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QUANTIFYING MODEL DISCREPANCY IN COUPLED MULTI-PHYSICS SYSTEMS

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ABSTRACT

Current design strategies for multi-physics systems seek to exploit synergistic interactions among disciplines in the system. However, when dealing with a multidisciplinary system with multiple physics represented, the use of high-fidelity computational models is often prohibitive. In this situation, recourse is often made to lower fidelity models that have potentially significant uncertainty associated with them. We present here a novel approach to quantifying the discipline level uncertainty in coupled multi-physics models, so that these individual models may later be used in isolation or coupled within other systems. Our approach is based off of a Gibbs sampling strategy and the identification of a necessary detailed balance condition that constrains the possible characteristics of individual model discrepancy distributions. We demonstrate our methodology on both a linear and nonlinear example problem.

1 INTRODUCTION

Complex, multi-physics systems, such as aerospace vehicles, often exhibit a great deal of uncertainty due to unexpected multi-physics interactions. To achieve greater performance, the design of such systems is usually aimed at exploiting these potential synergistic interactions. For this situation, it is often desired that high-fidelity computational models capable of precisely representing multi-physics interactions be used early in the design process. Typically, however, such models will carry significant computational expense. Recent work has thus focused on multi-fidelity approaches to the design and analysis of complex, multi-physics systems [1–3]. In general, for a particular design or analysis task, there will be many computational models that can be used to compute various quantities of interest in a multi-physics system. These computational models will generally vary in terms of fidelity because they will encompass different resolutions, physics, and modeling assumptions. These models will also vary in terms of computational expense. The goal then of multifidelity approaches in the design and analysis of complex multi-physics systems is to optimally exploit all available computational models for the task at hand. A critical aspect for enabling such multifidelity approaches is the rigorous quantification of uncertainty associated with the modeling capabilities themselves.

Multi-physics systems, such as aerospace systems, are often designed and developed by multiple teams within a given organization or set of organizations. As a result, the simulation of complex, multi-physics phenomena usually involves the execution of coupled disciplinary computational models. Such simulations can be computationally demanding, and recourse to lower fidelity models may be necessary. In these circumstances, the uncertainty, or model discrepancy, associated with each disciplinary model must be propagated through the coupled system. To ensure sufficiently reliable and robust estimates of quantities of interest in the system, rigorous quantification of the model discrepancy in the discipline level computational models used in coupled multi-physics simulations is essential. This is particularly important in the multifidelity setting, where we may desire

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to improve the fidelity of one discipline (e.g., by introducing a higher fidelity model) while keeping the fidelity of other modeling capabilities in the system fixed. For example, in the design of an aircraft wing, we may determine that aspects associated with a structural model are more important at a certain stage in the design process, so we use our computational budget to improve the structures model while keeping an aerodynamics model at lower fidelity.

In this paper we propose to estimate the model discrepancy of discipline level models within coupled multi-physics systems. We propose to do this by considering system level uncertainty information that is often available from experiments and historical databases (e.g., Jane's All the World's Aircraft [4] for the case of aerospace vehicles). From system level uncertainty information, we identify compatible discipline level uncertainty information pertaining to the individual models. By quantifying discipline level uncertainty, we enable the use of different couplings of multifidelity models as we seek to efficiently explore the design space. The rest of the paper is organized as follows: In Section 2, we present background on model discrepancy in coupled multi-physics systems. In Section 3, we setup the problem we use to demonstrate our methodology in this work. We follow this with a description of our problem statement in Section 4 and our methodology for solving our problem statement in Section 5. Section 6 then provides both a linear and nonlinear demonstration of our model discrepancy quantification procedure. Finally, conclusions and future work are presented in Section 7.

2 BACKGROUND

Model discrepancy arises because, even if all inputs and parameters of a mathematical model are known precisely, the mathematical model will not precisely estimate reality. The reason for this is that some aspects of reality may have been omitted, improperly modeled, or contain unrealistic assumptions. Following Ref. 5, we represent model discrepancy 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

$$\delta(\mathbf{x}) = f_r(\mathbf{x}) - f(\mathbf{x}), \tag{1}$$

where here we are assuming there are no parameters in the model to be calibrated. Typically, we will have available experimental data of reality (which will contain experimental variability), which can be used to create a stochastic process representation for $\delta(\mathbf{x})$. In this work, we assume that model discrepancy has been quantified previously for all available disciplinary models in the form of Gaussian processes. Thus, we add the Gaussian process model discrepancy term to the output of a disciplinary model. For example, for a given disciplinary model we have

$$Y(\mathbf{x}) = f(\mathbf{x}) + \delta(\mathbf{x}), \tag{2}$$

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

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. Previous work on multidisciplinary uncertainty analysis has focused on approximate methods, 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 [6]. 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 [7]. These approachs include implicit uncertainty propagation [8], reliability-based design optimization [9], robust moment matching [10–12], advanced mean value method [13], collaborative reliability analysis using most probable point estimation [14], and a multidisciplinary first-order reliability method [15].

