Preprint ANL/MCS P1397-0307

*Joint International Topical Meeting on Mathematics & Computation and Supercomputing in Nuclear Applications (M&C + SNA 2007)*
Monterey, California, April 15-19, 2007, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2007)

# STOCHASTIC FINITE-ELEMENT APPROXIMATION OF THE PARAMETRIC DEPENDENCE OF EIGENVALUE PROBLEM SOLUTION

**Mihai Anitescu, Giuseppe Palmiotti, and Won-Sik Yang**
Argonne National Laboratory
9700 S. Cass Ave., Argonne, IL, 60439
anitescu@mcs.anl.gov

**Monika Neda**
Department of Mathematics
University of Pittsburgh
Pittsburgh, PA, 15260

## ABSTRACT

We present a stochastic finite-element approach for characterizing parameter dependence of minimum eigenvalue problems encountered in neutronic calculations. Our formulation results in solving a nonlinear system of equations, that is $K$ times larger than the original problem and has $K$ constraints, where $K$ is the number of terms considered in the perturbative expansion of the solution. This approach allows us to calculate the behavior of the eigenvalue and the eigenvector in the entire parameter range, as opposed to a narrow region around a nominal value calculated by classical sensitivity analysis. Initial investigation for a small parameter space indicates that the method has the potential of substantial savings over Monte Carlo calculations that attempt to characterize the behavior of the eigenvector and eigenvalue over the entire parameter space.

*Key Words*: Stochastic finite element, eigenvalue problems, constrained optimization, uncertainty analysis

## 1 INTRODUCTION

This paper is concerned with the application of stochastic finite-element methods (SFEMs) for determining the parametric variation of the solution to minimum eigenvalue problems. Our main motivator is the issue of characterizing criticality of a nuclear reactor core in the presence of parameter uncertainty, although the methodology extends to parameter uncertainty questions beyond nuclear engineering.

## 2 BACKGROUND ON THE STOCHASTIC FINITE-ELEMENT METHOD

The stochastic finite-element method has emerged with substantial prominence in the past decade as a versatile tool for uncertainty quantification and uncertainty analysis [2]. In virtually every instance this method has been applied to the problem of parametric nonlinear equations, specifically, the parameter dependence of the solution of a nonlinear equation $F\left(x,\omega\right)=0$, where the function $F(\cdot,\cdot)$ is smooth in both its arguments. Under the assumption of non-singularity of $\nabla_x F(x,\omega)$ in a sufficiently large open set that contains $(x_0,\omega_0)$, one can determine a smooth mapping $x(\omega)$ that satisfies $x(\omega_0)=x_0$ and $F(x(\omega_0),\omega_0)$. The uniqueness of this

mapping, while crucial for classical analysis, is not addressed in this paper; we simply assume that this mapping also defines a unique solution to the nonlinear equation problem. The essence of parametric uncertainty analysis is to characterize the mapping $x(\omega)$ either by approximating it to an acceptable degree or by computing some of its integral characteristics, such as averages with appropriate weighting functions.

Perhaps the most widespread approach used for parametric uncertainty analysis is the Monte Carlo method. The parameter $\omega$ is interpreted as a random variable with an appropriate probability density function, and either the probability density function of $x(\omega)$ is approximated or computed, or appropriate averages $E_\alpha\left[g(x(\omega))\right]$ are computed for suitable expressions of the multidimensional merit function $g$. Values for $x(\omega)$ are produced for an appropriate set of sample points $\omega^i$, in which case for each sample point the original nonlinear problem must be solved for its argument $x$.

Recently, researchers have expressed renewed interest in carrying out the analytical computation as far as possible in order to characterize the mapping $x(\omega)$. Essentially, the mapping is approximated by a Fourier-type expansion with respect to a basis of polynomials $\psi_1(\omega), \psi_2(\omega), \ldots \psi_K(\omega)$ that are orthogonal with respect to the probability density function of $\alpha$, that is, $E_\alpha\left(\psi_i(\omega)\psi_j(\omega)\right) = \delta_{ij}, \quad 1 \le i, j \le K$. For $x_1, x_2, \ldots x_K \in R^n$, one defines the approximation $\tilde{x}\left(\omega; x_1, x_2, \ldots, x_K\right) = \sum_{i=1}^{K} x_i \psi_i(\omega)$, and the stochastic finite element formulation is obtained by determining the vectors $x_1^*, x_2^*, \ldots, x_K^*$ that satisfy the Galerkin projection conditions

$$E\left(F\left(\tilde{x}\left(\omega; x_1, x_2, \ldots, x_K\right), \omega\right)\psi_k(w)\right) = 0, k = 1, 2, \ldots, K.$$

