# EFFICIENT SHAPE OPTIMIZATION USING POLYNOMIAL CHAOS EXPANSION AND LOCAL SENSITIVITIES

Nam H. Kim and Haoyu Wang
*University of Florida, Gainesville, FL 32606*
*nkim@ufl.edu, hyw@ufl.edu*

Nestor V. Queipo
*University of Zulia, Venezuela*
*nqueipo@ufl.edu*

**Abstract**

This paper presents an efficient shape optimization technique based on stochastic response surfaces (polynomial chaos expansion) constructed using performance and local sensitivity data at heuristically selected collocation points. The cited expansion uses Hermite polynomial bases for the space of square-integrable probability density functions and provides a closed form solution of the performance. The focus is on calculating the uncertainty propagation using less number of function evaluations since the response surface needs to be reconstructed at each design cycle. Due to the continuum-based sensitivity analysis, the gradient information of performance is efficiently calculated and used in constructing the stochastic response surface. The efficiency and convergence of the proposed approach are demonstrated using a reliability-based shape optimization of a well-known structural problem.

## 1. Introduction

Uncertainty in the design parameters makes shape optimization of structural systems a computationally expensive task due to the significant number of structural analyses required by traditional methods. Critical issues for overcoming these difficulties are those related to uncertainty characterization, uncertainty propagation, and efficient optimization algorithms. Traditional approaches for these tasks often fail to meet constraints (computational resources, cost, time, etc.) typically present in industrial environments.

Reliability-based design optimization (RBDO) involving a computationally demanding model has been limited by the relatively high number of required analyses for uncertainty propagation during the design process. This paper presents an efficient shape optimization technique based on stochastic response surfaces (SRS) constructed using model outputs at heuristically selected collocation points. The efficiency of the uncertainty propagation approach is critical since the response surface needs to be reconstructed at each design cycle. In order to improve the efficiency, the performance gradient, calculated from sensitivity analysis, is used.

## 2. Uncertainty Quantification and SRS

Uncertainty quantification can be decomposed in three fundamental steps: i) uncertainty characterization of model inputs, ii) propagation of uncertainty, and iii) uncertainty management/decision making. The uncertainty in model inputs are represented in terms of standardized normal random variables (*srv*). We will assume that the model inputs are independent so each one is expressed directly as a function of a *srv* through a proper transformation. More arbitrary probability distributions can be approximated using algebraic manipulations or by series expansions (Devroye, 1986).

The uncertainty propagation is based on constructing a particular family of stochastic response surfaces known as polynomial chaos expansion. This kind of SRS (Tatang *et al*., 1997; Isukapalli *et al*., 2000) can be view as an extension of classical deterministic response surfaces for model outputs constructed using uncertain inputs and performance data collected at heuristically selected collocation points. Let $n$ be the number of random variables and $p$ the order of polynomial. The model output can then be expressed in terms of the *srv* $\{u_i\}$ as:

$$G^p = a_0^p + \sum_{i=1}^{n} a_i^p \Gamma_1(u_i) + \sum_{i=1}^{n}\sum_{j=1}^{i} a_{ij}^p \Gamma_2(u_i, u_j) + \sum_{i_1=1}^{n}\sum_{j=1}^{i}\sum_{k=1}^{j} a_{ijk}^p \Gamma_3(u_i, u_j, u_k) + \cdots, \qquad (1)$$

where $G^p$ is the model output, the $a_i^p, a_{ij}^p, \ldots$ are deterministic coefficients to be estimated, and the $\Gamma_p(u_1,\ldots,u_p)$ are multidimensional Hermite polynomials of degree $p$. In general, the approximation accuracy increases with the order of the polynomial, which should be selected reflecting accuracy needs and computational constraints.

The Hermite polynomials (orthogonal with respect to the Gaussian measure) provide this type of SRS with some attractive features, namely: more robust estimates of the coefficients with respect to those obtained using non-orthogonal polynomials (Gauthshi, 1996), it converges to any process with finite second order moments (Cameron and Martin, 1947), and the convergence is optimal (exponential) for Gaussian processes (Xiu and Karniadakis, 2002). In addition, the selected SRS approach includes a sampling scheme (collocation method) designed to provide a good approximation of the model output (inspired in the Gaussian quadrature approach) in the higher probability region with limited observations, and once the coefficients are calculated, statistical properties of the prediction, such as mean and variance can be analytically obtained, and sensitivity analyses can be readily conducted.

The number of simulations could be reduced even further when local sensitivity is available. Recently, Isukapalli *et al*. (2000) used an automatic differentiation program to calculate the local sensitivity of the model output with respect to random variables and used them to construct an SRS. Their results showed that local sensitivity can significantly reduce the number of sampling points as more information is available. The computational cost of the automatic differentiation, though, is often higher than that of direct analysis (Carle *et al*., 1998). However, local sensitivity can be obtained at a reasonable computational cost when using finite element analysis.