Other recent work has focused on exploiting the structure of a given multidisciplinary system. Ref. 16 presents a likelihood-based approach to decouple feedback loops, thus reducing the problem to a feed-forward system. Ref. 17 builds off the likelihood-based approach and incorporates an auxiliary variable approach based on the probability integral transform to quantify the distributions of coupling variables. 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 [18–20]. Coupling disciplinary models by representing coupling variables with truncated Karhunen-Loève expansions, has been studied for multi-physics systems [21]. A hybrid method that combines Monte Carlo sampling and spectral methods for solving stochastic coupled problems has also been proposed by Refs. 22 and 23.

In our approach we focus on sample based propagation of uncertainty through the coupled system. As discussed in the following section, our coupled system is modeled as a Markov Chain, and uncertainty is propagated through the system via Gibbs sampling. This approach is similar in concept to the use of fixed point iteration to ensure compatibility of coupling variables in a deterministic sense. Under the presence of model discrepancy, we seek compatibility in the coupling variables in a distributional sense.

3 PROBLEM SETUP

To demonstrate our sample based approach to quantifying discipline level model discrepancy in coupled multi-physics systems, we consider a two discipline system model with feedback coupling. This system is shown notionally in Fig. 1. The disciplines are represented by the functions $f(z)$ and $g(y)$. The model discrepancies are independent, normally distributed random variables, where $\delta_1 \sim \mathcal{N}(0,\sigma_1^2)$ and $\delta_2 \sim \mathcal{N}(0,\sigma_2^2)$. Here we are assuming that the model discrepancies are unbiased. This is due to our assumption that the discrepancies do not vary as a function of any variable in the system. Thus any bias in a given discrepancy term would be added to the associated model itself. The unbiased nature of the discrepancy terms can easily be relaxed if necessary.

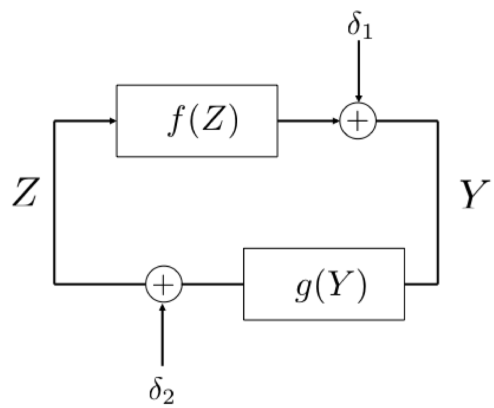

FIGURE 1. THE COUPLED TWO DISCIPLINE SYSTEM WITH MODEL DISCREPANCY

The goal of our work is to rigorously quantify the model discrepancies δ_1 and δ_2, using available system level information. That is, we wish to find δ_1 and δ_2 such that we can uncoupled the system and use our computational models, f and g, with their associated model discrepancies in other contexts (e.g., when coupled with other modeling capabilities or in isolation). This concept is shown notionally in Fig. 2. Our approach is based off of the assumption of the availability of a system level quantity of interest, for example, $Q(Y,Z)$, where the quantity is a function of the coupling variables. We aim to identify δ_1 and δ_2 such that the joint distribution of Y, and Z that results from resolving the system shown in Fig. 1, provides a close approximation to the real-world quantity of interest when passed through Q. Without loss of generality, in this work we will assume the quantity of interest from the system that we have real-world data for is one of the coupling variables (i.e., Z or Y). The conditional distributions of Y and Z that result from the coupled system are

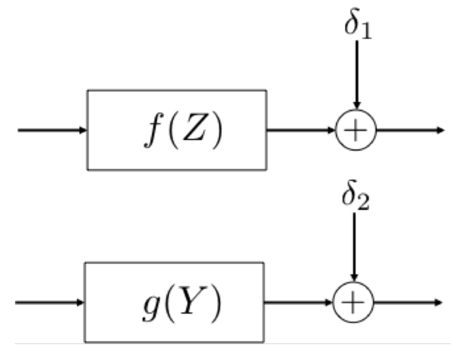

FIGURE 2. THE UNCOUPLED DISCIPLINES WITH ASSOCIATED MODEL DISCREPANCY.

$$Y = f(Z) + \delta_1 \tag{3}$$

$$Z = g(Y) + \delta_2. \tag{4}$$

The propagation of uncertainty through the coupled system can then be represented as a Markov chain that moves from one disciplinary output to the next. We represent this concept in Fig. 3, where we also present the concept of stopping the Markov chain at different points in the system. In the top portion of the figure, we stop the chain after evaluating $f(Z)$ and adding the associated discrepancy, δ_1. In the bottom portion, we stop the chain after evaluating $g(Y)$ and adding the associated discrepancy, δ_2. For a unique joint distribution of Y and Z, which we denote as $p_{Y,Z}(y,z)$, we require that the distributions of Y and Z be the same at either stopping point.

