

MULTISTEP INPUT REDUCTION FOR HIGH DIMENSIONAL UNCERTAINTY QUANTIFICATION IN RAVEN CODE

Paul W. Talbot, Congjian Wang, Cristian Rabiti

Nuclear Systems Design and Analysis Division

Idaho National Laboratory, Idaho Falls, Idaho, USA

paul.talbot@inl.gov; congjian.wang@inl.gov; cristian.rabiti@inl.gov

Anil K. Prinja

Department of Nuclear Engineering

MSC01 1120; 2009 Farris Engineering Center, Albuquerque, NM, USA

prinja@unm.edu

ABSTRACT

This manuscript focuses on the efficient construction of surrogates that can be employed in place of complex systems. The surrogates under consideration are fast to evaluate and yet accurate, which take the form of generalized polynomials chaos. Here, we utilize the principal component analysis (PCA) to reduce the number of input parameters, and we employ adaptive stochastic collocation (ASC) method to reduce the number of functions evaluations. Under the PCA and ASC methods, we propose a method that allow us to construct a surrogate that can effectively handle large number of input parameters and even more when adaptive high-dimensional model reduction (AHDMR) algorithm are employed to further reduce the dimensionality of input space. In the past year, this approach has been developed and implemented in RAVEN.

Key Words: Uncertainty Quantification, Principal Component Analysis, Adaptive Sparse Grid Collocation, Active Subspace, HDMR, RAVEN

1. INTRODUCTION

Uncertainty quantification (UQ) plays a fundamental role in the analyses of complex systems. In the past, many sampling-based approaches to UQ have been developed, such as Monte Carlo analysis, response surface methodology, generalized polynomial chaos method and high-dimensional model reduction (HDMR) [1]. Although these approaches are both effective and widely used, their determination usually requires a large number of model simulations that can be computationally expensive for large-scale complex systems with high-dimensional input space, i.e. the curse of dimensionality. To address this problem, one approach is to employ adjoint-based algorithms that can efficiently perform UQ with high-dimensional input space while minimizing the number of required function evaluations [2]. However, many simulation codes do not have this capability, and it is usually unfeasible to use them to calculate the first-order derivatives at different sampling points. Another approach is to identify the *active subspace* and *pseudo parameters* for the high-dimensional input space [3]. *Active subspace* is a low-dimensional subspace that captures all the important bases in the high-dimensional input space, and *pseudo parameters* are the projections of the original input parameters onto the active subspace; once identified, a surrogate model can be constructed with the active subspace and pseudo parameters.

In this study, we propose to construct a surrogate model of a complex code with low-dimensional parameterization that maintains the input/output representation. First, we employ the principal-component analysis (PCA) of the input space using the input covariance to identify the active subspace and pseudo parameters. The directions with small eigenvalues, usually several orders of magnitude smaller than the largest eigenvalue, can be neglected. Second, we construct a surrogate model with pre-identified pseudo parameters. In particular, we employ adaptive stochastic collocation for generalized polynomial chaos (ASCgPC) filtered using adaptive high-dimensional model reduction (AHDMR). Recently studies show that ASCgPC with HDMR approach can be more effective in comparison to Monte Carlo sampling for nearly a thousand input dimensions [4]. However, forward uncertainty propagation, even when performed adaptively, struggles to converge efficiently for thousands of input dimensions. A nuclear reactor criticality problem can exhibit tens of thousands of uncertain inputs, i.e. multi-group cross sections [5]. In this instance traditional methods such as ASCgPC can be much less effective than even traditional Monte Carlo sampling. For this case, the combination of input reduction and ASCgPC will be the most suitable candidate for high-dimensional uncertainty quantification.

The proposed approach has been developed and implemented in RAVEN. RAVEN [6] (**R**isk **A**nalysis and **V**irtual control **E**Nvironment) is a software framework under development at the Idaho National Laboratory (INL) since 2012. It can be used to perform parametric and stochastic analysis based on the response of complex systems. In this paper, we will employ RAVEN to perform the uncertainty quantification for neutron transport models.

