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A Methodology to Manage System-level Uncertainty During Conceptual Design

Current design decisions must be made while considering uncertainty in both models of the design and inputs to the design. In most cases, high fidelity models are used with the assumption that the resulting model uncertainties are insignificant to the decision making process. This paper presents a methodology for managing uncertainty during system-level conceptual design of complex multidisciplinary systems. This methodology is based upon quantifying the information available in a set of observations of computationally expensive subsystem models with more computationally efficient kriging models. By using kriging models, the computational expense of a Monte Carlo simulation to assess the impact of the sources of uncertainty on system-level performance parameters becomes tractable. The use of a kriging model as an approximation to an original computer model introduces model uncertainty, which is included as part of the methodology. The methodology is demonstrated as a decision-making tool for the design of a satellite system.
[DOI: 10.1115/1.2204975]

1 Introduction

The conceptual design of complex multidisciplinary systems requires the combination of information from many sources in order to make decisions between technology choices and sizing of subsystems [1]. The choice of a technology for a subsystem and the parametric sizes for that technology results in a corresponding performance measurement that is frequently estimated from a deterministic computer model [2]. Lewis and Mistree [3], in their review of the state of the art in multidisciplinary design optimization, discuss how design decisions need to be made with limited amounts of information, introducing uncertainty in all aspects of the design of real systems. Uncertainty exists in design from both a lack of knowledge about the specifications of the system and the models used to measure system-level performance being imperfect estimates of reality. In deterministic approaches, these uncertainties are ignored and not quantified. The need to include uncertainties in design has led to the introduction of *robust design*, the selection of a design that is insensitive to design uncertainties, and *reliability-based design optimization* (RBDO), the selection of a design that satisfies system and subsystem constraints with a specified probability.

The sources of uncertainty in a design can come from uncertainty in (1) the parameters that control the design or the inputs to the design (aleatoric) and (2) the models used to relate these inputs to system performance measurements (epistemic). Parametric uncertainties can include the uncertainty in a size in the system, the cost of an item in the system, or the requirement on a performance measurement of the system. The process of *uncertainty assessment* quantifies the uncertainty in the system performance by applying a probability distribution, such as normal, log-normal, or uniform, to the uncertain parameters and propagating this uncertainty through the system model.

The proposed methodology includes model uncertainty in its uncertainty assessment and quantifies the impact of model uncertainty along with input parameter uncertainty on the uncertainty of the system performance measurements. This is achieved by using a collection of probabilistic kriging models to estimate the performance of each subsystem. The kriging models are surrogates or approximations of more computationally expensive computer models [4]. The probabilistic nature of the kriging model is used to quantify the uncertainty that results from using it as an approximation to the original model. Using separate models for the many subsystem has two advantages: (1) it reduces the number of variables used as inputs to the kriging models and (2) it enables the identification of the sources of uncertainty within the system during sensitivity analysis [5].

The use of a kriging model as a metamodel during design is motivated by three factors. The first is its ability to reproduce nonlinear response surfaces by capturing the trend information across a surface in a manner similar to linear regression and by quantifying the spatial correlation that exists between nearby points in a manner similar to radial basis functions. The second is the ability of kriging model parameters to be estimated using statistical techniques based upon the set of observations, allowing the comparison of alternative forms of the kriging model to determine the most appropriate form given the current set of observations. The third motivating factor is its probabilistic model definition that enables it to quantify model uncertainty. In most applications of using a kriging model in design [6–11], it is used as a deterministic approximation of a computationally expensive model that does not quantify the model uncertainty introduced into the system by using an approximation to the original model. The probabilistic version of the kriging model that is traditionally used in geostatistics to simulate ore yield [12] or contamination level [13] is used in this work to quantify model uncertainty in the system-level uncertainty evaluation [14,15].

This paper is divided into five sections, the second of which provides background on the technical elements used in the methodology. An overview of the proposed methodology follows in Sec. 3. A case study on the uncertainty assessment and sensitivity analysis of a satellite using the proposed methodology is in Sec. 4. The paper finishes with some concluding remarks and future work in Sec. 5.

2 Background of Methodology

The use of metamodels in the proposed methodology is motivated by the idea that repeated evaluations of computationally expensive subsystem models during engineering design can be

Contributed by the Design Automation Committee of ASME for publication in the Journal of Mechanical Design. Manuscript received August 23, 2005; final manuscript received January 11, 2006. Review conducted by Shapour Azarm. Paper presented at the ASME 2005 Design Engineering Technical Conferences and Computers and Information in Engineering Conference (DETC2005), September 24–28, 2005, Long Beach, CA.

minimized. The information present in subsystem models that is used to make design decisions can be represented in a more computationally efficient manner with metamodels. During engineering design, subsystem models are evaluated many times while the design space is investigated to quantify the trade-offs that exist in the design. These evaluations are frequently used to make the current decision at hand, such as which direction to move the design, and are then forgotten. By using a metamodel during the investigation, all of the currently available observations are used to approximate the response of the original subsystem model.

The uncertainty that is introduced by using a kriging model as an approximation of the original computer model comes from two sources. The first and most often the largest of the uncertainty sources is the stochastic process that models the variation of the observations from the underlying trend surface model. The second source of uncertainty, and one that is seldom considered, is the uncertainty that results from using estimated model parameters. The estiamted model parameters are random variables. A Monte Carlo simulation (MCS) that takes into account all of the sources of uncertainty in the system—the uncertainty from the inputs to the design and the uncertainty that comes from using estimates of the model parameters—should be performed. Including all of these random variables in a MCS could potentially require the random sampling of a large number of random variables.

This proposed methodology simplifies the MCS by reducing the number of random variables that must be sampled. By sampling from the output distribution of the kriging model, using the best estimated of the kriging model parameters it is possible to eliminate the random sampling of the kriging model parameters. The output distribution of a kriging model that includes the uncertainty in model parameters that are estimated from the observations has its variance underestimated by the traditional mean square error (MSE) estimate [16] and is no longer multivariate Gaussian; rather, it is well approximated by a Student-*t* distribution [17]. The probability distribution of the model's output is estimated using a Bayesian analysis via a Markov chain Monte Carlo (MCMC) method [17,18]. The resulting estimate of the model's probability distribution includes both the structural and parametric uncertainty associated with the metamodel.