This leads to a set of general compatibility requirements that must be satisfied to ensure we have a unique distribution, $p_{Y,Z}(y,z)$. First, we may write the relation shown by the last two steps of the chain in the top portion of Fig. 3 as

$$Y = f(g(Y) + \delta_2) + \delta_1, \tag{5}$$

and the relation shown by the last two steps of the bottom portion of the figure as

$$Z = g(f(Z) + \delta_1) + \delta_2. \tag{6}$$

This establishes two requirements for compatibility. A third and crucial requirement, as will be demonstrated in Section 6, arises

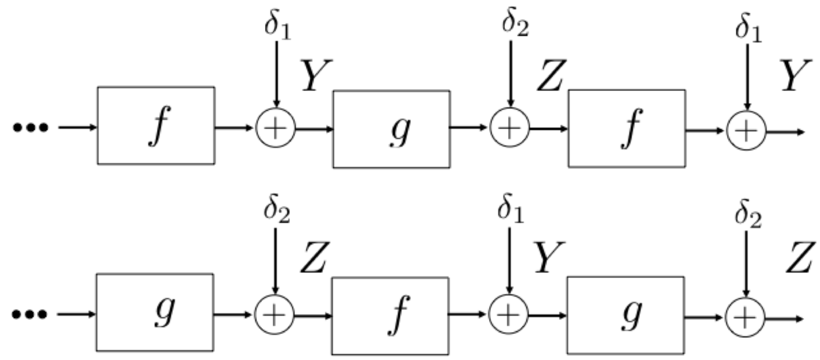

FIGURE 3. MARKOV CHAIN REPRESENTATION OF THE PROPAGATION OF UNCERTAINTY THROUGH A TWO DISCIPLINE FEEDBACK COUPLED SYSTEM.

from the definition of conditional probability [24]. Enforcing the same joint distribution of Y and Z in the top and bottom portion of Fig. 3 is equivalent to stating we require detailed balance to hold [25]. The condition is given as

$$p_{Y,Z}(y,z) = p_{Y|Z}(y,z)p_Z(z) = p_{Z|Y}(z,y)p_Y(y), \tag{7}$$

which is a probabilistic assertion that it should not matter where we stop the Markov chain in the propagation of uncertainty through the coupled system.

4 PROBLEM STATEMENT

In the context of the coupled system shown in Fig. 1, our problem is to find the distributions of δ_1 and δ_2, such that the joint distribution $p_{Y,Z}(y,z)$, produces accurate estimates of the system level quantity of interest, $Q(Y,Z)$, and satisfies Eqns. (5), (6), and (7). We note here that our two discipline coupled system is used for ease of the presentation, and is not a restriction on our approach. More disciplines can be added to our system with more complex couplings and still be adequately addressed by our approach described in Section 5.

In a general sense, the problem we seek a solution for may be written as,

$$\begin{aligned} (\sigma_1^*,\sigma_2^*) = \underset{\sigma_1,\sigma_2}{\arg\min} \quad & \mathscr{J} = \mathscr{D}_s(Q_r \| \hat{Q}(Y,Z)) + \\ & \mathscr{D}_s(p_{Y|Z}(y,z)p_Y(y) \| p_{Z|Y}(z,y)p_Z(z)) \\ \text{subject to} \quad & \sigma_1,\sigma_2 > 0. \end{aligned} \tag{8}$$

Here $\mathscr{D}_s(\cdot,\cdot)$ denotes a generic statistical distance measure (e.g., Kullback-Liebler divergence, Hellinger distance, sum of the squares of the differences in sufficient statistics, etc. [26]). Also in Problem 8, Q_r is the real-world estimated distribution of a quantity of interest and $\hat{Q}$ is the estimate of that quantity of interest from the joint distribution of Y and Z. In the following section we present a general methodology for finding the solution to Problem 8 under specific assumptions about Q_r.

5 METHODOLOGY

We approach the solution of Problem 8 by first recognizing that information regarding a real-world quantity of interest, Q_r, is often gathered experimentally and presented as a normal distribution. In this setting, sufficient statistics for Q_r are then the moments of the distribution. Without loss of generality, we assume that the quantity of interest we have available information for is Z. Thus, we have an approximation of the distribution of Z_r, the real-world random variable Z, which we assume is $Z_r \sim \mathscr{N}(\mu_{Z_r}, \sigma_{Z_r}^2)$. Our methodology is also based on a variational approach, where we seek a compatible multivariate normal distribution for $p_{Y,Z}(y,z)$, such that Problem 8 is solved. For the case of linear disciplines, normally distributed discrepancies, and normally distributed Z_r, this approach is exact. For the nonlinear case, this variational approach results in approximate solutions. An analysis of the impact of this assumption is a topic for future work.

