Quantifying the Impact of Different Model Discrepancy Formulations in Coupled Multidisciplinary Systems

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In this paper, we quantify the impact of different formulations of model discrepancy propagation in coupled multidisciplinary systems. Standard Gaussian process formulations of model discrepancy leave room for interpretation when incorporated into coupled system analyses. The objective of this work is to analyze resulting coupling variable distributions under different assumptions regarding these model discrepancy interpretations. The goal is to identify efficient, implementation independent, methods and rationale for the rigorous propagation of uncertainty in coupled systems. We demonstrate our methodology on an aerostructural wing analysis problem.

I. Introduction

The rise in complexity of engineering systems and the drive towards increasing performance has led to new challenges associated with uncertainty quantification. These challenges are the result of using imperfect models to analyze coupled systems in an effort to exploit interactions among disciplines. To ensure confidence in results obtained by such coupled system models, uncertainty must be completely and rigorously quantified. As described in Ref. 1, sources of uncertainty in such systems typically include parametric uncertainty, which involves uncertainty associated with model input parameters, parametric variability, which generally refers to variation that cannot be controlled (e.g., operating conditions), code uncertainty, which refers to the uncertainty associated with interpolating between known system responses, and model discrepancy, which is uncertainty associated with the fact that no model is perfect. It is this last form of uncertainty, model discrepancy, that poses the most significant challenges in coupled systems.

Multidisciplinary systems, such as aerospace systems, are often composed by integrating pre-existing disciplinary physics-based models. These complex, multi-physics systems also often exhibit feedback coupling between disciplines. In these systems, each disciplinary model has associated uncertainty that can have a substantial impact on system level uncertainty analysis results. A key challenge in these circumstances is the rigorous propagation of uncertainty through such systems in a manner that is not dependent on the implementation strategy chosen to resolve coupling variables (e.g., fixed point iteration in a deterministic setting takes on different meaning under uncertainty that may not be physically relevant). In this paper, the model discrepancy pertaining to each disciplinary model, which is the difference between the reality and simulation, is formulated as Gaussian process. The objective of our work is to analyze the resulting coupling distributions that arise given different assumptions regarding correlation in the model discrepancy terms. In the extremes, model discrepancy can either be viewed as independent, identically distributed (i.i.d.) noise that is passed back and forth in a coupled multidisciplinary system, or as a forcing term that is added outside of a fixed point iteration. We identify compatible discipline level uncertainty information pertaining to the individual models. By quantifying discipline level uncertainty, we study these extreme interpretations of model discrepancy formulations, as well as every formulation "in-between" these extremes. By using Gaussian process models of discrepancy, we accomplish this by varying the correlation length parameter for given discrepancy terms. With infinite correlation length, we arrive at the forcing term extreme. With zero correlation length, we arrive at the i.i.d. noise extreme.

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The rest of the paper is organized as follows. Section II presents background on related work. In Section IV, the approach is described. In Section V, we present results. In Section VI we describe our future work on this topic, and conclusions are drawn in Section VII.

II. Background

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.[2] These approaches include implicit uncertainty propagation,[3] reliability-based design optimization,[4] robust moment matching,[5–7] advanced mean value method,[8] collaborative reliability analysis using most probable point estimation,[9] and a multidisciplinary first-order reliability method.[10]

Other recent work has focused on exploiting the structure of a given multidisciplinary system. Ref. 11 presents 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.[12–14] Coupling disciplinary models by representing coupling variables with truncated Karhunen-Loève expansions, has been studied for multi-physics systems.[15] Refs. 16 and 17 have proposed a hybrid method that combines Monte Carlo sampling and spectral methods for solving stochastic coupled problems. Refs. 18 and 19 dealt with the challenges of uncertainty analysis for feed-forward multidisciplinary systems using a decomposition-based approach. Our earlier work[20] developed a compositional multidisciplinary uncertainty analysis methodology for systems with feedback couplings, and model discrepancy by incorporating aspects of importance resampling, density estimation, and Gibbs sampling.