Evaluating system-level uncertainty in design can be divided into two separate, yet related, tasks: *uncertainty assessment* and *sensitivity analysis*. Uncertainty assessment is concerned with quantifying the effect of input and model uncertainties on the output uncertainty. Sensitivity analysis determines the uncertainty factors that most influence the uncertainty of the output. Uncertainty assessment is a major task completed during reliability-based design optimization, whereas sensitivity analysis is the major task completed during robust design.

Uncertainty assessment methods can generally be divided into two techniques: (1) first-order (or second-order) reliability methods referred to as FORM (or SORM) and (2) Monte Carlo simulation methods [19]. FORM and Monte Carlo simulation are methods used by RBDO to find the point in the design space that satisfies all design constraints—given the uncertainty of the input variables—and to optimize the performance function of the system being designed.

In most FORM methods, the system uncertainty assessment consists of three steps. The system being assessed is linearized about the current design point of interest. The input uncertainties are transformed into independent standard normal, $N(0,1)$, random variables. The transformed variables are then projected into the output space by the linearized system. This approach is quite computationally efficient and accurate for systems that have input uncertainties that are nearly independent normal and have system-level responses that are nearly linear over the range of input uncertainties investigated. Unfortunately many systems do not have sensitivities that are linear throughout the region of variations of the design parameters, thus requiring the need to determine global sensitivities [20].

Monte Carlo simulation methods do not require any transformations of the random variables to an uncorrelated standard normal space. A Monte Carlo simulation draws samples directly from the probability distributions of the random variables and generates the probability space of the output variables through integration. Monte Carlo simulation requires a large number of performance evaluations in order to properly estimate the resulting probability distributions of the system performance. The result is that Monte Carlo simulation is often too computationally expensive to be used with detailed performance models. In this work, the detailed performance models are replaced with kriging models, using the probabilistic form of the kriging model to quantify the model uncertainty introduced by using the approximation to the original model. The output of each kriging model is sampled during the Monte Carlo simulation to include both the structural and parametric contributions to the model uncertainty with a single random variable rather than sample all of the kriging model parameters during the Monte Carlo simulation, greatly reducing the computational expense of including all of the sources of model uncertainty [21].

A sensitivity analysis (SA) is used to determine the sources of uncertainty that most influence the resulting uncertainty of the design [22,23]. This information is critical to understanding the robustness of a potential design to uncontrollable variability of the design parameters and to specifying tolerances on those parameters that can be controlled. Additionally, it is important during the design process to identify the design parameters that most directly control the system's overall performance. The large number of design parameters present in most complex system designs frequently makes it computationally infeasible to assess system uncertainty. Identifying the most important design parameters and using only those parameters in system uncertainty assessment enables a more computationally efficient method. This work is concerned with performing global sensitivity analysis using sampling-based methods with approximations to the original computer models to complete the SA for a complex system design by taking advantage of the computational efficiency and accuracy of kriging models along with the flexibility of Monte Carlo simulation [24,25].

3 Overview of the Methodology

The proposed methodology to evaluate system-level uncertainty is shown in Fig. 1. The input to the methodology is the information that is available to quantify the results of making design decisions. The output of the methodology is a probability distribution of the system performance to quantify the uncertainty that exists at a possible design point. The resulting uncertainty can be used to make decisions to: (1) reduce the model uncertainty, (2) improve the design, or (3) reduce the input uncertainty in the current design. The methodology is composed of six steps, which are described as follows.

Step 1: Establish a System Model. This step begins with identifying system requirements and constraints. From these requirements and constraints, the measurements of system performance are selected. Sources of information are gathered to evaluate the selected system performance measurements. These sources of information include relevant computer analysis models, previous design results, or best engineering judgements [26]. This step is common to many design problems and is not unique to this methodology [27].

Step 2: Create Probabilistic Kriging Models of Subsystems. Given the system model and sources of information, kriging models are created as approximations to the relationships between the input parameters and the performance measurements. Often, these mappings can be divided into a network of approximations with intermediate parameters that carry information from one subsystem to another. The creation of the probabilistic kriging models

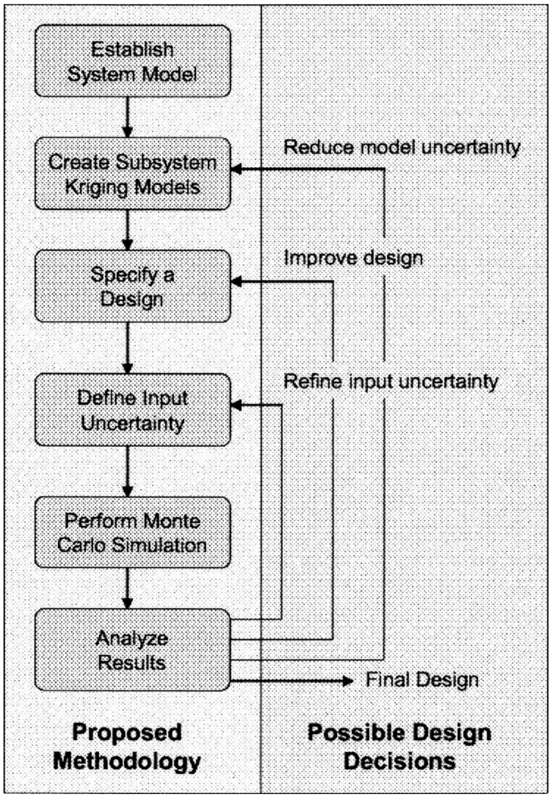

Fig. 1 Flowchart of proposed methodology

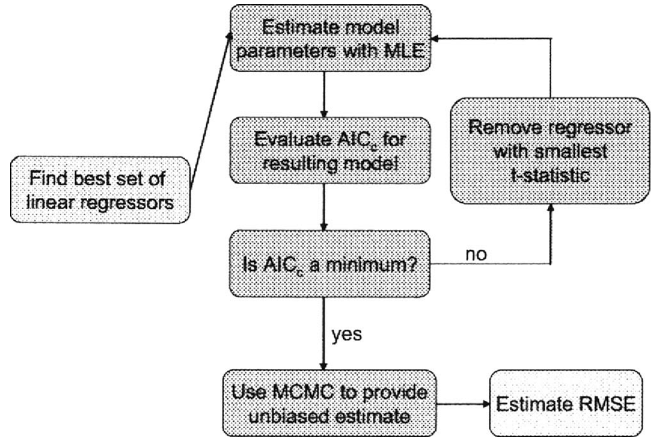

Fig. 2 Block diagram of the process

of the subsystems includes the following tasks.