Given our assumptions, we rewrite $\mathscr{J}$ in Problem 8 as

$$\mathscr{J}(\sigma_1,\sigma_2) = |\mu_{Z_r} - \mu_{\hat{Z}}| + |\sigma_{Z_r} - \sigma_{\hat{Z}}| + \|S_{Y|Z,Z} - S_{Z|Y,Y}\|, \tag{9}$$

where $\hat{Z}$ refers to the Z estimated by our sample based approach (described below), and S represents the sufficient statistics of a given distribution. For $p_{Y|Z,Y} = p_{Y|Z}p_Z$, these are the means and covariance matrix of the joint distribution. The same holds for $p_{Z|Y,Z} = p_{Z|Y}p_Y$.

With this objective function, we search for solutions using standard off-the-shelf optimization routines (e.g., pattern search) coupled with an uncertainty propagation methodology. This concept is shown notionally in Fig. 4, where the analysis block represents our uncertainty propagation approach through a coupled system.

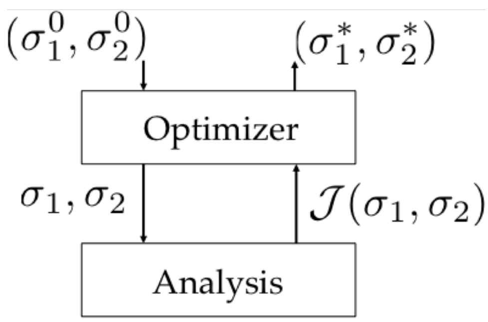

FIGURE 4. GENERAL APPROACH TO SOLVING PROBLEM 8.

To propagate uncertainty through the system represented by Fig. 1, and hence to evaluate $\mathcal{J}$ in Eqn. 9, we recognize the Markov chain nature of the system and the availability of the conditional distributions of $Y|Z$ and $Z|Y$. This enables us to use the Gibbs sampling algorithm to iteratively sample from the conditional distributions. Gibbs sampling was first described by Ref. 25 and has also been referred to as successive substitution sampling [27]. It is a Markov chain Monte Carlo based method for generating samples from a joint distribution that cannot be directly sampled. Following Refs. 27 and 28, suppose we have random variables $Y_1,\ldots,Y_k$, and we wish to generate samples from the joint distribution of those random variables, which we denote as $p_{Y_1,\ldots,Y_k}$. Assume we have a complete set of conditional distributions, $p_{Y_i|\{Y_j, j\neq i\}}$ for $i = 1,\ldots,k$, available for sampling. Then, starting from some initial arbitrary set of values, $y_1^{(0)},\ldots,y_k^{(0)}$, where the superscript denotes the iteration number of the Gibbs sampler, we draw a sample $y_1^{(1)}$ from $p_{Y_1|Y_2=y_2^{(0)},\ldots,Y_k=y_k^{(0)}}$. We then draw a sample $y_2^{(1)}$ from $p_{Y_2|Y_1=y_1^{(1)},Y_3=y_3^{(0)},\ldots,Y_k=y_k^{(0)}}$, and continue in this manner up to y_k from $p_{Y_k|Y_1=y_1^{(1)},\ldots,Y_{k-1}=y_{k-1}^{(1)}}$, which completes one iteration of the Gibbs sampler. After m iterations we obtain $(y_1^{(m)},\ldots,y_k^{(m)})$. For continuous distributions, Ref. 27 has shown, under mild assumptions, that this k-tuple converges in distribution to a random observation from $p_{Y_1,\ldots,Y_k}$ as $m \to \infty$.

The algorithm we use for our two discipline case is shown in Algorithm 1. In this algorithm, the subscript, t refers to the top Markov chain in Fig. 3 and the subscript, b, refers to the bottom Markov chain in the same figure. We recall here that for compatibility, these Markov chains must arrive at the same stationary distribution to ensure detailed balance is satisfied. In the algorithm, we are free to set the number of samples, M, of the joint distributions, which we use to estimate the sufficient statistics. We also must set a burn-in rate for the Markov chain Monte Carlo Gibbs sampling method, which refers to the number of samples we initially throw away to avoid autocorrelation in the samples [26]. In this work we set $M = 10,000$ and $B = 4,000$. The computational expense of our modeling capabilities in our demonstrations was negligible, thus, we oversampled to ensure converged results. It is a topic of future work to determine how to best select the parameters, M and B.