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,[21] physics-based deterministic function,[22] Gaussian random variable[20,23] which can be with fixed or input-dependent mean and variance, uncorrelated random vector,[24] random walk,[21] and Gaussian random process.[25–27] Ref. 28 investigates Bayesian calibration with different prior formulations of model discrepancy function and derives the corresponding likelihood functions.

II.A. Model Uncertainty Characterization

Following Ref. 1, a significant source of uncertainty is model discrepancy, which arises because mathematical models of reality are not perfect, and thus, some aspects of reality may have been improperly modeled, ignored, or contain unrealistic assumptions. Typically, experimental data of reality which contain experimental variability, are available which can be used to create a stochastic process representation for model discrepancy. We represent model discrepancy as an additive stochastic process as

$$Y(\mathbf{x}) = f(\mathbf{x}) + \delta(\mathbf{x}), \tag{1}$$

where $\mathbf{x}$ is an input vector to the model with function $f(\mathbf{x})$, $\delta(\mathbf{x})$ is the model discrepancy and $Y(\mathbf{x})$ is the estimate of reality with quantified model discrepancy. As discussed in Section II, model discrepancy can be formulated in different ways, and we will consider the implications of choosing representations different from Eq. 1 on our results. A key point to note here is that by assuming Eq. 1 for any given disciplinary model, we are assuming Y is a random variable. For a coupled system then, there is a question of whether δ should be sampled once, or resampled every time Y is sampled. This is the crux of our analysis, and leads to either infinite correlation length discrepancy or i.i.d. discrepancy respectively.

III. Motivation

Here we will discuss our motivation for enforcing the detailed balance when analyzing model uncertainty in a coupled system, regardless of the method used to implement uncertainty in the system. Figure 1 represents a two-discipline system where each discipline takes as input, an output from the other discipline which results in the coupling between disciplines. The output of each discipline has additive model uncertainty associated with it, denoted by δ_1 and δ_2 for discipline 1 and 2 respectively.

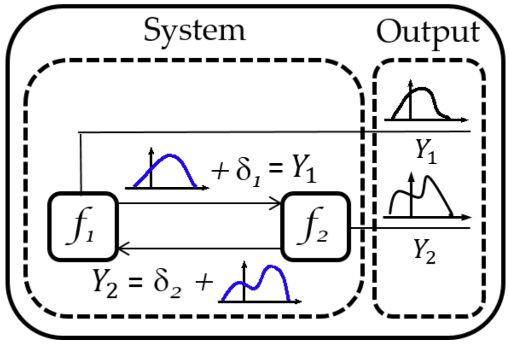


Figure 1: A two-discipline system with model discrepancy and feedback coupling. Here, f_1 and f_2 are the model functions, Y_1, Y_2 are the outputs of the respective disciplines which are the coupling variables, and δ_1 and δ_2 are the additive model discrepancies associated with the outputs.

One method to solve the coupled system under uncertainty is to take a single random sample from each model uncertainty distribution δ_1 and δ_2 and to treat those samples as constants in a fixed point iteration (FPI). The uncertainty sampling occurs "outside-the-loop" of the coupled system, before the system disciplines themselves are evaluated until the coupling variables converge. To obtain a conditional value, we simply perform an extra half iteration in the loop to get $Y_2 \mid Y_1 = y$. This procedure can be performed many times to obtain joint and conditional distributions of the coupling variables, which we then treat as our solution to the system under uncertainty. However, this outside-the-loop approach is closer to implementing parametric uncertainty into each of our disciplines rather than true model uncertainty as defined by Kennedy and O'Hagan.[1]

Model uncertainty defined by Kennedy and O'Hagan requires us to draw a new random sample from δ_1 and δ_2 each time we evaluate f_1 and f_2 during each iteration through the loop. In other words, model uncertainty is implemented "inside-the-loop". This implementation strategy can also be represented in the context of a Markov chain, where each event in the chain is a function output plus its related model uncertainty. Without loss of generality, we can pick either f_1 or f_2 as the point to start the chain and consequently stop the chain once the coupling variables have converged.