The result is a nonlinear system of equations $K$ times larger than the original nonlinear system of equations for a given choice of the parameter $\omega$. The advantage over the Monte Carlo method is that once this nonlinear system of equations is solved, the original nonlinear problem no longer needs to be solved. One explicitly has an approximation of the mapping $x(\omega)$; and if either several of its momentum or its probability density functions need to be evaluated, then a Monte Carlo method can be used on the explicit approximation $\tilde{x}(\omega) = \sum_{k=1}^{K} x_k^* \psi_k(\omega)$, without needing to solve any further system of nonlinear equations.

As an example, we discuss the case where $m = 1, \quad \Omega = [-1, 1]$, and the probability distribution function of the parameter $\alpha$ is uniform. In this case we have that $E_\alpha(g(\omega)) = \frac{1}{2}\int_{-1}^{1} g(\omega) d\alpha$. The appropriate polynomials are the normalized Legendre polynomial functions

$$P_k(\omega) = \frac{1}{\sqrt{2}}\sqrt{\frac{2k+1}{2}}\frac{1}{2^k k!}\frac{d^k}{d\omega^k}\left(\omega^2 - 1\right)^k, \quad k = 0,1,2,\ldots,K.$$

Because the polynomials are used as the generators of the space over which the approximation is carried out, given the stochastic interpretation of the parameter $\omega$, has led to the expansion defined by this approximation is called the chaos polynomial expansion.

Of course, the success of this method resides in the ability to choose a suitable set of polynomials $\psi_i$ ahead of time so that the residual decreases rapidly for relatively small values of $K$, before the size of the Galerkin projected problem explodes. A good way of choosing such polynomials is far from being settled for a very large value of $m$, the dimension of the parameter $\omega$. Nonetheless, for cases where $n$ is huge (e.g., cases originating in the discretization of partial differential equations) and $m$ is relatively moderate, the successes of the stochastic finite-element method have been spectacular compared to the Monte Carlo approach [2].

The object of this paper is to analyze some of the particularities of the stochastic finite-element method and new extensions of it when the original problems are optimization problems. In this work we are interested not in the stochastic aspect of the method per se, but in possible ways of generating the approximation $\tilde{x}(\omega)$ and in the properties of the resulting nonlinear problems. As an application we consider the eigenvalue problem associated to the solution of the neutron diffusion equation in a nuclear reactor.

## 3 STOCHASTIC FINITE-ELEMENT FORMULATION OF EIGENVALUE PROBLEMS

We consider the following structure of a generalized eigenvalue problem, depending on a parameter vector $\omega \in \Omega$.

$$\begin{aligned}
&Q^1(\omega)x^1(\omega) + Q^2(\omega)x^2(\omega) = Q^3(\omega)x^3(\omega)\\
&Q^5(\omega)x^2(\omega) = Q^4(\omega)x^1(\omega)\\
&x^3(\omega) = \lambda(\omega)x^1(\omega)\\
&x^1(\omega)^T x^1(\omega) = 1
\end{aligned} \tag{3.1}$$

The goal of the SFEM parametric analysis is to approximate $x(\omega)$ and $\lambda(\omega)$, where $\lambda(\omega)$ is the maximum eigenvalue mapping. At a first glance, one may think that the problem can be further reduced by explicitly replacing $x^2(\omega), x^3(\omega)$ in the first equation and inverting $\left\{Q^3(\omega)\right\}^{-1}$. However, this approach would involving applying $\left\{Q^3(\omega)\right\}^{-1}, \left\{Q^5(\omega)\right\}^{-1}$. The typical case of interest is the one in which $Q^3(\omega), Q^5(\omega)$ are linearly dependent on $\omega$, which is easy to represent efficiently in the spectral space, whereas $\left\{Q^3(\omega)\right\}$ has a rational function dependence that is much harder to represent in the spectral space.

