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Robust Hierarchical Multiscale Design Using PATC and PCE

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Abstract: Multiscale design for dealing with 2-scale material and product system is implemented by employing the probabilistic analytical target cascading (PATC) and polynomial chaos expansion (PCE) approaches in this paper. PATC allows design autonomy at each scale subsystem by formulating the multiscale design problem as a hierarchical structure. PCE ensures uncertainties to be propagated within and across each scale accurately and efficiently. In addition, correlation between the random inputs is also considered during uncertainty propagation. Comparative study on a multiscale bracket design problem shows that the results obtained by our strategy are very close to the reference values. It is demonstrated that PATC and PCE are effective and applicable on multiscale design.

Keywords: Multiscale design, material and product design, probabilistic analytical target cascading, polynomial chaos expansion.

1. INTRODUCTION

Multiscale design is an emerging research topic that is built upon multiscale simulations to design systems at different scales (length and time) for achieving the required system performances [1]. From the design research point of view, multiscale design deals with the efficient utilization of information from multiscale models that may be associated with design explorations at different scales and by different engineering disciplines [1]. The widely existing uncertainties often cause unexpected quality loss or even catastrophic failure which stresses the necessity to consider the design robustness during multiscale design. Recently, there have seen lots of works about the robust multiscale design. In [2], some of the pending challenges for applications of robust design to multiscale systems and materials were highlighted. An inductive design exploration method for robust multi-scale material design was proposed to support integrated multiscale materials and product design under uncertainty [3].

One of the challenges in robust multiscale design is that multiscale analyses usually involve multiple scales/disciplines, various physical elements, and coupled information exchanges, which dramatically increase the demand of computation. The complexity of multiscale analysis places a critical obstacle in the employment of conventional design methods, which integrate the entire analysis models into single system and solve it in an all-in-one fashion. Recent years have seen work that views multiscale design as a multidisciplinary design activity where design decisions are made by each individual discipline (e.g., material design, product design, and manufacturing process design) with a common objective of achieving the desired product performance [2]. Due to the hierarchical structure of scale decomposition in multiscale systems, there is a great potential to exploit the existing hierarchical multidisciplinary design optimization techniques for making design decisions at various scales. As a classical multilevel design formulation, the probabilistic analytical target cascading (PATC) [4] method has been applied to various probabilistic hierarchical design optimization problems such as vehicle and aircraft designs, however there does not exist any applications of PATC to robust multiscale design.

The second challenge in robust multiscale design is associated with the various uncertainties in multiscale systems. It is well known that one of the key components of robust optimization is how to effectively propagate the input uncertainties to outputs (named as uncertainty propagation, UP for short). In multistage systems, the uncertainties may exist at each scale in the hierarchy, which would be further propagated to the upper scales and finally to the system probabilistic performance. It is crucial to develop efficient UP approaches that can manage the challenge in propagating various uncertainties within and across multiple scales to quickly assess the probabilistic product performance in the hierarchical materials and product design. Lots of UP approaches have been proposed among which the polynomial chaos expansion (PCE) method with attractive attributes has demonstrated to be effective in many applications. In addition, some output responses from the lower scales in the hierarchical multiscale systems which act as input to the upper scales may be correlated due to the common uncertainty sources which exerts great difficulty on UP in multi-scale design. Ignoring the correlation in the multiscale hierarchy would induce errors to the probabilistic performance estimations in the upper scale and finally to the system optimal design solution.

It is our interest in this work to address the aforementioned two challenges by employing PATC and PCE to support the robust multiscale design process involving material and product design. The remainder of this paper is organized as follows: the proposed robust hierarchical multiscale design framework is introduced in Section 2, where the PATC and PCE approaches are first briefly reviewed. In Section 3, the material and product design of a bracket

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multiscale problem which is formulated in a hierarchical design structure is presented to demonstrate the effectiveness of our approach. Conclusions are drawn in Section 4.

