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DESIGN OPTIMIZATION OF HIERARCHICALLY DECOMPOSED MULTILEVEL SYSTEMS UNDER UNCERTAINTY

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ABSTRACT

This paper presents a methodology for design optimization of decomposed systems in the presence of uncertainties. We extend the analytical target cascading (ATC) formulation to probabilistic design by treating stochastic quantities as random variables and parameters and posing reliability-based design constraints. We model the propagation of uncertainty throughout the multilevel hierarchy of elements that comprise the decomposed system by using the advanced mean value (AMV) method to generate the required probability distributions of nonlinear responses. We utilize appropriate metamodeling techniques for simulation-based design problems. A simple yet illustrative hierarchical bi-level engine design problem is used to demonstrate the proposed methodology.

1 INTRODUCTION

Design optimization of complex engineering systems can be accomplished only by decomposition. The system is partitioned into subsystems, the subsystems are partitioned into components, the components into parts, and so on. This decomposition process results in a multilevel hierarchy of elements that comprise the system.

Hierarchical decomposition facilitates employing decentralized optimization approaches that aid systems engineers to identify interactions among elements at lower levels and to transfer this information to higher levels, and has in fact become standard design practice, as evidenced by the organizational structure of engineering companies [1].

In this paper we consider such hierarchically decomposed multilevel systems. In particular, we extend previous deterministic methodologies for optimal and consistent design of such systems to account for the presence of uncertainties. Our objective is to introduce the concept of uncertainty, model its propagation through the multilevel hierarchy, set the ground for the application of "single-element" optimization under uncertainty methods in multilevel systems, and identify needs for future research.

Our motivation is that deterministic approaches assume that complete information of the problem is available, and that design decisions can be implemented. These assumptions imply that optimization results are as good (and therefore useful) as the design and simulation/analysis models used to obtain them, and that they are meaningful only if they can be realized exactly. In reality, these assumptions do not hold. We are rarely in a position to represent a physical system without using approximations, have complete knowledge on all of its parameters, or control the design variables with high accuracy. It is therefore necessary to treat all quantities associated with uncertainty as stochastic.

It is important to differentiate our research work from that related to multidisciplinary design optimization (MDO). Multidisciplinary systems design approaches are used when considering the system as consisting of multiple interacting disciplines.

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Several approaches for MDO have been developed during the 1990's, all of which had as an objective the coordination of the interacting disciplines during the design optimization process, mostly using single- or bi-level formulations [2, 3]. These approaches are non-hierarchical in the sense that the disciplines are not decomposed into multilevel hierarchies. Discipline outputs are inputs to other disciplines and *vice versa*. This is the significant difference between MDO and our work. In hierarchically decomposed multilevel systems outputs of lower-level elements are inputs to higher-level elements, but not *vice versa*. An additional difference between design optimization of hierarchical multilevel systems and MDO is the type of decomposition, distinguished in [4] as object and aspect-based, respectively. Nevertheless, if it is possible to define a discipline-based hierarchy where lower-level discipline outputs are inputs to higher-level disciplines, our methodology would then provide an MDO approach to optimal design of hierarchical multilevel systems.

To the best of our knowledge, no research work on addressing the presence of uncertainties in hierarchically decomposed multilevel systems has been reported in the literature. However, there is ongoing work to take uncertainties into consideration in the MDO framework [5–14].

Most of these references utilize a simple first-order Taylor expansion [5, 7, 8] to calculate the mean and variance of the response in robust multidisciplinary design [14]. A "worst case" concept based on first-order sensitivity has been used to evaluate the performance range of a multidisciplinary system [9].

Although the calculation of the response mean and variance using first-order sensitivity may be adequate for robustness calculations, it does not provide enough statistical information to consider design feasibility under uncertainty. As will be illustrated in this paper, probabilistic representation of the constraints requires complete probabilistic distributions of the system output. Reliability analysis using probabilistic distributions has been used in MDO [15–17]. Reliability analysis introduces an additional iteration loop resulting in coupled optimization problems that are computationally expensive. Response surfaces have been used to reduce the computational effort [5]. Decoupled reliability and optimization procedures in an MDO framework have been also proposed using approximate probabilistic constraint representations [16]. In general, a double-loop optimization process exists in reliability-based MDO analysis, which repeatedly calls expensive system-level multidisciplinary analyses. A single-loop collaborative reliability analysis method has been recently proposed in [15]. A Most Probable Point (MPP) reliability analysis method is combined with the collaborative disciplinary analyses to automatically satisfy the interdisciplinary consistency in reliability analyses. A single reliability optimization loop uses equality constraints to enforce disciplinary compatibility. Despite the use of a single optimization loop, it is a computationally expensive, "all-at-once" procedure due to the presence of the equality discipline constraints.

The paper is organized as follows. In the next section we present a methodology for optimal design of hierarchical multilevel systems, and extend its formulation to account for uncertainties. In Section 3 we address the issue of modeling uncertainty propagation in multilevel hierarchies and present some analytical examples. In Section 4 we present an efficient methodology to develop highly accurate metamodels. A simple yet illustrative simulation-based example is used in Section 5 to demonstrate our methodology for hierarchical multilevel system design. Finally, concluding remarks are summarized in Section 6.

2 OPTIMAL DESIGN OF HIERARCHICALLY DECOMPOSED MULTILEVEL SYSTEMS

Our framework for hierarchical multilevel system optimization under uncertainty is based on analytical target cascading (ATC). In this section we first review the deterministic formulation of ATC, and then we present its extension to account for uncertainties.

2.1 Deterministic Formulation

ATC is a mathematical methodology for translating ("cascading") overall system design targets to element specifications based on a hierarchical multilevel decomposition [18–20]. The objective is to assess relations and identify possible trade-offs among elements early in the design development process, and to determine specifications that yield consistent system design with minimized deviation from design targets. For an engineering corporation, ATC provides a means to dictate technical objectives to different design teams, knowing *a-priori* that these goals can be achieved without conflicting with those of other teams. Consistent system design can then be accomplished with minimum communication overhead, i.e., maximum efficiency, avoiding costly iterations late in the process.

The ATC process is proven to be convergent when using a specific class of coordination strategies [21], and has been successfully applied to a variety of optimal design problems, e.g., [22–25].

We refer the reader to the above references for a detailed description of ATC. Here, we will briefly present the concept and the general mathematical formulation. In ATC a minimum deviation optimization problem is formulated and solved for each element in the multilevel hierarchy that reflects the decomposed optimal system design problem, *cf.* Figure 1. Therefore, responses of lower-level elements are inputs into higher-level elements. The ATC process aims at minimizing the gap between what higher-level elements "want" and what lower-level elements "can". If design variables are shared among some elements at the same level, their consistency is coordinated by their parent element at the level above.