2. METHODOLOGIES AND IMPLEMENTATION

2.1 Principal Component Analysis of Nuclear Data Covariance

Nuclear data undergoes a series of pre-processing steps to arrive in the suitable format, such as multigroup covariance matrices, for nuclear applications. In the following analysis, we will assume the multigroup covariance matrices are available for given nuclear data. In addition, the nuclear data, represented hereinafter by $\mathbf{x} \in \mathbb{R}^n$, is assumed to have a multivariate normal distribution with mean $\boldsymbol{\mu}_0$ and covariance matrix $\mathbf{C}_x \in \mathbb{R}^{n \times n}$, where n is the size of the nuclear data. To model the uncertainties and correlations presented in the nuclear data, we must transform the set of correlated nuclear data to a set of uncorrelated standard Gaussian variables $\xi(\theta) = \{\xi_1(\theta), \xi_2(\theta), \dots, \xi_r(\theta)\}$ via the following:

$$\mathbf{x} = \boldsymbol{\mu}_0 + \mathbf{L}\xi \quad (1)$$

where \mathbf{L} is a lower-triangular matrix obtained via the Cholesky decomposition of $\mathbf{C}_x = \mathbf{L}\mathbf{L}^T$. In addition, PCA or singular value decomposition (SVD) in linear algebra can be used to identify the principal components in the covariance matrix [7]. In this work, the SVD technique is employed to compute the principal components as follows:

$$\mathbf{C}_x = \mathbf{U}\mathbf{S}\mathbf{U}^T \quad (2)$$

where \mathbf{U} is $n \times n$ real unitary matrix and \mathbf{S} is $n \times n$ diagonal matrix with non-negative real entries. The diagonal entries $\mathbf{S}_{i,i}$ of \mathbf{S} are known as the singular values of \mathbf{C}_x . The components directions, i.e. the columns of matrix \mathbf{U} , associated with small singular values, usually several orders of magnitude smaller than the largest singular values, can be neglected so that the dimensionality of the transformed data, i.e. ξ , is reduced. Based on this transformation, stochastic collocation methods and generalized Polynomial Chaos methods can be used to build a surrogate model with respect to the reduced input parameters ξ .

2.2 Adaptive Stochastic Collocation for generalized Polynomial Chaos Expansion

Generalized Polynomial Chaos expansion methods (gPC) expand a function in a series of orthogonal multidimensional polynomials. Because of the uncorrelated pseudo parameters obtained using PCA, the multidimensional polynomials are the product of polynomials in each pseudo parameter. The polynomial orders used make up a multi-index set Λ . The gPC expansion is described by

$$\mathbf{u}(\xi) = \sum_{\mathbf{k} \in \Lambda} \mathbf{u}_k \Phi_{\mathbf{k}}(\xi) \quad (3)$$

where $\mathbf{u}(\xi)$ is the quantity of interest as a function of the pseudo parameters, \mathbf{k} is a multi-index representing polynomial orders, and $\Phi_{\mathbf{k}}$ is a multidimensional polynomial composed of the product of single-dimension polynomials with orders \mathbf{k} [4]. The coefficients \mathbf{u}_k are obtained using the orthonormality of the multidimensional polynomials,

$$\mathbf{u}_k = \langle \mathbf{u}(\xi), \Phi_{\mathbf{k}}(\xi) \rangle \quad (4)$$

where angle brackets denote the probability-weighted integral over the domain space. To evaluate this integral numerically, we make use of Smolyak-like sparse grid quadrature [8]. We refer to this gPC expansion using collocation points as stochastic collocation for generalized polynomial chaos expansion (SCgPC).

While static isotropic methods exist for determining the polynomial set to use in the gPC expansion, adaptive techniques can be employed to more efficiently explore an optimal set. This expands from the algorithm given in [4], where a suitable expansion is determined by constructing the full expansion for each potential polynomial to include. In this work, we use a predictive method to select polynomials to add to the expansion as the polynomial set grows. This prediction is made by considering the contribution of immediate lower neighbors in the polynomial Hilbert space. For instance, a multipolynomial with orders (3,2) being considered for inclusion has its benefit predicted by the impact of multipolynomials already in the set, namely (2,2) and (3,1). For brevity we refer to this as ASCgPC.