In our previous work, we explored the Markov chain concept of detailed balance and how it enforces that our coupled system will converge to a unique stationary joint distribution regardless of where we start and stop the chain.[29] In the context of probability distributions of two random variables, the detailed balance requirement is equivalent to finding the same joint distribution between variables obtained by using either conditional distribution,[30] seen in the relation

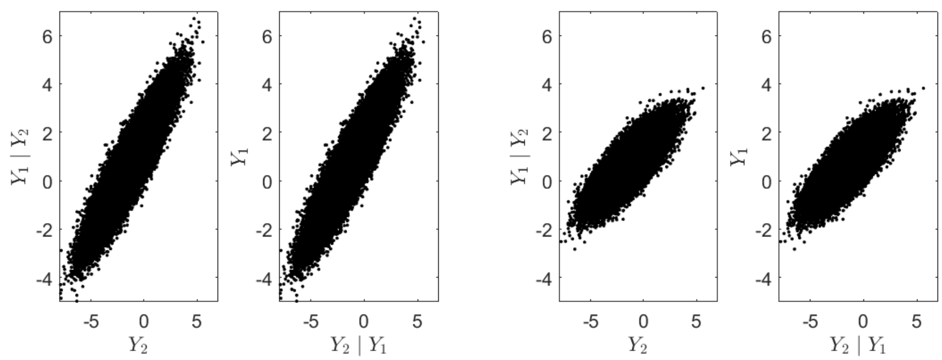
$$p_{Y_1,Y_2} = p_{Y_2,Y_1} \quad \implies \quad p_{Y_1|Y_2} p_{Y_2} = p_{Y_2|Y_1} p_{Y_1} \tag{2}$$

This relationship between the marginal and conditional distributions of the coupling variables is also known as compatibility. We have previously shown how, when model uncertainty is sampled inside-the-loop, the uncertainty distributions should be chosen such that detailed balance is enforced. On the contrary, since the FPI implementation is deterministic for each individual sample, there is no difference between the coupling variables' marginal and conditional distributions, so detailed balance is enforced automatically. However, when joint distributions obtained via FPI are then fed through system operating in an inside-the-loop scheme where new samples are drawn from the uncertainty distributions, the joint distribution of the coupling variables begin to shift toward those obtained in an inside-the-loop manner in which detailed balance is significant.

To demonstrate the importance of considering detailed balance even when using FPI, the linear example demonstrated in Ref. 29 is re-examined here, where the solution obtained though FPI is fed through one iteration of a Gibbs sampler to get a completely different joint distribution for our coupling variables. Using Fig. 1 as a template, the coupled system is $f_1(y_2) = ay_2 + b$ and $f_2(y_1) = cy_1 + d$ with $a = 1/4$, $b = 1$, $c = 1$, and $d = -2$. The uncertainty terms were unbiased normal distributions $\delta_1 \sim \mathcal{N}(0, \sigma_1^2)$ and $\delta_2 \sim \mathcal{N}(0, \sigma_2^2)$. For the case without detailed balance, $\sigma_1^2 = 1$ and $\sigma_2^2 = 1/2$. For the case with detailed balance, $\sigma_1^2 = 1/4$