2. A ROBUST HIERRCHICAL MULTISCALE DESIGN FRAMEWORK

In this paper, we propose to apply the existing PATC multilevel design formulation to hierarchical multiscale system design. Different from the original PATC approach where Monte Carlo Simulation (MCS) is simply used for UP, in this work PCE is employed for propagating uncertainties within and across different scales in the hierarchy. To further address the correlation between some properties at certain scale in the hierarchical multiscale system, correlated PCE models for these stochastic properties are constructed with the introduction of Gaussian bases which comprise the marginal PCE's.

2.1. Multilevel Optimization for Multiscale Design

A generalized 2-level multiscale modeling pattern is displayed in Fig. (**1**) and the corresponding multilevel design

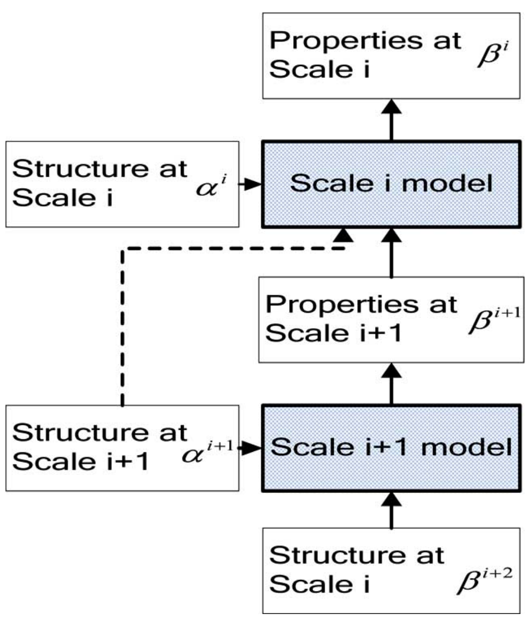

Fig. (1). A generalized 2-level multiscale modeling pattern.

pattern following a target cascading process at the neighboring levels in this paper is illustrated in Fig. (**2**). Within the PATC design framework, the design for each scale (material and product) is implemented at one level, and different levels (scales) are interrelated by the output properties. The probabilistic characteristics of the properties β are represented by the first two statistic moments (mean μ_β and variance σ^2_β). The optimal solutions of β^i (μ_{β^i} and σ_{β^i}) from Level *i*-1 design are assigned as targets ($\mu^T_{\beta^i}$ and $\sigma^T_{\beta^i}$) to Level *i* design. At Level *i*, the design goal is to find optimal solutions of α^i and β^{i+1} that yield the responses of β^i ($\mu^R_{\beta^i}$ and $\sigma^R_{\beta^i}$) that best match their targets ($\mu^T_{\beta^i}$ and $\sigma^T_{\beta^i}$). The optimal solutions of β^{i+1} ($\mu_{\beta^{i+1}}$ and $\sigma_{\beta^{i+1}}$) are further passed as targets ($\mu^T_{\beta^{i+1}}$ and $\sigma^T_{\beta^{i+1}}$) to a lower Level *i*+1 design. The whole target cascading process terminates once the solutions converge to values within a specified tolerance.

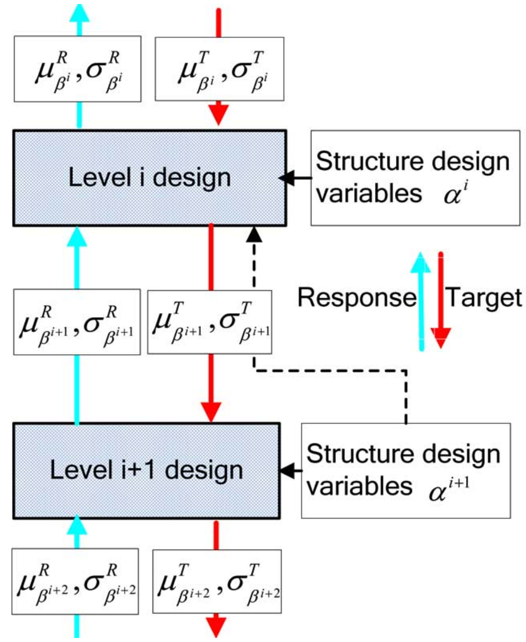

Fig. (2). Robust design pattern of multilevel optimization.