2.3 Adaptive High-Dimension Model Reduction (AHDMR)

Even with the strengths of adaptive polynomial expansions as in ASCgPC, the curse of dimensionality makes it impractical for more than a dozen inputs on even highly regular response surfaces. To further mitigate this limitation, Cut-HDMR (hereafter HDMR) can be used to divide

the input space into constituent subspaces [4]. That is, we can expand our quantity of interest as a function of the pseudo parameters as

$$\mathbf{u}(\xi) = \mathbf{u}_0 + \sum_{i=1}^N \mathbf{u}_i + \sum_{i_1=1}^N \sum_{i_2=1}^{i_1-1} \mathbf{u}_{i_1 i_2} + \cdots + \mathbf{u}_{i_1 \cdots i_N} \quad (5)$$

where N is the cardinality of the input space, and the subspace contributions \mathbf{u}_i are

$$\mathbf{u}_i = \mathbf{u}(\xi_i) - \mathbf{u}_0 \quad (6)$$

and $\mathbf{u}(\xi_i)$ denotes holding all ξ_j where $j \neq i$ at a constant reference value, usually the mean. The expansion is exact when all terms are included, but can often be truncated to include only first-order and second-order terms without introducing significant error.

2.4 Impact Parameters for ASCgPC and AHDMR

We treat each subset \mathbf{u}_i in Eq. (5) using ASCgPC, since by definition the subspace of each subset is small for the first terms in the HDMR expansion. In other words, we use this synergy of HDMR using ASCgPC to adaptively pick terms to include in the HDMR expansion. In order to do this, we define expected impact parameters for improving both SCgPC and HDMR expansions.

To predict the impact of extending a SCgPC expansion, we use variance-based consideration. Because of the orthonormality of the polynomials used in the SCgPC expansion, the variance of the expansion is given by the sum of the squares of the polynomial coefficients,

$$\text{var}[\mathbf{u}(\xi)] = \sum_{k \in \Lambda} c_k^2 \quad (7)$$

where $\{c_k\}_{k \in \Lambda}$ are the coefficients associated with the multidimensional polynomials $\{\Phi_k\}_{k \in \Lambda}$. The impact η_k of any polynomial k on the total variance is the ratio of the square of the coefficient to the total variance,

$$\eta_k = \frac{c_k^2}{\text{var}[\mathbf{u}(\xi)]} \quad (8)$$

The predicted value of a polynomial not yet included in the expansion is given by the product of subset-included polynomials. For example, for a three-dimension input space,

$$\tilde{\eta}_{(i,j,k)} = (\eta_{(i-1,j,k)} \eta_{(i,j-1,k)} \eta_{(i,j,k-1)})^{1/N}$$

with the exception of when any i, j, k are zero, in which case the exponent is reduced by one and the associated term is removed from the product.

To predict the impact of extending the HDMR expansion to include additional subsets, we introduce an HDMR impact parameter κ ,

$$\kappa_\ell = \frac{\text{var}[\mathbf{u}_\ell]}{\sum_h \text{var}[\mathbf{u}_h]} \quad (9)$$

where \mathbf{h} indexes over all existing terms in the HDMR expansion. We note this is similar in form but not equivalent to the Sobol' sensitivity indices, as it neglects non-zero cross-terms in the variance sum. When predicting the impact of an additional HDMR term, we take the product of constituent terms. For example, when considering adding a three-dimension subset, the expected impact parameter is

$$\tilde{\kappa}_{a,b,c} = \kappa_a \kappa_b \kappa_c.$$

To compare the impact of extending the HDMR expansion to extending any given SCgPC expansion, we weight the SCgPC expansion impact parameter with the HDMR impact parameter for the corresponding subset. In order to select the next term to resolve in the adaptive algorithm, the impact parameters are sorted and the highest overall impact is used.

3. NUMERICAL RESULTS

3.1 Preliminary Multistage Input Reduction

We use a simple 2-D pin-cell model based on a 17 by 17 Westinghouse standard PWR assembly model to examine multistage reduction technique. Figure 1 shows the model layout. The input-input correlation is featured by the input covariance matrix, while the input-output correlation can be identified by the sensitivities of the response of interest to the input cross sections. For this study, the dimension of parametric input space is 11308, and TSUNAMI-2D [9] was employed to compute the sensitivities and standard derivation of k_{eff} , i.e. $\sigma(k_{eff})/k = 534 \text{pcm}$, via “sandwich-equation”.

