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14. ABSTRACT The major accomplishments include: - Development of a new and more rigorous variability measure for robust optimization - Development of an efficient algorithm for robust optimization - Development of a highly efficient numerical method for computing rare failure probability. It is better than any of the existing methods by several orders. - Development of the first-ever numerical method for epistemic uncertainty analysis.					
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1 Project Objectives

The research objectives of the project revolve around the development of a rigorous mathematical framework for uncertainty-based design optimization, with an emphasis on the construction and analysis of a set of efficient numerical methods applicable for complex systems. The objectives include the following major components:

1. Constructing a mathematical framework, using generalized polynomial chaos (gPC) theory, to facilitate the analysis of uncertainty-based design optimization.
2. Developing novel and efficient numerical algorithms.
3. Conducting rigorous analysis and error estimates for the new algorithms.

The work is performed on two kinds of uncertainty-based design optimization:

- Robust design optimization, where the objective is to optimize the system performance while minimizing its sensitivity to uncertainty.
- Reliability-based design optimization, where the objective is to optimize the system performance while keeping its failure probability under control.

2 Major Achievements

We report here that we have made significant progresses and accomplished notable achievements in all fronts of the project objectives. To facilitate the discussion, we employ the following notation: let x be a set of design variables for a system $\mathcal{S}$, and Z be a set of random variables representing uncertainty in the system, and $f(x, Z)$ be a cost function to be minimized. The underlying assumption is that the system $\mathcal{S}$ is highly complex, and consequently the cost function f is time consuming to simulate.

2.1 Robust Design Optimization

In robust optimization the goal is to minimize the cost function and simultaneously its sensitivity to the uncertainty input. The most widely adopted formulation takes the following form

$$\min_x (\mu_f(x) + \alpha \cdot V_f(x)), \quad (1)$$

where μ_f is the mean of the cost function and V_f its variance, α is a parameter specifying the significance of the variance in this formulation. It is clear that this formulation seeks to minimize both the average behavior of the cost function and its variance.

2.1.1 Theoretical Achievement

It was proposed in this project that the traditional formulation (1) is not sufficient to guarantee that the optimal solution is “least sensitive”. This is because the use of variance V_f , which is a weak measure of variability. For example, the objective functions shown in Fig. 1 all have the same variance, but their sensitivity towards randomness are obviously drastically different.

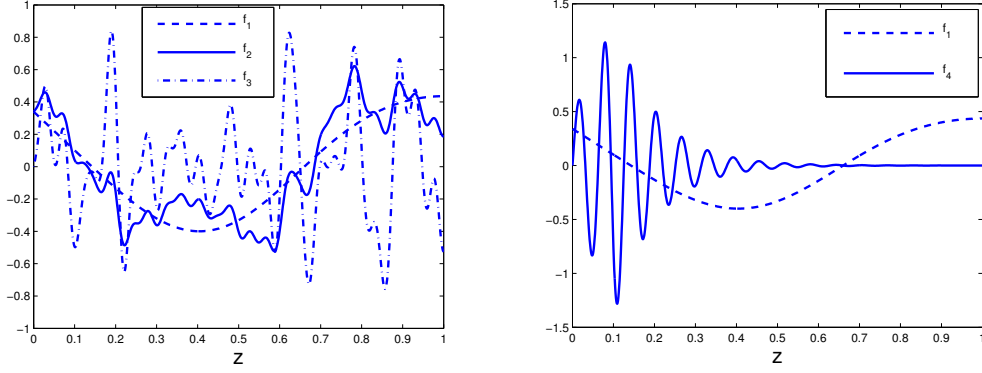


Fig. 1: Illustrative examples of objective functions f in term of random parameter Z . All responses $f_i(Z), i = 1, 2, 3, 4$ have same mean (~ 0) and STD $\sigma \sim 0.3$, but the “sensitiveness” with respect to Z is drastically different. f_1 is obviously the most “robust” choice.

To circumvent the difficulty, a set of “strong” measures for robustness are proposed in [4]. Instead of defining V_f by the variance as in (1), we define

$$V_f \equiv \mathbb{E} \left[\left\| \frac{\partial f}{\partial Z} \right\|_p \right], \quad (2)$$

where the p -norm can be the standard ∞ -norm, 1-norm, and 2-norm. These measures can more

Measure	f_1	f_2	f_3	f_4
STD	0.3	0.3	0.3	0.3
$p = 0$	2.4	20.0	65.7	111.1
$p = 2$	1.6	5.3	19.6	14.7

Table 1: Different measures of the variability of the illustrative response functions in Fig. 1, using the p -norm from (2).

accurately reflect the variability of a given response function. And this is demonstrated by applying these measures to the illustrative functions f_1, f_2, f_3 , and f_4 in Fig. 1. The results are summarized in Table 1. Clearly, the “least robust” objective function f_3 and f_4 are easily identified.