The mathematical formulation of problem p_{ij}, where i and j

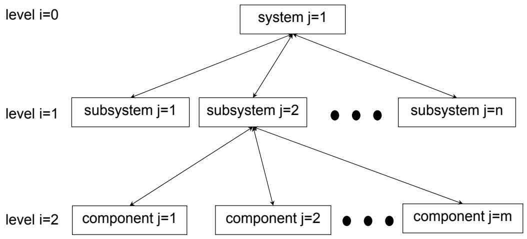

Figure 1. Example of hierarchically decomposed multilevel system

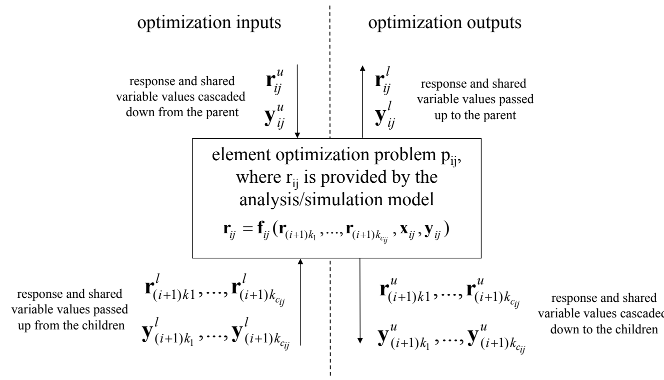

Figure 2. ATC information flow at element j of level i

denote level and element, respectively, is

$$
\begin{aligned}
\min_{\tilde{\mathbf{x}}_{ij}, \varepsilon^r_{ij}, \varepsilon^y_{ij}} \quad & \|\mathbf{r}_{ij} - \mathbf{r}^u_{ij}\|_2^2 + \|\mathbf{y}_{ij} - \mathbf{y}^u_{ij}\|_2^2 + \varepsilon^r_{ij} + \varepsilon^y_{ij} \qquad (1)\\
\text{subject to} \quad & \textstyle\sum_{k=1}^{n_{ij}} \|\mathbf{r}_{(i+1)k} - \mathbf{r}^l_{(i+1)k}\|_2^2 \leq \varepsilon^r_{ij} \\
& \textstyle\sum_{k=1}^{n_{ij}} \|\mathbf{y}_{(i+1)k} - \mathbf{y}^l_{(i+1)k}\|_2^2 \leq \varepsilon^y_{ij} \\
& \mathbf{g}_{ij}(\mathbf{r}_{(i+1)1}, \ldots, \mathbf{r}_{(i+1)n_{ij}}, \mathbf{x}_{ij}, \mathbf{y}_{ij}) \leq \mathbf{0} \\
& \mathbf{h}_{ij}(\mathbf{r}_{(i+1)1}, \ldots, \mathbf{r}_{(i+1)n_{ij}}, \mathbf{x}_{ij}, \mathbf{y}_{ij}) = \mathbf{0} \\
\text{with} \quad & \mathbf{r}_{ij} = \mathbf{f}_{ij}(\mathbf{r}_{(i+1)1}, \ldots, \mathbf{r}_{(i+1)n_{ij}}, \mathbf{x}_{ij}, \mathbf{y}_{ij}),
\end{aligned}
$$

where the vector of optimization variables $\tilde{\mathbf{x}}_{ij}$ consists of (n_{ij}) children response design variables $\mathbf{r}_{(i+1)1}, \ldots, \mathbf{r}_{(i+1)n_{ij}}$, local design variables $\mathbf{x}_{ij}$, local shared design variables $\mathbf{y}_{ij}$ (i.e., design variables that this element shares with other elements at the same level), and coordinating variables for the shared design variables of the children $\mathbf{y}_{(i+1)1}, \ldots, \mathbf{y}_{(i+1)n_{ij}}$, and where $\mathbf{g}_{ij}$ and $\mathbf{h}_{ij}$ denote local design inequality and equality constraints, respectively. Tolerance optimization variables ε^r and ε^y are introduced to coordinate responses and shared variables, respectively. Superscripts u (l) are used to denote response and shared variable values that have been obtained at the parent (children) problem(s), and have been cascaded down (passed up) as design targets (consistency parameters), *cf.* Figure 2. Note that although communication among levels, i.e., updating parameter values associated with the ATC process, is bi-directional, functional dependency is strictly hierarchical (as we emphasized in the introduction section). Higher-level responses are functions of lower-level responses, but not *vice versa*.

Assuming that all the parameters have been updated using the solutions obtained at the parent- and children-problems, Problem (1) is solved to update the parameters of the parent- and children-problems. This process is repeated until the tolerance optimization variables in all problems cannot be reduced any further.

2.2 Non-deterministic Formulations

In this section, the ATC formulation is modified to account for uncertainties. Stochastic quantities are represented by random variables and parameters (denoted by upper case latin symbols). We present two alternative non-deterministic formulations for solving the hierarchical multilevel optimization problem in the presence of uncertainties. The stochastic formulation does not use a probabilistic representation of the design constraints, while the probabilistic one does. For the sake of simplicity, in the following formulations we will assume that all design variables are random and that there are no random parameters.

2.2.1 Stochastic Formulation In the stochastic formulation, each random variable is represented by a parameter that describes its probabilistic characteristics. Typically, this parameter is the first moment, or mean, of the random variable. Responses and other functions of random variables are expressed as expected values. Thus, Problem (1) becomes