1. Design of Experiments. A Latin Hypercube Sampling (LHS) [28] design is employed to sample the subsystem's region of interest (domain) for the design if a set of observations of the subsystem do not already exist. LHS is used due to its excellent projective properties, good space-filing properties, and the unnecessary need to use replications [29,30].

2. Establish Kriging Model Inputs and Output. At times, the evaluation of the system performance is simplified by switching an input and an output for a subsystem model, removing the need to iterate to resolve subsystem constraints. Every attempt should be made to create a system model that can be evaluated with a single pass through the kriging models of the subsystems. The input parameters may also need to be transformed in such a way to that the observations fill a hypercube space. Finally, the output may also need to be transformed in a way that can be better represented by a kriging model [31].

3. Estimate Kriging Model Parameters. The process of estimating the kriging model parameters [17,32] is shown in Fig. 2. The first step is to select the best form of a linear regression model using backward elimination [33]. In backward elimination, a full second-order model is first created, and regressors are then removed, one at a time, based upon their p value from an analysis of variance of the results from fitting the model.

In general, a kriging model requires fewer regressors than a linear regression model. Regressors are removed from the kriging model by estimating the model parameters using maximum likelihood estimation (MLE), evaluating the model parameter covariance matrix to determine the model parameter variances [21], and then removing the regressor that has the smallest absolute *t statistic* ($|b_k|/s_{b_k}$). This cycle continues until the smallest corrected Akaike's information criterion (AIC$_c$) [34] is obtained. During this process of elimination, second-order and cross terms are typically removed before the first-order terms. This process of minimizing the AIC$_c$—while using the MLE parameter estimation method—is expected to find the model form that has the least amount of uncertainty in the estimation of its parameters.

The MCMC method is used to provide an unbiased estimate of the model parameters for the best form as determined by using MLE and the AIC$_c$ criterion. The MCMC method also provides an estimate of the best shape parameter to use when estimating the probability of the output of the kriging model that includes model uncertainty in order to create a probabilistic kriging model that quantifies what is known about the subsystem—based upon the observations used—and what is not known—based upon the resulting uncertainty or probability distribution estimated by the kriging model. The last step is to estimate the root mean square error (RMSE) of prediction for the kriging model.

4. Assess Model Quality. Evaluate the kriging model's RMSE of the prediction using the cross-validation (CV) method to estimate the model's actual RMSE. Confirm that the $R^2_{\text{prediction}} > 0.95$ requirement [32] is satisfied.

5. Improve Kriging Model (If Needed). If the resulting kriging model does not have the predictive capabilities required to evaluate the system performance, then more observations are needed to improve its resulting predictions (reduce model uncertainty). Model uncertainty can be reduced through the following four operations: (1) take advantage of the knowledge of neighborhood of the design point (as defined by the extent of the uncertainties) to reduce the domain of the kriging model, (2) sample the computer model's new domain, reusing the observations used in the prior kriging model that are still within the domain, (3) fit the revised kriging model, and (4) perform a new uncertainty analysis with the revised probabilistic kriging model.

Step 3: Specify a System Design. Based upon the current knowledge of the system, a system design is selected to evaluate the system-level uncertainty. The decision made in this step can either be made by a designer in an interactive design environment or through the use of an optimization algorithm that quantifies the preferences of the designer and executes autonomously.

Step 4: Define Input Uncertainty for the System Design. The input uncertainty for a system in this work is defined by the probability distributions of the system inputs. The input distributions are typically a function of the design specified in the previous step. The selection of input probability distributions will always be a stumbling block in uncertainty-based methods [35]. The best one can do is to make a best guess, most often a conservative estimate, of the uncertainty of the system noise factors. Another alternative is to use a fuzzy approach to quantify the uncertainty or vagueness in the system [36]. The intent of the input uncertainties is to quantify what is *not* known about the system or what cannot be controlled. This proposed methodology, due to its relative computational efficiency can permit many different input uncertainties to be assessed as more information becomes available about the input distributions. One reasonable result of this methodology is: given the current design information and the expected uncertainty of the input factors, there is too much uncertainty to support making a decision, an alternative design needs to be selected, the models need to be improved, or the input uncertainties need to be refined.

Step 5: Perform Monte Carlo Simulation of System Model. A Monte Carlo simulation of the system model is actually an integration problem [18, Chap. 3]. The probability distributions of the random variables defined in the previous step must be integrated through the system model to obtain the probability distributions of the system performance (output) parameters. The integral is evaluated by drawing samples of the random variables based upon their probability distributions. These samples are evaluated by the system model, and the resulting distribution of the performance parameters is an estimate of the actual distribution of the performance parameters. By using simple random sampling, the resulting distributions are always unbiased estimates [37, p. 111]. The precision of the resulting probability distributions is a function of the number of samples used to estimate them. Precise results may require the use of large numbers of samples (greater than 10,000): future work should investigate rules to select the number of samples that will result in a good approximation of the performance parameter probability distributions. Other researchers have also published computationally efficient alternatives to Monte Carlo simulation for uncertainty assessments including: stochastic analysis with minimal sampling (SAMS) [38], saddlepoint approximations [19], and analytical variance-based global sensitivity analysis [23].

The unique aspect of our methodology is that the computationally expensive subsystem analyses are approximated with a probabilistic kriging model that quantifies the uncertainty associated with using the metamodel. The system model network of kriging models is evaluated for all of the samples generated from the input parameter distributions. The output of each subsystem kriging model is a random variable with a probability distribution described with a student-*t* distribution. The output of the kriging model is sampled simply based upon its probability distribution in order to include the model uncertainty introduced by using kriging models to approximate the original analyses.