2.1.2 Development of Efficient Algorithms

A set of highly efficient numerical algorithms were developed using the theory of generalized polynomial chaos (gPC), for both the traditional weak measure of robustness and the new strong measure of robustness. The gPC theory, an extension of the earlier work of polynomial chaos (PC) [1], is

first proposed in [5]. It is an orthogonal polynomial approximation in multi-dimensional space. In gPC, the cost function can be approximated by

$$f(x, Z) \approx f_N(x, Z) = \sum_{j=0}^N a_j(x) \Phi_j(Z), \quad (3)$$

where a_j are the coefficients and Φ_j are orthogonal polynomials satisfying

$$\mathbb{E}[\Phi_i(Z) \Phi_j(Z)] = \delta_{ij}, \quad (4)$$

where the operator $\mathbb{E}[\cdot]$ stands for expectation (or, mean, average). Due to the orthogonality, we have

$$\mu_f = a_0(x), \quad V_f = \sum_{j=1}^N a_j^2(x). \quad (5)$$

The robust optimization problem (1) can then be reformulated entirely in term of the gPC expansion coefficients. And all other statistical quantities, including those required by the strong robustness measure (2), can be easily evaluated by the gPC approximation without simulating the system. For examples, let the objective function to be

$$f(u, w) = \frac{1}{2} \int_{\Omega} (u - u_d)^2 dx + \frac{\delta}{2} \int_{\partial\Omega} (w - w_d)^2 dx \quad (6)$$

subject to a stochastic diffusion equation

$$\begin{aligned} Lu(x, \mathbf{z}) &= f(x), & x &\in \Omega \\ u &= w, & x &\in \partial\Omega. \end{aligned} \quad (7)$$

A representative result is shown in Fig. 2. We observe significant efficiency gain obtained by stochastic collocation (SC) based gPC solver.

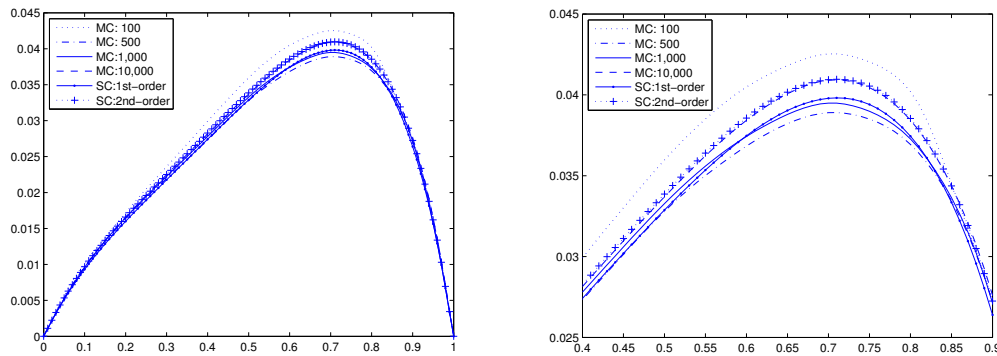


Fig. 2: Comparison of the solution of (7) between Monte Carlo (MC) method and stochastic collocation (SC) gPC method. Left: standard deviation; right: zoomed view of standard deviation. The 1st-order SC requires 41 samples and the 2nd-order requires 841 samples. Both are much smaller than 10,000 MC samples. Details are in [4].

2.2 Reliability-based Design Optimization

In a very general setting, the basic formulation for reliability-based design optimization (RBDO) takes the following form.

$$\begin{aligned} \min_x & f(x, Z), \\ \text{subject to } & P_f < \epsilon, \end{aligned} \quad (8)$$

where P_f is the failure probability of the system and $\epsilon \geq 0$ is a small number. The failure probability is defined as

$$P_f = \text{Prob}[g(Z) \leq 0] = \int_{g(z) \leq 0} \rho(z) dz, \quad (9)$$

where $\rho(z)$ is the probability distribution of the random variables Z , and g is the so-called “limit state function” or “failure function” of the system $\mathcal{S}$. The design space is separated into two regions by $g = 0$, the safe region $g > 0$ and the failure region $g \leq 0$.

