and/or decision criteria.

The recent trends in computational optimization move away from the traditional methods to contemporary nature-inspired metaheuristic algorithms [2,7,8], though traditional methods can still be an important part of the solution techniques. However, new studies and research tend to focus on the development of novel techniques that primarily based on swarm intelligence. New algorithms such as particle swarm optimization, cuckoo search and firefly algorithm have become hugely popular. One of the reasons for such popularity is that these metaheuristic algorithms are simple and easy to implement, and yet they can solve very diverse, often highly nonlinear problems. This partly meets the need to deal with nonlinearity in a non-conventional way.

Multimodality in many design problems mean the true global optimality is not easy to reach. In fact, there is no guarantee if the global optimality can be reached in a finite number of iterations. However, there is sufficient evidence that the global optimum can be found using nature-inspired algorithms in a vast majority of the cases. There are many reasons for good success rates in searching for optimality, a main reason is that metaheuristic algorithms use stochastic components or randomization techniques to increase the ergodicity of the iterative search path.

Nature-inspired algorithms have the advantages of simplicity, flexibility, and ergodicity [2,8]. These algorithms are typically very simple to understand and easy to implement, which requires little efforts for new users to learn. Therefore, researchers with diverse backgrounds can relatively easily use them in their own research. At the same, nature-inspired are quite flexible; that is, these seemingly simple algorithms can solve highly complex, high nonlinear optimization problems. In addition, nature-inspired metaheuristic algorithms can often find the global optimum solution within a relatively small, finite number of iterations. Some algorithms such as simulated annealing and cuckoo search can have guaranteed global convergence. That means that they can find the true global solution with a practically acceptable time scale. Such high ergodicity is common for the new nature-inspired algorithms, although it is not for the traditional algorithms such as gradient-based methods (unless in the special case of convex optimization where global optimality is also guaranteed).