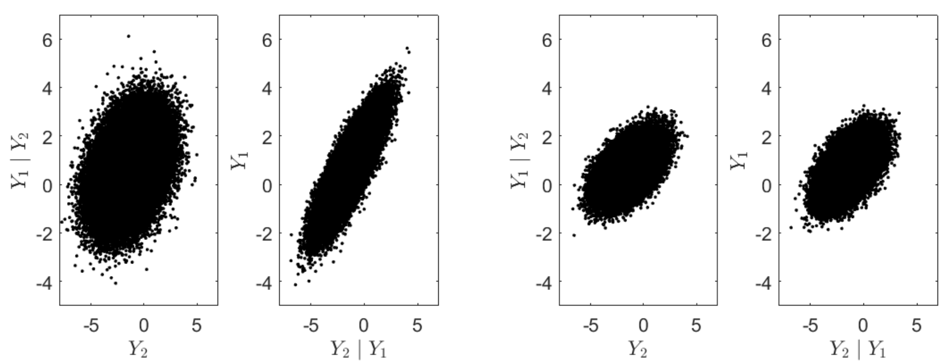
and $\sigma_2^2 = 1$. Samples from the conditional distributions $p_{Y_1|Y_2}$ and $p_{Y_2|Y_1}$ were calculated using Markov chain Monte Carlo (MCMC) with Gibbs sampling.

Note that all six pairs of joint distribution plots shown in Fig. 2-4 are calculated from the same coupled system, with only the uncertainty distributions and implementation of that uncertainty changing. This problem has only two linear disciplines coupled together with scalar coupling variables connecting them. Yet a solution resulting in a stationary joint distribution of coupling variables is elusive without the consideration of detailed balance. More applied problems, like the aerostructural example discussed in Sec. IV, have nonlinear disciplines that pass high dimensional field coupling variables between them. We wish to view these problems through the same lens as this simple example, where we focus on model uncertainty sampled directly inside the coupled system loop and restricting the uncertainty functions such that detailed balance is enforced in order to maintain a stationary distribution for our coupled system.



(a) Without Detailed Balance   (b) With Detailed Balance

Figure 2: Parametric uncertainty evaluated outside-the-loop via 100,000 samples of fixed point iteration.

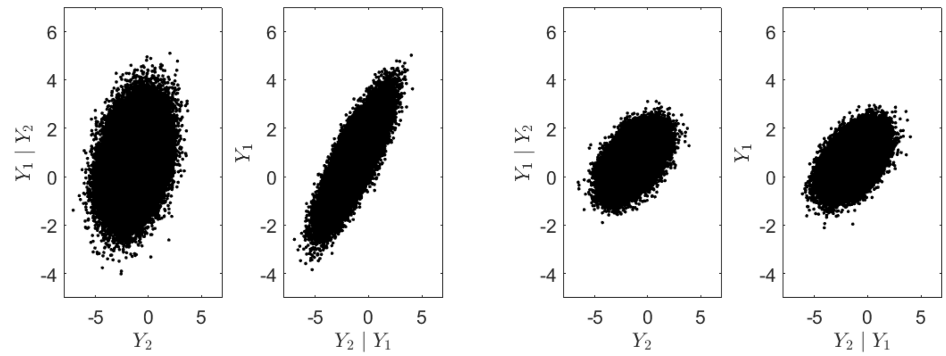


(a) Without Detailed Balance   (b) With Detailed Balance

Figure 3: Joint distributions shown in Fig. 2 passed through one iteration of the coupled system under model uncertainty.

IV. Approach

In this section, we first present our aerostructural model with high dimensional coupling field variables, followed by our characterization of model discrepancy in those variables, and finally our methodology to propagate this uncertainty when solving the system.



(a) Without Detailed Balance (b) With Detailed Balance

Figure 4: Model uncertainty evaluated inside-the-loop via Markov chain Monte Carlo with 100,000 Gibbs samples.

IV.A. Aerostructural Example

The aerostructural model of the wing is based on the NASA Common Research Model (CRM)[31] implementation of Ref. 32. The advantage to using the CRM in our model is that it is a commonly used representation of a long-range commercial airliner wing operating in transonic flight, with many benchmarking CFD and wind tunnel test results available for validation.[33]

The aerostructural model is made of three main components: a wing geometry module which takes the CRM geometric parameters and creates the mesh to be analyzed, the aerodynamics module that takes that mesh and the flight parameters and calculates the loads produced by aerodynamic lift based on that geometry, and the structures module that calculates the deformations on the wing based upon those applied loads. A general overview of the system is seen in Fig. 5. The model geometry generates a mesh for wing based on a user-specified number of spanwise inboard and outboard points. The coupled variable **loads** shown in Fig. 5 is a matrix of the point load vectors and moments due to aerodynamic lift applied to each wing section in the wing mesh geometry. The coupled variable **deformed mesh** shown in the same figure is a matrix of node position coordinates for the deformed mesh that result from the displacement and rotation of each section of the wing caused by the applied aerodynamic forces and moments. The deformed mesh is then provided to the aerodynamics discipline to calculate updated load forces and moments.

