

**UNCERTAINTY ANALYSIS FOR COUPLED  
MULTIDISCIPLINARY SYSTEMS USING SEQUENTIAL  
IMPORTANCE RESAMPLING**

A Thesis

by

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## **ABSTRACT**

In this thesis, a novel compositional multidisciplinary uncertainty analysis methodology is presented for systems with feedback couplings and model discrepancy. The approach incorporates aspects of importance resampling, density estimation, and Gibbs sampling to ensure that, under mild assumptions, the method is provably convergent in distribution. A key feature of the approach is that disciplinary models can all be executed offline and independently. Offline data is synthesized in an online phase that does not require any further model evaluations or any full coupled system level evaluations. The approach is demonstrated on an aerodynamics-structures system, and a comparison to brute force Monte Carlo simulation results is presented. The results demonstrate that our method has captured the joint distribution of interest. This was achieved without any online evaluations of models separately or as a coupled system.

## **ACKNOWLEDGMENTS**

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# 1 INTRODUCTION AND BACKGROUND

## 1.1 Motivation

In response to progress in science and technology, demands on modern aerospace vehicles to have better performance, higher reliability and robustness, and lower cost and risk are ever increasing [3]. This demand has led to the development of highly coupled systems designed to exploit interactions among disciplines to achieve greater performance. There is typically a great deal of uncertainty associated with such systems due to potential new regimes of system behavior arising from unexpected multi-physics interactions. In traditional design practice, to account for such uncertainties, constraints imposed on the design are often reformulated deterministically, with pre-defined safety factors and margins, to ensure the reliability of a design. This approach will typically result in an overly conservative design that cannot meet the demands placed on today's modern aerospace systems. Thus, there is a critical need for the development of advanced, scalable technologies aimed at rigorously quantifying uncertainty in multi-physics aerospace systems.

Multidisciplinary uncertainty analysis of numerical simulation models entails the propagation of uncertainty from model inputs to model outputs. Often, multidisciplinary simulation capabilities are composed by integrating pre-existing disciplinary physics-based models. For such composed multi-physics systems, the task of uncertainty analysis can be challenging owing to the disciplinary models being managed by separate entities or housed in separate locations, analysis capabilities running on different computational platforms,

models with significantly different analysis run times, and the sheer number of disciplines required for a given analysis. An engineering system may contain feedforward coupling in which the output of an upstream discipline becomes an input to a downstream discipline (one-directional coupling), or feedback coupling in which the two disciplines are interconnected in such a way that the output of one becomes an input to the other (bi-directional coupling). Complex, multi-physics systems often exhibit feedback coupling (e.g., aeroelastic coupling in an aero-structural analysis of a wing) that can have a substantial impact on system level uncertainty analysis results. Further, the coupled nature of multi-physics systems necessitates an iterative uncertainty analysis procedure in traditional Monte Carlo based system level uncertainty analysis approaches that can be computationally prohibitive.

## **1.2 Sources of Uncertainty**

The sources of uncertainty in engineering systems are broadly classified into two types of 'Aleatory' and 'Epistemic' uncertainty. Aleatory uncertainty refers to the uncertainty which is due to the presence of physical variability and inherent randomness in nature. This type of uncertainty is irreducible. Epistemic uncertainty arises because of lack of knowledge regarding a particular quantity and/or a physical phenomenon. This type of uncertainty can be reduced by gathering more information if available.

Kennedy and O'Hagan proposed the following classification of uncertainty sources in computer models, as described in Ref. 4.

*Parametric Uncertainty* refers to uncertainty associated with inputs or parameters of a model such as coefficients representing the physical properties of a model.

*Parametric Variability* is the uncertainty due to uncontrolled and/or unspecified input conditions. Uncertain wind loading on an engineering structure, and uncertain operating conditions for an aircraft (e.g., atmospheric conditions, gust encounters, etc.) can be examples of this type of uncertainty.

*Residual Variability* results from the uncertainty due to intrinsic random variation in the process being modeled or in a lack of model detail to discriminate between conditions that lead to different process values. Some examples of these conditions are chaotic flows and turbulence in weather models.

*Model Discrepancy* is another source of uncertainty which results from underlying missing physics, numerical approximations, and/or other inaccuracies of the computer model that would exist even if all the parameters were known. This uncertainty is associated with the fact that no model is perfect, and an example of that can be in potential flow solvers that ignore boundary layer effects and turbulence.

*Observation Error* is the uncertainty in experimentally measured data that may be used for calibration or for solving an inverse problem.

*Code Uncertainty* refers to the uncertainty associated with not knowing the output of a computer model given any particular input configuration until the code is run. For example, this uncertainty arises when Gaussian process emulator is used as a surrogate model to interpolate between known system responses.

### 1.3 Research Objectives

The overall objectives of this thesis are to formulate the problem of propagating uncertainty through a coupled system, and to create an efficient methodology for propagating the uncertainty, and to demonstrate the methodology on a realistic example.

To alleviate the computational burden of multidisciplinary uncertainty analysis in coupled systems composed of integrated disciplinary models, this thesis proposes a probabilistic, sample-based compositional uncertainty analysis methodology. The presented approach in this thesis builds off of the work of Refs. 5 and 1, where a decomposition-based uncertainty analysis methodology is developed for feedforward systems with parametric input uncertainty. Recognizing that the disciplinary models composing the system are imperfect, the method in this thesis takes into account the model discrepancy associated with coupling variables in the system.

A key feature of this thesis is an offline/online approach to uncertainty analysis enabled by the compositional nature of an integrated multidisciplinary system. Specifically, the approach is designed to use offline *independent* uncertainty analysis results for each discipline of the composed system in an online synthesis procedure. Offline results can be generated at any time (e.g., from a previous use of a disciplinary model) and do not require knowledge of the specific input probability distributions that will be used in the composed system level analysis. Further, the proposed online synthesis of offline data from the disciplinary models does not require any coupled system level evaluations. The result is that the computational expense of coupled multidisciplinary uncertainty analysis is moved offline,

allowing for substantial gains in computational efficiency. The proposed methodology incorporates aspects of density estimation, Radon-Nikodym importance weights, and ensemble Gibbs sampling to ensure convergence in distribution of system level uncertainty analysis results under mild assumptions on the disciplinary models and probabilistic distributions. The proposed methodology is demonstrated on an aero-structural system adapted from Ref. 2.

#### **1.4 Background**

Multidisciplinary systems analysis and optimization is a wide area of research, and numerous studies have dealt with the various aspects of coupled multidisciplinary analysis in several engineering disciplines. Researchers have focused both on the development of computational methods and on the application of these methods to several types of multidisciplinary systems such as fluid–structure [6], thermal–structural [7], fluid–thermal–structural [8].

Computational methods for multidisciplinary analysis can be classified into three different groups of approaches [9]. The first approach, known as the field elimination method, eliminates one or more coupling variables (referred to as “field”) by techniques such as integral transforms or model reduction. This approach is restricted to special linear problems that permit efficient decoupling. The second approach, known as the monolithic or simultaneous method, treats the problem as a monolithic entity, and solves the coupled analysis simultaneously using a single solver such as Newton–Raphson. The third approach, known

as the partitioned method, solves the individual analyses separately with different solvers. The field elimination and monolithic methods tightly couple the multidisciplinary analyses together, the partitioned method does not.