We can immediately use the ansatz above in order to obtain a set of nonlinear equations. Once we carry out this formulation, however, it is not clear how to extend to this problem some of the very useful algorithms of eigenvalue calculations, in particular, power methods. In order to derive an algorithm similar to the power method, we interpret the normalizing step of the power method as a projection onto the space of the constraint $x^T x = 1$, and rewrite the problem above as

$$\begin{aligned}
&Q^1(\omega)x^1(\omega) + Q^2(\omega)x^2(\omega) = Q^3(\omega)x^3(\omega) \\
&Q^5 x^2(\omega) = Q^4(\omega)x^1(\omega) \\
&x^1(\omega) = \arg\min_{z, z(\omega)^T z(\omega)=1} \left(x^3(\omega) - z(\omega)\right)^T \left(x^3(\omega) - z(\omega)\right).
\end{aligned}$$

Indeed, rewriting the optimality conditions for the optimization problem below, we obtain that $x_3(\omega) - x_1(\omega) = \theta(\omega)x_1(\omega)$ which in turn results in $\lambda(\omega) = 1 + \theta(\omega)$.

Using the SFEM decomposition presented above, we approximate the mappings $x^i(\omega)$, $i = 1,2,3,\ \lambda(\omega), z(\omega)$ by a Fourier type expansion with respect to a basis of polynomials $\psi_1(\omega), \psi_2(\omega), \ldots \psi_K(\omega)$ that are orthogonal with respect to the probability density function of $\omega$. The mapping coefficients satisfy $x_j^i \in R^n,\ z_j \in R^n,\ \lambda_j \in R,\ i = 1,2,3,\ j = 1,2,\ldots,K$, and we define the approximations in the $K$-dimensional space as

$$\begin{aligned}
&\tilde{x}^i(\omega) = \sum_{j=1}^{K} x_j^i \psi_j(\omega),\ i = 1,2,3 \\
&\tilde{z}(\omega) = \sum_{j=1}^{K} z_j \psi_j(\omega),\ \tilde{\lambda}(\omega) = \sum_{j=1}^{K} \lambda_j \psi_j(\omega)
\end{aligned}$$

### 3.1 Expressing the Lower-Level Optimization Problem in SFEM

$$\begin{aligned}
\tilde{x}_1(\omega) = \arg\min_{z_1, z_2, \ldots, z_k} \quad & E_\omega\left[\left(\sum_{i=1}^{K}\left(x_i^3 - z_i\right)\psi_i(\omega)\right)^T \left(\sum_{i=1}^{K}\left(x_i^3 - z_i\right)\psi_i(\omega)\right)\right] \\
\text{s.t.} \quad & E_\omega\left[\left(\sum_{i=1}^{K} z_i \psi_i(\omega)\right)^T \left(\sum_{i=1}^{K} z_i \psi_i(\omega)\right)\psi_k(\omega)\right] = E_\omega\left[\psi_k(\omega)\right] \quad k = 1,2,\ldots,K.
\end{aligned} \tag{3.2}$$

The Lagrange multipliers $\theta_1, \theta_2, \ldots \theta_K$ of the constraints at optimality are the coefficients of the approximation to the mapping $\theta(\omega)$, $\tilde{\theta}(\omega) = \sum_{i=1}^{K} \theta_i \psi_i(\omega)$ as detailed in [1].

Expressing The Parametric Linear Constraints For Linear Parametric Dependence

Expressing the two linear constraints in the eigenvalue problem in the generic format of (3.1) is , to a large extent, uninformative. Therefore we formulate the problem for a special but widely encountered case in which the matrices appearing in (3.1) have the following expression :

$$Q^i(\omega) = Q_0^i + \sum_{j=1}^{m} Q_j^i \zeta_i, i = 1, 2, \ldots 5,$$

where we have defined by $\zeta_i$ the components of the vector $\omega$, that is, $\omega = (\zeta_1, \zeta_2, \ldots, \zeta_m)$. Replacing in the SFEM formulation, we obtain the following.