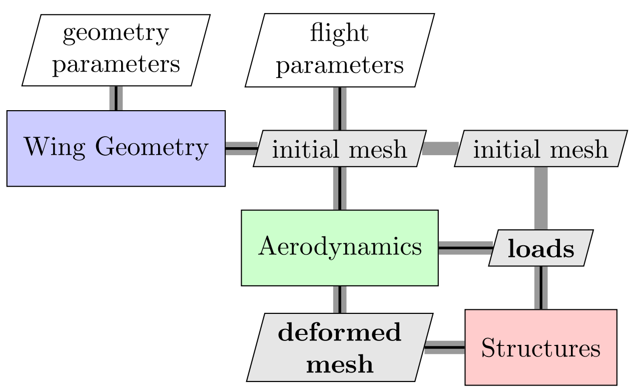


Figure 5: Aerostructural Model Diagram[34]

The aerodynamics discipline uses a modified vortex lattice method (VLM) approach by modeling the velocity potential distribution as a single row of infinite, discrete horseshoe vortices along the quarter-chord line of the wing.[35] Lifting forces are computed using the VLM at the collocation points located at the three-quarter-chord line. The matrix of section forces is then converted to a mesh of applied loads to be used in the finite element model in the structures discipline.

The structures discipline applies those sectional forces to the wing via a 6-degree of freedom Euler-Bernoulli beam finite element method (FEM). For the finite element model, the wing is modeled as a mesh of connected aluminum tubes based upon the original wing geometry mesh defined earlier. When the FEM converges, the resulting section displacements and rotations are added to the current wing mesh to create a deformation mesh, which is then fed back into the aerodynamics discipline.

IV.B. Uncertainty Propagation in High Dimensional Coupled Variables

To propagate the uncertainty in coupled multidisciplinary systems, we need to formulate the model discrepancy and function model corresponding to each discipline.

In this work, we assume that disciplinary model discrepancy functions depend on input, and also there may be a correlation between the model discrepancies at different points in the input space. This correlation implies that when there is a high discrepancy from the model at one input point, the model is not well predicted at a nearby input point too. Based on these assumptions, we formulate the model discrepancy as a Gaussian process with mean function $m(x)$ and covariance function $K(x, x')$ as

$$\delta(\mathbf{x}) \sim \mathcal{GP}(m(\mathbf{x}), K(\mathbf{x}, \mathbf{x}')). \tag{3}$$

Here, we assume the model discrepancies to be unbiased, i.e. zero mean function, and the covariance function is considered to be squared exponential function which is the most widely used covariance function in the machine learning literature, due to the fact that it is infinitely differentiable.[36] The squared exponential covariance function with noise-free observations can be written as

$$K(\mathbf{x}, \mathbf{x}') = \sigma_f^2 \exp(-\sum_{i=1}^{d} \frac{(x_i - x_i')^2}{2l_i^2}), \tag{4}$$