Given the presence of model discrepancy in a coupled multidisciplinary system, we must be capable of propagating that uncertainty to system level quantities of interest. While most of the methods for deterministic multidisciplinary analysis can easily be extended to non-deterministic multidisciplinary analysis using Monte Carlo sampling, this may be computationally expensive due to repeated evaluations of disciplinary analyses. Hence, researchers have focused on developing more efficient alternatives. Previous work on multidisciplinary uncertainty analysis has focused on approximations such as surrogate modeling and simplified representations of system uncertainty. The use of surrogates for disciplinary models in a composed system can provide computational savings, as well as simplify the task of integrating components [10]. Approximate representations of uncertainty, such as using mean and variance information in place of a full probability distribution have been used to avoid the need to propagate uncertainty between disciplines. Such simplifications are commonly used in uncertainty-based multidisciplinary design optimization methods as a way to avoid a system-level uncertainty analysis [3]. These approaches include implicit uncertainty propagation [11], reliability-based design optimization [12], robust moment matching [13–15], advanced mean value method [16], collaborative reliability analysis using most probable point estimation [17], and a multidisciplinary first-order reliability method [18]. Ref. 19 proposed worst case uncertainty propagation using

derivative-based sensitivities.

Other recent work has focused on exploiting the structure of a given multidisciplinary system. Ref. 20 present a likelihood-based approach to decouple feedback loops, thus reducing the problem to a feed-forward system. Dimension reduction and measure transformation to reduce the dimensionality and propagate the coupling variables between coupled components have been performed in a coupled feedback problem with polynomial chaos expansions [21–23]. Coupling disciplinary models by representing coupling variables with truncated Karhunen-Loève expansions, has been studied for multi-physics systems [24]. A hybrid method that combines Monte Carlo sampling and spectral methods for solving stochastic coupled problems has also been proposed by Refs. 25 and 26. In addition to the probabilistic techniques, non-probabilistic techniques based on fuzzy methods [27], evidence theory [28], interval analysis [29] have also been studied for multidisciplinary analysis under uncertainty.

Despite the extensive work on multidisciplinary uncertainty analysis, the formulation of the model discrepancy function is still a challenging issue. Different prior formulations have been assumed for model discrepancy in previous work. These formulations include constant bias [30], physics-based deterministic function [31], Gaussian random variable [32, 33] which can be with fixed or input-dependent mean and variance, uncorrelated random vector [34], random walk [30], and Gaussian random process [35–37]. Ref. 38 investigates Bayesian calibration with different prior formulations of model discrepancy function and derives the corresponding likelihood functions.

Review of the above studies reveals that the existing methods for multidisciplinary uncertainty analysis are either computationally expensive or based on several approximations. Computational expense results from using deterministic methods with Monte Carlo simulation which requires several thousands of evaluations of the individual disciplinary analyses, and also non-probabilistic techniques use interval-analysis-based approaches which require substantial computational effort. Approximations may come from approximating the probability distributions with the first two moments, or approximations of individual disciplinary analyses may be considered using derivative-based sensitivities or linearizations at most probable point for reliability analysis.

In this thesis, the approach builds on the work of Refs. 5 and 1, where the challenges of uncertainty analysis for feed-forward multidisciplinary systems were dealt with using a decomposition-based approach. As shown notionally in Figure 1.1, the multidisciplinary

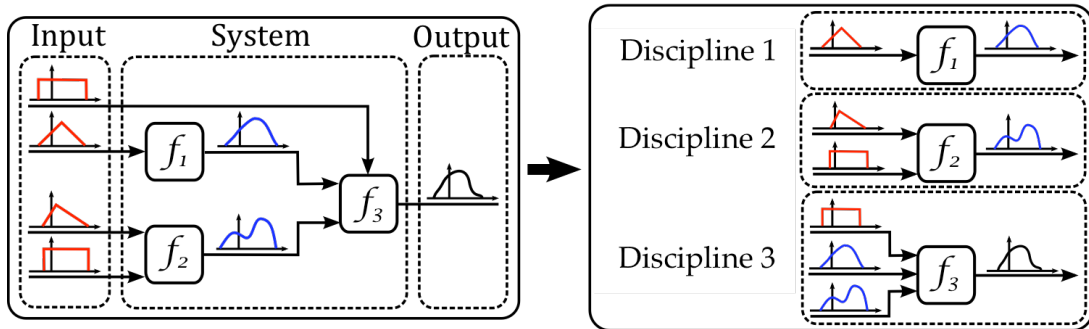


Figure 1.1: The decomposition-based feed-forward multidisciplinary uncertainty analysis method of Ref. 1. The method decomposes the problem into manageable components and synthesizes the system level uncertainty analysis without needing to evaluate the system in its entirety.  $f_1$ ,  $f_2$  and  $f_3$  are the input-output functions associated with each component.

uncertainty analysis is decomposed into individual discipline level uncertainty analyses.

These analyses are then assembled in a provably convergent manner to the desired mul-



tidisciplinary uncertainty analysis results. Taking this approach leads to several benefits, such as enabling offline disciplinary analyses to be conducted when suitable, enabling concurrent evaluation of the disciplinary models for online uncertainty analysis, avoiding the challenges of integrating various disciplinary models that may have been created on different computational platforms, and being consistent with many organizational structures. In the work presented in this thesis, the methodology of Ref. 1 is extended to handle feedback coupling between disciplines, as well as model discrepancy associated with each discipline. This concept is presented notionally in Figure 1.2, where a two-discipline system is represented. It should be noted that the term compositional is used rather than the term decompositional to stress the concept of integrating a set of information sources rather than beginning with a monolithic system that is to be decomposed.

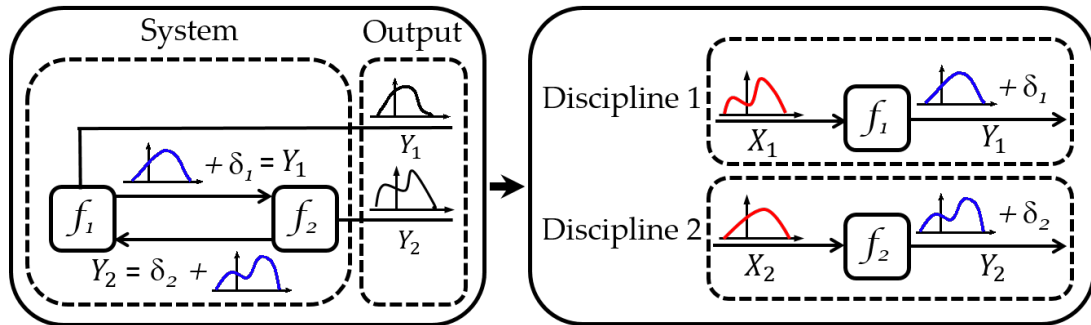


Figure 1.2: A depiction of the concept of a compositional multidisciplinary uncertainty analysis approach for a two-discipline system with model discrepancy and feedback coupling. Here,  $f_1$  and  $f_2$  are the model functions,  $X_1, X_2$  and  $Y_1, Y_2$  are the inputs and outputs of the respective disciplines, and  $\delta_1$  and  $\delta_2$  are the additive model discrepancies associated with the outputs. The approach composes disciplinary uncertainty analysis results without needing to evaluate the coupled system.

In this example, each discipline takes as input, an output from the other discipline. The output of each discipline has additive model discrepancy associated with it, denoted

by  $\delta_1$  and  $\delta_2$  for discipline 1 and 2 respectively. This source of uncertainty will be discussed in more detail in the following chapters. Note that it is this source of uncertainty that necessitates an iterative approach to uncertainty quantification as discussed in Ref. 14, which leads to substantial computational expense for multidisciplinary uncertainty analysis. The remainder of this thesis is organized as follows. Chapter 2 presents the approach, its key ingredients followed by the presentation of the algorithm and convergence analysis of the approach. Chapter 3 presents the application of the approach and its results, and conclusions are drawn in chapter 4.

## 2 APPROACH

In this chapter, characterization of model discrepancy is presented. Then, the proposed approach in this thesis, compositional multidisciplinary uncertainty analysis approach, is presented followed by a discussion of the methodological key ingredients of importance resampling and Gibbs sampling. The use of effective sample size as a heuristic indicator of the quality of a proposal distribution and as a means of identifying stationarity is also discussed. Finally, the algorithm and convergence properties of the proposed method are presented.