ALGORITHM 1: GIBBS SAMPLING FOR UNCERTAINTY PROPAGATION

Data: Model discipline functions $f(z)$ and $g(y)$, discrepancy standard deviations σ_1 and σ_2, number of samples M, Burn-in, B.
Result: Joint densities $P_{Z|Y,Y}$ and $P_{Y|Z,Z}$.

for $i = 1 : M$ **do**
  Initialize $y_t^{(0)} = y_b^{(0)} = z_t^{(0)} = z_t^{(0)} = 0$.
  for $j = 1 : B$ **do**
    Let $z_t^{(j)} = g(y_t^{(j-1)}) + \delta_2^{(j)}$
    Let $y_t^{(j)} = f(z_t^{(j)}) + \delta_1^{(j)}$
    Let $y_b^{(j)} = f(z_b^{(j-1)}) + \delta_1^{(j)}$
    Let $z_b^{(j)} = g(y_b^{(j)}) + \delta_2^{(j)}$
  end
  Let $y_t^i = y_t^{(B)}$
  Let $z_t^i = z_t^{(B)}$
  Let $y_b^i = y_t^{(B)}$
  Let $z_b^i = z_t^{(B)}$
end
Estimate the sufficient statistics of $p_{Z|Y,Y}$ from $\{y_t^i, z_t^i\}_{i=1}^M$
Estimate the sufficient statistics of $p_{Y|Z,Z}$ from $\{y_b^i, z_b^i\}_{i=1}^M$

We couple our uncertainty propagation algorithm with a pattern search based optimization routine to search the space of possible σ_1 and σ_2 values that are compatible and lead to an accurate estimate of Z_r sufficient statistics. In the following section we present our results for a linear and nonlinear demonstration case.

6 ANALYSIS

We present in this section, an analytic solution to the linear case to provide a clear description of what we are seeking to accomplish in terms of compatibility of the discrepancy terms. Here we show both a compatible and an incompatible solution. We then demonstrate our numerical approach using Gibbs sampling on a nonlinear problem.

6.1 Linear Case

For the linear case, we define two disciplines as

$$f(z) = az + b \tag{10}$$
$$g(y) = cy + d \tag{11}$$

with $a,b,c,d \in \mathbb{R}$. Furthermore, we define the outputs for these disciplines with model discrepancy as

$$Y = f(Z) + \delta_1 \tag{12}$$
$$Z = g(Y) + \delta_2 \tag{13}$$

where Z is the input to f and Y is the input to g. Since our disciplines $f(Z)$ and $g(Y)$ are linear, we can analytically evaluate the marginal conditional probability distributions to find the conditions under which compatibility, as described by Eqn. (7) is satisfied. Although we are assuming that the discrepancies δ_1 and δ_2 are unbiased, we maintain the μ_1 and μ_2 variables for completeness. Since the discrepancies and the functions are linear, the marginal distributions are normally distributed and given by

$$Z \sim \mathcal{N}(\mu_Z, \sigma_Z^2)$$
$$Y \sim \mathcal{N}(\mu_Y, \sigma_Y^2).$$

The conditional distributions are also normally distributed and are given by

$$Y \mid \{Z = z\} \sim \mathcal{N}(az + b + \mu_1, \sigma_1^2) \tag{14}$$
$$Z \mid \{Y = y\} \sim \mathcal{N}(cy + d + \mu_2, \sigma_2^2). \tag{15}$$

Our task is then to find μ_Z, σ_Z, μ_Y, and σ_Y. Here, we are not yet considering a specific Z_r, and are instead looking to derive conditions on σ_1 and σ_2 for any Z_r.

The first step we take is to find the conditions such that the system will converge, which is to satisfy Eqns. (5) and (6). Once the marginal distributions converge, the distributions of Z and Y cannot change between each iteration. We begin by finding implicit equations for Z and Y following the output once around the loop shown in Fig. 1 to arrive at

$$Z = g(f(Z) + \delta_1) + \delta_2 = c(az + b + \delta_1) + d + \delta_2$$
$$Y = f(g(Y) + \delta_2) + \delta_1 = a(cy + d + \delta_2) + b + \delta_1.$$

By inspection, the statistics of the distribution for Z are

$$\mu_Z = c(a\mu_Z + b + \mu_1) + d + \mu_2 \tag{16}$$
$$\sigma_Z^2 = c^2(a^2\sigma_Z^2 + \sigma_1^2) + \sigma_2^2. \tag{17}$$

By rearranging Eqns. 16 and 17 we have

$$\mu_Z = \frac{c(b + \mu_1) + d + \mu_2}{1 - ac}$$
$$\sigma_Z^2 = \frac{c^2\sigma_1^2 + \sigma_2^2}{1 - a^2c^2}$$

Since by definition $\sigma_Z, \sigma_1, \sigma_2 > 0$, then

$$1 - a^2c^2 > 0$$
$$\implies ac < 1. \tag{18}$$

This condition ensures that the marginal distributions do not grow without bound.