Step 6: Analyze the Results. The results of the Monte Carlo simulation are first analyzed as part of an uncertainty assessment. The uncertainty assessment quantifies the resulting probability distributions of the system's performance measurements. The probability distributions can be summarized with their mean and standard deviations or by prediction intervals. A sensitivity analysis can also be completed to identify and quantify the contribution of the input and model uncertainty sources to the observed performance uncertainty. From these results, decisions are made. Often these decisions may result in three choices: (1) changing the current design to be less influenced by the input parameter uncertainty, (2) limiting the variability in the input parameters, or (3) improving the quality of the kriging models to reduce model uncertainty. This final decision indicates that additional information is required to make a decision, thus improving the predictive capabilities of the kriging models used in the system model.

4 Demonstration of the Methodology

A case study is used to demonstrate the methodology as a tool to manage uncertainty in the conceptual design of a satellite orbiting Mars.

Step 1: Establish a System Model. A Mars orbiting satellite is designed using the proposed methodology. Most of the design rules presented in this section are based upon the research of Yukish [39]. This hypothetical satellite is sized to deliver an instrumentation package into orbit around the planet Mars. The satellite design rules used in this case study permits the choice of payload mass, orbit radius, rocket engine sizing parameters, and tank capacities. The satellite system design variables are identified in Table 1. The inputs to the system analysis are indicated in the top portion of Table 1. The bold design variables are permitted to vary during the design process, while the other variables are held constant, indicating mission specific parameters. The outputs are indicated in the bottom portion of Table 1. The design process establishes the total mass of the system and determines if the design is feasible as determined by the remaining fuel and oxidizer.

Table 1 Satellite system design variables and values

Parameter	Value	Units
Payload mass	600	kg
Orbit radius	400	km
Trajectory velocity	3	km/s
Throat diameter (diam Throat)	**0.037**	**m**
Exit diameter	0.2	m
Mass flow rate fuel (mdotF)	**0.666**	**kg/s**
Mass flow rate oxidizer (mdotO)	**1.930**	**kg/s**
Tank volume (tankV)	**0.864**	**m^3**
Power/weight ratio	**37**	**kJ/kg**
Remaining fuel	*325.84*	*kg*
Remaining oxidizer	*20.114*	*kg*
Total system mass (mass Total)	*2999.9*	*kg*

The system is divided into three subsystems: (1) rocket engine, (2) fuel and oxidizer tanks, and (3) orbit mechanics. These subsystems are placed together in a single system and result in cumulative system mass (massTotal) and the engine burn time (burnTime) as shown in Fig. 3. The system diagram that is shown in Fig. 3 identifies the variables that are varied in the case study and the connectivity between subsystem models. The payload is taken as a given mass that must be delivered to an orbit around Mars.

The system model cannot be solved with a single pass of the inputs through the subsystem models due to the circular dependency in the calculation of the burnTime, the amount of time the rocket engines must fire to slow the satellite enough to enter the specified orbit. The subsystem models calculate their results quite quickly (1 s or less), but due to the circular dependency, the actual time to solve the system equations can take up to 2 min. The code is executed on a Pentium M 1.8 GHz Dell laptop computer. Details can be found in Ref. [21].

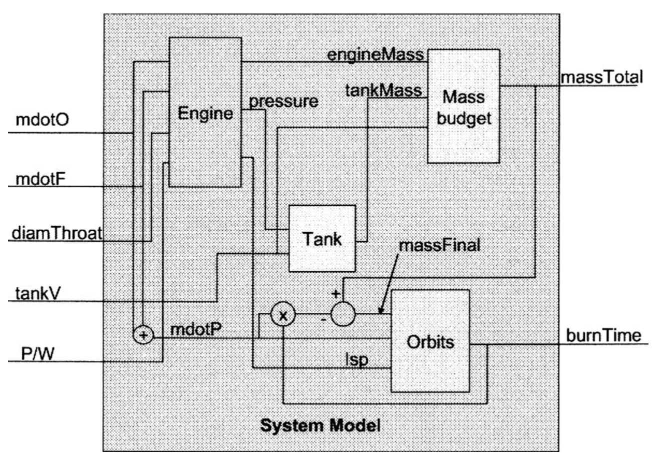

Fig. 3 Diagram of system and subsystem models

Table 2 Input ranges for the subsystem models

Model	Input	Min		Max	
Engine	Mass flow rate	0.5	kg/s	5	kg/s
	Mixture ratio	1		3	
	Area ratio	20		80	
Tank	Max pressure	2.69	MPa	22.20	MPa
	Tank volume	0.2	m^3	1	m^3
Orbit	Mass flow rate	0.5	kg/s	5	kg/s
	Isp	260	s	325	s
	Final mass	1000	kg	3000	kg

Step 2: Create Probabilistic Kriging Models for Subsystems.

1. Design of Experiments. The first task in creating probabilistic kriging models of subsystem models is to create sets of observations of each subsystem. In this work, an LHS design of experiments (DoE) is used to sample the subsystem models. The requirements and constraints of the subsystem model input parameters for the satellite system design are known before the DoE is created and are used to restrict the parameter ranges that are investigated. The minimum and maximum values for the input parameters are shown in Table 2.

The engine subsystem model is sampled using a 20-point LHS centered design. The engine model DoE is based upon the total mass flow rate, the mixture ratio, and the area ratio of the nozzle. These three parameters provide a feasible space that is better described by a hypercube than sampling over the mass flow rates of the oxidizer and fuel and the nozzle diameter. The tank model is sampled using a 15-point LHS design. The orbit model is sampled using a 20-point LHS design.

2. Establish Kriging Model Inputs and Outputs. The engine analysis model results in observations of six parameters that describe the different rocket engine designs. The list of inputs to the kriging model is: (1) mass flow rate, (2) mixture ratio, and (3) area ratio. The use of these three parameters results in a better mapping of the feasible design space to a unit hypercube than by using the mass flow rates of the fuel and oxidizer and diameter of the throat directly. Three kriging models are created to estimate the specific impluse (ISP), chamber pressure, and power generated by the engine.

The tank analysis model calculates the mass of the tank that can hold liquid at the specified pressure and volume. The kriging model that estimates the mass of the tank is a direct replacement for the original analysis, using the two inputs—maximum pressure and tank volume—to estimate the one output, tank mass.