As discussed by van Keulen *et al*. (2004), finite element-based sensitivity analysis provides an efficient tool for calculating gradient information. In the context of structural analysis, for example, the discrete system is often represented using a matrix equation of the form $[\mathbf{K}]\{\mathbf{D}\}=\{\mathbf{F}\}$. The model output in Eq. (1) can be expressed as a function of the nodal solution. Thus, the local sensitivity of the model output can be easily calculated if that of the nodal solution is available. When design parameters are defined, the matrix equation can be differentiated with respect to them to obtain

$$[\mathbf{K}]\left\{\partial\mathbf{D}/\partial u_{i_p}\right\}=\left\{\partial\mathbf{F}/\partial u_{i_p}\right\}-\left[\partial\mathbf{K}/\partial u_{i_p}\right]\{\mathbf{D}\}. \tag{2}$$

Equation (2) can be solved inexpensively because the matrix [**K**] is already factorized. The computational cost of sensitivity analysis is usually less than 20% of the original analysis cost so local sensitivity can in fact be obtained efficiently and the number of simulations for constructing the SRS at each design cycle can be consequently reduced.

As an illustration of the effectiveness, efficiency and convergence properties of the SRS approach, consider the construction of the probability density function (*pdf*) associated with a simple analytical function represented by $G(x) = e^x$, with $x$ being a random variable normally distributed as $N(0,0.4^2)$; note that in this case the exact *pdf* is known. The SRS for second and third order polynomials constructed using three and five collocation points are shown in Eq. (3). Figure 1 shows the *pdf* obtained through Monte Carlo simulation on the SRS and the exact solution. Observe the good agreement in the *pdf* approximation and how the $L^2$-norm (0.03835 for $p$=2; 0.00969 for $p$=3) of the errors decreases with higher order polynomials.

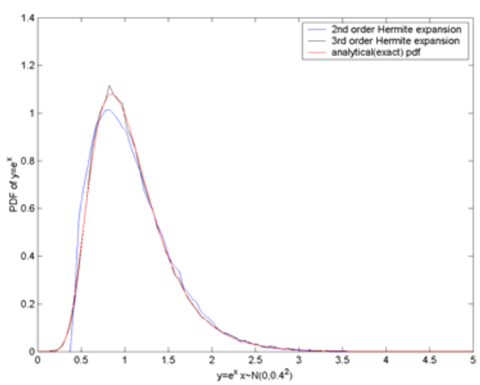



Figure 1. Probability density function obtained using SRSs and exact solution for the performance function $G(x) = e^x$(Illustrative example)

$$\begin{aligned} G^2 &= 1.005 + 0.1005x + 0.005(x^2-1) \\ G^3 &= 1.005 + 0.1005x + 0.005(x^2-1) + 0.0001671(x^3-3x) \end{aligned} \tag{3}$$

## 3. Reliability-Based Design Optimization – Problem Formulation

In general, the RBDO problem (Enevoldsen and Sorensen, 1994) can be defined as,

$$\begin{aligned} &\text{minimize} && c(\mathbf{d}) \\ &\text{subject to} && P(G_j(\mathbf{x}) < 0) \le \overline{P}_{f,j}, \quad j = 1, 2, \ldots, np \,. \\ & && \mathbf{d}_L \le \mathbf{d} \le \mathbf{d}_U \end{aligned} \tag{4}$$

where $\mathbf{x} = [x_i]^T$ ($i$ = 1, 2,…, $n$) denotes the vector of random parameters, $\mathbf{d} = [d_i]^T = [\mu_i]^T$ represent the design variables chosen as the mean values of $\mathbf{x}$, and $c(\mathbf{d})$ identifies a cost function. The system performance criteria are described by the performance functions $G_j(\mathbf{x})$ such that the system fails if $G_j(\mathbf{x}) < 0$. Each $G_j(\mathbf{x})$ is characterized by its cumulative distribution function $F_G(g)$:

$$F_{G_j}(g) = P(G_j(\mathbf{x}) < g) = \int_{G_j(\mathbf{x}) < g} \cdots \int f_{\mathbf{X}}(\mathbf{x})\, dx_1 \cdots dx_n \,, \tag{5}$$

where $f_{\mathbf{X}}(\mathbf{x})$ is the joint *pdf* of all random system parameters and $g$ is named the probabilistic performance measure. The reliability analysis of the performance function requires evaluating the non-decreasing $F_G(g) \sim g$ relationship (Tu *et al.*, 1999), which is performed in the probability integration domain bounded by the system parameter tolerance limits. Each prescribed failure probability limit $\overline{P}_f$ is often represented by the reliability target index as $\beta_t = -\Phi^{-1}(\overline{P}_f)$. The *pdf* estimated using the proposed uncertainty propagation scheme is used for evaluating reliability constraints hence providing better approximations than traditional linearization and thus significantly improving the rate of convergence of RBDO.