Continuing the analysis, for any independent and normally distributed δ_1 and δ_2, we can also find the conditional probability density functions for Eqns. (14) and (15), which we write as

$$p_{Y|Z}(y,z) = \frac{1}{\sqrt{2\pi}\sigma_1} \exp\left\{ -\frac{1}{2}\left(\frac{y - (az + b + \mu_1)}{\sigma_1}\right)^2 \right\}$$
$$p_{Z|Y}(z,y) = \frac{1}{\sqrt{2\pi}\sigma_2} \exp\left\{ -\frac{1}{2}\left(\frac{z - (cy + d + \mu_2)}{\sigma_2}\right)^2 \right\}.$$

Then the product of the conditional densities and the marginal densities yields the joint densities as

$$P_{Y|Z}(y,z)P_Z(z) = (2\pi\sigma_1\sigma_Z)^{-1} \exp\left\{ -\frac{1}{2}\left[\left(\frac{y - (az + b + \mu_1)}{\sigma_1}\right)^2 + \left(\frac{z - \mu_z}{\sigma_z}\right)^2\right] \right\} \tag{19}$$

$$P_{Z|Y}(z,y)P_Y(y) = (2\pi\sigma_2\sigma_Y)^{-1} \exp\left\{ -\frac{1}{2}\left[\left(\frac{z - (cy + d + \mu_2)}{\sigma_2}\right)^2 + \left(\frac{y - \mu_Y}{\sigma_Y}\right)^2\right] \right\}. \tag{20}$$

Equations (19) and (20) are the joint densities associated with our linear system and the top and bottom of Fig. 3. Detailed balance requires that these joint distributions be equal to each other. Therefore, the arguments of each exponent must be equal to each other. This leads to

$$\left(\frac{y-(az+b+\mu_1)}{\sigma_1}\right)^2+\left(\frac{z-\mu_z}{\sigma_z}\right)^2= \left(\frac{z-(cy+d+\mu_2)}{\sigma_2}\right)^2+\left(\frac{y-\mu_Y}{\sigma_Y}\right)^2. \quad (21)$$

Carrying through the multiplication and comparing the coefficients of the terms y^2, z^2, yz, y, and z we find the conditions required for detailed balance. For the case of a linear system, the conditions we require are that given by Eqn. (18) and the following condition:

$$\frac{-2a}{\sigma_1^2}=\frac{-2c}{\sigma_2^2}$$
$$\implies \frac{\sigma_1^2}{\sigma_2^2}=\frac{a}{c}. \quad (22)$$

As long as the ratio of variances to our model discrepancies abide by Eqn. (22), then detailed balance will hold between our resulting design variables.

To demonstrate the difference in joint densities with and without detailed balance, we compute two examples of this linear case in which $a=1/4$, $b=1$, $c=1$, and $d=-2$. From Eqn. (18), we know that the Gibbs sampler will converge. We draw 10,000 samples and run the Gibbs sampler as presented in Algorithm 1 using two different pairs of discrepancy variances. First, we let $\sigma_1^2=1$ and $\sigma_2^2=1/2$. Since $\sigma_1^2/\sigma_2^2\neq a/c$, the joint densities do not meet the detailed balance condition. Using our algorithm to produce samples in this case results in the scatterplots shown in Fig. 5. As can clearly be seen from the figure, the joint distributions that result from stopping a different point in the Markov chain are not the same.

To demonstrate the importance of the detailed balance condition, we perform our Gibbs sampling procedure with $\sigma_1^2=1/4$ and $\sigma_2^2=1$. The results of this analysis are shown in Fig. 6. From visual inspection of the figure, it is clear that these scatterplots represent the same joint density functions. In this case, $\sigma_1^2/\sigma_2^2=a/c$. Quantitative evidence of the importance of the detailed balance condition are presented in Tab. 1, where the sufficient statistics of the distributions are presented for both the without detailed balance (Without DB) and with detailed balance (With DB) satisfied cases. These statistics correspond to Figs. 5 and 6, respectively.