$$
\begin{aligned}
\min_{\mu_{\tilde{\mathbf{X}}_{ij}}, \varepsilon^R_{ij}, \varepsilon^Y_{ij}} \quad & \|E[\mathbf{R}_{ij}] - \mu^u_{\mathbf{R}_{ij}}\|_2^2 + \|\mu_{\mathbf{Y}_{ij}} - \mu^u_{\mathbf{Y}_{ij}}\|_2^2 + \varepsilon^R_{ij} + \varepsilon^Y_{ij} \qquad (2)\\
\text{subject to} \quad & \textstyle\sum_{k=1}^{n_{ij}} \|\mu_{\mathbf{R}_{(i+1)k}} - E[\mathbf{R}_{ij}]^l\|_2^2 \leq \varepsilon^R_{ij} \\
& \textstyle\sum_{k=1}^{n_{ij}} \|\mu_{\mathbf{Y}_{(i+1)k}} - \mu^l_{\mathbf{Y}_{(i+1)k}}\|_2^2 \leq \varepsilon^Y_{ij} \\
& E[\mathbf{g}_{ij}(\mathbf{R}_{(i+1)1}, \ldots, \mathbf{R}_{(i+1)n_{ij}}, \mathbf{X}_{ij}, \mathbf{Y}_{ij})] \leq \mathbf{0} \\
& E[\mathbf{h}_{ij}(\mathbf{R}_{(i+1)1}, \ldots, \mathbf{R}_{(i+1)n_{ij}}, \mathbf{X}_{ij}, \mathbf{Y}_{ij})] = \mathbf{0} \\
\text{with} \quad & \mathbf{R}_{ij} = \mathbf{f}_{ij}(\mathbf{R}_{(i+1)1}, \ldots, \mathbf{R}_{(i+1)n_{ij}}, \mathbf{X}_{ij}, \mathbf{Y}_{ij}),
\end{aligned}
$$

where $E[\cdot]$ denotes the expectation operator.

In words, this formulation attempts to

1. Match the expected values of the local responses with the targets cascaded from the higher level; these targets are the optimal values of the random design variables, i.e., the means, of the higher-level problem.
2. Match the optimal values of the random response design variables, i.e., the means, with the expected values of the children responses.

3. Match the optimal values of the local and children random shared variables, i.e., the means, with the target values cascaded from the higher and lower levels, respectively.

The challenge in solving stochastic optimization problems such as Problem (2) is that evaluating expectations requires knowledge of the probability density functions of the random variables and evaluation of multidimensional integrals.

The solution of Problem (2) satisfies the design inequality and equality constraints in an average sense, but does not provide any information on the percentage of constraint violations due to uncertainty. In practical applications, however, there is a need to satisfy the constraints at a specified target reliability level.

2.2.2 Probabilistic Formulation

The constraints are thus reformulated. We now require that the probability of satisfying a constraint under the presence of uncertainties greater than some appropriately selected threshold, or, alternatively, that the probability of violating a constraint is less than some prespecified probability of failure. The formulation of Problem (2) becomes

$$\begin{aligned}
\min_{\mu_{\tilde{\mathbf{X}}_{ij}},\varepsilon^R_{ij},\varepsilon^Y_{ij}} \quad & \|E[\mathbf{R}_{ij}]-\mu^u_{\mathbf{R}_{ij}}\|_2^2+\|\mu_{\mathbf{Y}_{ij}}-\mu^u_{\mathbf{Y}_{ij}}\|_2^2+\varepsilon^R_{ij}+\varepsilon^Y_{ij} \qquad (3)\\
\text{subject to} \quad & \textstyle\sum_{k=1}^{n_{ij}}\|\mu_{\mathbf{R}_{(i+1)k}}-E[\mathbf{R}_{ij}]^l\|_2^2\le\varepsilon^R_{ij}\\
& \textstyle\sum_{k=1}^{n_{ij}}\|\mu_{\mathbf{Y}_{(i+1)k}}-\mu^l_{\mathbf{Y}_{(i+1)k}}\|_2^2\le\varepsilon^Y_{ij}\\
& P[\tilde{\mathbf{g}}_{ij}(\mathbf{R}_{(i+1)1},\ldots,\mathbf{R}_{(i+1)n_{ij}},\mathbf{X}_{ij},\mathbf{Y}_{ij})>0]\le\mathbf{P}_f,\\
\text{with} \quad & \mathbf{R}_{ij}=\mathbf{f}_{ij}(\mathbf{R}_{(i+1)1},\ldots,\mathbf{R}_{(i+1)n_{ij}},\mathbf{X}_{ij},\mathbf{Y}_{ij}),
\end{aligned}$$

where $P[\cdot]$ denotes probability measure and $\mathbf{P}_f$ is a vector of prespecified probability of failure thresholds.

Note that the mathematical formulation of Problem (3) does not contain equality constraints. Equality constraints do not make sense in a probabilistic framework (it is meaningless to require that a function takes exactly a specific value under the presence of uncertainty, since the probability of a continuous random variable taking an exact value ois zero), one has to introduce some slack and treat equality constraints as inequality constraints. For example, if in a deterministic framework it is required that $h(\mathbf{x})=0$, in a probabilistic framework it is required that $|\ h(\mathbf{X})\ |\le\delta$, where δ is a small positive constant, so that the constraint is formulated as $P[|\ h(\mathbf{X})\ |-\delta>0]\le P_f$. Therefore, we rewrite equality constraints as inequality constraints and unite the two constraint function vectors into one, denoted by $\tilde{\mathbf{g}}$.

Of course, there are applications where certain equality constraints are “more” important than others. For example, equality constraints representing governing equations of physical phenomena must be satisfied *almost surely*, i.e., with a probability close to one. For such “hard” constraints, the δ value and the acceptable probability of failure P_f must be small, as opposed to “soft” constraints, where these values can be relaxed at the designer’s discretion. A more elaborate discussion on this subject can be found in [26].

Problem (3) can be solved with any of the available commercial software packages or the methods reported recently in the literatures, e.g., the hybrid mean value (HMV) method or the sequential optimization and reliability assessment (SORA) method [27, 28]. We adopt a recently developed single-loop method that is as accurate as the HMV and the SORA methods, but much more efficient [29].

3 PROPAGATION OF UNCERTAINTIES

The responses of the elements in the multilevel hierarchy are typically nonlinear functions of the elements’ inputs, which include random variables and parameters. Thus, responses are themselves random variables, whose expected value must be computed to evaluate objective and constraints when solving probabilistic optimization problems. Moreover, estimated variance of responses is required if robustness considerations are included.

Finally, in a multilevel hierarchy, responses of lower-level subsystems are inputs to higher-level subsystems. Therefore, it is necessary to obtain probability distribution information required for the solution of the higher-level problems. This is an issue of outmost importance in design optimization of hierarchically decomposed multilevel systems. An efficient and accurate mechanism is required for propagating probabilistic information in the form of cumulative distribution and probability density functions throughout the hierarchy.