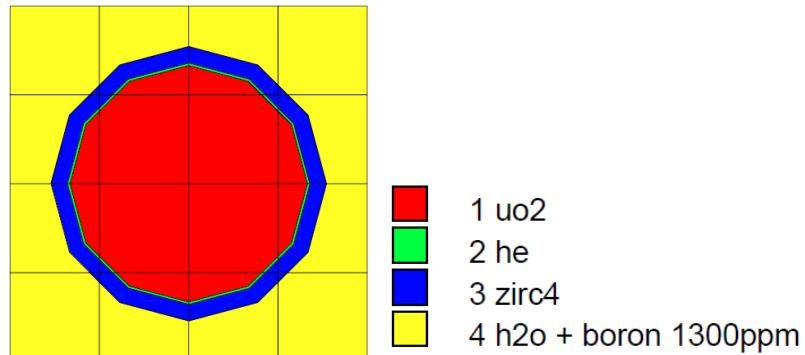


Figure 1. Model Layout

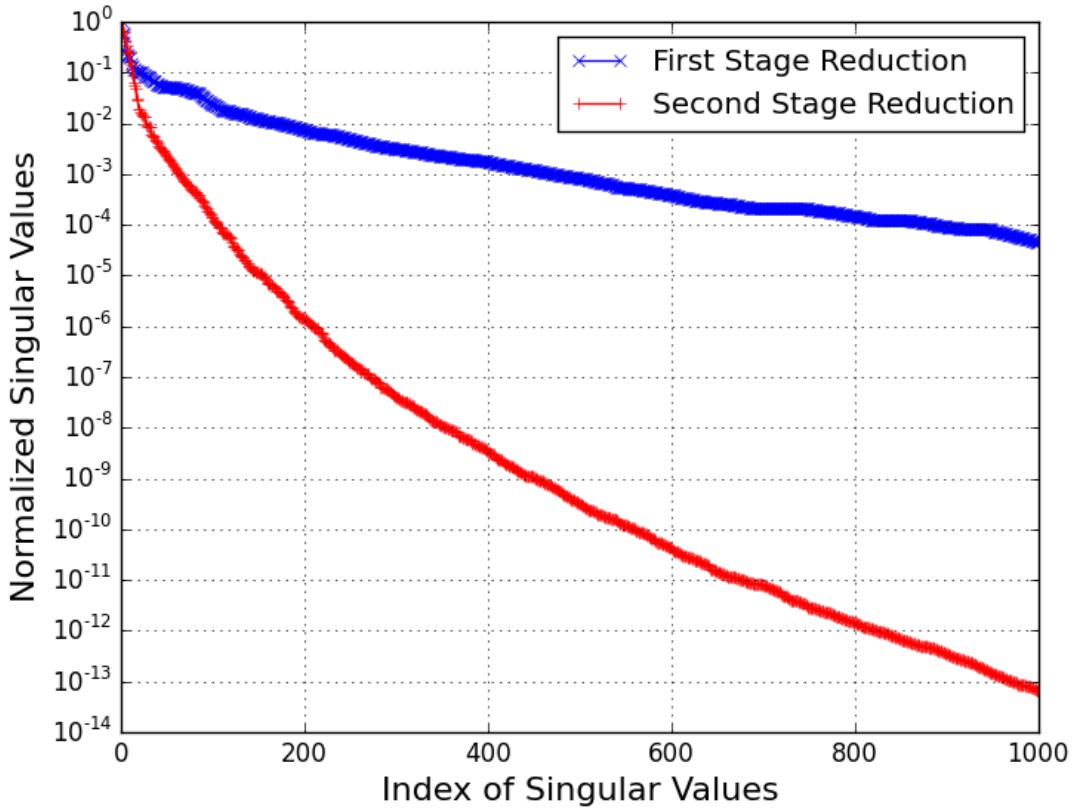


Figure 2. Multistage Input Reduction

First, PCA/SVD is employed to do the first stage reduction in the input space using input-input correlation. Second, input-output correlations, i.e. sensitivities, are used to identify the directions in the active subspace with the strongest variability in the multiplication factor. Figure 2 plots the normalized singular values for both the first stage and second stage reductions. For the first stage reduction, the number of principal directions needs to be 1110 in order to keep discrepancy in the approximation of $\sigma(k_{\text{eff}})/k$ below 10 pcm. For the second stage reduction, the number of principal directions can be significantly reduced to 20 while still keeping the discrepancy below 10 pcm.

3.2 Uncertainty Quantification for IAEA 2D PWR Benchmark

In this case study, we employ the IAEA-2D PWR benchmark to examine the accuracy and efficiency of our proposed approach when propagating the uncertainties of input cross sections. The benchmark is documented in reference [10], and the results are computed via RATTES_NAKE [11]. Several methods inside RAVEN are used to propagate the uncertainties, such as Monte Carlo, HDMR, and ASCgPC with AHDMR acceleration. In order to propagate the uncertainties for this benchmark, we have introduced 5% relative uncertainties, i.e. $\sigma/E = 5\%$, in capture, scattering, and fission cross-sections, and neutron multiplication factor v . In addition, we have introduced 10% correlation between the energy group cross sections for each material. The reference fast and thermal flux computed via RATTES_NAKE is shown in Figure 3.