$$\begin{aligned} &Q_0^1(\omega) x_i^1 + \sum_{k=1}^{K} \sum_{j=1}^{m} Q_j^1 x_k^1 E_\omega\left[\psi_i(\omega)\psi_k(\omega)\omega_j\right] + Q_0^2(\omega) x_i^2 + \sum_{k=1}^{K} \sum_{j=1}^{m} Q_j^2 x_k^2 E_\omega\left[\psi_i(\omega)\psi_k(\omega)\omega_j\right] = \\ &Q_0^3(\omega) x_i^3 + \sum_{k=1}^{K} \sum_{j=1}^{m} Q_j^3 x_k^3 E_\omega\left[\psi_i(\omega)\psi_k(\omega)\omega_j\right], i = 1, 2, \ldots K \end{aligned} \tag{3.3}$$

$$Q_0^5(\omega) x_i^2 + \sum_{k=1}^{K} \sum_{j=1}^{m} Q_j^5 x_k^2 E_\omega\left[\psi_i(\omega)\psi_k(\omega)\zeta_j\right] = Q_0^4(\omega) x_i^1 + \sum_{k=1}^{K} \sum_{j=1}^{m} Q_j^4 x_k^1 E_\omega\left[\psi_i(\omega)\psi_k(\omega)\zeta_j\right] \tag{3.4}$$

We can write these equations in matrix form, where we use the notation $\hat{x}^i = \left(\left[\hat{x}_1^i\right]^T, \left[\hat{x}_2^i\right]^T, \ldots, \left[\hat{x}_K^i\right]^T\right)^T, \quad i = 1, 2, 3$, as

$$\hat{Q}^1 \hat{x}^1 + \hat{Q}^2 \hat{x}^2 = \hat{Q}^3 \hat{x}^3, \quad \hat{Q}^5 \hat{x}^2 = \hat{Q}^4 \hat{x}^1. \tag{3.5}$$

## 3.2 Iterative Scheme.

We can then define our iterative scheme as follows:

- Choose the vector coefficients $x_k^1 \in R^n, k = 1, 2, \ldots, K,$ which are the block components of $\tilde{x}^1(\omega)$
- Compute the vector $\hat{x}^2$ by solving the equation (3.5) with matrix $\hat{Q}^5(\omega)$.
- Compute the vector $\hat{x}^3$ by solving the equation (3.5) with matrix $\hat{Q}^3(\omega)$.
- Compute the solution of the constrained optimization problem (3.5), which provides the new $\hat{x}^1$ and the Lagrange multipliers $\theta^k, k = 1, 2, \ldots, K,$ which are the coefficients of the approximation $\tilde{\theta}(\omega)$. We obtain the approximation $\tilde{\lambda}(\omega)$ of the eigenvalue map.
- Repeat the process.

Clearly, as $Q_j^i, i = 1, 2, \ldots, 5, \; j = 1, 2, \ldots, m$ approach 0, this algorithms approaches precisely the power method applied to the matrix $\left\{Q_0^3\right\}^{-1}\left(Q_0^1 - Q_0^2\left\{Q_0^5\right\}^{-1} Q_0^4\right)$, provided that it is started with $x_i^1 = 0_n, i = 2, 3, \ldots, K$.