The orbit analysis model calculates the shortest burn time required to insert the satellite into its final orbit. The analysis uses the final mass of the satellite as an input since the analysis uses final mass as an initial condition to integrate back in time, adding mass to the system. The total mass is determined by adding the propellant mass flow rate times the burn time to the final mass. The total mass is used to replace the final mass as an input to the kriging model estimate of burn time in order to remove the circular dependency in the system performance calculations (see Fig. 3). From this burn time and the mass flow rate of the propellant, the system calculation for the remaining fuel and oxidizer is determined.

The burn time is a nonlinear function of mass flow rate, Isp, and final mass. The Isp in all of these cases is taken as a constant 312 s. In an effort to improve the ability of the kriging model to fit the observations, the logarithm of the burn time is taken, and the kriging model is fit to the resulting values.

3. Estimate Kriging Model Parameters. The revised system model that uses kriging models—instead of the original analyses

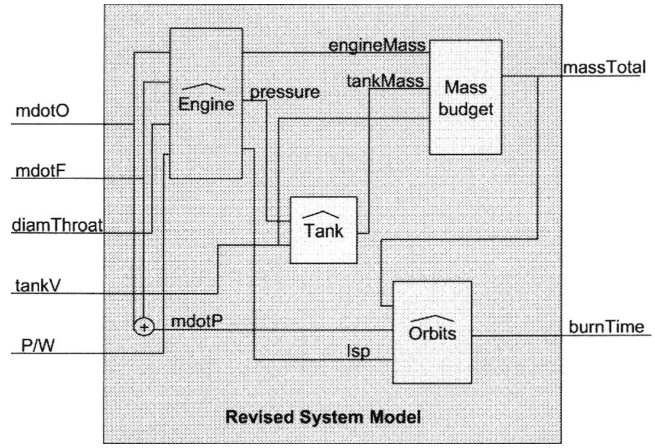

Fig. 4 Revised system diagram using kriging models

(see Fig. 3)—is shown in Fig. 4. The subsystems that use kriging models as approximations to the original computer subsystem models are indicated with hats. Three kriging models are created to approximate the three outputs of the engine subsystem model, and one kriging model is created for each of the tank and orbits subsystem models. The major difference between this system model and the original system model in Fig. 3 is that the circular dependency of the burnTime in the orbits model has been removed. This permits the system performance to be evaluated with a single pass through the subsystem models, reducing the computational expense of the system evaluation.

4. Assess Model Quality. The quality of the resulting kriging models is provided in Table 3 by reporting the $RMSE_{CV}$ measurements. The coefficients of multiple determination are calculated to quantify the amount of variability captured by the kriging model. All of the kriging models appear to be very good representations of the original analyses. The log (burn time) model appears to perform the worst, but it is still acceptable for use in this demonstration of the proposed methodology.

Step 3: Specify a System Design. To demonstrate the methodology, a design is specified that appears to be feasible—given the original models—but it is not an optimal design by any measure. The inputs to the system and their corresponding values are listed in the top portion of Table 1. The bold parameters indicate the random input variables in this study. Their probability distributions are defined in the next section. The outputs from the system model are listed in the bottom portion of Table 1. The values listed in Table 1 are the deterministic results from the original analysis models.

Step 4: Define Input Uncertainty for the Design. Uncertainty is introduced into the design by defining probability distributions for five of the inputs to the model (see Table 1): the mass flow rates of the fuel and oxidizer, the volume of the tanks, the diameter of the throat, and the ratio of the engine power to weight ratio. In order to simplify this case study, all of the inputs are

Table 3 Predictive capability of the kriging models

Model	$RMSE_{CV}$	$R^2_{prediction}$
Isp	1.0418	0.9945
Pressure	0.085	0.9996
Power	79.199	0.9998
Tank mass	1.8419	0.9987
Log (burn time)	0.061910	0.9904

Table 4 Input parameter distribution

Parameter	Mean	Standard deviation	Unit
Mass flow rate oxidizer	1.93	0.05	kg/s
Mass flow rate fuel	0.666	0.03	kg/s
Tank volume	0.864	0.01	m^3
Diameter throat	0.037	0.001	m
Power/weight ratio	37	1	kJ/kg

assumed to have independent Gaussian distributions with means specified by the design values and standard deviations as given in Table 4. The standard deviations in Table 4 are chosen for demonstration purposes only; the proposed methodology permits the use of any distribution of the input parameters. Alternatively, any distribution that best matches the known uncertainty of the input parameters could have been chosen.

The distributions are truncated after $\pm 3\sigma$. Allowing the parameters to be sampled from a true Gaussian distribution causes troubles with the analysis models since it will permit infeasible results such as negative values of the parameters. At this conceptual level of a design, measurements of $\pm 2\sigma$ or 95% prediction intervals of the system performance parameters are good enough to make decisions. By sampling the input parameters to $\pm 3\sigma$, an adequate estimate of the 95% prediction intervals will result.

Step 5: Perform Monte Carlo Simulation of System. The proposed methodology presumes that the propagation of uncertainty through the system models can be well approximated by using kriging models as computationally efficient surrogates of the original subsystem models. This use of kriging models introduces model uncertainty into the resulting probability distributions of the system performance parameters. In order to validate the use of kriging models in this methodology, a Monte Carlo simulation of the original subsystem models using simple random sampling and the input distributions is completed. These results are compared to the system uncertainty assessment completed using the deterministic version of the kriging models and the probabilistic version of the kriging models as approximations to the original subsystem models in the next section (see Table 5). The deterministic version of the kriging model uses only the expected value of the kriging model as its output. The results from using the deterministic kriging model should be similar to those using the original subsystem models, since they both include the same sources of input uncertainty. The deterministic version of the kriging model ignores the model uncertainty that is introduced by using the kriging model approximation to the original subsystem models. A third case is evaluated that uses the probabilistic version of the kriging models to include the model uncertainty in the resulting probability distributions of the system performance measurements. The model uncertainty introduced by using a kriging model as an approximation to the original computer model for a subsystem is included in the Monte Carlo simulation by using simple random sampling from the output probability distribution from each probabilistic kriging model rather than always using the expected value as is the case for the deterministic kriging models.