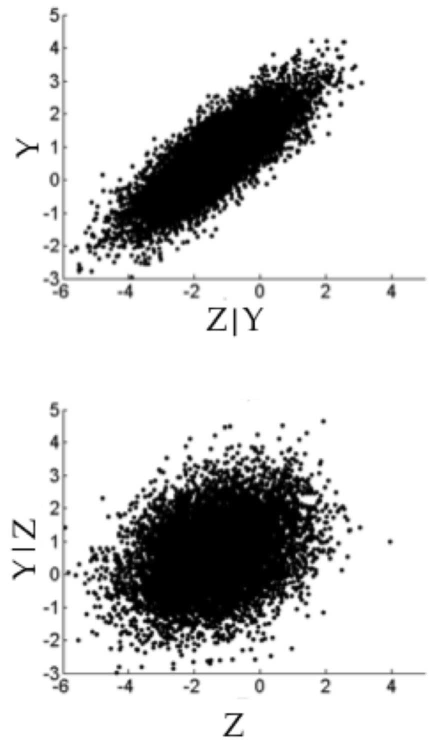

FIGURE 5. LINEAR DISCIPLINE JOINT DENSITIES WITHOUT DETAILED BALANCE

TABLE 1. LINEAR DISCIPLINE JOINT DENSITY STATISTICS

Statistic	Without DB.	With DB.
μ_Z	-1.32520	-1.31487
$\mu_{Z\|Y}$	-1.32963	-1.32518
μ_Y	0.66374	0.67129
$\mu_{Y\|Z}$	0.66241	0.67155
σ_Z^2	1.60245	1.31144
$\sigma_{Z\|Y}^2$	1.60549	1.31786
σ_Y^2	1.09224	0.32569
$\sigma_{Y\|Z}^2$	1.09772	0.33019
$\rho(Z,\, Y\mid Z)$	0.82719	0.49711
$\rho(Y,\, Z\mid Y)$	0.29484	0.50401

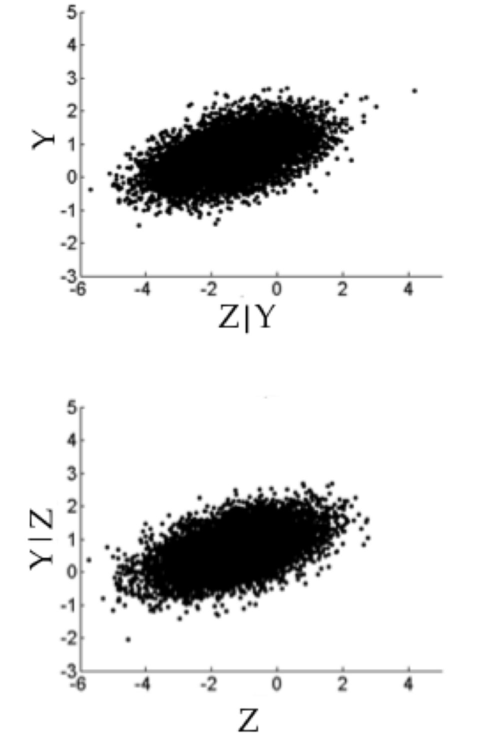

FIGURE 6. LINEAR DISCIPLINE JOINT DENSITIES WITH DETAILED BALANCE

We end the discussion of the linear case by noting that if we had information about a system level quantity of interest, Q_r, here related to Z for example, we could ensure that we match the statistics of the system level quantity of interest by simply matching the statistics of Z. For a more complex quantity of interest, say something that is a function of Z and Y, we could proceed with our optimization approach described in Section 5.

6.2 Nonlinear Case

The nonlinear example problem we use to demonstrate our method for quantifying model discrepancy in a coupled multi-physics system is a two-dimensional airfoil in airflow from Ref. 29 and shown in Fig. 7. As described in Ref. 29, the airfoil 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, ϕ, are the coupling variables and also the outputs in this system. A complete description of the problem can be found in Ref. 29 and for the sake of completeness, the equations and variable values are presented in the appendix.

For this demonstration, we assume we have real-world data regarding the lift of the airfoil. This information suggests that the distribution of the lift is, $L_r \sim \mathcal{N}(502, 345)$, where the units

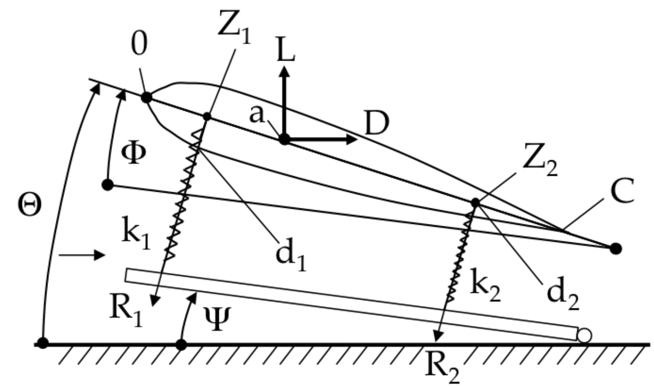

FIGURE 7. SIMPLE COUPLED AERODYNAMICS-STRUCTURES SYSTEM ADAPTED FROM REF. 29.

are in Newtons. Using Algorithm 1, coupled with an optimization routine, we solve Problem 8, with $\mathscr{J}$ set as in Eqn. (9). The results of this process are shown in Fig. 8. The figure presents scatterplots of the joint distributions arrived at by stopping after the aerodynamics model and after the structures model respectively. By inspecting the figures, we see that the detailed balance condition has resulted in joint densities that are approximately the same. We present quantitative results of the statistics of the coupling variables, L and Φ, as well as the values of the discrepancy variances, σ_1 and σ_2, in Tab. 2. Here we see that the normal distribution of L approximated by our method is approximately the same as that of the real-world data associated with that quantity of interest. We further note that, though this system is nonlinear, our variational approach, staying with the family of normal distributions, is still able to ensure approximate satisfaction of detailed balance and match the real-world information. A more careful look at the limitations associated with assumed normality in the coupling variables is a topic of future work.

