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Quantification of model-form and predictive uncertainty for multi-physics simulation

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ABSTRACT

Traditional uncertainty quantification in multi-physics design problems involves the propagation of parametric uncertainties in input variables such as structural or aerodynamic properties through a single, or series of models constructed to represent the given physical scenario. These models are inherently imprecise, and thus introduce additional sources of error to the design problem. In addition, there often exists multiple models to represent the given situation, and complete confidence in selecting the most accurate model among the model set considered is beyond the capability of the user. Thus, quantification of the errors introduced by this modeling process is a necessary step in the complete quantification of the uncertainties in multi-physics design problems. In this work, a modeling uncertainty quantification framework was developed to quantify to quantify both the model-form and predictive uncertainty in a design problem through the use of existing methods as well as newly developed modifications to existing methods in the literature. The applicability of this framework to a problem involving full-scale simulation was then demonstrated using the AGARD 445.6 Weakened Wing and three different aeroelastic simulation packages to quantify the flutter conditions of the wing.

1. Introduction

In many multi-physics design problems, such as aeroelasticity, multiple models often exist to represent the given physical scenario. Examples of this are numerous in the variety of aeroelastic simulation packages that are available to users ranging from panel methods, such as those available in Nastran [1] or ASTROS [2], to full CFD simulations coupled with dynamic structural responses such as ZEUS [3] or Navier–Stokes solvers [4]. Often, these models produce different results for the same set of design parameters. This variation in results is due to the different assumptions that are made in the mathematical formulations of the individual models. Traditional uncertainty quantification methods in aeroelastic design involve selecting the best model among the model set being considered and then propagating the uncertain input variables through the model to calculate a non-deterministic response of the system. However, one primary flaw with this methodology in that it is beyond the capability of the designer to select with complete certainty the model which is most accurate in all areas of the design space. Although a particular model might be shown to be most accurate, or ever fully correct, at a particular point in the design space, this result cannot be inherently translated to all regions of the design space. A simple example of this could be that although a model might be shown to be accurate in the subsonic Mach regime, there is no guarantee that it will maintain its accuracy in the transonic or supersonic Mach regimes. It is thus proposed that instead of utilizing only a single model in the uncertainty quantification of the design process, that multiple models be considered, in a systematic fashion, so that the additional uncertainty introduced to the design problem through the modeling process can be quantified and mitigated, and the total uncertainty in the problem can be completely quantified. This work introduces an uncertainty quantification framework that quantifies the uncertainties introduced through the modeling process by utilizing existing methods in the literature – with relevant modifications in particular methods – to construct a complete and accurate representation of the modeling uncertainty that is present in an analysis.

2. Background and methods

2.1. Uncertainty definition

In the process of discretizing a physical scenario for modeling, assumptions are made to achieve a simplified representation of the problem. As it is beyond the capability of the designer to completely understand any true engineering problem in its full complexity, these assumptions can produce a discrepancy between

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Nomenclature

$E[\blacksquare]$	expected value of a variable	FEM	finite element method
$Cov[\blacksquare]$	covariance of a variable	PDF	probability density function
AGARD	Advisory Group for Aerospace Research and Development	BMA	Bayesian model averaging
		AFA	adjustment factors approach
CFD	computational fluid dynamics	MAFA	modified adjustment factors approach

the physical scenario and the results produced by the model, meaning that the resulting model is merely a partial representation of reality. This discrepancy between the result of the model and the true physical scenario is referred to as predictive uncertainty [5], and the degree of this uncertainty is often a function of the ability of the model to capture the phenomena in the physical scenario of interest.

It is also very common in engineering problems for multiple models to be constructed to represent the same given scenario. Guedes Soares states that in situations such as this, there exists only one correct model [6]. However, it is beyond the capability of the designer to select the model which is correct in every given situation. Thus, there exists uncertainty in the selection of the model which best represents the physical scenario of interest. This uncertainty in the identification of the best model among a model set that is being considered is referred to as model-form uncertainty [7].