The corresponding PATC formulation for Level *i* design is given in (1). The completion of all the optimizations of each level in the hierarchy is considered as one cycle.

$$
\begin{aligned}
&\text{Given} && \mu^T_{\beta^i}, \sigma^T_{\beta i} \\
&\text{find} && \alpha^i, \mu_{\beta^{i+1}}, \sigma_{\beta^{i+1}} \\
&\min && \left\| \mu_{\beta^i} - \mu^T_{\beta^i} \right\| + \left\| \sigma_{\beta^i} - \sigma^T_{\beta^i} \right\| + \varepsilon^i, \\
&\text{s.t.} && \left\| \mu_{\beta^{i+1}} - \mu^R_{\beta^{i+1}} \right\| \le \varepsilon^i, \\
& && \mu_{g^i} + k\sigma_{g^i} \le 0
\end{aligned} \tag{1}
$$

where $\beta^i = \beta^i(\alpha^i, \beta^{i+1})$ and $g^i = g^i(\alpha^i, \beta^{i+1})$ which are functions of local design variables in Level *i* and the properties from lower Level *i*+1, and g^i are local constraints at Level *i*, ε^i is the tolerance to control design consistency.

2.2. Uncertainty Propagation in Robust Multiscale Design

In the robust multiscale design framework, PCE is used to implement UP both in and across different scales. At each level, robust design is carried out independently with PCE as the UP technique for robustness assessment (mean and variance). In addition, PCE is also used to propagate uncertainties from the lower levels to the upper levels. A brief step-by-step description of PCE is given below and the reader can refer to [5, 6] for more detailed introduction.

Step 1. Represent the inputs as functions of standard random variables.

$$X_i = T_i(\xi_i) = F^{-1}(\phi(\xi_i)), \quad i = 1, 2, ..., d \tag{2}$$

where d is the dimension of random input variables, F and ϕ represent the cumulative density function (CDF) and standard random distribution respectively. In this paper, we only consider the situation that ξ_i follows standard normal distribution, although other standard non-normal distributions can also be used.

Step 2. Expand the output response as a function of random variables using PCE model. For Gaussian (normal) variable, the Hermite orthogonal polynomials are correspondingly used to construct PCE model. In our paper, Hermite orthogonal polynomials since only random normal variables are considered in Step 1. As for variables with other probabilistic distributions, other types of orthogonal polynomials can be used. See Table **1** for detailed information.

Table 1. Random Variables and the Corresponding Orthogonal Polynomials

Random Variables	Gaussian	Gamma	Beta	Uniform
Orthogonal polynomial functions	Hermite	Laguerre	Jacobi	Legendre

The same set of standard random variables that are used to represent input randomness can then be used for the representation of outputs. An equivalent reduced model for an output is expressed in the form of a series expansion consisting of multi-dimensional Hermite polynomials of normal random variables as,

$$y = \alpha_0 \Gamma_0 + \sum_{i_1=1}^{\infty} \alpha_{i_1} \Gamma_1(\xi_{i_1}) + \sum_{i_1=1}^{\infty} \sum_{i_2=1}^{i_1} \alpha_{i_1 i_2} \Gamma_2(\xi_{i_1}, \xi_{i_2}) + \sum_{i_1=1}^{\infty} \sum_{i_2=1}^{i_1} \sum_{i_3=1}^{i_2} \alpha_{i_1 i_2 i_3} \Gamma_3(\xi_{i_1}, \xi_{i_2} \xi_{i_3}) + \ldots \quad (3)$$