3.1 Estimating Moments Using the Mean-Value First-Order Second-Moment Method

In an initial effort, a mean-value first-order second-moment (MVFOSM) approach was adopted to estimate the mean and standard deviation of a nonlinear function of random variables [30]. Specifically, a first-order Taylor expansion about the current design, represented by the mean vector $\mu_{\mathbf{X}}$ of the random variables $\mathbf{X}$, was used to linearize a nonlinear random response R:

$$R=f(\mathbf{X})\approx f(\mu_{\mathbf{X}})+\sum_{i=1}^{n}\frac{\partial f(\mu_{\mathbf{X}})}{\partial X_i}(X_i-\mu_{X_i}), \qquad (4)$$

where n is the dimension of the vector $\mathbf{X}$. Assuming that all the random variables are statistically independent (uncorrelated), the first-order approximations of the mean and the variance of R were given by

$$E[R]=\mu_R\approx f(\mu_{\mathbf{X}}) \qquad (5)$$

and

$$Var[R] = \sigma_R^2 \approx \sum_{i=1}^{n} \left(\frac{\partial f(\mu_{\mathbf{X}})}{\partial X_i} \right)^2 \sigma_{X_i}^2, \tag{6}$$

respectively.

The advantage of this approach, besides efficiency, is that it allowed us to assume that the responses are normally distributed if all input random variables and parameters were normal. Therefore, propagation of uncertainty in ATC was modeled as a linear process. With the distribution information known, all that was necessary was the estimation of the first two moments, which characterize a normal distribution completely. The validity of the successive linearizations during the ATC process was ensured by virtue of the ATC consistency constraints that do not allow large deviations from current designs.

To our knowledge, this linearization approach is currently embedded in all state-of-the-art software packages for optimization under uncertainty. As will be demonstrated shortly, the linearization approach does a fairly good job in estimating the expected value of nonlinear functions of random variables. However, it can be quite inaccurate in estimating higher moments, e.g., the standard deviation. Moreover, it is limiting in that it does not provide us with the correct probability distribution information of the random nonlinear responses.

It is also important to note that if the linearization approach is used to compute expectations in the stochastic formulation, Problems (1) and (2) generate identical solutions. There is no value in solving the stochastic ATC formulation if expectations are not computed exactly, which requires accurate probability distribution information and multidimensional integrations. This is an additional reason that may explain why the probabilistic constraint formulation is used universally today to solve nondeterministic problems.

3.2 Generating Distributions Using the Advanced Mean Value Method

In this paper, we utilize the advanced mean value (AMV) method to generate the cumulative distribution function (CDF) of a nonlinear response. The AMV method [31] is a computationally efficient method for generating the CDF of nonlinear functions of random variables. It improves the Mean Value (MV) prediction (Section 3.1) by using a simple correction to compensate for errors introduced from the Taylor series truncation. A response performance function $R = f(\mathbf{X})$ is linearized as shown in Eq. (4) and its first and second order moments μ_R and σ_R are calculated using Eqs. (5) and (6), respectively.

A limit state function is then defined as

$$g(\mathbf{X}) = f(\mathbf{X}) - f_0, \tag{7}$$

where f_0 is a particular value of the performance function. The reliability index β is then given by

$$\beta = \frac{\mu_g}{\sigma_g}, \tag{8}$$

where $\mu_g = \mu_R - f_0$ and $\sigma_g = \sigma_R$. The CDF value of f at f_0 is calculated from the first-order relation

$$P[f \le f_0] = P[g \le 0] = \Phi(-\beta), \tag{9}$$

where Φ is the standard normal cumulative distribution function. It is emphasized that Eq. (8) is equivalent to calculating the most probable point (MPP) using the linear approximation of Eq. (4). The MPP in the standard normal space is given by

$$\mathbf{U}^* = -\beta \frac{\nabla g(\mathbf{X})}{|\nabla g(\mathbf{X})|}. \tag{10}$$

In the original X space, the MPP coordinates vector is

$$\mathbf{X}^* = \mathbf{U}^* \sigma_{\mathbf{x}} + \mu_{\mathbf{x}}, \tag{11}$$

where $\mu_{\mathbf{x}}$ and $\sigma_{\mathbf{x}}$ are the mean and standard deviation vectors, respectively, of the vector of random variables $\mathbf{X}$.

In the AMV method, the following relation is used instead of Eq. (9):

$$P[f \le f(\mathbf{X}^*)] = \Phi(-\beta), \tag{12}$$

i.e., the f_0 value at which the reliability index β is calculated is replaced by $f(\mathbf{X}^*)$.

To generate the CDF of $R = f(\mathbf{X})$, the Most Probable Point Locus (MPPL) is first calculated using the simple MV method. The MPPL is defined by connecting all MPP's for a discretized appropriate range of the performance function at points f_i. Subsequently, a single function evaluation $f(\mathbf{X}^*)$ is used at each CDF level to correct the CDF value obtained with the MV method. The AMV method is computationally efficient since it requires only a single linearization of the performance function at the mean value and an additional function evaluation at each CDF level (discretized f range at values f_i). It is also very accurate as repeatedly demonstrated in the literature [32–34]. Note that the MPPL-based CFD generation concept has been reported before, but is was based on a less efficient MPP determining procedure [35].

With the CDF available, one can differentiate numerically to obtain the probability density function (PDF). We use central differences to obtain second-order accurate approximations.

Finally, to compute moments, we integrate numerically, using spline interpolation to estimate response values that lie between the available PDF values. As will be shown by means of several analytical examples, this method is quite accurate.

3.3 Examples

The MVFOSM-based and AMV-based methods were used to estimate the first two moments of several nonlinear analytical expressions. All random variables were assumed to be normal. Test functions and input statistics are presented in Table 1 and results are summarized in Table 2. One million samples were used for the Monte Carlo simulations.

Table 1. Test functions and input statistics

#	Expression	Input Statistics
1	$X_1^2+X_2^2$	$X_1 \sim N(10,2)$, $X_2 \sim N(10,1)$
2	$-\exp(X_1-7)-X_2+10$	$X_{1,2} \sim N(6,0.8)$
3	$1-\frac{X_1^2X_2}{20}$	$X_{1,2} \sim N(5,0.3)$
4	$1-\frac{(X_1+X_2-5)^2}{30}-\frac{(X_1-X_2-12)^2}{30}$	$X_{1,2} \sim N(5,0.3)$
5	$1-\frac{80}{X_1^2+8X_2+5}$	$X_{1,2} \sim N(5,0.3)$

Table 2. Estimated moments and errors relative to Monte Carlo simulation (MCS) results