2.2.1 Theoretical Achievement

The key component in RBDO is the evaluation of the failure probability P_f in (9). The most reliable method is the Monte Carlo sampling (MCS), where the failure probability is estimated by

$$P_f^{mc} = \frac{\text{Number of samples in failure domain}}{\text{Total number of samples}}. \quad (10)$$

Though simple to implement, the method poses numerical challenge. It requires about at least 10 failed samples to reliably estimate the failure probability. This usually translates into a large number of total samples. For example, for $P_f \sim 10^{-5}$, it is quite common to require 10^6 samples. Even with the most sophisticated important sampling (IS) method, a minimal of 10^4 samples are required. For any practical large-scale systems, the required number of samples is completely out of reach.

In this project, we have developed a novel method to estimate failure probability. The key features of the new method include

- *High accuracy.* The method is accurate and does not have any approximation. It can reproduce exactly the result obtained by traditional MCS. In many examples the new method with $\sim 10^2$ samples can match every single digit of the MCS results obtained by $\sim 10^6$ samples.
- *Rigorousness.* The theoretical foundation is established rigorously by our convergence theorem in [3].

2.2.2 Development of Efficient Algorithms

To successfully implement the new method for practical complex system, we developed a highly efficient predictor-correction algorithm. The feature of the algorithm includes

- *Unparalleled efficiency.* This method allows us to compute rare failure probability as low as $P_f \sim 10^{-6}$ with only a few hundred samples. This capability is superior than any of the existing methods in the world by several orders.
- *Ease of implementation.* The coding effort of the new algorithm is close to zero. One can easily adopt the algorithm for complex systems which are simulated by legacy codes.

A typical example is shown in Table 2. Here the state-of-the-art importance sampling (IS) method, the cross-entropy method, is employed. And it produces rare failure probability more accurate than the brute-force MC and uses only 25,000 samples. Our new algorithm can exactly reproduce this accurate result with only 400 samples! Extensive numerical tests were conducted for a variety of problems and all results are very similar. *The new method makes accurate computation of rare failure probability possible for practical systems.*

	MC	MC+IS	New method
P_f	2.02×10^{-6}	2.025×10^{-6}	2.025×10^{-6}
# of samples	10^8	25,000	400

Table 2: Example of computing rare failure probability. The Important sampling (MC+IS) produces a better result than MC and requires 25,000 samples. Our new method can reproduce exactly the same result with only 400 samples. Details are in [3].

2.3 Other Aspects: Epistemic Uncertainty

Other notable accomplishments made during the project include the development of a computational strategy for epistemic uncertainty analysis. Epistemic uncertainty refers to the uncertainty without sufficient knowledge to specify its probability. And this is frequently encountered in design and optimization. Owing to its difficulty, there has been no systematical study. In this project, we have produced *the very first systematical numerical framework to quantify epistemic uncertainty.*

This work, published in [2], consists of the following major steps.

- Encapsulation of the epistemic uncertainty. Here a bound of the epistemic uncertainty is estimated so that all epistemic uncertainty can be encapsulated in a sufficiently large hypercube.
- Solution of the governing PDE in the hypercube. Here no probability distribution is imposed.
- Post-processing the result. If a posterior probability information about the epistemic uncertainty is available, we can then post-process the simulation result to obtain better understanding of the solution.

An example is shown in Fig. 3. This is a result of an oscillator, which is an ODE with six parameters. Two of the parameters are epistemic variables. The results here show the CDF of the final solution. Note the CDF is a function of the two epistemic variables, and here we plot 25 ensembles of the CDF.

This work will certainly lead the way of the study of epistemic uncertainty analysis and play a key role in design and optimization under uncertainty.

3 Student support

During the course of the project, the research fund is used to support one graduate student, Ms Jing Li. Since the fund is for one semester and summer each year, other funds (e.g. from NSF) is used to leverage the support.