where $\{\xi_i\}_{i=1}^{\infty}$ is a set of standard normal variables, Γ_P is a generic element in the set of multidimensional Hermite polynomial of order p, and α_i is the deterministic PCE coefficient. We can rewrite Eq. (3) in a simpler form as,

$$y = \sum_{i=0}^{\infty} b_i \psi_i(\xi_{i_1}) \quad (4)$$

where b_i and ψ_i ψ correspond to $\alpha_{i_1 i_2 \ldots i_p}$ and $\Gamma_p(\xi_{i_1}, \ldots, \xi_{i_p})$ in Eq. (3) respectively. For example, a two dimensional PCE with 2[nd] order (p=2) can be written as,

$$y = b_0 + b_1 \xi_1 + b_2 \xi_2 + b_3(\xi_1^2 - 1) + b_4 \xi_1 \xi_2 + b_5(\xi_2^2 - 1) \quad (5)$$

If we only consider PCE of p^{th} order, the total number of orthogonal polynomial terms, i.e. the number of PCE coefficients P, can be expressed as a function of order p and input dimension d

$$\mathrm{P} = 1 + \sum_{s=1}^{p} \frac{1}{s!} \prod_{r=0}^{s-1} (n + r) = \frac{(d+p)!}{d!\,p!} \quad (6)$$

Then, the PCE model is now approximated as,

$$y \approx y^{(p)}(\xi) = \sum_{i=1}^{\mathrm{P}} b_i \psi_i(\xi) \quad (7)$$

Step 3. Estimate the PCE coefficients $b_i (i = 1, \ldots, \mathrm{P})$ by the weighted least square regression. In this work, we adopt the weighted stochastic response surface method (WSRSM) developed in our previous work to achieve this goal [7]. As an enhanced technique based on stochastic response surface method (SRSM), WSRSM aims at improving the accuracy of UP with the consideration of the sample probabilistic weights during the regression process. Within WSRSM, the PCE coefficients can be estimated as below. Choose N effective sample points $\hat{\mathbf{\imath}} = [\xi_1, \ldots, \xi_j, \ldots, \xi_N]^T$, obtain the real output function values $y = [y(\xi_1), \ldots, y(\xi_j), \ldots, y(\xi_N)]^T$ and the sample probabilistic weights $w = [w_1, \ldots, w_j, \ldots, w_N]^T$ at these sample points. Plug the inputs and output into the PCE model,

$$\begin{bmatrix} \psi_1(\xi_1)\ \psi_2(\xi_1)\ \ldots \psi_P(\xi_1) \\ \psi_1(\xi_2)\ \psi_2(\xi_2)\ \ldots \psi_P(\xi_2) \\ \vdots \quad \vdots \quad \vdots \\ \psi_1(\xi_N)\ \psi_2(\xi_N) \ldots \psi_P(\xi_N) \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_P \end{bmatrix} = \begin{bmatrix} Y(\xi_1) \\ Y(\xi_2) \\ \vdots \\ Y(\xi_N) \end{bmatrix} \quad (8)$$

The coefficients $b = [b_1, \ldots, b_{\mathrm{P}}]^T$ are calculated using the regression approach with the weighted least square method based on a set of sample points, the corresponding real function evaluations as well as the probabilistic weights.

$$\min J(b) = \sum_{i=1}^{N} w_i \varepsilon_i^2 = \sum_{i=1}^{N} w_i (Y(\xi_i) - Y^h(\xi_i))^2 \quad (9)$$

We can rewrite Eq. (8) in the matrix formulation by taking W into account

$$AWb = Y \quad (10)$$

where

$$W = \begin{bmatrix} w_1\ 0 \cdots 0 \\ 0\ w_2 \cdots 0 \\ \vdots\ \vdots \ddots \vdots \\ 0\ 0 \cdots w_N \end{bmatrix} \quad (11)$$