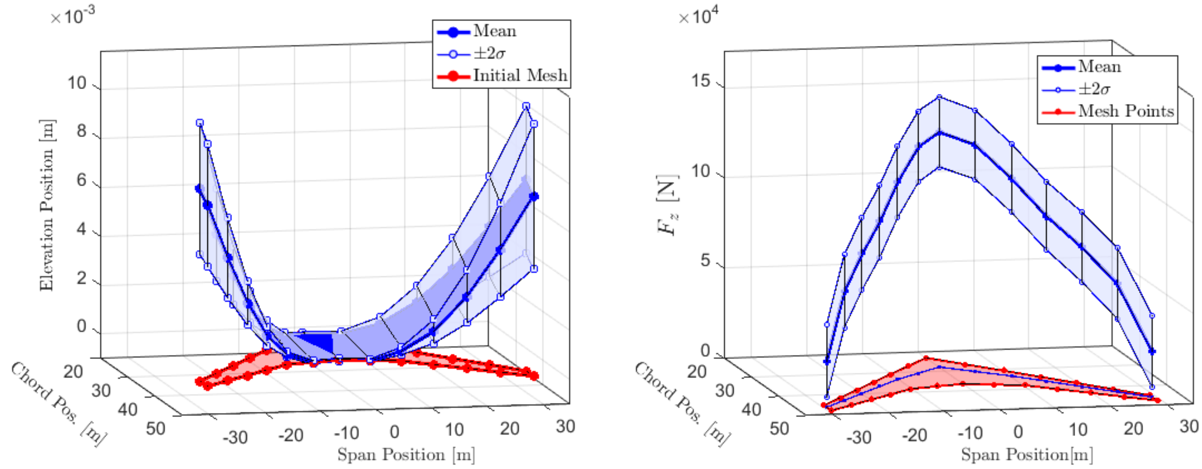
where d is the dimension of the inputs, σ_f^2 is the variance of the Gaussian process, and l_i is the characteristic length-scale of the process associated with the input variable x_i which specifies the degree of correlation between the input points. For very large values of the length-scale, the covariance becomes almost independent of that input, and for very small values of the length-scale, the points get quite uncorrelated and the sample function varies more rapidly.

We also draw a posterior sample from the Gaussian process model discrepancy terms, which is a function of the variable's defined variance, correlation length, and is evaluated at the spanwise mesh points along the airplane wing. The discrepancy drawn from the Gaussian process at a point along the wing span is applied to each variable located at that span length.

V. Results

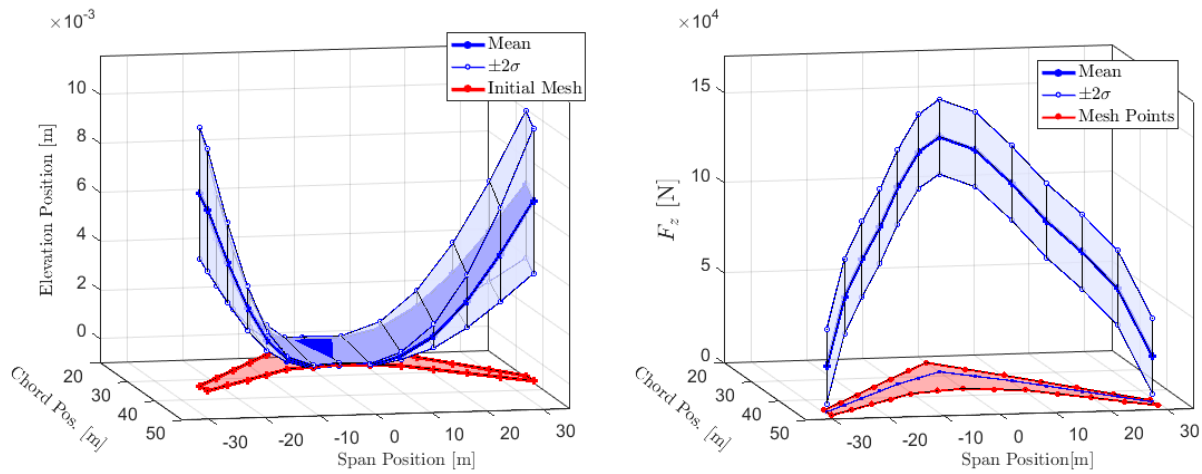
In this section, we present the preliminary results of our approach applied to the aerostructural system. The aerostructural system was run through a Gibbs sampler with 750 samples. The wing mesh was generated using 3 inboard points and 5 outboard points across the span of one side of the airplane wing and then mirrored to create the full mesh. This mesh produced coupling field variables with 78 dimensions each. A design of experiments was performed using the Gaussian process uncertainty function parameters σ_L^2, l_L, σ_M^2, and l_M as design variables. The uncertainty terms were drawn from a posterior sample from the Gaussian process evaluated at the spanwise mesh coordinates of the wing. Those discrepancies were equally added to all variable dimensions physically located at that spanwise coordinate on the wing.