#	1	2	3	4	5
μ_{lin}	200.0	3.6321	−5.25	−1.0333	−0.1428
μ_{AMV}	203.4	3.6029	−5.3495	−1.0380	−0.1454
μ_{MCS}	205.0	3.4921	−5.3114	−1.0404	−0.1448
ε_{lin} [%]	−2.44	4.00	−1.15	−0.68	−1.30
ε_{AMV} [%]	−0.78	3.17	0.71	−0.23	0.41
σ_{lin}	44.72	1.9386	0.8385	0.1166	0.00627
σ_{AMV}	45.20	0.9013	0.8423	0.1653	0.00631
σ_{MCS}	45.10	0.9327	0.8407	0.1653	0.00630
ε_{lin} [%]	−0.84	107.85	−0.26	29.46	−0.47
ε_{AMV} [%]	0.22	−3.36	0.19	0	0.15

By inspecting Table 2, it can be seen that while the mean-related errors of the linearization approach are within acceptable limits, standard deviation errors can be quite large. The AMV-based moment estimation method performs always better, and never exhibits unacceptable errors. Moreover, the AMV-method provides accurate probability distribution information of nonlinear responses. For example, Figures 3 and 4 depict the CDFs and PDFs, respectively, of function # 1, obtained using both the MVFOSM-based and the AMV-based method. It can be seen that, using the linearization approach, the nonlinear response would be incorrectly assumed as normally distributed.

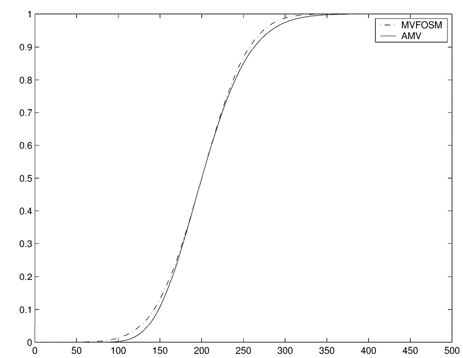

Figure 3. Cumulative distribution function of function #1

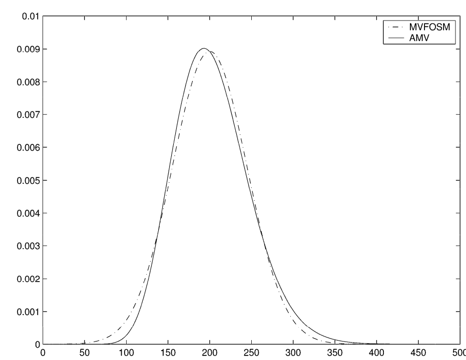

Figure 4. Probability density function of function #1

3.4 Propagating Uncertainty in ATC

Our methodology for propagating uncertainty information during the ATC process can be summarized in the following steps:

1. Start at the bottom level of the hierarchy, where probability distribution on the input random variables and parameters is assumed as known. If such information is not available at the bottom level, start at the lowest level possible where such information is available.
2. Solve the probabilistic design optimization problems for the level specified in step 1.

3. Use the approach described in Section 3.2 to obtain distribution information for the response variables that are inputs to higher-level ("parent") problems.
4. Using the information obtained at step 3, solve the parent problems. Note that the CDFs and PDFs of lower-level ("children") responses that constitute optimization variables in the parent problems are required for solving these problems correctly. Second moment (variance) information alone is inadequate to guarantee proper solution process and uncertainty propagation throughout the hierarchy (as opposed, e.g., to "single"-element robust design optimization).
5. Move your way to the top of the hierarchy.
6. Once you have reached the top-level problem start moving towards the bottom using previous solutions to update parameters as shown in Figure 2.
7. Keep iterating until all ε values in all problems in the hierarchy have been reduced as much as possible, i.e., have converged to a steady state value. Note that the ε variables are deterministic, as are the constraints they appear in. While uncertainties are taken into account in the probabilistic design constraints, the non-deterministic ATC process aims at coordinating values of shared variables and responses in an average sense.

Note that since the linearization approach is sufficiently accurate for estimating expected values, it can be used to reduce computational cost. However, the AMV-based method is so efficient, that it is suggested for use in estimating expected values to improve accuracy and thus, possibly, the convergence rate of the ATC process.

4 METAMODELING FOR SIMULATION-BASED DESIGN UNDER UNCERTAINTY

The state-of-the-art analytical reliability analysis methods are gradient based. When simulations are used to compute responses, as is the case in our following example (Section 5), numerical noise can occur. In addition, simulations tend to be computationally expensive. Computational cost is then aggregated during optimization and reliability analysis.

Use of metamodels (or surrogate models, or response surfaces) is the established remedy to address the above issues. However, metamodels introduce additional errors to the ones already existing due to lack of knowledge, inability to represent physics with mathematical expressions, incomplete information, numerical arithmetic errors, uncertainty, and its propagation, as illustrated in the following expression

$$R = f(\mathbf{x}) + \varepsilon_{\text{physics}} + \varepsilon_{\text{modeling}} + \varepsilon_{\text{metamodeling}} + \varepsilon_{\text{data}} + \varepsilon_{\text{numerics}} + \varepsilon_{\text{uncertainty}} + \varepsilon_{\text{uncertainty propagation}}.$$

Approximations and errors are a reality that we must acknowledge even if we are not in a position to eliminate completely. There is no meaning in driving just one error down to zero if any of the remaining ones are still relatively large [36]. Our point is that if metamodels must be used, they must be associated with small errors relative to other error sources.

Traditional response surface methodology using Design of Experiments (DOE) techniques [37, 38], such as fractional factorials, central composite, Plackett-Burman, and Box-Behnken designs, is usually computationally efficient. However, it often becomes inadequate in nonlinear multivariate metamodeling of complex simulation models. In traditional parametric regression, the metamodel functional form is assumed known (e.g., polynomials in the conventional least-squares regression). The goal of regression analysis is to determine the parameter values of the assumed functional form, so that the generated metamodel best fits the provided data set. A linear or nonlinear parametric metamodel is likely to produce good approximations only when the assumed functional form is close to the true underlying function.

For this reason, nonparametric regression techniques [39, 40], along with the progressive space-filling sampling [41, 42], have attracted a growing interest. They only use a few general assumptions about the functional form of the metamodel, such as its smoothness properties. The functional form is not prespecified, but determined instead from the available data. The nonparametric approach is therefore, more flexible and is likely to produce accurate nonlinear approximations even if the true underlying function form is totally unknown.

Many nonparametric techniques have been proposed for univariate modeling, such as smoothing splines and local polynomial fitting [43, 44]. They can be easily extended to multivariate cases. As a more general case of smoothing splines, nonparametric regression methods using Gaussian process models (similar to Kriging in spatial statistics) and radial basis functions (RBF), have been used to fit data from computer experiments [45–47]. The local polynomial fitting and Kriging/RBF techniques have demonstrated better predictive performance than the parametric regression techniques [48]. Their main advantage is an automated metamodeling process, in which the hyper-parameters in local polynomial fitting and Kriging can be determined by minimizing the metamodel cross-validation error and maximizing the likelihood function, respectively. Local polynomial fitting, using the cross-validated moving least squares (CVMLS) method [39, 40], is used in this paper.