For this demonstration, the time to evaluate 10,000 samples using the deterministic kriging models is about 20.1 ± 0.1 s. The time to evaluate the probabilistic kriging models is about 43.2 ± 0.2 s. The mean time for a *single* system evaluation using the original subsystem models is about 20.4 s with a standard deviation of about 7.5 s. All execution times are determined using an evaluation timing function built into MATHEMATICA.

Step 6: Analyze the Results

Uncertainty Assessment. There are two tasks involved in analyzing the results of the Monte Carlo simulation. The first task is to quantify the resulting probability distributions of the uncertainty assessments. Table 5 summarizes these results for the three cases of subsystem models: (1) original model, (2) deterministic kriging, and (3) probabilistic kriging. The design used is that listed in Table 1. For each of the three cases of subsystem models, the mean, standard deviation, and 5% and 95% prediction intervals are provided for comparison of the resulting probability distributions. The three system performance parameters are reported first. The next five are intermediate parameters that connect the inputs and outputs of subsystem models.

From the resulting performance parameter distributions shown in Table 5, it appears that using a deterministic kriging model as an approximation of the original model produces very similar results. The case of using probabilistic kriging models of the subsystems has nearly the same expected values as using deterministic kriging models of the subsystems. This is anticipated since the expected value of the probability distribution from the probabilistic kriging model is the same value that is used in the deterministic kriging model, and, for a system that is nearly linear about its design point, the symmetric distributions from the probabilistic kriging models do not change the expected values of the system performance probability distributions. The variances of the system performance probability distributions are larger and their prediction intervals extend further from the mean, as would be expected for the case of using probabilistic kriging models. This increase is due to the inclusion of model uncertainty in the Monte Carlo simulation. In most cases the prediction intervals predicted by the probabilistic kriging model contain the prediction intervals of the original model.

The level of agreement seen in this study indicates the need for excellent quality in the kriging models used to approximate the subsystem models. From the results shown in Table 3, the smallest $R^2_{\text{prediction}}$ value is 0.9904, which can be considered excellent given the large domains covered by the kriging models and small number of observations used to determine the kriging parameters. The results from Ref. [21] indicate that, in general, the cross-validation estimate of the RMSE provides an upper bound esti-

Table 5 System uncertainty assessment of selected design

	Original model				Deterministic kriging				Probabilistic kriging			
	Mean	Standard deviation	5%	95%	Mean	Standard deviation	5%	95%	Mean	Standard deviation	5%	95%
Total mass	3056.4	31.96	3002.4	3107.5	3062.7	28.69	3015.4	3110.4	3063.2	29.43	3014.1	3112.3
Oxidizer left	30.43	17.73	1.24	58.50	26.26	16.30	−0.60	53.38	26.11	26.24	−17.94	69.02
Fuel left	338.30	16.74	310.32	366.12	337.11	17.64	308.38	366.28	337.04	18.71	306.14	367.75
Burn time	633.87	13.60	611.72	657.16	635.70	13.38	614.14	658.13	635.74	17.09	608.32	664.54
pressure (MPa)	4.26	0.25	3.86	4.69	4.29	0.25	3.89	4.71	4.29	0.26	3.87	4.74
Isp	299.49	2.431	294.84	302.23	298.65	2.740	293.55	301.96	298.68	2.868	293.21	302.04
Mass engine	291.98	16.180	262.36	314.98	297.48	12.298	277.54	317.98	297.72	12.639	276.77	318.29
Mass tanks	151.16	6.268	141.05	161.68	151.96	6.269	142.05	162.74	152.07	6.755	141.32	163.49

mate of the actual RMSE. As a result, $R^2_{\text{prediction}}$ provides a lower bound to R^2_{actual}. $R^2_{\text{prediction}}$ of 0.9904 indicates that over 99% of the variability is explained by the kriging model.

Sensitivity Analysis. The SA of the results is used to identify which of the sources of uncertainty are the most important ones in explaining the observed system performance variability. The results of this assessment can be used by the designer to make design decisions. For this work, a very simple SA method, using Pearson correlation coefficients (PCC), was chosen in order to demonstrate the effectiveness of using metamodels during SA. A more rigorous and precise method is offered by McKay [40]. The PCC between m observations of two parameters is calculated as:

$$r[\mathbf{x},\mathbf{y}] = \frac{\sum_{i=1}^{m} (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{m} (x_i - \bar{x})^2}\sqrt{\sum_{i=1}^{m} (y_i - \bar{y})^2}} \tag{1}$$

The PCC can also be interpreted as providing a measure of the linear relationship between the input/output (I/O) parameters [37]. The correlations between the five inputs and three outputs to the system are shown in Fig. 5. Correlations are always between −1 and 1 with positive values indicating a positive correlations and negative values indicating a negative correlation. More extreme values indicate that the I/O parameters are more correlated. Correlations cannot be used to determine causation; that must always come from other sources. In this example, it is known which parameters are inputs and which parameters are outputs, thus indicating the causation.

There are two important conclusions to draw from Fig. 5. The first is the general conclusion that deterministic kriging model approximations to the original subsystem models provide a very good estimate of the I/O correlations. The results from using probabilistic kriging models, as specified in the proposed methodology, provide similar results on the magnitudes and relative rankings of the correlations. The results from using the probabilistic kriging models give larger system uncertainty measurements and (by definition) smaller correlation coefficients than the original subsystem models and the deterministic kriging models. This is due to the former results including the model uncertainty introduced by using the probabilistic kriging as an approximation to the original subsystem models.

The second conclusion to draw from Fig. 5 and Tables 6–8 is that the results of using the probabilistic kriging models as approximations to the original subsystem models provide the information needed to make design decisions on how to refine the input parameters' uncertainties in order to manage the output uncertainties. For this satellite case study, it appears that in order to reduce the uncertainty in the system outputs, the uncertainty of the mass flow rate of fuel (mdotF) has the largest influence; so, it must be reduced. The uncertainty of the tank volume (tankV) and the mass flow rate of oxidizer (mdotO) also appear to have large influences on the three outputs. The uncertainty of the power to weight ratio (pw) and the throat diameter (diamT) appear to have little influence. The uncertainty of pw that is used in the engine mass model does not appear to be an influential parameter; as a result, an improved kriging model of the engine does not appear to be needed yet at this point in the design to reduce this source of uncertainty.