A pattern search optimization is proposed to return the Gaussian process uncertainty arguments that minimize the difference between each variable's marginal and conditional distribution in order to satisfy detailed balance, thereby finding a stationary joint distribution of the multivariate coupling variables. Limitations to this approach include the high computational expense to evaluating the aerostructural model for many thousands of Gibbs samples. Evaluating the coupled system with our uncertainty analysis shows that the statistics of the marginal and conditional multivariate coupling variables are similar. Data for one of these analyses is shown in Table 1 and Figs 6 and 7. This similarity implies that compatibility for the coupled system may be satisfied. Further analysis of the difference or divergence between two multivariate distributions can confirm if the uncertainty in the system has indeed satisfied detailed balance.



(a) Mesh Deformation (b) Force Load

Figure 6: Marginal distributions of the **loads** and **deformed mesh** coupling variables of the aerostructural model under uncertainty. Uncertainty calculated via Gaussian process with $\sigma_L^2 = 100$, $l_L = 15$, $\sigma_M^2 = 1e-8$, $l_M = 15$. Evaluated using 750 Gibbs samples.



(a) Mesh Deformation (b) Force Load

Figure 7: Conditional distributions of the **loads** and **deformed mesh** coupling variables of the aerostructural model under uncertainty. Uncertainty calculated via Gaussian process with $\sigma_L^2 = 100$, $l_L = 15$, $\sigma_M^2 = 1e-8$, $l_M = 15$. Evaluated using 750 Gibbs samples.

VI. Future Work

Our future work will adapt our Gibbs sampling algorithm to take advantage of parallel processing to reduce computation time such that optimization can be reasonably run with additional Gibbs samples and over additional Gibbs iterations. We will look to alternative methods to quantify model uncertainty, including copulas, without adding a high number of design variables to the optimization problem. We will also explore ways to incorporate this type of analysis into more complex aerostructural systems, such as CFD analyses with full finite element meshes of the wing structure. Surrogate models will most likely need to be used to further reduce computation time.

Table 1: Statistics of the joint distribution of **loads** (L) and **deformed mesh** (M) coupled variables under uncertainty shown in Figs. 6 and 7. Gaussian processes calculated from $\sigma_L^2 = 100$, $l_L = 15$, $\sigma_M^2 = 1\text{e} - 8$, $l_M = 15$.

Statistic	L	$L \mid M$	M	$M \mid L$
$\|\mu\|$	4.4594e+5	4.4594e+5	2.1996e+2	2.1996e+2
$\|cov(\Sigma)\|$	3.6269e+9	3.9855e+9	2.1543e–5	2.1583e–5
$\|var(\Sigma)\|$	8.5447e+8	9.4606e+8	7.3094e–6	7.3119e–6

VII. Conclusion

This paper has presented an uncertainty analysis methodology for multidisciplinary systems with feedback couplings. The distinction between sampling from uncertainty distributions outside and inside the coupled system loop was made. The goal is to identify efficient, implementation independent methods and rationale for the rigorous propagation of uncertainty in these systems. The proposed method uses Gaussian processes for model discrepancy functions of disciplines, and identifies the desired discipline level uncertainty information pertaining to the individual models that will satisfy compatibility. This method propagates the model discrepancy through the system. The coupling distributions that result from different model discrepancy assumptions are the focus of this paper. We demonstrated the results on an aerostructural wing analysis problem.

Acknowledgments

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