### 2.1 Model Discrepancy Characterization

Model discrepancy arises because mathematical models of reality are not perfect, and thus, some aspects of reality may have been omitted, improperly modeled, or contain unrealistic assumptions. Following Ref. 4, model discrepancy is represented here as an additive stochastic process. For example, if we have a model that consists of a function  $f(\mathbf{x})$ , where  $\mathbf{x}$  is an input vector to the model, and reality is denoted as  $f_r(\mathbf{x})$ , then the model discrepancy of the model can be represented as

$$\delta(\mathbf{x}) = f_r(\mathbf{x}) - f(\mathbf{x}), \quad (2.1)$$

where here it is assumed that there are no parameters in the model to be calibrated. Typically, experimental data of reality (which will contain experimental variability) will be available, which can be used to create a stochastic process representation for  $\delta(\mathbf{x})$ . In this

thesis, it is assumed that model discrepancy has been quantified previously for all available disciplinary models in the form of Gaussian processes. Thus, the Gaussian process model discrepancy term will be added to the output of a disciplinary model, as shown notionally in Figure 1.2. For example, for Discipline 1 in Figure 1.2, we have

$$Y_1(\mathbf{x}) = f_1(\mathbf{x}) + \delta_1(\mathbf{x}), \quad (2.2)$$

where  $\delta_1(\mathbf{x})$  is the Gaussian process representation of the model discrepancy of Discipline 1 and  $Y_1(\mathbf{x})$  is the estimate of reality from Discipline 1 with quantified model discrepancy. In this thesis, without loss of generality, the focus is on discrepancies that are not a function of an input.

## 2.2 Compositional Multidisciplinary Uncertainty Analysis

The proposed compositional multidisciplinary uncertainty analysis approach for systems with feedback coupling, and model discrepancy, consists of an offline and online phase. To make the discussion more concrete but without loss of generality, the aspects of the approach are developed with the system presented in Figure 1.2 in mind. The approach begins offline, by performing uncertainty analysis independently for each discipline of the system. To do this, distributions must be proposed for inputs for each discipline, since the distributions of the coupling variables are not known in advance. These distributions are defined as proposals which are represented by  $\pi_{X_1}$  and  $\pi_{X_2}$ . This process is shown notionally in Figure 2.1. As it is shown, the samples generated from the proposal distributions are propagated through the disciplines with functions  $f_1$  and  $f_2$  to generate the corresponding

samples of the discipline outputs. The underlying densities of the output samples are then approximated as  $\pi_{Y_1}$  and  $\pi_{Y_2}$  using a density estimation technique such as kernel density estimation [39].

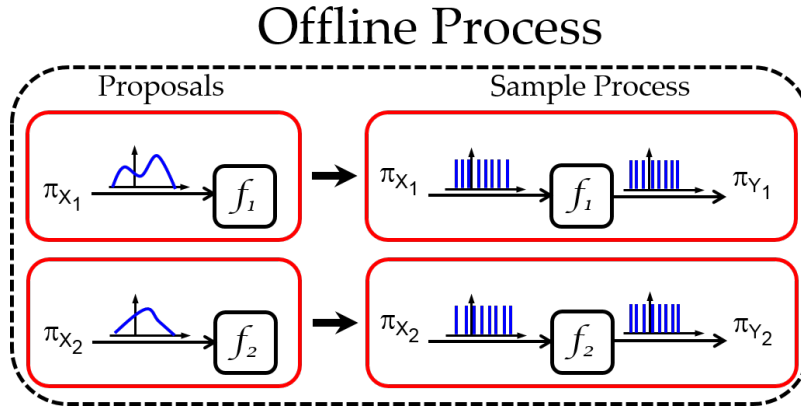


Figure 2.1: A depiction of the offline uncertainty analysis process adapted from Ref. 1. Here,  $\pi_{X_1}$ ,  $\pi_{X_2}$ ,  $\pi_{Y_1}$ , and  $\pi_{Y_2}$  are the densities associated with the inputs (proposals) and outputs of the respective disciplines.

The online process consists of a Gibbs sampling procedure that is enabled by iteratively re-weighting the samples generated offline for each discipline through a combination of density estimation and sequential importance resampling. The use of importance weights allows us to change underlying input probability distributions to each discipline. These weights can then be used on the output probability distributions of each discipline. The weighted output distributions converge in distribution to the output distributions that would have resulted from the modified input probability distributions sampled from in the first place. The overall online process is presented notionally in Figure 2.2 for the system presented in Figure 1.2. Here, it is assumed that each discipline contains model discrepancy, and the output of the systems (e.g., the quantity of interest) is the joint distribution

of the coupling variables. The online process evolves this joint distribution iteratively via Gibbs sampling of the conditional densities. For example, in Figure 2.2, the process begins with the joint distributions  $\pi_{X_1|Y_2}$ ,  $\pi_{Y_1|X_1}$ ,  $\pi_{X_2|Y_1}$ , and  $\pi_{Y_2|X_2}$ . The initial distribution assumed for each conditional distribution is given by the offline uncertainty analysis. From these proposed distributions ( $\pi_{X_1}$  and  $\pi_{X_2}$ ), some samples are drawn to pass through each discipline independently to produce the initial samples from the target distributions ( $\pi_{Y_1|X_1}$  and  $\pi_{Y_2|X_2}$ ). In the online process, the joint distribution of each conditional distribution is updated sequentially and iteratively using Radon-Nikodym importance weights. To do so, the samples from  $\pi_{X_1|Y_2}$  and  $\pi_{X_2|Y_1}$  are re-weighted and updated followed by a density estimation technique and using the ratio of densities of target and proposal distributions as the Radon-Nikodym weights. By sequential importance resampling,  $\pi_{X_1|Y_2}$  and  $\pi_{X_2|Y_1}$  match  $\pi_{Y_2|X_2}$  and  $\pi_{Y_1|X_1}$  respectively, so the target distributions are simulated and propagated without rerunning the model online. This iterative process results in the convergence in distribution of the joint distribution of  $Y_1$  and  $Y_2$  as the number of iterations grows. Hence, the joint distribution of the two sources of uncertainty in the system is recovered without ever performing a coupled system level analysis.

### 2.3 Key Ingredients of the Approach

As mentioned, the two key ingredients of the proposed approach are sequential importance resampling and Gibbs sampling.

## Online Process

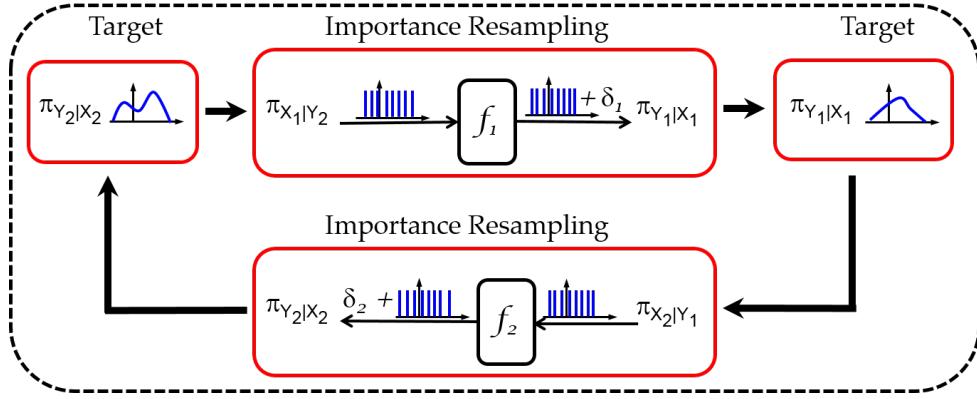


Figure 2.2: A depiction of the online uncertainty analysis process. It should be noted that the models  $f_1$  and  $f_2$  are not actually executed in the online process. Instead, the Radon-Nikodym importance weights found for re-weighting the input proposal distribution are passed on to the output distributions.