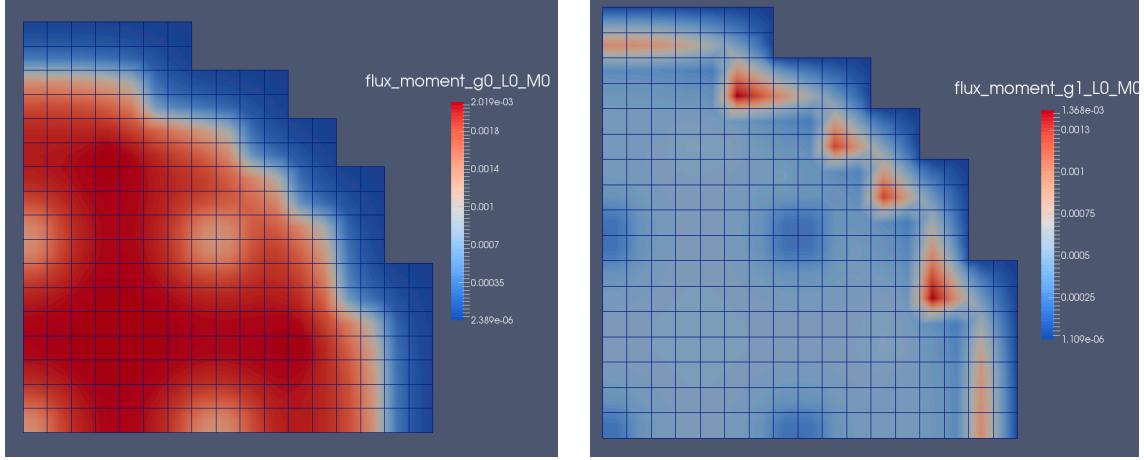


Figure 3. Reference Fast (Left) and Thermal Flux (Right) from RATTLESNAKE

In this case study, we employ RAVEN to compute the uncertainty in the k -eigenvalue due to the input uncertainties. First, we employ HDMR method to compute the first-order Sobol' indices. As shown in Figure 4, the relative contributions to the total variance in k -eigenvalue are computed for each principal components of input space. As observed from Figure 4, only few of the principal components will have the major contributions to the total variance. Moreover, there are components that are important with respect to the input space, i.e. principal components with index 3, 6-14, but their contributions to the total variance (around 0.23%) can be neglected. This implies that AHDMR-ASCgPC can be more effective in constructing the surrogate model. As depicted in Figure 5, multiple surrogate models are constructed using AHDMR-ASCgPC based on the number of original model evaluations. The accuracy in each surrogate model is currently examined via 10000 random samples. The uncertainties in the k -eigenvalue evaluated via the surrogate models are compared with original model with Monte Carlo method. Each evaluation of the original model took an average of 5.112 seconds on a 2.5 GHz Intel Core i7 Macbook Pro, while each evaluation of the 3000-run surrogate model took an average of 0.315 seconds on the same machine, for a speedup of approximately 16 times.