The analytical solution by least square method is

$$b = (AWA^T)^{-1} A^T WY \quad (12)$$

W is a diagonal matrix of probabilistic weights and w_i is the weight at the i^{th} sample point ξ_i. It's then the probabilistic weight (or importance) w_i that reflects the relative frequency of input random variable taking the value at the particular sampling site. Although various sampling techniques, i.e., Gaussian Quadrature point (GQ), Monomial Cubature rule (MCR) and Latin Hypercube Design (LHD), and the corresponding techniques to determine the sample probabilistic weights have been studied and demonstrated to be effective in WSRSM, only LHD sampling method is employed to estimate the PCE coefficients in this paper. We follow the method in [7] and use the joint probability density function values as the sample probabilistic weights.

Step 4. Evaluate the PCE model with MCS to obtain the probabilistic characteristics of the output response y.

Steps 1-4 briefly describe the process of UP in multiscale design. The only difference between UP in and across levels lies in Step 4. For the formal one, sample points are generated randomly according to the distribution type of random variables. However, when propagating uncertainties from lower levels to upper levels, it is foremost to generate the equivalent correlated coefficient matrix of the Gaussian bases which comprise the marginal PCE's characterized by a set of PCE coefficients. In this work, we follow the approach proposed in [8] to accomplish this task. After the optimization of a lower level, the PCE models are established for the stochastic property functions following Steps 1-3 at the current optimal design points. Based on the PCE coefficients of stochastic property functions, the equivalent correlated coefficient matrix of the Gaussian bases are constructed [8]. Large amount of correlated standard random normal sample points can be generated using the correlated standard Guassian bases.

3. BRACKET PROBLEM DESCRIPTION AND ROBUST MULTISCALE DESIGN IMPLEMENTATION

The multiscale design problem studied in this work is considered as a multilevel multidisciplinary design problem to design the optimal material microstructure and product geometry that yields the minimum volume of material, subject to the stress constraint. Fig. (**3**) illustrates the framework and information flow in the bi-level PATC formulation. At Scale 1 (product model), the left vertical surface of bracket is fixed on the wall and the displacement boundary condition is applied to the upper surface. The three product design variables (C_X, C_Y, R) represent the location and radius of the hole. The finite element modeling and analysis is implemented in ABAQUS© to predict the maximum stress in terms of C_X, C_Y, R, k and n when the boundary conditions are fully applied. The strength index (k) and strain hardening index (n) are material design parameters from the power model to represent the material constitutive property. At Scale 2 (material model), a Representative Volume Element (RVE) material model [9] is employed to construct the microstructure-constitutive property relation of an aluminum alloy material. The aluminum alloy material contains micro silicon particles uniformly distributed in the aluminum matrix. Silicon Particle Volume Fraction (PVF) and Particle Density (N) which quantitatively characterize the material microstructure are introduced as material design variables. A power model is employed to fit the strain-stress curve from RVE simulations following the way introduced in Ref. [10]. Due to the high computational cost of RVE simulations, Kriging are constructed for material property responses (k and n) as functions of PVF and N.

The design objective is to minimize the material volume used in the bracket product, which is equivalent to maximizing the radius of the hole. The maximum stress occurred in the bracket should be less than the critical stress (Smax_C). Additional geometry constraints (g_2–g_4) are applied to ensure the hole remain within the bracket external contour. The deterministic All-In-One optimization formulation of this problem is shown in (13).