## 4. Numerical Example – Torque Arm RBDO Problem

Consider a torque arm model in Fig. 2 that is often used in shape optimization (Kim *et al*., 2003). The locations of boundary curves have associated uncertainties modeled as probabilistic distributions due to manufacturing tolerances. Thus, the relative locations of corner points of the boundary curves are defined as random variables with $\mathbf{x} \sim N(0, 0.1^2)$. The mean values of these random variables are chosen as design parameters, while the standard deviation remains constant during the design process.

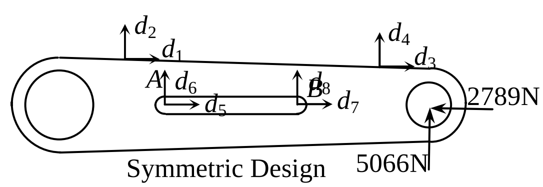
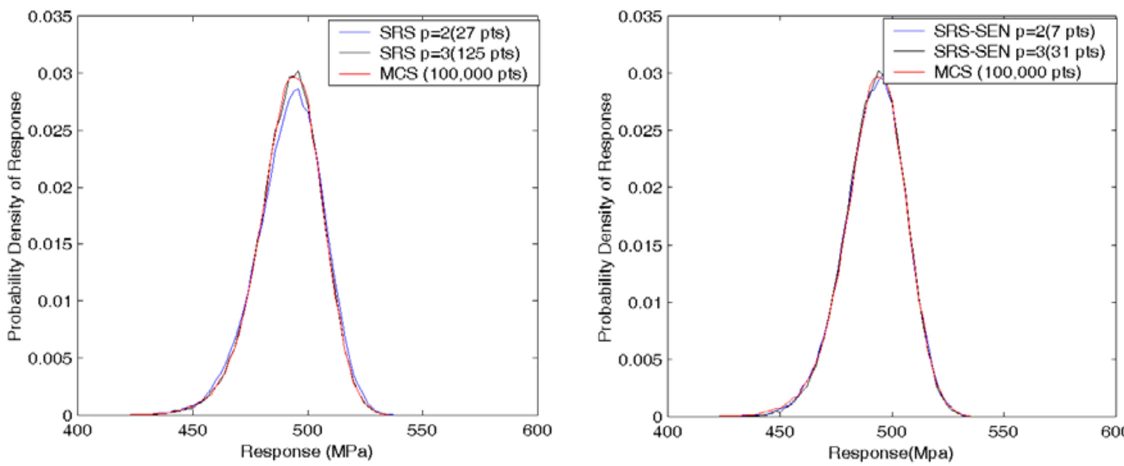


Figure 2. Shape design parameters for the torque arm

The initial model consists of eight design parameters. In order to show how the SRS is constructed and the *pdf* of the model output is calculated, we choose the five design parameters ($d_1$, $d_2$, $d_3$, $d_6$, and $d_8$) that are known to most significantly contribute to the stress performance at points $A$ and $B$ in the figure. In the initial design, the maximum stress of $\sigma_A$ = 319MPa occurs at location $A$. The stress limit is established to be $\sigma_{max}$ = 800MPa. In the reliability analysis the performance function is defined such that $G \leq 0$ is considered failure. Thus, the performance function can be defined as $G(\mathbf{x}) = \sigma_{max} - \sigma_A(\mathbf{x})$.

The number of unknown coefficients is a function of the dimension of the design space *n*. For 2nd- and 3rd-order expansion, the numbers of coefficients, denoted by $N_2$ and $N_3$, are 10 and 20, respectively. There are 27 possible collocation points and 10 unknown coefficients in the case of 2nd-order expansion. For robust estimation, the number of collocation points in general should be at least twice the number of coefficients. Fig. 3(a) shows the *pdf* associated with $G(\mathbf{x})$ when different polynomial approximations are used. The accuracy and the convergence of the stochastic response surfaces are compared with the *pdf* obtained using Monte Carlo simulation with 100,000 sample points. As expected, the square-root error is smaller for the higher-order polynomial.




(a) Only function values are used (b) Function values and local sensitivities are used

Figure 3. PDF of performance function $G(\mathbf{x})$ – Torque Arm Problem

In order to reduce the required number of sampling points, local sensitivities can be used for constructing the SRS. Then, in addition to the function value, the gradients of the performance function with respect to the random variables at each sampling point are also available. Hence, in the case of the torque arm problem, the data which can be obtained from each sampling point is increased from one to six. Fig. 3(b) shows the *pdf* of the performance function for different polynomial approximations and that obtained from direct Monte Carlo simulation. When local sensitivities are used, the polynomial approximations can be obtained with four times lower number of sampling points. In general, theoretically, the number of sampling points can be reduced *n*+1 times with *n* being the number of random variables.