4.1 Optimal Symmetric Latin Hypercube Sampling

In order to construct a metamodel using the CVMLS method, an appropriate sampling technique is necessary, which preferably uses a modest number of samples with the potential to explore nonlinear input/output relationships. Previous studies have found that uniformity is the most important criterion, while the space-filling uniform design is preferable [41, 42]. The optimal symmetric Latin hypercube (OSLH) technique is used here. It is an efficient space-filling sampling method for constructing high quality metamodels with very few samples.

A Latin hypercube is a set of n points in d dimensions with the property that the projections on any axis form a uniform grid. A Latin hypercube design (LHD) is an $n \times d$ matrix, in which each column is a random permutation of $(1,2,\ldots,n)$. An LHD has uniform projection properties on any single dimension, and is much more efficient than conventional designs for problems with large number of design variables. An LHD is called a symmetric Latin hypercube design (SLHD) if the i-th row is the symmetric point of the $(n+1-i)$-th row about the center, i.e., the design is symmetric about the midpoint.

A randomly selected LHD may act poorly in estimation and prediction if its uniformity in higher than one dimensions is not good. One approach is to use optimal designs according to some criteria such as entropy [49], integrated mean-squared error [45] or minimum inter-site distance [50]. The entropy criterion is equivalent to the minimization of $-\log \mid C \mid$, where C is the covariance between two d-dimensional vectors $\mathbf{s}$ and $\mathbf{t}$ of a zero-mean Gaussian process $Z(x)$; it is defined as

$$C(\mathbf{s},\mathbf{t}) = \sigma^2 \exp\left(-\theta \sum_{i=1}^{d} \mid s_i - t_i \mid^p\right), \tag{13}$$

where σ, θ and p are parameters that determine the properties of $Z(x)$. A design with a smaller entropy value has better uniformity and is thus considered better.

Finding OSLH designs requires searching the space of all Latin hypercubes for a design that optimizes some measure of “uniformity” in two and higher dimensions. The exchange algorithm in [40] has been used in this example for constructing OSLH designs.

4.2 Cross-Validated Moving Least Squares

The moving least squares (MLS) method originated in curve and surface fitting [51]. An advanced CVMLS method was recently developed [39, 40], and is used in this paper.

For a multivariate function $f(\mathbf{x})$, $\mathbf{x}^i = [x_1^i x_2^i \ldots x_d^i]^T$, $i = 1,2,\ldots,n$, represents the i-th point of n known sample points scattered in the d-dimensional space. The corresponding function value is denoted by $f^i = f(\mathbf{x}^i)$ for $i = 1,\ldots,n$. The function $f(\mathbf{x})$ can be approximated by $g(\mathbf{x})$ using a linear combination of basis functions. The fundamental assumption in MLS is that the predicted function value at a point $\mathbf{x}$ should be most strongly influenced by the values of f^i at the points $\mathbf{x}^i$ that are closest to $\mathbf{x}$. Therefore, a weighting function is necessary, which decreases monotonically as the distance from $\mathbf{x}$ to $\mathbf{x}^i$ increases. A commonly used form for the weighting function in MLS is

$$w(\mathrm{dist}(\mathbf{x},\mathbf{x}^i)) = \exp\left(-\alpha \sum_{j=1}^{d} (x_j - x_j^i)^2\right), \tag{14}$$

where dist denotes distance, represented here by the square of the Euclidean norm. The positive tuning parameter α controls the degree of localization in MLS regression by scaling the slope of the weighting function.

The prediction $f(\mathbf{x})$ at point $\mathbf{x}$ is

$$f(\mathbf{x}) \approx g_{\mathrm{mls}}(\mathbf{x}) = \sum_{k=1}^{m} a_k(\mathbf{x}) b_k(\mathbf{x}) = \mathbf{a}^T(\mathbf{x})\mathbf{b}(\mathbf{x}), \tag{15}$$

where $\mathbf{b}$ is a basis with a full set of linear polynomials. Since the weights w^i are functions of $\mathbf{x}$, the coefficients $\mathbf{a}$ also depend on $\mathbf{x}$, and are obtained by solving m normal equations $\frac{\partial I_{\mathbf{x}}(g)}{\partial a_j} = 0$, where

$$I_{\mathbf{x}}(g) = \sum_{i=1}^{n} w^i(\mathbf{x})(g(\mathbf{x}^i) - f^i)^2 \tag{16}$$

is a residual error functional.

The localized regression using the MLS procedure can be tuned by adjusting α in Eq. (14). In addition, since the performance function could have a different relationship with each input variable, the square of the Euclidean distance in Eq. (14) is usually replaced by a general parameterized distance formula

$$\mathrm{dist}(\mathbf{x},\mathbf{x}^i) = \sum_{j=1}^{d} \gamma_j (x_j - x_j^i)^2, \tag{17}$$

Thus, the weight function in Eq. (16) can be expressed as

$$w(\mathrm{dist}(\mathbf{x},\mathbf{x}^i))\big|_{\gamma_1,\ldots,\gamma_d} = \exp\left(-\alpha \sum_{j=1}^{d} \gamma_j (x_j - x_j^i)^2\right), \tag{18}$$

where d positive weight function parameters $gamma_1,\ldots,\gamma_d$ are calculated from minimizing the metamodel prediction error.

A leave-one-out cross-validation procedure is used to compute a metamodel prediction error metric such as the cross-validation root mean square error (CV-RMSE) or the cross-validation average absolute error (CV-AAE). Every known sample $\mathbf{x}^i$ is left out successively, and its value is predicted based on the remaining known samples. The MLS parameters can be thus estimated from solving an unconstrained optimization problem that minimizes the cross-validation error.

The CVMLS method is used in the simulation-based example presented in the next section for its simplicity, computational efficiency, and effectiveness. Uniformly spaced OSLH samples are used in order to ensure the robustness of the cross-validation error estimate and also to avoid redundant samples.

5 EXAMPLE

The probabilistic formulation of the ATC process (Problem (3)) is used to solve a simple yet illustrative simulation example. We consider a V6 gasoline engine as the system, which is "decomposed" into a subsystem that represents the piston-ring/cylinder-liner subassembly of a single cylinder. The system simulation predicts engine performance in terms of brake-specific fuel consumption. Although the engine has six cylinders, they are all designed to be identical. For this reason, we only consider one subsystem.