$$
\begin{aligned}
\min \quad & -x_3^2 \\
\text{s.t.} \quad & g_1 = \text{Smax}/\text{Smax}_C - 1 \le 0 \\
& g_2 = (x_2 + x_3)/20 + 1 \le 0 \\
& g_3 = 1 - (x_1 - x_3)/20 \le 0 \\
& g_4 = 0.5387x_1 - x_2 + 1.1359x_3 \le 0 \\
& k = \text{model}^k(x_4, x_5),\ n = \text{model}^n(x_4, x_5) \\
& lb \le X \le ub
\end{aligned}
\qquad (13)
$$

where

$X = \{x_1, x_2, x_3, x_4, x_5\} = \{C_X, C_Y, R, PVF, N\}$,

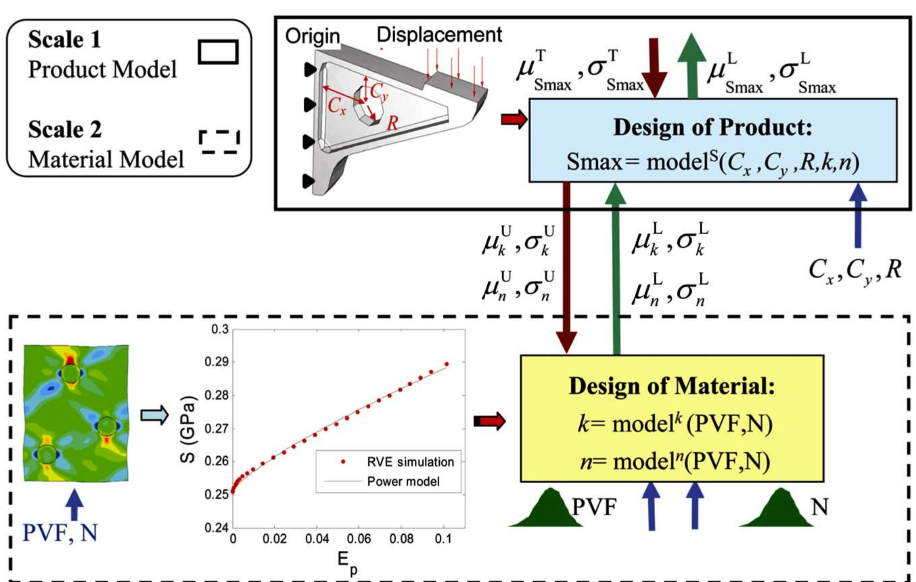

Fig. (3). Framework and information flow in PATC of the multiscale bracket problem.

Table 2. Optimal Design Variables and Confirmed Objective

	X					e_X	*f*	e_f
PATC	52.0000	-50.3268	30.3268	0.0500	4.0646	1.5883	919.7148	0.0060
PAIO	50.4183	-50.4183	30.4183	0.0500	4.0000	---	925.2730	---

$\text{Smax} = \text{model}^{S}(x_1, x_2, x_3, k, n)$, model^k and model^n are Kriging metamodels for the two interrelated responses *k* and *n*; model^s stands for the Kriging metamodel of the structure maximum stress (Smax); g_1 is the maximum stress constraint. Due to the random nature of material, the microstructure design variables *PVF* and *N* are considered as random design variables. During our study, it is found that *k* and *n* are highly correlated which is expected to have large impact on the optimal design solution. Therefore the enhanced PATC formulation [11] with the consideration of the covariance between *k* and *n* is applied to the multiscale bracket design problem formulated in (14) and (15). Following the target cascading fashion, targets of the desired material design parameters *k* and *n* are determined at Scale 1 (see (14)) and assigned to the Scale 2 (see (15)). The Scale 2 design optimization is carried out to match the targets.

Top level (Scale 1):

$$\begin{aligned} \min \quad & x_3^2 + w_1\varepsilon^{\mu} + w_2\varepsilon^{\sigma} \\ s.t. \quad & P(g_1 \le 0) \ge \alpha,\ g_1 = \text{model}^{S}(x_1, x_2, x_3, k, n)/\text{Smax}_C - 1 \\ & g_2 = (x_2 + x_3)/20 + 1 \le 0 \\ & g_3 = 1 - (x_1 - x_3)/20 \le 0 \\ & g_4 = 0.5387x_1 - x_2 + 1.1359x_3 \le 0 \\ & (\mu_k - \mu_k^{L})^2 + (\mu_n - \mu_n^{L})^2 \le \varepsilon^{\mu},\ (\sigma_k - \sigma_k^{L})^2 + (\sigma_n - \sigma_n^{L})^2 \le \varepsilon^{\sigma} \\ & lb \le X \le ub, X = (x_1, x_2, x_3, \mu_k, \sigma_k, \mu_n, \sigma_n, \varepsilon^{\mu}, \varepsilon^{\sigma}) \end{aligned} \tag{14}$$