The square of the correlation coefficient, from Eq. (1), is the same as the coefficient of determination in simple linear regression [41, pp. 539–540]. In this setting of correlation, it may be used to describe the fraction of observed variability of the output that is due to the variability of the input. Given this fact, it is known that the only sources of uncertainty in the original models and deterministic kriging models are the uncertainty of the five input parameters. The total r^2 (sum of the five input sources)

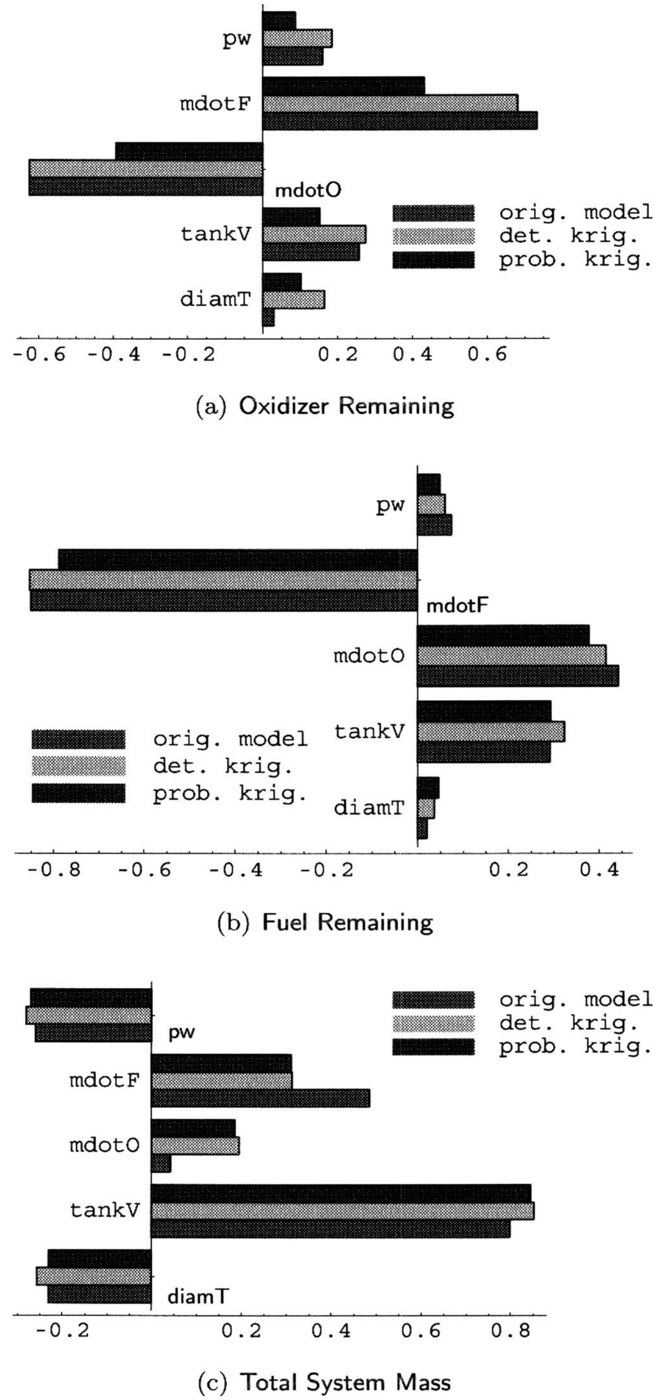

Fig. 5 Bar charts of the system input/output correlations

Table 6 Sources of uncertainty (r^2) for the remaining oxidizer

Inputs	Original model	Deterministic kriging	Probabilistic kriging
Diam. throat	0.001	0.027	0.010
Tank volume	0.066	0.075	0.023
$\dot{m}_{\text{oxidizer}}$	0.390	0.390	0.154
$\dot{m}_{\text{fuel}}$	0.539	0.465	0.185
p/w ratio	0.026	0.034	0.008
Total	1.023	0.992	0.381

shown in Tables 6–8 are approximately equal to one, appearing to confirm that the five sources of uncertainty do account for all of the uncertainty seen in the three outputs. The r^2 values do not sum exactly to one due to the limited precision of a 10,000 sample Monte Carlo simulation used for each case.

The five inputs do not account for all of the uncertainty seen in the outputs of the system made up of probabilistic kriging models. The remaining uncertainty in the outputs is caused by the model uncertainty introduced by using the probabilistic kriging models. The model uncertainty present in the estimation of the total mass (see Table 8) is the smallest source of uncertainty (total amount of uncertainty-input uncertainty=model uncertainty$\Rightarrow 1 - 0.972 - 0.028$). The model uncertainty in the remaining fuel is the second largest source of uncertainty and is about the same magnitude as the mass flow rate of oxidizer (see Table 7). The model uncertainty in the remaining oxidizer is by far the largest source of uncertainty. Given the amount of model uncertainty present in the remaining oxidizer system performance parameter, it is understandable why the deterministic and probabilistic kriging model cases performed the worst at estimating the remaining oxidizer.

The result of measuring the sources of uncertainty through the use of probabilistic kriging models, as shown in Tables 6–8, is that very little reduction in the uncertainty of the remaining oxidizer can be achieved by reducing the uncertainty of the inputs. In order to reduce the uncertainty in the remaining oxidizer, the model uncertainty must be reduced. This uncertainty can be reduced by improving the current kriging models used to approximate the subsystems within the system. The first step is to identify which model or models are the largest source of model uncertainty. The source of the model uncertainty for the remaining oxidizer is shown here as an example of the procedure.

The remaining oxidizer (oxiLeft) after the orbit insertion burn (burnTime) is defined by the following relationship

$$\text{oxiLeft} = \text{tankV}\rho_{\text{oxidizer}} - \dot{m}_{\text{oxidizer}}\text{burnTime} \tag{2}$$

where tankV is the volume of the oxidizer tank and ρ_{oxidizer} is the density of the oxidizer, which is assumed to be a constant value. The input parameters tankV and $\dot{m}_{\text{oxidizer}}$ to Eq. (2) are system-level inputs. The burnTime parameter is the result of the orbit kriging model. The inputs to the orbit model and their corresponding contributions to the uncertainty of the burnTime output are shown in Table 9. A little over half of the uncertainty in the burnTime output is due to the uncertainty in $\dot{m}_{\text{propellant}}$, which is defined as the sum of the system inputs the mass flow rates of fuel and oxidizer.