4 Other Synthetic Activities

The PI has attended almost all major conferences and workshops on UQ, and presented numerous invited lectures. Notable ones include

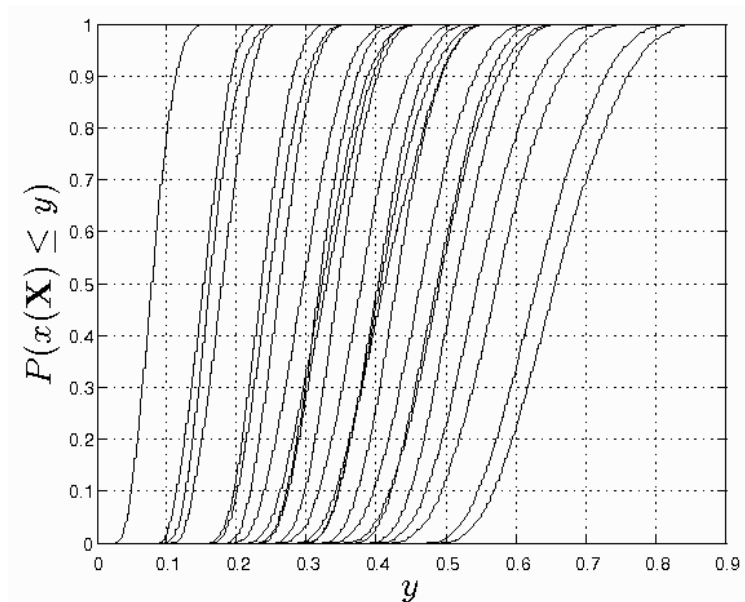


Fig. 3: An ensemble of 25 CDFs of the solution to the damped harmonic oscillator subject to mixed aleatory and epistemic uncertainty. Each CDF corresponds to one particular set of epistemic variables values.

- Plenary Talk, High Order Methods for Stochastic Computations, International Conference On Spectral and High Order Methods (ICOSAHOM07), Chinese Academy of Sciences, Beijing, China, June 18-22, 2007.
- Plenary talk. Ecole Doctorale sur la Quantification des Incertitudes, Paris, November 24-27, 2008.
- Plenary talk. The Third International Conference on Scientific Computing and Partial Differential Equations, Hong Kong, December 8-13, 2008.
- Invited speaker. Workshop on Numerical Solution of Stochastic Partial Differential Equations, Dipartimento di Matematica, Politecnico di Torino, Italy, May 10-13, 2010.
- Invited speaker. Workshop on Uncertainty Quantification, The Royal Society of Edinburgh, Scotland, May 24-28, 2010.
- Colloquium and seminar. University of Buffalo, Arizona State University, Stanford University, Lawrence Livermore National Lab, George Mason University, Northwestern University, University of Southern California, Brown University, etc.

Also, the PI has become the first Associate editor-in-chief for the first journal dedicated to UQ, the *International Journal for Uncertainty Quantification*.

5 Publications

Under the grant, the following papers have been published.

1. D. Xiu, “Fast Numerical Methods for Robust Optimal Design”, *Engineering Optimization*, Vol. 40, 489-504 2008.
2. D. Xiu and J. Shen, “Efficient Stochastic Galerkin Methods for Random Diffusion Equations”, *Journal of Computational Physics*, Vol. 228, 266-281, 2009.

3. R. Archibald, A. Gelb, R. Saxena and D. Xiu, “Discontinuity Detection in Multivariate Space for Stochastic Simulations”, *Journal of Computational Physics*, Vol. 228, 2676-2689, 2009.
4. Y. Marzouk and D. Xiu, “A Stochastic Collocation Approach to Bayesian Inference in Inverse Problems”, *Communications in Computational Physics*, Vol. 6, 826-847, 2009.
5. J. Li and D. Xiu, “A Generalized Polynomial Chaos Based Ensemble Kalman Filter with High Accuracy”, *Journal of Computational Physics*, Vol. 228, 5454-5469, 2009.
6. J. Jakeman, M. Eldred and D. Xiu, “Numerical Approach for Quantification of Epistemic Uncertainty”, *Journal of Computational Physics*, Vol. 229, 4648-4663, 2010.
7. Jing Li and D. Xiu, “Evaluation of Failure Probability via Surrogate Models”, *Journal Computational Physics*, Vol. 229, 8966-8980, 2010.
8. P. Tsuji, D. Xiu and L. Ying, “A Fast Method for High-frequency Acoustic Scattering from Random Scatterers”, *International Journal for Uncertainty Quantification*, Vol. 1, 99-117, 2011.

The PI also published the first-ever graduate-level textbook on stochastic simulation and uncertainty quantification.

- D. Xiu, *Numerical Methods for Stochastic Computations: a Spectral Method Approach*, Princeton University Press, July 21, 2010. Hard cover: 152 pages. ISBN-10: 0691142122, ISBN-13: 978-0691142128.

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