Bottom level (Scale 2):

$$\begin{aligned} \min \quad & (\mu_k - \mu_k^{U})^2 + (\mu_n - \mu_n^{U})^2 + (\sigma_k - \sigma_k^{U})^2 + (\sigma_n - \sigma_n^{U})^2 \\ & k = \text{model}^k(x_1, x_2),\ n = \text{model}^n(x_1, x_2) \\ & lb \le X \le ub,\ X = (x_1, x_2) = (PVF, N) \end{aligned} \tag{15}$$

Within the PCE method, the stochastic response is represented as a PCE model, which is implemented using the weighted least square regression approach at a set of sample points. In our work, the LHD sampling technique is employed in the regression process to establish the PCE models for the probabilistic outputs responses (*k*, *n* and Smax) in each subsystem optimization at every scale. The uncertainties can be propagated with PCE during optimization in and across different scales.

The standard deviation values for random design variables (*PVF* and *N*) are set as $\sigma_{PVF} = 0.0067, \sigma_N = 0.3$ in this study. The results solved by the Probabilistic All-In-One (PAIO) method integrating Monte Carlo Simulation (MCS) as UP strategy are used as reference values to verify the accuracy of the obtained results. For simplicity, we denote the results produced by our scheme and PAIO combining MCS respectively as PATC and PAIO, which are shown in Table **2**. The confirmed *f* and the confirmed mean and standard deviation values of *k* and *n* are displayed in Table **3**, which are obtained by plugging the obtained optimal design variables into the PAIO formulation. In Table **2**, e_X is the square sum of the absolute error of *X* and e_f is the absolute error of *f* relative to the solutions of PAIO.

Table 3. Comparison of the Confirmed Interrelated Responses

	μ_k	σ_k	μ_n	σ_n
PATC	0.2560	0.0035	0.8667	0.0166
PAIO	0.2557	0.0033	0.8663	0.0163

It is found that the optimal design variables and objective values obtained by PATC are almost identical to the ones using PAIO. Meanwhile, the mean and standard deviation values of the two interrelated responses also show great agreement to those of PAIO. Compared to PAIO that treats all analysis models at the material and product scale levels as an integrated complicated system, PATC follows the hierarchical decomposition strategy where a complex system is divided into subsystems at different levels, and each subsystem design problem is solved in a target cascading iterative fashion. Such a method maintains the design autonomy of each scale at different levels and greatly facilitates the implement of parallel process. Meanwhile, PCE yields efficient and accurate results for propagating uncertainties within or across multiple scales, while at a much smaller fraction of the cost of MCS. As is well-know that PCE suffers from the “curse of dimension” problem, it is only useful for small to middle sized problems. In the future, techniques such as “dimension adaptivity” will be investigated to deal with this problem.

4. CONCLUSIONS

Conventional design methods for multiscale design integrate all the models from multiple scales into single system and solve it in an all-in-one fashion, which greatly limit the autonomy of each individual scale and bring about intensive complexity. By applying the PATC method, the complicated multiscale design problem is formulated as a multilevel design structure within which each scale can achieve independent design. The introduction of PCE as UP strategy in the PATC design formulation ensures accurate and efficient uncertainty propagation within and across different scales. The comparative study on the engineering bracket design problem associated with material and product design evidently demonstrates the effectiveness and applicability of PATC and PCE on multiscale design.

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