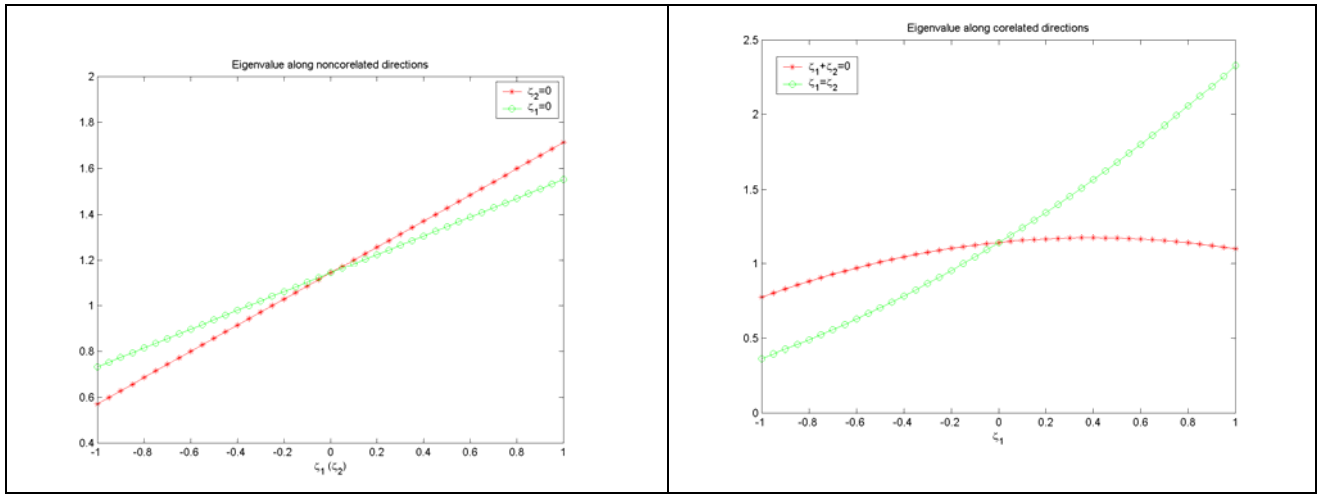


**Figure 1: Eigenvalue and error of SFEM approximation.**

## 4 NUMERICAL EXAMPLE

We use the one-dimensional multigroup diffusion equation

$$-\frac{d}{dz}D_g\frac{d}{dz}\phi_g(z)+\Sigma_{tg}(z)\phi_g(z)-\sum_{g'\neq g}\Sigma_{s,g'\to g}(z)\phi_{g'}(z)=$$
$$\frac{1}{k}\chi_g\sum_{g'}\nu\Sigma_{fg'}(z)\phi_{g'}(z),\quad 0\le z\le L$$

with boundary conditions $\phi_g(z)=0,\quad z=0,L$ [1]. We have used a 2-group configuration with nominal parameters from Table 7-2 of [1], where the energy groups are directly coupled. The model was discretized with finite differences on 200 nodes in MATLAB. We assume that we have uncertainty in the cross sections as follows: $\Sigma_{s,1\to 2}=\Sigma^0{}_{s,1\to 2}(1+\varepsilon\zeta_2)$ and $\Sigma_{f1}=\Sigma_{f1}(1+\varepsilon\zeta_1)$ $\Sigma_{f2}=\Sigma_{f2}(1+\varepsilon\zeta_1)$ (that is, the two fission cross sections have correlation 1). Here the random variables $\zeta_1$ and $\zeta_2$ are independent uniformly distributed on the interval $[-1,1]$. Note that we have chosen two variables primarily because it is easier to display functions of two variables as opposed to more variables; there is no conceptual impediment to applying our method to larger configurations.

If we denote the Laplacian by $L$ and the identity matrix by $I$, our equation above applies with the following matrices, where $\omega=(\zeta_1,\zeta_2)$:

