

A Variable-Size Local Domain Approach to Computer Model Validation in Design Optimization

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ABSTRACT

A common approach to the validation of simulation models focuses on validation throughout the entire design space. A more recent methodology validates designs as they are generated during a simulation-based optimization process. The latter method relies on validating the simulation model in a sequence of local domains. To improve its computational efficiency, this paper proposes an iterative process, where the size and shape of local domains at the current step are determined from a parametric bootstrap methodology involving maximum likelihood estimators of unknown model parameters from the previous step. Validation is carried out in the local domain at each step. The iterative process continues until the local domain does not change from iteration to iteration during the optimization process ensuring that a converged design optimum has been obtained. The proposed methodology is illustrated using a thermal, one-dimensional, linear heat conduction problem in a solid slab with heat flux boundary conditions.

1. INTRODUCTION

Design optimization often requires computational analysis or simulation models. These models quantify functional input-output relations contained in the objective and constraints. Such models are inexact approximations of the physical world, and so we need to quantify our confidence that designs obtained using simulations will perform as expected when produced. Current practice uses computational models for

optimization studies in relatively large design spaces even though the models have been validated only in a small subset of the design space. Within this paradigm, computational models need to be validated in the entire feasible design space in order to obtain high confidence in the results. Computational models are usually validated by calibrating a number of parameters the model is a function of. There is however, inherent uncertainty in both the model calibration parameters and the tests that are conducted to obtain the data to be used in the validation comparisons. For this reason, the model validation procedure can be time consuming and resource intensive.

Due to limited resources, the simulation models are usually validated only at a relatively small number of points in the design space and are then used for optimization studies in the entire design space. This approach can compromise local model accuracy in order to use a single global model which is not calibrated throughout the input space. [Li et al. \(2010\)](#) demonstrated that design optimization using a global model can yield a different and potentially worse optimal design relative to the one obtained by using a model that is calibrated when necessary as the optimization process progresses.

The motivation for the present work is that the aforementioned global model validation may not be necessary. A numerical optimization process creates a sequence of design iterates, whose validity is important only at the optimum. One way to concentrate on the validity of the

optimal design rather than that of the model is to validate the simulation model at the design iterates as they are generated during the optimization process.

In this paper, we propose a methodology for sequential, calibration-based validation of the simulation model at, and in the vicinity of, the design candidates as they are generated during the optimization process. The goal of such validation is confidence in the resulting design and all intermediate design iterates, rather than in the global performance of the underlying simulation model. A sequential optimization approach is used where the design space at each iteration is much smaller than the entire feasible space. The proposed approach utilizes available testing resources more effectively as it determines the minimum amount of tests required for validation in targeted local domains. It can be also applied to parametric studies to ensure that a design is valid for different operating conditions.

Statistical methods to computer model calibration are available in the literature ([Kennedy and O'Hagan, 2001](#); [Bayarri et al., 2007](#); [Higdon et al., 2008](#); [Drignei et al., 2008](#); [Drignei et al., 2010](#)). However, none of these works addresses the number of required test data and a sequential approach to collecting the test data as we propose in this article.

The surrogate management framework by [Booker et al. \(1999\)](#) offers a variation of the main idea presented and implemented here. [Booker et al. \(1999\)](#) generate a sequence of calibrated approximations (metamodels or surrogate models) of the objective function only, which they manage for direct surrogate optimization. They do not assess the validity of their approximations; they simply improve it by calibration during optimization. In the present work, we assess the validity of the design iterates generated by sequential optimization in subsets of the design space by validating the simulation model at these subsets and improving it only if necessary, provided testing can be performed at these points.

1.1. Background and Previous Research

Verification and validation (V&V) of simulation models has been extensively studied during the past decade from researchers, practitioners, professional societies, and government agencies (DoD; [Oberkampf and Barone, 2004](#); [Gu and Yang, 2003](#)). A National Science Foundation (NSF) panel on simulation-based engineering science ([Oden, 2006](#)), identified V&V as a core topic. It should be noted that verification is related to computing the simulation model correctly, while validation refers to computing the correct simulation model ([Roache, 1998](#)). Verification of a simulation model is an assessment of the accuracy of the solution of simulation model, compared to the mathematical model on which the simulation model is based. Verification is

typically done by comparing the solution of the simulation model to the known solution of a particular mathematical model. Verification also provides confidence levels on the accuracy of the simulation models as they are refined, relative to the validity of the underlying mathematical model.

The validation of a simulation model can be viewed as an assessment of accuracy of a simulation model to represent the physical system, in accordance with the user's intentions. This requires an appropriate, well-defined validation metric. [Oberkampf, Trucano and Hirsch \(2004\)](#) provide an excellent review of the state-of-the-art in V&V methods in computational engineering and physics. They advocate that the validation metric should consider confidence (uncertainty) levels in the computational model, the mathematical model, the tests, and the experimental and model parameters. Validation relies critically on physical test and experimental data and is most effective when validation experiments are constructed carefully to determine the agreement between the simulation model and the experimentally tested physical system, under a well-defined set of conditions.