### 2.3.1 Sequential Importance Resampling

A key ingredient of the online approach is the iterative re-weighting of offline sample information. This is achieved using sequential importance resampling [40]. The method is used as follows. Consider a bivariate density of the random variables  $Y_1$  and  $Y_2$  and assume a bivariate normal distribution have been sampled where  $Y_1 \sim \mathcal{N}(0, 2)$ ,  $Y_2 \sim \mathcal{N}(0, 2)$ , and the random variables are independent. Contours of this density are shown in red on the left in Figure 2.3 and samples of this distribution are shown with red dots on the same figure. These samples could then be propagated through a model, say  $f(Y_1, Y_2)$  to compute statistics of interest such as the expectation,  $\mathbb{E}[f(Y_1, Y_2)]$ . Now suppose that instead of the distribution represented by the red contours on the left in Figure 2.3, we wished to compute the expectation of  $f(Y_1, Y_2)$  with  $Y_1$  and  $Y_2$  distributed jointly according to the distribution

represented by the blue contours on the left in Figure 2.3. A traditional approach would require sampling from this distribution and then propagating these samples through the model. However, importance resampling, which is based on the Radon-Nikodym theorem [41], allows us to compute this information by simply re-weighting the samples from the original distribution, which we can then resample from with replacement.

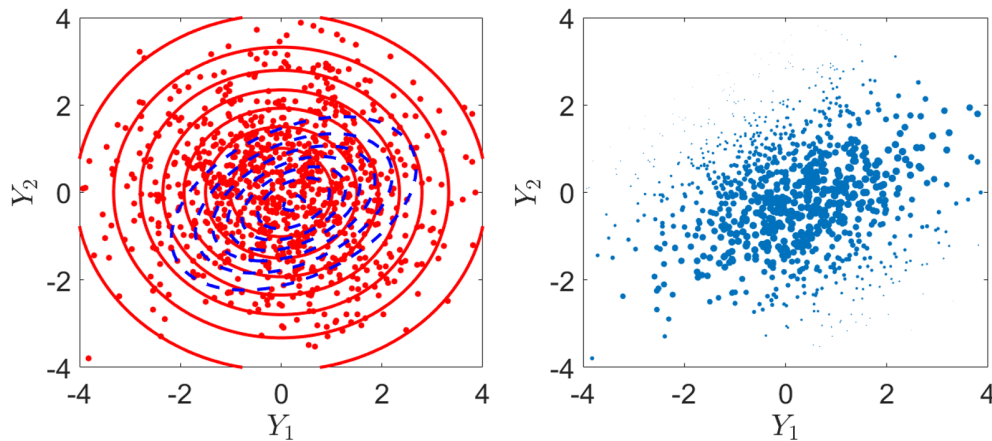


Figure 2.3: The importance resampling process uses the realizations shown by red dots on left figure, generated from a proposal distribution  $P(Y_1, Y_2)$  (corresponding density shown as red solid contour on left figure) to approximate a target distribution  $Q(Y_1, Y_2)$  (blue dash contour on left figure), by weighting the proposal realizations shown by blue dots on right figure (adapted from Ref. 1).

The concept is demonstrated in Figure 2.3, where Radon-Nikodym importance weights are used to re-weight the samples given by the red dots on the left figure. The result is the blue dots on the right figure, where the size of the dots denotes the relative weights given to the samples. These weights are the Radon-Nikodym derivatives of the desired distribution with respect to the original distribution evaluated at the original sample points. Mathematically, if we wished to compute the expected value of some function



$f(Y_1, Y_2)$  using the density represented by the blue contours but had only samples of the density represented by the red contours, we would proceed as follows. Referring to the original distribution as the *proposal* distribution and denoting its density by  $p(Y_1, Y_2)$  and referring to the desired distribution as the *target* distribution and denoting its density by  $q(Y_1, Y_2)$ , the expected value of  $f(Y_1, Y_2)$  with respect to the target distribution is given as

$$\mathbb{E}_Q[f(Y_1, Y_2)] = \int_{\mathcal{P}} \frac{q(Y_1, Y_2)}{p(Y_1, Y_2)} f(Y_1, Y_2) p(Y_1, Y_2) dY, \quad (2.3)$$

where  $\mathcal{P}$  is the support of the proposal density and the target distribution is absolutely continuous with respect to the proposal distribution. This integral can be evaluated with Monte Carlo simulation as

$$\mathbb{E}_Q[f(Y_1, Y_2)] \approx \frac{1}{N} \sum_{i=1}^N f(Y_1^i, Y_2^i) \frac{q(Y_1^i, Y_2^i)}{p(Y_1^i, Y_2^i)}, \quad (2.4)$$

where the samples  $\{Y_1^i, Y_2^i\}$  are drawn from the proposal distribution (i.e., the red contours in Figure 2.3). This is the key aspect of the method. The proposal samples are propagated through a model offline. Online, these samples are re-weighted so as to simulate a target distribution being propagated through a model. Importance resampling allows us to achieve this simulation *without rerunning the model online*. It should be noted here that sequential importance resampling (sampling from the discrete distribution given by the Radon-Nikodym importance weights) is done followed by a density estimation technique to update the joint densities in the online process. This is required because the Radon-Nikodym weights are density ratios.

### 2.3.2 Gibbs Sampling

The second key ingredient of the approach is Gibbs sampling. The presence of model discrepancy in a multidisciplinary system with feedback coupling requires the addition of that model discrepancy iteratively. That is, considering the system in Figure 1.2, if we first evaluate Discipline 1 (with an initial estimate of the input to this discipline from Discipline 2), we have an estimate of the output of Discipline 1 that feeds into Discipline 2. To this output, we add the discrepancy term denoted by  $\delta_1$  in the figure. Discipline 2 can then be evaluated and to its output that feeds back into Discipline 1, we must add the discrepancy term denoted by  $\delta_2$  in the figure. This process must be repeated until some form of convergence is achieved. Here, the convergence that is required is convergence in distribution. That is, an iterative process is required that, when enough iterations have occurred, the joint distribution of the coupling variables is stationary. One method for achieving this is through the use of Gibbs sampling.

Gibbs sampling was first described by Ref. 46 and has also been referred to as successive substitution sampling [47]. It is a Markov chain Monte Carlo based method for generating samples from a joint distribution that cannot be directly sampled. Following Refs. 47 and 48, suppose we have random variables (which can be vector-valued)  $Y_1, \dots, Y_k$ , and we wish to generate samples from the joint distribution of those random variables, which we denote as  $\pi_{Y_1, \dots, Y_k}$ . Assume we have a complete set of conditional distributions,  $\pi_{Y_i | \{Y_j, j \neq i\}}$  for  $i = 1, \dots, k$ , available for sampling. Then, starting from some initial arbitrary set of values,  $y_1^{(0)}, \dots, y_k^{(0)}$ , where the superscript denotes the iteration num-

ber of the Gibbs sampler, we draw a sample  $y_1^{(1)}$  from  $\pi_{Y_1|Y_2=y_2^{(0)}, \dots, Y_k=y_k^{(0)}}$ . We then draw a sample  $y_2^{(1)}$  from  $\pi_{Y_2|Y_1=y_1^{(1)}, Y_3=y_3^{(0)}, \dots, Y_k=y_k^{(0)}}$ , and continue in this manner up to  $y_k$  from  $\pi_{Y_k|Y_1=y_1^{(1)}, \dots, Y_{k-1}=y_{k-1}^{(1)}}$ , which completes one iteration of the Gibbs sampler. After  $m$  iterations, we obtain  $(y_1^{(m)}, \dots, y_k^{(m)})$ . For continuous distributions, Ref. 47 has shown, under mild assumptions, that this  $k$ -tuple converges in distribution to a random observation from  $\pi_{Y_1, \dots, Y_k}$  as  $m \rightarrow \infty$ .