7 CONCLUSIONS

We have presented an approach to quantifying model discrepancy in disciplinary models of coupled multi-physics systems using system level discrepancy information. Our approach was based on a Gibbs sampling procedure and our analysis revealed the significance of considering a detailed balance condition in our Markov chain model of uncertainty propagation through a coupled system. We employed a variational approach to quantifying model discrepancy in disciplinary outputs and assumed the discrepancies and the coupling variables to be normally distributed. Our results for a nonlinear, feedback coupled system suggest that there are times when these assumptions are reasonable. It is a topic of future work to examine when assumptions of normality are too restrictive.

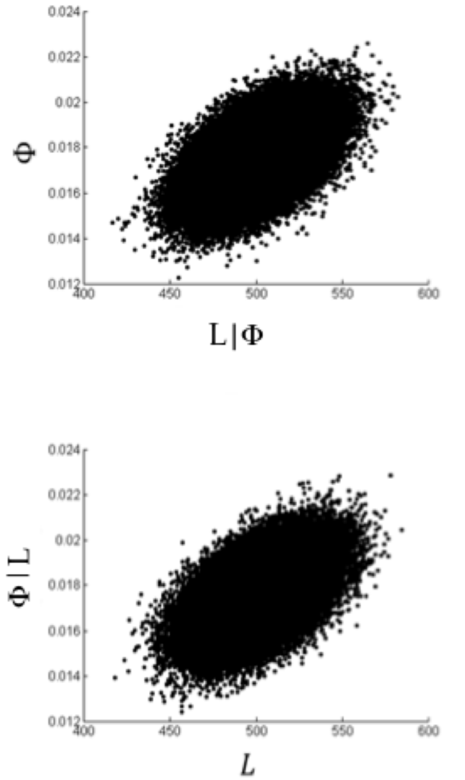

FIGURE 8. AERODYNAMICS-STRUCTURES NONLINEAR DISCIPLINE JOINT DENSITIES WITH DETAILED BALANCE

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TABLE 2. AERODYNAMICS-STRUCTURES DISCIPLINE JOINT DENSITY STATISTICS

Statistic	Result of Our Methodology
σ_1^2	242.9290
σ_2^2	9.968973e-7
μ_L	502.0375
$\mu_{L\|\Phi}$	502.0473
μ_Φ	0.01757051
$\mu_{\Phi\|L}$	0.01757442
σ_L^2	347.59021
$\sigma_{L\|\Phi}^2$	349.94898
σ_Φ^2	1.4276724e-6
$\sigma_{\Phi\|L}^2$	1.4263481e-6
$\rho\big(L, (\Phi \mid L = l)\big)$	0.54807928
$\rho\big(\Phi, (L \mid \Phi = \phi)\big)$	0.54944618

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Appendix A: Aerodynamics-Structures System

Aerodynamics Model

$$L = qSC_L$$
$$\theta = \phi + \psi$$
$$C_L = u\theta + r\Big[1 - \cos\big[(\pi/2)(\theta/\theta_0)\big]\Big]$$

Structures Model

$$R_1 = L/(1+p) \qquad R_2 = Lp/(1+p)$$
$$d_1 = R_1/k_1 \qquad d_2 = R_2/k_2$$
$$\phi = (d_1 - d_2)/[C(\overline{z_2} - \overline{z_1})]$$

Aerodynamics-Structures Data

$\bar{z}_1 = z_1/C$	$\bar{z}_2 = z_2/C$	$\bar{a} = a/C$
$\bar{h}_1 = \bar{a} - \bar{z}_1$	$\bar{h}_2 = \bar{z}_1 - \bar{a}$	$p = \bar{h}_1/\bar{h}_2$
$S = BC$	$B = 100\,\mathrm{cm}$	$C = 10\,\mathrm{cm}$
$\bar{z}_1 = 0.2$	$\bar{z}_2 = 0.7$	$k_1 = 4000\,\mathrm{N\,cm^{-1}}$
$k_2 = 2000\,\mathrm{N\,cm^{-1}}$	$\bar{a} = 0.25$	$q = 1\,\mathrm{N\,cm^{-2}}$
$\theta_0 = 0.26\,\mathrm{rad}$	$\psi = 0.05\,\mathrm{rad}$	$u = 2\pi$
$r = 0.9425$		