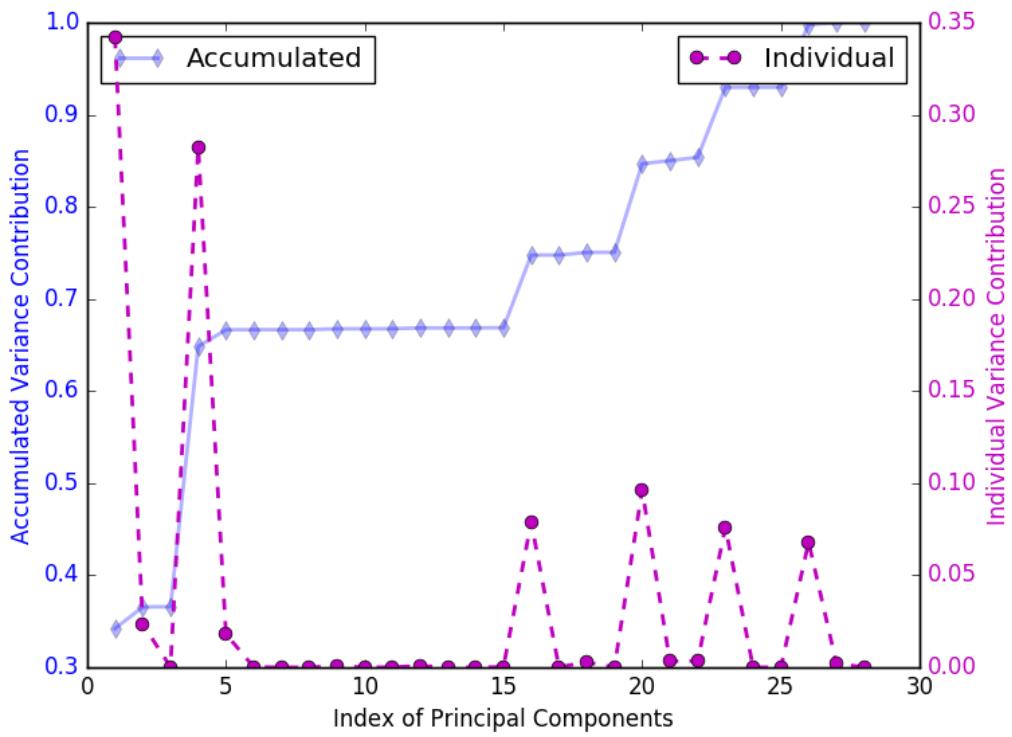


Figure 4. First-Order Sobol Indices Contributions

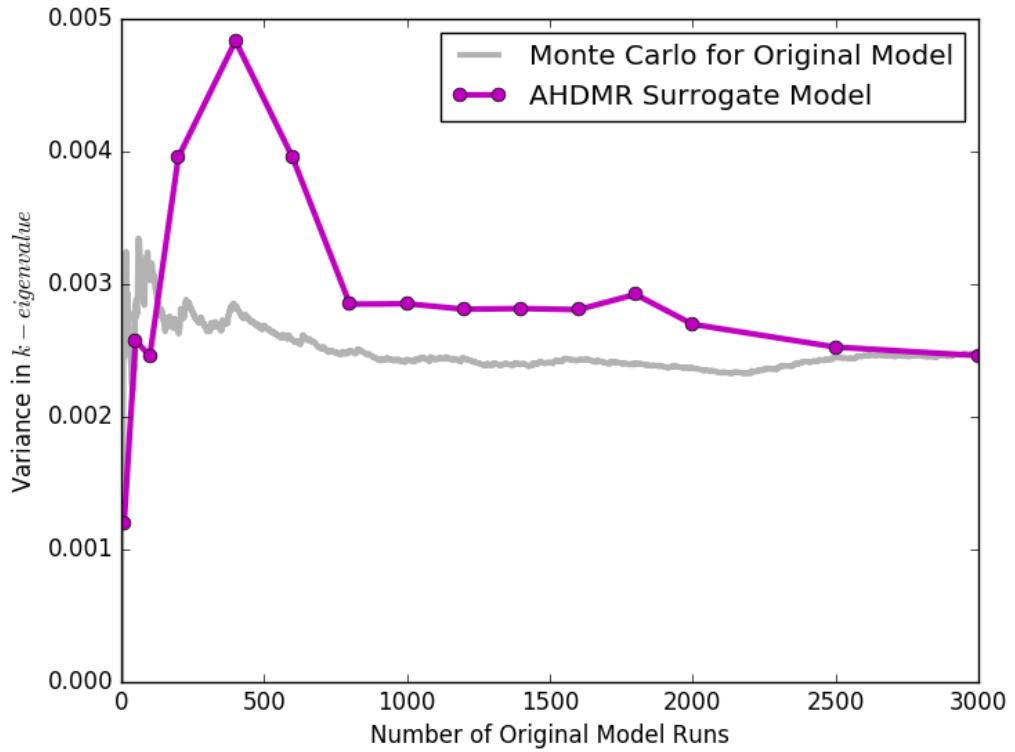


Figure 5. Uncertainty Propagation via AHDMR-ASCgPC Surrogate Model

4. CONCLUSIONS

While recent advances in forward uncertainty quantification have expanded the reach of sampling-based methodologies, there are still engineering applications with input dimensions too large for forward methods. As demonstrated in the pin cell model, significant reduction in input dimensionality can be achieved through input-input correlation as well as input-output correlation. These together can serve to reduce dimensionality sufficiently for adaptive, sparse sampling-based strategies such as SCgPC to compete in efficiency with traditional Monte Carlo methods.

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