To demonstrate the applicability of Gibbs sampling to multidisciplinary uncertainty analysis, consider again the system shown in Figure 1.2. Let  $y_1^{(0)}$  be an initial estimate from Discipline 1, where an arbitrary estimate from Discipline 2 has been assumed. This sample then can be propagated through Discipline 2, which generates a sample from the conditional distribution,  $\pi_{Y_2|Y_1=y_1^{(0)}}$ , which is denoted as  $y_2^{(1)}$ . Then this sample can be propagated through Discipline 1 to generate a sample from the conditional distribution  $\pi_{Y_1|Y_2=y_2^{(1)}}$ , and so on. By repeating this process many times, we ensure that the random sample,  $(y_1^{(m)}, y_2^{(m)})$  converges in distribution to a random observation from the true joint distribution of  $Y_1$  and  $Y_2$ .

For compositional multidisciplinary uncertainty analysis approach and the system represented by Figures 1.2 and 2.2, Gibbs sampling is performed over the conditional joint distributions of  $X_1|Y_2, Y_1|X_1, X_2|Y_1$ , and  $Y_2|X_2$ . This begins with initial distributions,  $\pi_{X_1^{(0)}}, \pi_{Y_1^{(0)}}, \pi_{X_2^{(0)}}$ , and  $\pi_{Y_2^{(0)}}$ , which were generated offline. Then Radon-Nikodym importance weights from the ratio of  $\pi_{Y_2^{(0)}}$  to  $\pi_{X_1^{(0)}}$  are used to generate the distribution  $\pi_{X_1^{(1)}|Y_2^{(0)}}$  as well as  $\pi_{Y_1^{(1)}|X_1^{(1)}}$ . Then Radon-Nikodym importance weights from the ratio of  $\pi_{Y_1^{(1)}}$  to

$\pi_{X_2^{(0)}}$  can be used to generate the distribution  $\pi_{X_2^{(1)}|Y_1^{(1)}}$  and  $\pi_{Y_2^{(1)}|X_2^{(1)}}$ , which completes one iteration of the importance weighted Gibbs sampler.

## 2.4 Kernel Density Estimation

For applying sequential importance resampling, the importance weights that are the ratio of the target density to the proposal density are computed for a given sample. Since a sample-based approach is employed here to propagate uncertainty, a means of estimating proposal and target densities from a set of samples is required. In particular for some continuous random variable  $x$  with density function  $f(x)$ , we require that for any density estimate,  $\hat{f}(x)$ ,

$$\lim_{n \rightarrow \infty} \hat{f}(x) = f(x) \quad (2.5)$$

at all points of continuity of the density  $f(x)$ . For this, we use kernel density estimation,

$$\hat{f}(x) := \frac{1}{nL^d} \sum_{i=1}^n K\left(\frac{x-x^j}{L}\right) \quad (2.6)$$

where  $L > 0$  is a smoothing parameter called the bandwidth with the property that  $\lim_{n \rightarrow \infty} L = 0$  and  $K$  is a kernel function satisfying

$$0 \leq K(t) \leq \infty \quad (2.7)$$

$$\int_{\mathbb{R}^d} K(t) dt = 1 \quad (2.8)$$

$$\int_{\mathbb{R}^d} K(t)x dt = 0 \quad (2.9)$$

$$\int_{\mathbb{R}^d} K(t)\|t\|^2 dt < \infty \quad (2.10)$$

where  $t \in \mathbb{R}^d$  and  $\|\cdot\|$  is the Euclidean norm. Then,  $\lim_{n \rightarrow \infty} \hat{f}(x) = f(x)$  at every point  $x$  of continuity of  $f(\cdot)$  [50].

## 2.5 Effective Sample Size

As noted in Section 2.2, since the joint distributions of the coupled variables are not known in advance, distributions must be proposed for the inputs of each discipline. These proposal distributions come from the previous knowledge about the system, and can impact the convergence performance of the compositional multidisciplinary uncertainty analysis approach. In general, the quality of the proposal distributions cannot be evaluated before executing the approach; but after knowing the importance weights, it can be done by computing the effective sample size as

$$n_{\text{eff}} = \frac{1}{\sum_{i=1}^N (w(x_i))^2}, \quad (2.11)$$

where  $N$  is the number of samples and  $w(x_i)$  is the normalized importance weight assigned to the proposal sample  $x_i$  [42–44]. The effective sample size ranges from  $n_{\text{eff}} = 1$  to  $n_{\text{eff}} =$

$N$ . We have  $n_{\text{eff}} = N$  when all the samples have the same weights ( $\frac{1}{N}$ ), so the proposal and target distributions are equal to each other, while  $n_{\text{eff}} = 1$  shows that the weight of all the samples except one sample is 0. Thus, effective sample size is often used as a heuristic for determining when the proposal distribution adequately captures the target distribution [45]. This approach is taken here as discussed in Section 2.2, where the use of an unchanging effective sample size is also considered as a heuristic indicator of stationarity in a target distribution.

## 2.6 Algorithm

The proposed compositional multidisciplinary uncertainty analysis method for coupled systems with model discrepancy is presented in Algorithm 1. The data necessary for this algorithm are the samples generated from the proposal distributions as inputs and the output samples of each discipline obtained independently in the offline process. The number of samples and the number of disciplines are represented as  $N$  and  $N_d$  respectively. Since this approach is based on samples, to be able to compute the importance weights, the densities of the inputs,  $\pi_X$ , and outputs,  $\pi_Y$ , of the disciplines need to be estimated. The algorithm starts from the first discipline, and computes the unnormalized weights ( $w_{i,j}^{un}$ ) for each sample of disciplines ( $\{x_{i,j}\}_{i=1,\dots,N}^{j=1,\dots,N_d}$ ) as  $w_{i,j}^{un} = \frac{\pi_{Y_{j-1}}(x_{i,j})}{\pi_{X_j}(x_{i,j})}$ , which is the ratio of the target input density (output from the upstream discipline) and the proposal input density computed at each sample previously simulated from the proposal input distribution. After assigning weights to all the samples,  $N$  samples are drawn with replacement from the out-

put samples, and the model discrepancy corresponding to the current discipline is added to the importance resampled samples. From these updated samples, the probability density of the output, which is the new target input distribution for the downstream discipline, is updated. To compute the effective sample size, the weights assigned to the samples need to be normalized to sum to unity. After repeating these steps for all the disciplines, one iteration of the Gibbs sampler is completed, and  $M$ , which represents the number of Gibbs iterations and is initialized to 0, is updated to  $M + 1$ . The algorithm stops when the relative difference between the effective sample size in the current Gibbs iteration and the previous one,  $\left| \frac{n_{\text{eff}}^j(M) - n_{\text{eff}}^j(M-1)}{n_{\text{eff}}^j(M)} \right|$ , for all the disciplines is less than a user-defined threshold ( $\epsilon$ ), which shows that the approach has converged to a stationary joint distribution of the coupling variables.

---

**Algorithm 1:** Compositional Multidisciplinary Uncertainty Analysis.

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**Data:** Offline sample sets of inputs  $\{\mathbf{x}_{i,j}\}_{i=1,\dots,N}^{j=1,\dots,N_d}$  and outputs  $\{\mathbf{y}_{i,j}\}_{i=1,\dots,N}^{j=1,\dots,N_d}$  obtained from offline Monte Carlo based individual discipline analyses.

**Result:** The joint distribution of outputs of all the disciplines  $\{Y_j\}_{j=1,\dots,N_d}$  and their statistics.

**Parameters:**  $N$  = number of samples;  $N_d$  = number of disciplines;  $M$  = number of Gibbs iterations;  $\delta_j$  = additive model discrepancy of discipline  $j$ ;  $n_{\text{eff}}$  = effective sample size;  $\varepsilon$  = user-defined threshold for the iteration stopping criterion;  $w_{i,j}^{un}$  = unnormalized weights;  $w_{i,j}$  = normalized weights

Initialize input and output distributions of  $\{X_j\}_{j=1,\dots,N_d}$  ( $\pi_{X_j}$ ) and  $\{Y_j\}_{j=1,\dots,N_d}$  ( $\pi_{Y_j}$ ) using offline sample sets, and  $M = 0$ .