The associated bi-level hierarchy, shown in Figure 5, includes the engine as a system at the top level and the piston-ring/cylinder-liner subbassembly as a subsystem at the bottom level. The ring/line subassembly simulation takes as inputs the

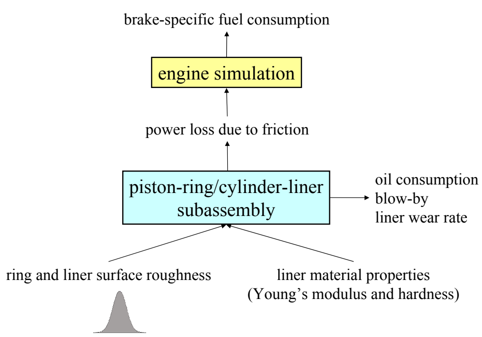

Figure 5. Hierarchical bi-level system

surface roughness of the ring and the liner and the Young's modulus and hardness and computes power loss due to friction, oil consumption, blow-by, and liner wear rate. The root mean square (RMS) of asperity height is used to represent asperity roughness, which is assumed to be normally distributed. The engine simulation takes then as input the power loss and computes brake-specific fuel consumption of the engine. Commercial software packages were used to perform the simulations. A detailed description of the problem can be found in [30].

5.1 Problem Formulation

Due to the simplicity of the given problem structure, we will use here a modified version of the notation introduced earlier. Since there are only two levels with only one element in each, we skip element indices and denote the upper-level element with subscript 0 and the lower-level element with subscript 1. We use second indices to denote entries in the design variable vector of the lower-level element optimization problem. The design problem is to find optimal mean values $\mu_{X_{11}}$ and $\mu_{X_{12}}$ for the piston-ring and cylinder-liner surface roughness random variables X_{11} and X_{12}, respectively, and optimal values for the deterministic design variables representing the material properties (Young's modulus x_{13} and hardness x_{14}) of the liner that yield minimized expected value of brake-specific fuel consumption R_0. The optimal design is subject to constraints on liner wear rate, oil consumption, and blow-by. The power loss due to friction R_1 links the two levels.

The top- and bottom-level ATC problems are formulated as

$$\begin{aligned} \min_{\mu_{R_1},\varepsilon^R} \quad & (E[R_0]-T)^2+\varepsilon^R \\ \text{subject to } & (\mu_{R_1}-E[R_1]^l)^2 \leq \varepsilon^R \\ \text{with } \quad & R_0 = f_0(R_1) \end{aligned} \tag{19}$$

and

$$\begin{aligned} \min_{\mu_{X_{11}},\mu_{X_{12}},x_{13},x_{14}} \quad & (E[R_1]-\mu^u_{R_1})^2 \\ \text{subject to} \quad & P[\text{liner wear rate} > 2.4\times 10^{-12}\ m^3/s] \leq P_f \\ & P[\text{blow-by} > 4.25\times 10^{-5}\ kg/s] \leq P_f \\ & P[\text{oil consumption} > 15.3\times 10^{-3}\ kg/hr] \leq P_f \\ & P[X_{11} < 1\mu m] \leq P_f \\ & P[X_{11} > 10\mu m] \leq P_f \\ & P[X_{12} < 1\mu m] \leq P_f \\ & P[X_{12} > 10\mu m] \leq P_f \\ & 340\ GPa \geq x_{13} \geq 80\ GPa \\ & 240\ BHV \geq x_{14} \geq 150\ BHV \\ \text{with} \quad & R_1 = f_1(X_{11},X_{12},x_{13},x_{14}), \end{aligned} \tag{20}$$

respectively. The standard deviation of the surface roughnesses was assumed to be 1.0 μm, and remained constant throughout the ATC process. The assigned probability of failure P_f was 0.13%, which corresponds to the target reliability index $\beta = 3$. The fuel consumption target T was simply set to zero to achieve the best fuel economy possible.

Note that since the random variables are normally distributed, the associated linear probabilistic bound constraints can be reformulated as deterministic. For example,

$$P[X_{11} < 1\mu m] \leq P_f \Leftrightarrow P[X_{11} - 1\mu m < 0] \leq P_f \Leftrightarrow$$
$$\Phi(0 - \frac{\mu_{X_{11}} - 1\mu m}{\sigma_{X_{11}}}) \leq \Phi(-\beta) \Rightarrow -\frac{\mu_{X_{11}} - 1\mu m}{\sigma_{X_{11}}} \leq -\beta \Leftrightarrow$$
$$\frac{\mu_{X_{11}} - 1\mu m}{\sigma_{X_{11}}} \geq \beta \Leftrightarrow \mu_{X_{11}} - 1\mu m \geq \beta\sigma_{X_{11}} \Leftrightarrow$$
$$\mu_{X_{11}} \geq 1\mu m + \beta\sigma_{X_{11}} \Leftrightarrow \mu_{X_{11}} \geq 4\mu m$$

Similarly, the other three probabilistic bound constraints in Problem (20) can be reformulated as

$$\mu_{X_{11}} \leq 7\mu m; \quad \mu_{X_{12}} \geq 4\mu m; \quad \mu_{X_{12}} \leq 7\mu m.$$

5.2 Metamodeling and Error Analysis

Five metamodels were developed according to the methodology described in Section 4 to replace the system and subsystem simulations and to predict power loss due to friction, liner wear rate, blow-by, and oil consumption, and brake-specific fuel consumption, respectively. An OSLH design with 250 points was used to create the four different, four-dimensional subsystem metamodels, while a 50-point OSLH design was used for the one-dimensional system metamodel.

Additional optimal symmetric Latin hypercubes were generated to validate the surrogate models generated based on the initial ones. Specifically, an OSLH design with 150 points was generated for the ring-liner simulation and an OSLH design with 40 points was generated for the engine simulation. Both the simulation models and the CVMLS metamodels were then executed at the OSLH sample points, and the relative errors were computed according to the formula

$$\varepsilon = \left| \frac{\text{response}_{\text{simulation}} - \text{response}_{\text{metamodel}}}{\text{response}_{\text{simulation}}} \right| \times 100.$$

The means and standard deviations of the relative errors are summarized in Table 3. The oil consumption metamodel exhibits the largest errors. However, it was found that this is due to one extreme outlier in the data. Once this data point is removed, the error values drop dramatically. It can be concluded that the accuracy of the metamodels is more than acceptable. In fact, the additional error they introduce is negligible considering the assumptions and approximations used in the simulation modeling work.