Given the results of this sensitivity analysis performed during the last step of the proposed method, the best design decision appears to be to reduce model uncertainty of the orbit model. The model uncertainty introduced by the other four kriging models does not appear to have an important impact on the resulting uncertainty of the system model. A strategy to improve the orbit kriging model is identified in step 2 of the proposed methodology. Some published strategies [9,42] for improving the kriging model may require that the domain be reduced if the correlation matrices become ill-conditioned, but other strategies [43] do not appear to have the same problem. The loss of information that occurs by not reusing observations that are not within the neighborhood of the current design point is negligible due to the spatial correlation function that decreases their influence as the points become further apart.

Table 7 Sources of uncertainty (r^2) for the remaining fuel

Inputs	Original model	Deterministic kriging	Probabilistic kriging
Diam throat	0.0004	0.001	0.002
Tank volume	0.085	0.105	0.086
$\dot{m}_{\text{oxidizer}}$	0.196	0.172	0.143
$\dot{m}_{\text{fuel}}$	0.721	0.725	0.620
p/w ratio	0.006	0.004	0.002
Total	1.008	1.008	0.854

Table 8 Sources of uncertainty (r^2) for the total mass

Inputs	Original model	Deterministic kriging	Probabilistic kriging
Diam throat	0.053	0.065	0.053
Tank volume	0.638	0.726	0.715
$\dot{m}_{\text{oxidizer}}$	0.002	0.038	0.035
$\dot{m}_{\text{fuel}}$	0.235	0.098	0.097
p/w ratio	0.067	0.079	0.073
Total	0.995	1.006	0.972

5 Conclusions

In this work a methodology is proposed to evaluate system-level uncertainty in the design of complex multidisciplinary systems. The methodology is based upon the uncertainty assessment of the system model by performing a Monte Carlo simulation, which is made computationally feasible through the use of kriging model approximations to the original subsystem models used to create the system model. Through the use of these surrogates, model uncertainty can be incorporated into the resulting performance uncertainty. The proposed methodology relies heavily upon the probabilistic kriging model and the model uncertainty estimates presented in Ref. [17].

By analyzing the results of the Monte Carlo simulation with an uncertainty assessment and a sensitivity analysis, the amount of uncertainty present in the system performance parameters and the impact of the sources of uncertainty (input and model) on the system performance parameters are quantified. Given these results, four design decisions can be made: (1) accept the system design, (2) improve the system design, (3) reduce the input uncertainty, or (4) reduce model uncertainty (see Fig. 1). The proposed methodology helps manage uncertainty by providing a basis to make decisions under uncertainty. The methodology identifies the largest sources of uncertainty in the design and provides a means to reduce them until a final design can be accepted.

The main benefit of the proposed methodology is that *it provides a means to manage uncertainty during system-level design*. Further benefits of the proposed methodology include:

1. The system-level uncertainty evaluations are done in the original parameter space. The methodology does not require transformation of variables to uncorrelated standard normal. The system-level uncertainty evaluation is completed using the parameters that make more sense to a designer.

2. The methodology is computationally efficient. The repeated evaluations of the original subsystem model are replaced by kriging models during subsequent Monte Carlo simulations. Design options can be traded off—without having to reevaluate the original subsystem models.

3. The methodology includes model uncertainty in its system-level uncertainty evaluations. Through the use of probabilistic

Table 9 Sources of uncertainty (r^2) for burn Time

Inputs	Probabilistic kriging
$\dot{m}_{\text{propellant}}$	0.516
Isp	0.0007
Total mass	0.006
Total	0.523

kriging models, the model uncertainty introduced by using approximations to the original computer subsystem models is incorporated into the system-level uncertainty evaluations.

4. The methodology reports the sources of system-level uncertainty. During the sensitivity analysis step, the results of the Monte Carlo simulation provide the information needed to quantify the sources that contribute to the system-level uncertainties. With this information, design decisions can be made on how best to reduce the system-level uncertainty, by selecting a different design, reducing the input uncertainties, or reducing model uncertainty.

5. The methodology provides a probability distribution of the system performance parameters. From this probability distribution, it is easy to determine the mean, variance (or higher moments), and prediction intervals to be used as part of an optimization algorithm.

The proposed methodology can also be used as a tool during RBDO. The resulting probability distributions from the uncertainty assessment can be used to estimate prediction intervals. The difficulty involved with using the results of a Monte Carlo simulation to calculate the objective function for an optimization problem is that they are not deterministic, rendering most optimization algorithms useless. A stochastic optimization algorithm such as simulated annealing is required to deal with the stochastic nature of the objective function [21,44].

The primary limitation of the proposed methodology is its heavy reliance upon the capabilities of the kriging model to quantify what is known (the observations of subsystems) and what is not known (model uncertainty). The use of kriging models have not gained widespread acceptance in engineering design due to a lack of off-the-shelf software for parameter estimation and for model error assessment-other than that of Lophaven et al. [45]. Based upon the results presented elsewhere [17,31,32], the proper use of kriging models in engineering design requires a significant background in statistics and in engineering design.

Future work on this methodology should investigate more precise methods for sensitivity analysis such as those presented by McKay [40]. Additionally, future work is needed to quantify the accuracy of the prediction intervals resulting from the method as a function of the number of samples used in the MCS. A sample size of 10,000 was used only to demonstrate the proposed methodology. Finally, future work should address applying this methodology as part of a RBDO algorithm. Specifically, research is needed to use the estimates of the prediction intervals from the methodology to efficiently drive an optimization algorithm. The prediction intervals are random variables that are estimated from the Monte Carlo simulation. The precisions of the estimates are a function of the number of samples taken during the simulation. Taking too many samples during the Monte Carlo simulation to achieve precise results may result in a method that is too computationally expensive to use in practice.

Acknowledgment

The authors would like to thank Dr. Kam Ng of The Office of Naval Research 332 for his generous support on Contract No. N00014-00-G-0058.

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