**while**  $\max_{j \in \{1,\dots,N_d\}} (\varepsilon_j) > \varepsilon$  **do**

**for**  $j = 1 : N_d$  **do**

**for**  $i = 1 : N$  **do**

**if**  $j = 1$  **then**

$$w_{i,j}^{un} = \frac{\pi_{Y_{N_d}}(x_{i,j})}{\pi_{X_j}(x_{i,j})}$$

**else**

$$w_{i,j}^{un} = \frac{\pi_{Y_{j-1}}(x_{i,j})}{\pi_{X_j}(x_{i,j})}$$

            Importance resample from the discrete distribution given by the computed weights.

            Add the model discrepancy associated with the current discipline ( $\delta_j$ ) to the respective importance resampled samples.

            Update the probability density of  $Y_j$  ( $\pi_{Y_j}$ ) from the updated samples.

            Normalize the unnormalized weights  $\{w_{i,j}^{un}\}$  to obtain the normalized weights  $\{w_{i,j}\}_{i=1,\dots,N}$ .

$$n_{\text{eff}}^j(M) = \frac{1}{\sum_{i=1}^N (w_{i,j})^2}$$

$$\varepsilon_j = \left| \frac{n_{\text{eff}}^j(M) - n_{\text{eff}}^j(M-1)}{n_{\text{eff}}^j(M)} \right|$$

**$M = M + 1$**

---



## 2.7 Convergence Analysis

In this section, the convergence properties of the proposed compositional multidisciplinary uncertainty analysis method are discussed. Convergence results from applications of the law of large numbers, Skorokhod's representation theorem, and the convergence of kernel density estimation, importance weighted empirical distributions, and the Gibbs sampler.

In the offline process of the compositional multidisciplinary uncertainty analysis method, Monte Carlo analysis is performed and samples are generated from the input proposal distributions of each discipline. The convergence of these input proposal samples to their respective input proposal distributions follows from the law of large numbers [49]. From the generated input samples, the output samples are obtained independently for each discipline, so the output variances and other distributional quantities can similarly be estimated using Monte Carlo simulation results. By assuming that the function model of each discipline,  $f_j$ , is bounded and continuous, then as an application of Skorokhod's representation theorem, the output empirical distribution converges to the true output proposal distribution of each discipline [49].

In the online process of the compositional multidisciplinary uncertainty analysis method, importance sampling is used to weight the proposal samples, so as to approximate the target input distribution, using the samples previously simulated from the proposal input distributions. The convergence of the sampling and importance resampling (SIR) algorithm is discussed in Ref. 40. To apply SIR, the proposal and target densities

need to be estimated from the corresponding samples to compute the importance weights. By using a kernel density estimation method that is strongly uniformly convergent [50,51], pointwise estimates of the densities are obtained where we are ensured to converge pointwise as the number of samples increases to the true density [52]. Then, by an application of Skorokhod's representation theorem [49], the weighted empirical output proposal distribution converges to the true output target distribution. As can be seen in Figure 2.2, these target distributions are conditional distributions for each coupling variable conditioned on all other coupling variables. Hence, iteratively sampling via the process of re-weighting offline samples constitutes a Gibbs sampling process, which has been shown to converge under certain conditions (i.e., compatible conditional distributions) to samples from the true joint distribution of the coupling variables [53].

Thus, the proposed compositional multidisciplinary uncertainty analysis approach can perform the uncertainty analysis for coupled systems with model discrepancy in a provably convergent manner under mild assumptions on the disciplinary functions and the model discrepancy terms.

### 3 APPLICATION AND RESULTS

#### 3.1 Application

In this chapter, a demonstration of the effectiveness of the proposed compositional multidisciplinary uncertainty analysis approach is presented. The application system of interest is adapted from Ref. 2. The application is discussed followed by the description of the results.

##### 3.1.1 Aerodynamics-Structures System

The example problem that is used to demonstrate the method is a two-dimensional airfoil in airflow from Ref. 2 and shown in Figure 3.1. As described in Ref. 2, the airfoil

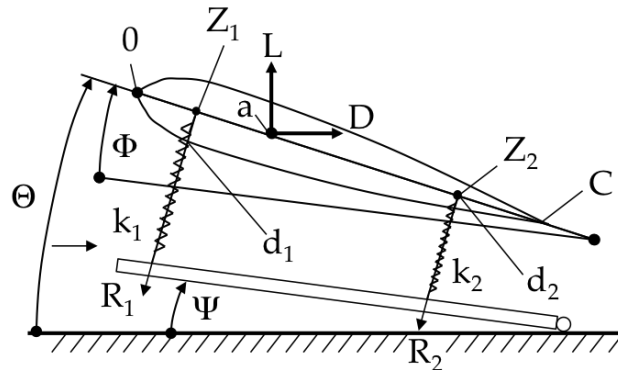


Figure 3.1: Coupled aerodynamics-structures system adapted from Ref. 2.

is supported by two linear springs attached to a ramp. The airfoil is permitted to pitch and plunge. The lift,  $L$ , and the elastic pitch angle,  $\phi$ , are the coupling variables and also the outputs in this system. A complete description of the problem can be found in Ref. 2

and for the sake of completeness, the equations and variable values are presented in the appendix. A block diagram of the system is shown in Figure 3.2, where the considered model discrepancies are highlighted. For this demonstration, the distribution of model discrepancies are assumed to be  $\delta_1 \sim \mathcal{N}(0, 250)$  (N) and  $\delta_2 \sim \mathcal{N}(0, 1e-6)$  (rad), where  $\mathcal{N}(\mu, \sigma^2)$  represents a normal distribution with mean  $\mu$  and variance  $\sigma^2$ . The objective then is to correctly estimate the joint distribution of  $L$  and  $\phi$  using the compositional multidisciplinary uncertainty analysis methodology.

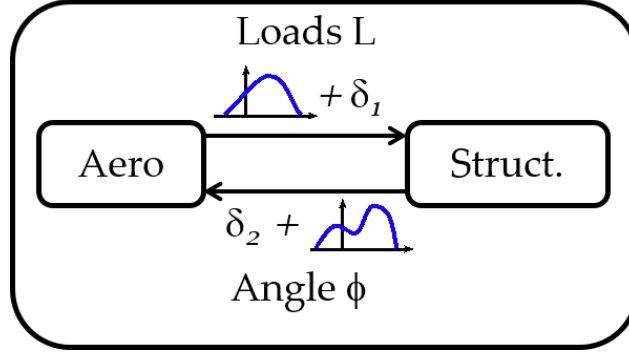


Figure 3.2: Block diagram of the coupled aerodynamics-structures system adapted from Ref. 2 showing the model discrepancies considered.  $L$  is the lift and  $\phi$  is the elastic pitch angle.

### 3.2 Results

In this section, the results of the compositional multidisciplinary uncertainty analysis (CUA) approach applied to the coupled aerodynamics-structures system are presented. A comparison to brute force Monte Carlo simulation results, the evolution of the joint distribution of  $L$  and  $\phi$  using the compositional multidisciplinary uncertainty analysis methodology, and convergence results for both increasing Gibbs iterations and increasing sample

size for statistics of interest are presented.

The Monte Carlo results that are compared to the proposed methodology consisted of generating 100,000 samples from the joint distribution of  $L$  and  $\phi$  using Gibbs sampling. The Gibbs sampler underwent 15 iterations for each sample, thus the models were evaluated 1,500,000 times each. The compositional multidisciplinary uncertainty analysis approach used 200,000 offline evaluations of each model independently. For the aerodynamics model of the example problem, an input distribution of  $\phi \sim \mathcal{N}(0.017, 4e-6)$  was used as the proposal. For the structures model, the independent input distribution,  $L \sim \mathcal{N}(500, 400)$ , was used as the proposal. It should be noted here that these proposals were completely independent (that is, all off-diagonal terms in the covariance matrix of the joint distribution of the variables were zero), and that the offline evaluations of the aerodynamics and structures models were run in isolation of each other. That is, there was never any coupled system evaluation conducted offline.