Model validation approaches can be classified as frequentist (e.g., [Oberkampf and Barone, 2004](#); [Esterling and Berger, 2002](#)) or Bayesian (e.g., [Kennedy and O'Hagan, 2001](#); [Bayarri et al., 2002](#)). The frequentist approach assumes distributions of model calibration parameters and uses collected data on model predictions to estimate, within confidence intervals, the parameters of the assumed distributions of the model calibration parameters by means of statistical inference. The Bayesian approach assumes an initial prior of the distributions of model calibration parameters and uses observations and predictions to update the previous prior distributions. Typically, the frequentist approach requires much more data to reduce the otherwise unreasonably large confidence intervals. The Bayesian approach does not require large amount of data, and it can be used to incrementally improve distribution approximations as new data become available. For this reason, the Bayesian approach is typically preferred in engineering design.

There are only few methods that focus on model validity for design optimization purposes. The work of [Zhang and Mahadevan \(2003\)](#) initiated a large body of literature ([Mahadevan and Rebba, 2005](#); [Rebba and Mahadevan, 2006](#); [Jiang and Mahadevan, 2008a](#); [Jiang and Mahadevan, 2008b](#); [Jiang and Mahadevan, 2009](#)), which uses Bayesian hypothesis testing to accept or reject a design based on model validity. They investigated the effect of model inaccuracies on the reliability requirements of a design using Bayesian formulations to calculate the posterior probability of a design being valid or invalid. Although their approach provides a novel way for design validation, it is limited to design validation with respect to design reliability, and does not

address the use of validated simulation models in design optimization.

Gunawan and Papalambros (2006) looked into the inaccuracy of a model due to external factors and developed a design confidence metric utilizing Bayesian inference of a binomial process. They then used the metric in reliability-based optimization in order to link confidence, amount of data, and reliability requirement of a potential optimum. There are notable advantages in this approach. First, the availability of a confidence measure enables designers to perform explicit trade-offs between optimality and confidence. Second, the confidence is also directly linked with the amount of data available, and hence the cost associated with it. This can be a valuable tool for the designer conducting a certification effort. Despite these benefits, the method is limited to tackling reliability requirements.

A so-called design-driven approach to validation has been proposed by Chen et al. (2008) using test and model data sampled throughout the design domain. It introduces a statistical prediction model $\hat{Y}$ that associates the test and model data, including a bias term, and it assumes that the design objective f depends on $\hat{Y}$. Because the latter is a random variable, f is also a random variable. For a candidate design $\mathbf{x}^*$ to be declared design-valid, it must lead to an improved design objective with high confidence, when compared with the design objective of any other design candidate $\mathbf{x}$. For example, the probabilistic relation

$$P[f(\hat{Y}(\mathbf{x}^*)) < f(\hat{Y}(\mathbf{x}_i))] > 0.95, \quad \forall \mathbf{x}_i \in D, \quad \mathbf{x}_i \neq \mathbf{x}^*$$

will indicate that the design candidate $\mathbf{x}^*$ is the design-driven optimum with a 95% confidence. This is an attractive approach. However, it does not provide a metric of statistical agreement between test and model prediction at a particular design candidate. Also, it does not provide a formal measure to ensure that the number of required tests is kept at a minimum.

It should be emphasized that the methodologies of Gunawan and Papalambros (2006) and Chen et al., (2008) are global in the sense that validation is conducted in the entire design domain. In addition, the issues of minimum number of tests at a design candidate and the number of design sites, where designs are conducted, in the global domain are not addressed. We believe that these issues are essential in order to reduce the required resources. Our proposed research addresses both issues.

The paper is organized as follows. Section 2 describes the proposed approach, including the description of the test and prediction models and the definition of the local domains. To illustrate the methodology, Section 3 presents an example

involving heat conduction in a solid. Section 4 presents a summary and conclusions.

2. PROPOSED APPROACH

This paper proposes a sequential, trust-region-like design optimization methodology, where the simulation model is validated through calibration. Starting with an initial design we conduct optimization within a local domain around that design in which we consider the simulation model to be valid within a given confidence level. Our approach reduces the number of required tests, which are carefully chosen at each design point. In this manner, available resources are utilized effectively while ensuring the validity of the simulation model in the vicinity of the design candidates generated by the optimization process.

The proposed methodology is sequential in that optimization occurs at stages using local, trust-region-like domains; optimization and validation are conducted concurrently in that the model is not validated globally before optimization. The contributions and benefits of the proposed approach include 1) an efficient and effective utilization of available testing resources, 2) an explicit treatment of and accounting for test uncertainty in the validation-driven calibration process, and 3) a quantification of the tradeoff between validation confidence level and local domain size.

Consider a two-dimensional design optimization problem (Figure 1). We start with an initial design $\mathbf{d}=(d_1, d_2)$ and determine the minimum number of tests at $\mathbf{d}$ in order to calibrate the simulation model used for analysis so that model predictions match a statistical model of available test data under uncertainty. Minimizing the number of tests is important because tests are usually expensive and time consuming. Subsequently, we determine the size of a local domain around $\mathbf{d}$, so that the simulation model can be considered valid for a certain confidence level. Validation of the simulation model within the local domain means that we are, for example, 95% confident that there is statistical similarity between the model prediction at each design in the local domain and the test data at the center design $\mathbf{d}$. Each local domain is in general, of rectangular shape with a different range for each design variable.

Ideally, we should compare the model prediction at each design in the local domain with test data at the same design. This is however, impractical because it requires expensive tests at many designs. For this reason, we rely on statistical methods to infer the statistical agreement between model prediction at each design within the local domain and tests at the center design. After the size of the local domain is determined, optimization is performed to obtain the optimal design within the local domain, which completes the first stage of the sequential approach. We then initiate the second stage of the sequential approach using the optimal design of