5.3 Results

It is desired to minimize power loss due to friction in order to optimize engine operation and thus maximize fuel economy.

Table 3. Means and standard deviations of the metamodel relative errors

Response	Mean	Standard deviation
Power loss	0.37 %	0.77 %
Liner wear rate	0.72 %	1.32 %
Blow-by	0.37 %	0.63 %
Oil consumption	1.74 %	3.68 %
Fuel consumption	0.005 %	0.004 %

Therefore, it was anticipated that the bottom-level optimization problem would yield a design with as smooth surfaces (low surface roughnesses) as possible.

The probabilistic ATC process of solving Problems (20) and (19) iteratively converged after two iterations. The obtained optimal ring/liner subassembly design is shown in Table 4. The

Table 4. Optimal ring/liner subassembly design

Variable	Description	Value
X_{11}	Ring surface roughness, [μm]	4.00
X_{12}	Liner surface roughness, [μm]	6.15
x_{13}	Liner Young's modulus, [GPa]	80
x_{14}	Liner hardness, [BHV]	240

ring surface roughness optimal value is at its probabilistic lower minimum, while the liner's Young's modulus and hardness optimal values are at their deterministic lower and upper bounds, respectively.

The liner surface roughness is not, however, at its lower bound because the problem is bounded by the oil consumption constraint. A certain degree of surface roughness is required to maintain an optimal oil film thickness in order to avoid excessive oil consumption. For this reason, the associated constraint is active, and the surface roughness of the liner is an interior optimizing argument.

An interesting theoretical issue arises. How do we define activity for probabilistic constraints? The definition of constraint activity in deterministic optimization is the following: A constraint is active if removing it or moving its boundary affects the location of the optimum. In probabilistic design, a constraint is active if the reliability index associated with the constraint's MPP is equal to the target reliability index. In other words, the constraint's MPP lies on the target reliability circle.

A Monte Carlo simulation was performed to assess the accuracy of the reliability analyses of the probabilistic constraints.

One million samples were generated using the mean and standard deviation values of the design variables, and the constraints were evaluated using these samples to calculate the probability of failure. Results are summarized in Table 5. The obtained design

Table 5. Reliability analysis results

Constraint	Active	P_f	MCS P_f
Liner wear rate	No	$\leq$ 0.13 %	0 %
Blow-by	No	$\leq$ 0.13 %	0 %
Oil consumption	Yes	0.13 %	0.16 %

is actually 0.03% less reliable than found. This error is due to the first-order reliability approximation used in the probabilistic optimization problem.

Propagation of uncertainty was modeled using the approach described in Section 3.2. Table 6 summarizes the estimated moments for the two responses of the bi-level hierarchy. The linearization approach results are included to illustrate the large error that this approach introduces to the top-level problem. This happens because the power loss function is highly nonlinear. In fact, its PDF is multi-modal, as illustrated in Figure 6. Figure 7 depicts the histogram obtained by Monte Carlo simulation using one million samples; note that the perpendicular axis of the histogram must be divided by 1,000,000 to obtain the probability density relative to the sample size. The agreement is quite satisfactory and illustrates the usefulness of the AMV-based approach to propagate uncertainty for highly nonlinear functions. The fuel consumption is almost a linear function of the power loss.

Table 6. Estimated moments and errors relative to Monte Carlo simulation (MCS) results for the simulation example

Response	Power loss	Fuel consumption
μ_{lin}	0.3950	0.5341
μ_{AMV}	0.3922	0.5431
μ_{MCS}	0.3932	0.5432
ε_{lin} [%]	0.45	-0.01
ε_{AMV} [%]	-0.25	-0.01
σ_{lin}	0.0481	0.00757
σ_{AMV}	0.0309	0.00760
σ_{MCS}	0.0311	0.00759
ε_{lin} [%]	54.6	-0.25
ε_{AMV} [%]	-0.64	0.13

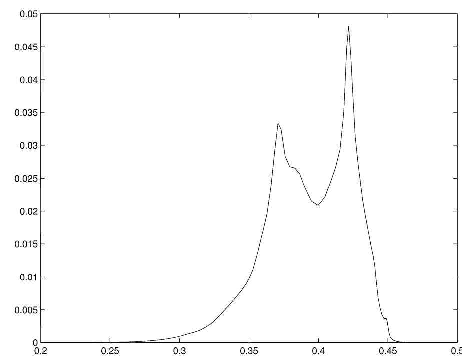

Figure 6. PDF of power loss obtained using the AMV-based method

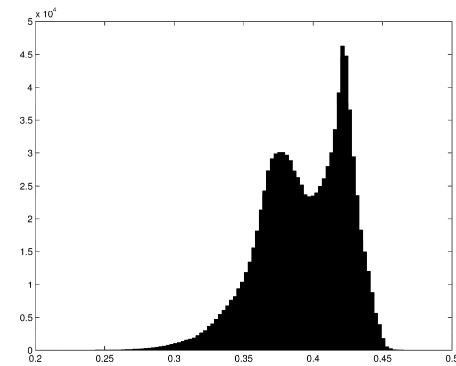

Figure 7. Power loss histogram obtained using Monte Carlo simulation (perpendicular axis must be divided by 1,000,000 to obtain probability density relative to sample size)

6 SUMMARY AND CONCLUSIONS

We have presented a methodology for design optimization of hierarchically decomposed multilevel systems under uncertainty. We extended the deterministic formulation of analytical target cascading (ATC) to account for uncertainties. We modeled the propagation of uncertainty in the ATC process by using the advanced mean value (AMV) method to generate accurate probability distributions of nonlinear responses. The cross-validated moving least squares (CVMLS) metamodeling technique was used based on optimal symmetric Latin hypercube (OSLH) sampling. Finally, we demonstrated the presented methodology by means of a simple yet illustrative engine design example.

The following issues deserve special attention.

The proposed methodology for simulation-based optimal system design by decomposition is not related to multidisciplinary design optimization (MDO) methods in either its deterministic or its probabilistic formulation.

Stochastic formulations are meaningful only if expectations of nonlinear responses are computed exactly, which requires probability distribution information of the input random variables and parameters and accurate multidimensional integrations. Probabilistic formulations are suggested for practical applications.

The linearization approach for propagating uncertainties yields inaccurate second moment estimations and is inadequate for multilevel optimization under uncertainty since it does not provide probability distribution information that is necessary for solving higher-level problems.

Use of metamodels should be exercised only if their accuracy is sufficient relative to the accuracy of utilized modeling techniques and numerical methods.

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