To analyze the discretization of the physical scenario, parameters are defined within the models to represent aspects of the physics, such as dimensions, material properties, environmental conditions, or modeling constants. Although these parameters are often represented as deterministic values within the model, they rarely can be considered deterministic in the true physical scenario. As a result, there exists a third type of uncertainty in the modeling process – parametric uncertainty – which refers to the uncertainty inherent to the parameters that are input into a model [5]. These parametric uncertainties are commonly split into two distinct categories: aleatory and epistemic uncertainty [8]. Aleatory uncertainty is defined as the uncertainty that arises as a result of natural, unpredictable variation in the performance of the system [9]. This type of uncertainty is commonly thought of as the type of uncertainty of which enough information is known to assign probability density functions to represent the random nature of the variable. Epistemic uncertainty, on the other hand, is defined as the type of uncertainty that is due to the lack of knowledge regarding the behavior of a system that could, in theory, be resolved through the introduction of additional information [10]. Epistemic uncertainty is commonly referred to as incomplete uncertainty; or more simply put, inherent variability of which not enough is known to accurately approximate the uncertainty.

Model-form, predictive, and parametric uncertainties are all present in modeling problems. Eq. (1) shows the general formulation of a modeling problem as the function of three variables, $\tilde{f}_i, \tilde{x}$, and $\hat{\varepsilon}$:

$$y = \tilde{f}_i(\bar{x}) + \hat{\varepsilon}_i \tag{1}$$

$\tilde{f}_i(\bar{x})$ represents the result of a particular model, model i, to a set of input parameters, $\bar{x}$. $\hat{\varepsilon}_i$ represents the discrepancy between the result of model i, and the true physical scenario, y. In this regard, the possibility of disagreement between multiple $\tilde{f}_i(\bar{x})$ can be said to represent model-form uncertainty, the variation in $\tilde{f}_i(\bar{x})$ due to uncertainties in the set of input parameters, $\bar{x}$ can be shown to represent parametric uncertainty, and $\hat{\varepsilon}$ represents the predictive uncertainty inherent to model i.

Although the above three types of uncertainty are defined uniquely, they are not necessarily independent of each other. Methods that exist in the literature to quantify uncertainty of a particular form – such as parametric uncertainty – are not necessary applicable, or even valid, to quantify model-form or predictive uncertainty. In aeroelastic design, extensive work has been done working on the quantification of parametric uncertainty. Kurdi et al. explored the effects of uncertainty on structural finite element parameters, such as rib and skin sizes, in the transonic aeroelastic regime using sampling based uncertainty quantification methods for aleatory uncertainties in the parameters of an aeroelastic model [11]. Ueda also explored the effects of aleatory uncertainties on calculating the sensitivities of a structure to the uncertain variables [12]. Tonon et al. further explored the uncertainties in the structural parameters in aeroelastic design, but explored the effects of considering epistemic uncertainties in the problem outside of simply uncertainties in the individual parameters using random set theory [13]. Pettit and Grandhi further quantified the epistemic uncertainty in aerodynamic parameters, such as gust loads, to perform a reliability based optimization [14]. Although much work has been done in the aeroelastic community regarding the quantification of parametric uncertainties, represented as both aleatory and epistemic, little work has been done on the quantification of the model-form and predictive uncertainty in these problems. Due to the increasing complexity of aeroelastic models being constructed, as well as the advancement of aeroelastic modeling into complex regions of the design space, it is important to quantify these additional uncertainties in order to maintain a robust design that accurately considers potential uncertainties in the design problem from all possible sources, including the modeling process itself.

2.2. Model-form and predictive uncertainty quantification methods

To quantify the uncertainties introduced in a modeling process, multiple approaches have been developed that consider the results of multiple models – and the presence of any available experimental data – to develop a non-deterministic representation of a composite model. The first proposal of model combination as a method to quantify the uncertainty between models was made by Barnard [15], a rudimentary combination of multiple airline passenger models. Roberts later suggested an aggregate distribution that combines the opinions of two models using weighting factors [16]. Leamer expanded on this idea, developing the basic paradigm for what is now known as Bayesian model averaging by accounting for the uncertainty in the selection of the model itself [17].

2.2.1. Bayesian model averaging

As opposed to basing a prediction of a physical scenario of interest upon the results of a singular model, Bayesian model averaging constructs a distribution for the adjusted model, $\Pr(y|D)$, as an average of the posterior distributions of each of the N models considered, weighted by its posterior model probability. If y is considered as the adjusted model of interest, then its posterior distribution given experimental data, D, is shown in Eq. (2):