Statistics of the joint distribution of  $L$  and  $\phi$  are presented in Table 3.1 for both the full Monte Carlo simulation approach (MCS) and the compositional multidisciplinary uncertainty analysis (CUA) approach proposed here. The results demonstrate the mean, vari-

Table 3.1: Quantities of interest computed in MCS and CUA methods

Variable	MCS	CUA
$\mu_L$	502.0265	502.0563
$\sigma_L^2$	352.2087	353.0435
$\mu_\phi$	0.0176	0.0176
$\sigma_\phi^2$	$1.4240e-06$	$1.4318e-06$
$cov(L, \phi)$	0.0122	0.0123
$cor(L, \phi)$	0.5447	0.5476

ance, covariance, and correlation coefficient of the joint distribution are being estimated well by the proposed approach. The joint distribution of the variables using each method is shown in Figure 3.3 as contour plots. The left side of the plot is the MCS result whereas the right side is the result of the proposed approach. Graphically it is clear that CUA method has captured the joint distribution of interest. This was achieved without any online evaluations of either model separately or as a coupled system. Thus, the online cost of using CUA method to propagate uncertainty through this system was negligible, whereas the MCS approach incurred substantial computational cost.

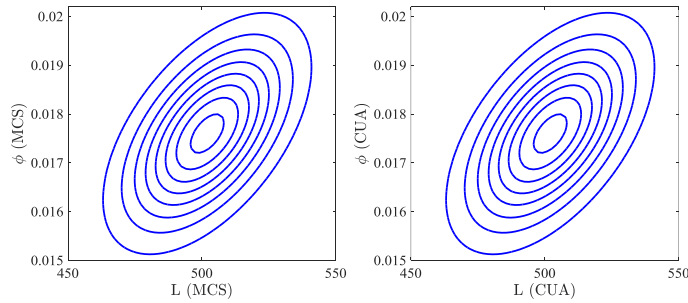


Figure 3.3: Joint distributions represented with contour plots for both the MCS and CUA methods. The MCS approach used 1,500,000 samples and the CUA approach used 200,000.

Figure 3.4 shows the evolution of the joint distribution of  $L$  and  $\phi$  using the proposed approach after one, three, and five Gibbs iterations. Red samples are generated from the proposal distributions shown as red solid contours which are re-weighted to capture the evolving target distribution, shown as blue dashed contours, and the weighted samples are shown in blue dots in the plots below the distributions.

To demonstrate the convergence of the joint distribution of  $L$  and  $\phi$  obtained using

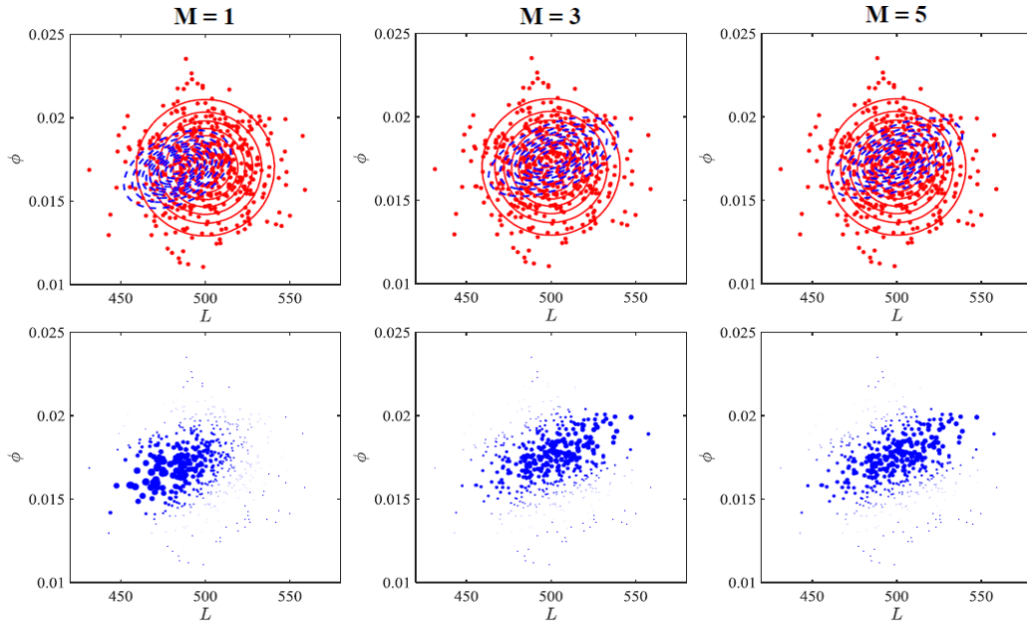


Figure 3.4: Evolution of the joint distribution of  $L$  and  $\phi$  using the proposed approach after one, three, and five Gibbs iterations. Red samples are generated from a proposal distribution shown as red solid contours which are re-weighted (weighted blue dots in below plots) to capture the evolving target distribution, shown as blue dashed contours.

the compositional methodology, the Cramer von-Mises criterion [54] is computed between the empirical joint distribution obtained by the proposed approach and that recovered by brute force Monte Carlo simulation. The Cramer von-Mises criterion is defined as

$$\omega = \int_{-\infty}^{+\infty} [F_n(x) - F^*(x)]^2 dF^*(x), \quad (3.1)$$

where  $F_n$  and  $F^*$  are the cumulative distribution functions of the empirical distribution and a desired distribution, respectively. Figure 3.5 presents the Cramer von-Mises criterion as a function of the number of offline samples used in the proposed approach averaged over 100 independent simulations. Also, the effective sample size is shown as a function of the number of offline samples averaged over the 100 independent simulations. The results

show that the Cramer von-Mises criterion converges with the number of samples, and the rate of convergence is  $1/N$ , where  $N$  is the number of samples, which is expected based on the dependence of the convergence analysis of the approach on the law of large numbers.

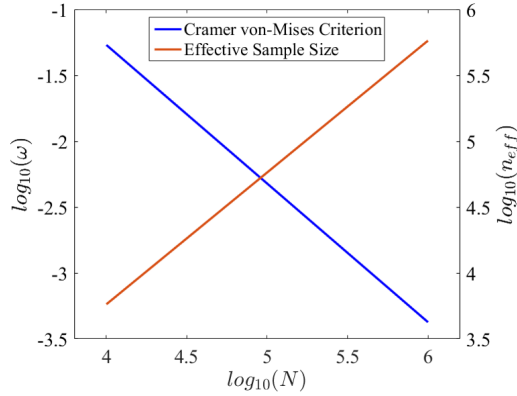


Figure 3.5: Average Cramer von-Mises criterion and effective sample size over 100 runs of the CUA approach as a function of the number of offline samples.

Certain quantities of interest, such as means, variances, and the covariance of the joint distribution of  $L$  and  $\phi$  also converge to their true values as shown in the following numerical results. The expected value of the relative error of the mean and variance estimates are computed as,  $\mathbb{E}\left[\frac{|\hat{\mu}_q - \mu_q|}{\hat{\mu}_q}\right]$  and  $\mathbb{E}\left[\frac{|\hat{\sigma}_q^2 - \sigma_q^2|}{\hat{\sigma}_q^2}\right]$  respectively, in which  $q$  refers to  $L$  or  $\phi$ . The expected value of the relative error of the covariance of  $L$  and  $\phi$  is computed as,  $\mathbb{E}\left[\frac{|c\hat{ov}(L, \phi) - cov(L, \phi)|}{c\hat{ov}(L, \phi)}\right]$ . The expectation is computed as the average of 100 independent uncertainty analysis trials. The mean and variance,  $\hat{\mu}_q$  and  $\hat{\sigma}_q^2$ , are obtained using the full Monte Carlo simulation uncertainty analysis results, and  $\mu_q$  and  $\sigma_q^2$ , are the mean and variance estimates (for  $L$  and  $\phi$ ) obtained from the compositional multidisciplinary uncertainty analysis approach. To assess the quality of the proposal distributions, the effective sample size is computed once the target distribution is known after each Gibbs iteration.



