OBJECTIVE OF THE PROJECT

Computer-aided analysis is nowadays the most widely used and efficient tool for handling complex scientific and engineering problems. Its fundamental advantage is high accuracy of representing the system at hand as well as possibility of dynamic adjustment of the physical parameters of the model or the operating conditions without the necessity of re-constructing a virtual representation of the phenomenon or the object under analysis. Typical examples of practical application of numerical modeling is computer-aided design of complex engineering systems such as structures in civil and material engineering, aircraft wings in aerospace engineering, or wireless communication systems in microwave and antenna engineering.

Reliable modeling of physical phenomena is possible by means of complex mathematical equations, the solution of which is only possible through numerical procedures. Consequently, the use of accurate simulation models that adequately represent real-world engineering systems requires considerable computational resources, often exceeding capabilities of the standard personal computers. For example, a single simulation of a three-dimensional model of an aircraft wing requires from a few dozen to a few hundreds of gigabytes of RAM memory and takes several dozen of hours. On the other hand, analytical representation of complex physical systems using explicit formulas is merely an approximation of the reality—typically of a very limited accuracy—and it is therefore not applicable for solving realistic problems in science and engineering.

The excessive computational cost associated with accurate computer simulations is therefore a fundamental obstacle in effective automation of the design processes when realized using conventional numerical optimization procedures and algorithms. A solution to the optimization task is a set of designable parameters for which an objective function—formulated according to given design specifications—assumes its minimum. In case of problems with a single design objective, a typical optimization process requires from a few dozen or a few hundred (in case of relatively simple problems with a small number of designable parameters) to thousands of objective function evaluations (for complex problems in highly-dimensional spaces). It is worth emphasizing that real-world engineering problems require simultaneous handling of several design criteria which are usually conflicting with each other. The most popular solution approaches for multi-objective optimization include population-based metaheuristics (genetic algorithms, particle swarm optimizers), whose computational cost is typically at least an order of magnitude higher—in terms of the number of required system simulations—than for single-objective optimization. Assuming, for the sake of example, multi-criterial optimization using conventional means, the evaluation time of a simulation model to be ten hours, and ten thousands of model evaluation to converge, the entire process would exceed ten years. This indicates that conventional computer modeling and optimization methods are not sufficient for handling engineering problems that involve realistic design requirements and accurate simulation models, particularly from the point of view of design automation.

The proposed research aims at alleviating the aforementioned difficulties by means of the development of novel modeling and optimization methodologies for interdisciplinary design of complex systems. To this end, we will exploit a surrogate-based optimization (SBO) paradigm, in which the subject of the numerical optimization process is—instead of the accurate simulation model—its computationally cheap representation, which is iteratively corrected using the available (yet sparse) data from the original (expensive) model. The main tasks of the proposed project include: development of a systematic methodologies for constructing fast replacement models (both simplified physics-based ones, e.g., obtained through coarse discretization of the structure under design, as well as hybrid ones, e.g., corrected approximation models obtained using data sampled from simplified physics-based models), as well as development of efficient optimization algorithms for realistic engineering design problems of high complexity. It is expected that accomplishment of the project goals will considerably influence those areas of science and engineering that heavily rely on simulation-driven design; in particular it will significantly push forward the state of the art in the development of surrogate-based modeling and optimization techniques.

BASIC RESEARCH DESCRIPTION

The objective of the proposed research is development of efficient modeling and optimization methods with application to automated design of complex systems, involving expensive computational models.

The first stage of the project will be development of versatile an efficient algorithms for solving numerically demanding numerical problems of realistic settings and specifications. The proposed approaches will exploit surrogate-assisted principles and corrected fast replacement models. As opposed to many known surrogate-based techniques, our algorithms will feature: guaranteed convergence, low computational cost, (to some extent) immunity to inaccuracies of the underlying low-fidelity model, as well as low number of the control parameters. Termination conditions will account for the trade-off between the efficiency of the numerical optimization process and the quality of the final design obtained. Small number of control parameters will make the use of the algorithms convenient even for designers and engineers who do not have extensive experience in numerical optimization.

The second stage of the proposed research will be focused on the development of methodologies and algorithms for constructing corrected low-fidelity models for surrogate-assisted optimization. The low-fidelity model is the fundamental component of any surrogate-based optimization process. It is a computationally cheap representation of the accurate simulation model of the system under design. The efficiency of the optimization procedure depends on both the low-fidelity model accuracy and its computational cost. The proposed model construction methodologies will take these two aspects into account. Furthermore, they will contain procedures for model quality verification, as well as the mechanisms for predicting the performance of the surrogate-based optimization process based on partial information from the original (expensive) simulation model accumulated during the algorithm run, as well as techniques for selection of the low-fidelity model and its correction methods in the course of optimization. At this stage, the emphasis will be put, first of all, on simplified physics-based models constructed using available data on the system at hand (obtained, e.g., through fast simulation using coarse discretization of the structure). The model correction will utilize various types of space mapping techniques and similar methods.

The third stage of the project will be development of the methods and surrogate-based optimization algorithms exploiting hybrid replacement models (surrogates). Operation of the available surrogate-assisted optimization techniques is mostly based on the replacement models of a specific type, i.e., either physics-based or data-driven (function-approximation) ones. The major issues of either approach are limitations of the particular classes of the models. For example, low-fidelity simulation models are relatively expensive (although much faster than the high-fidelity ones). Approximation models, on the other hand, are very fast but their setup may be computationally prohibitive due to the necessity of acquiring sufficient number of training data from the original simulation model. This issue is especially pronounced for higher-dimensional design spaces. Consequently, an important goal of the project is to development of systematic procedures for construction of the hybrid replacement models, in particular approximation surrogates that utilize low-fidelity simulation data samples with subsequent correction using limited amount of high-fidelity data.
The last, yet very important part of the project will be computer implementation and validation of the modeling and optimization methods developed in the previous stages of the proposed research.

JUSTIFICATION FOR CHOOSING THE RESEARCH TOPIC

The state-of-the-art analysis indicates serious limitations of the current paradigms of solving computationally demanding problems in contemporary engineering and science. In particular, it can be observed that reliable and efficient tools (especially in terms of computational efficiency) for modeling and automated design of real-world engineering systems are still lacking. The most important and still open methodological problems can be characterized as follows:

1. Available numerical optimization techniques are not applicable for solving complex simulation-driven problems of contemporary science and engineering. On one hand, analytical descriptions are inadequate due to complexity of the systems, which calls for using accurate (but expensive) simulation models. On the other hand, conventional optimization algorithms based solely on expensive simulation models are often computationally prohibitive.
2. Existing methods, particularly global optimization techniques inspired by nature, such as population-based metaheuristics (especially in multi-objective optimization context), require large numbers of objective function evaluations (up to thousands and tens of thousands), which make them unusable for handling computer simulation models (regardless of the structure discretization density).
3. Available commercial software packages for design automation are normally equipped with only basic algorithms for direct optimization (typically gradient-based ones). This is mostly a result of the fact that many methodological issues concerning surrogate-assisted optimization are yet to be solved, including convergence issues, robustness, sensitivity to the underlying low-fidelity model quality, as well as a large number of the control parameters of the algorithms.

It should be emphasized that solving the above research problems may lead to alleviating difficulties related to handling simulation models in many areas of engineering and sciences where computer-aided modeling and optimization are of primary importance. As a matter of fact, simulation-driven design is ubiquitous in majority of disciplines. Examples include aerospace engineering (optimization of aircraft wings), hydrodynamics (optimization of underwater vehicles), climate science (ocean/climate model calibration), electrical engineering (microwave system and antenna design), to name just a few.