The RBDO problem requires minimizing the mass of the torque arm while the reliability constraints on stress are satisfied. Formally, it can then be defined as,

$$\begin{aligned} &\text{Minimize} && Mass(\mathbf{d}) \\ &\text{subject to} && P(G_i(\mathbf{x}) \le 0) \le \Phi(-\beta_{t_i}), \quad i = 1,\ldots,NC, \\ & && \mathbf{d}^L \le \mathbf{d} \le \mathbf{d}^U \end{aligned} \tag{6}$$

where $\beta_t$ is the target reliability indices and Φ denotes the cumulative density function of *srv*. Table 2 shows the properties of the random variables and the lower and upper bounds of the design parameters. Figure 4 shows the optimal result when $\beta_t$ is set equal to 3 (0.13% chances of failure). Figure 5 provides the cost function optimization history. The solution of the RBDO problem using the proposed approach resulted in a reduction of the mass of the torque arm from 0.878kg to 0.509kg (about 42.01%) after about twelve (12) design cycles.

Table 2. Definition of random design variables and their bounds – Torque arm model

| Random Variables | $\mathbf{d}^L$ | $\mathbf{d}$ (Initial) | $\mathbf{d}^U$ | $\mathbf{d}^{opt}$ (optimum) | Standard Deviation | Distribution type |
|---|---|---|---|---|---|---|
| $d_1$ | –3.0 | 0.0 | 1.0 | -3.8202E-01 | 0.1 | Normal |
| $d_2$ | –0.5 | 0.0 | 1.0 | -5.0000E-01 | 0.1 | Normal |
| $d_3$ | –1.0 | 0.0 | 1.0 | 8.1976E-01 | 0.1 | Normal |
| $d_4$ | –2.7 | 0.0 | 1.0 | -2.7000E+00 | - | Deterministic |
| $d_5$ | –5.5 | 0.0 | 1.0 | -5.1980E-01 | - | Deterministic |
| $d_6$ | –0.5 | 0.0 | 2.0 | 2.0000E+00 | 0.1 | Normal |
| $d_7$ | –1.0 | 0.0 | 7.0 | -4.1962E-02 | - | Deterministic |
| $d_8$ | –0.5 | 0.0 | 1.0 | 3.7534E-01 | 0.1 | Normal |

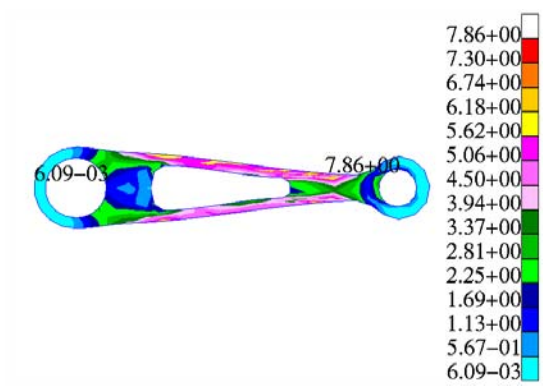



Figure 4. Stress contour plot at optimum design of torque arm RBDO model

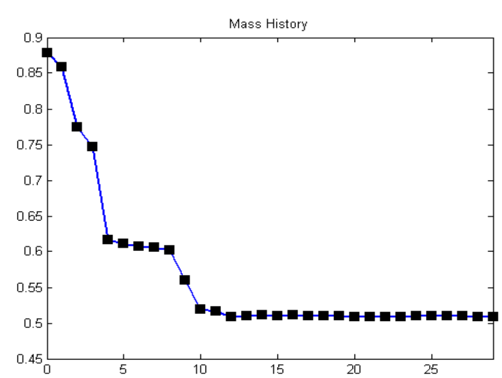



Figure 5. Design optimization history for the mass of torque arm RBDO model

## Conclusions

In this paper, we presented a more effective and efficient approach for RBDO through the use of polynomial chaos expansions (modeling reliability restrictions) and local sensitivity information. It has been shown that in the context of a shape optimization problem with five uncertain inputs (torque arm RBDO), twenty seven (27) – hundred and twenty five (125) sampling points were necessary for 2nd- and 3rd-order polynomial approximations (without using local sensitivities) to accurately represent the probability distribution of the model output, while when gradient information is available the corresponding sampling points are reduced to seven (7) and thirty one (31), respectively, which represents a reduction of about 75% in the computational effort.

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