Figure 3.6 shows the expected error in estimating the covariance of  $L$  and  $\phi$ , and also the effective sample size as the number of Gibbs iterations increases. As it is seen, in this par-

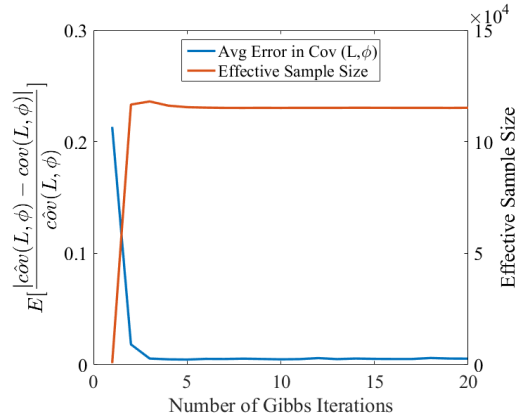


Figure 3.6: Average effective sample size and the expected value of the relative error of the covariance of  $L$  and  $\phi$  using the CUA method with 200,000 samples and averaged over 100 runs versus the number of Gibbs iterations.

ticular example, the joint distribution is captured after a few Gibbs iterations. As shown in the figure, the effective sample size and relative error in the covariance estimate level off around the same number of Gibbs iterations. As discussed earlier, the leveling off of the effective sample size is used as a heuristic to indicate that the approximation of the target distribution is stationary. In this situation, the only mechanism for obtaining a better estimate of the target is the introduction of more samples, which is a topic of future work.

Figure 3.7 shows the expected value of the relative error of the means and variances of  $L$  and  $\phi$ , as well as the effective sample size as the number of offline samples increases. The results show that the proposed approach is effectively estimating the statistics of  $L$  and  $\phi$ .

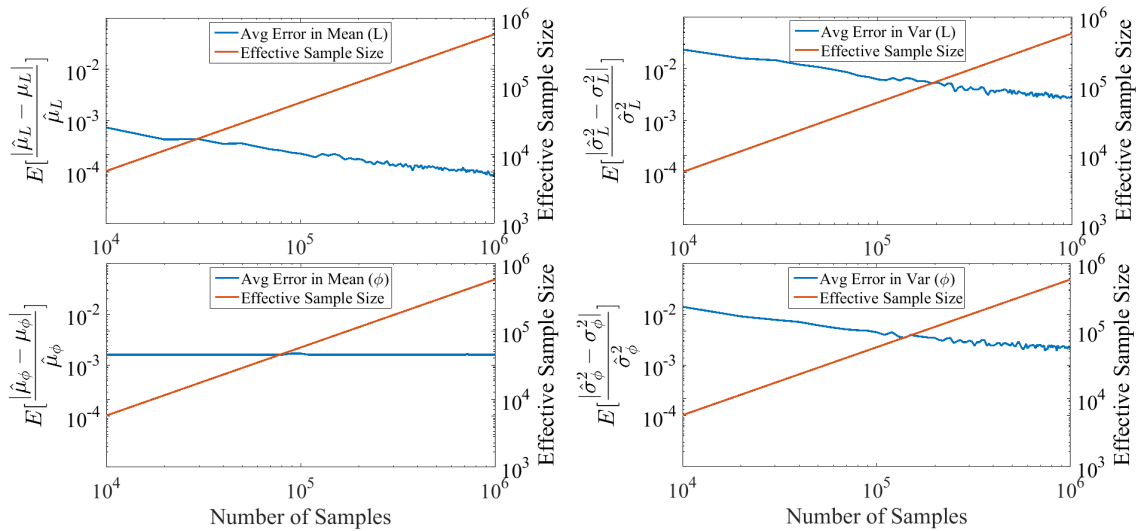


Figure 3.7: Average effective sample size and expected value of the relative error of the mean and variance of  $L$  and  $\phi$  computed using CUA approach averaged over 100 runs versus number of samples on a logarithmic scale

## 4 SUMMARY AND CONCLUSIONS

This thesis has presented a compositional multidisciplinary uncertainty analysis methodology. The approach was motivated by the fact that often, multidisciplinary simulation capabilities are composed by integrating pre-existing disciplinary physics-based models. For such composed multi-physics systems, the task of uncertainty analysis can be challenging owing to the disciplinary models being managed by separate entities or housed in separate locations, analysis capabilities running on different computational platforms, models with significantly different analysis run times, and the sheer number of disciplines required for a given analysis. Further, it is also often the case for such systems to exhibit feedback couplings, which can lead to computationally prohibitive expense for uncertainty analysis tasks. To ensure confidence in results obtained by such coupled system models, uncertainty must be completely and rigorously quantified. Thus, there is a need to alleviate the computational burden of multidisciplinary uncertainty analysis in coupled systems composed of integrated disciplinary models. This was achieved by moving most of the computational expense of multidisciplinary uncertainty analysis to an offline phase, that can be conducted whenever there is the opportunity to do so. The key advantage of the proposed approach is that there is no need to do system level uncertainty analysis, and all the disciplinary analyses can be performed independently in the offline process. Offline data is used in an online process that does not require any further model evaluations or any system level analysis. The approach is demonstrated on a coupled aerodynamics-structures

system with model discrepancies.

So, the first objective of this thesis which was formulating the problem of propagating uncertainty through a coupled system is achieved by the use of Gibbs sampling to sample from the conditional distributions of each discipline conditioned on the output of the other discipline. The other objective which was to create an efficient methodology for propagating the uncertainty is achieved by the use of sequential importance resampling which allows to modify the offline information intelligently without rerunning the models, and the last objective is achieved by demonstrating the methodology on a coupled aerodynamics-structures system which was used in Ref. 2 to demonstrate the global sensitivity equations for coupled systems.

In future research, the approach needs to be extended to systems with parametric uncertainty, and also some methods need to be investigated for adaptively introducing new samples online, for situations where proposals are inadequately capturing targets.

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**APPENDIX A**  
**MISCELLANEOUS**

**Aerodynamics-Structures System**

**Aerodynamics Model**

$$L = q \cdot S \cdot C_L$$

$$\theta = \phi + \psi$$

$$C_L = u\theta + r[1 - \cos[(\pi/2)(\theta/\theta_0)]]$$

**Structures Model**

$$R_1 = L/(1+p) \quad R_2 = Lp/(1+p)$$

$$d_1 = R_1/k_1 \quad d_2 = R_2/k_2$$

$$\phi = (d_1 - d_2)/[C \cdot (\bar{z}_2 - \bar{z}_1)]$$

**Data**

$$\bar{z}_1 = z_1/C \quad \bar{z}_2 = z_2/C \quad \bar{a} = a/C$$

$$\bar{h}_1 = \bar{a} - \bar{z}_1 \quad \bar{h}_2 = \bar{z}_1 - \bar{a} \quad p = \bar{h}_1/\bar{h}_2$$

$$S = B \cdot C$$

$$B = 100 \text{ cm}; \quad C = 10 \text{ cm}; \quad \bar{z}_1 = 0.2; \quad \bar{z}_2 = 0.7$$

$$k_1 = 4000 \text{ N/cm}; \quad k_2 = 2000 \text{ N/cm}$$

$$\bar{a} = 0.25; \quad q = 1 \text{ N/cm}^2; \quad \theta_0 = 0.26 \text{ rad}; \quad \psi = 0.05 \text{ rad}$$

$$u = 2\pi; \quad r = 0.9425$$