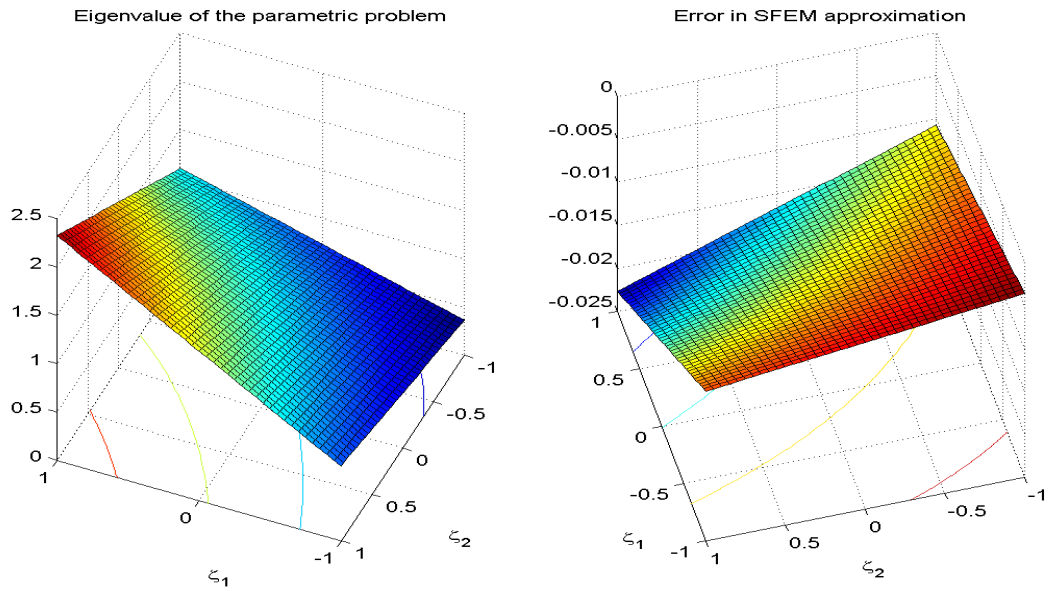


**Figure 2: Eigenvalue computed by direct numerical simulation and error of SFEM approximation.**

Here we consider only the case of the constant diffusion parameter, which allows us to write the previous algebraic expressions. We choose the parameter $\varepsilon = 0.5$, which corresponds to a 50% uncertainty in the fission and scattering cross-sections.

A nonlinear Gauss-Newton method is used to solve the optimization inner loop (a projection on a manifold problem). The iteration is stopped when the 2-norm of the vector of Lagrange multipliers $\theta_1, \theta_2, \ldots, \theta_K$ obtained from the projection process did not vary for more than 1e-4.

## 4.1 SFEM Results

As the polynomial basis, we consider the tensor product basis with maximum degrees $N_1$ and $N_2$, $\psi_{(i-1)N_2+j}(\zeta_1, \zeta_2) = P_i(\zeta_1) P_j(\zeta_2), \quad i = 0,1,\ldots,N_1,\ j = 0,1,\ldots,N_2$ In our simulations, we have used $N_1 = N_2 = 3$, which results in 16 polynomials.

The results require 104 seconds to generate with SFEM and 480 seconds to generate by direct calculation on a 41x41 grid: almost 5 times larger time . In the left panel of Figure 1, we show the results from direct calculation on a 41x41 grid. In the right panel, we display the error on the same grid points of the SFEM approach. We can see that the maximum relative error is less than 1%.

We also note that the computed model exhibits substantial nonlinearity, which would nonetheless be invisible on a parameter-by-parameter basis. Indeed, in the left panel of Figure 2,

where the graph of the eigenvalue is plotted along the directions $\zeta_i, i = 1,2$, we see that the graph is nearly perfectly linear, and could be well captured by sensitivity.On the other hand, along the correlated directions $\zeta_1 + \zeta_2 = 0, \zeta_1 = \zeta_2$ the eigenvalue exhibits substantial nonlinearity, that is well captured by our model and that could not be captured by sensitivity calculations alone. Nonetheless, sensitivity coefficients (that here have a global least squares meaning) can be computed from the linear term of the SFEM model.

### 4.2 Considering Subsets of the Full Tensor Product Set

One of the problems with our approach is the curse of dimensionality, since degree of up to 3 in each variable results in $4^d$ coefficients to be calculated, where $d$ is the dimension of the parameter set. We expect that this will be alleviated by considering only subsets of the full tensor product of orthogonal polynomials in two variables. In Figure 3 we plot the logarithm of the SFEM coefficients of the solution $\tilde{\lambda}(\omega)$ as a function of the degrees $i, j$ of the component polynomials in the individual variables $\zeta_1$ and $\zeta_2$ that define the basis. Clearly only 4 coefficients are significant: the ones of $P_0^2, P_0P_1(\zeta_1), P_0P_1(\zeta_2), P_1(\zeta_1)P_1(\zeta_2)$. If we consider only those in our approximation, the time of calculation of the SFEM approximation drops to 40 s, with virtually no change in the quality of the solution (see Table I). *In this case the ratio of the time of grid exploration to simulation exceeds 12!* Of course, in doing so we have the advantage of hindsight, but this shows that the reach of the method can be substantially expanded by considering well chosen subsets of the complete polynomial set of a given degree.

**Table I. Timing results and error for SFEM and direct calculation**

| Method | Time to Completion | Average Error |
|---|---|---|
| **SFEM,** $N_1 = N_2 = 1$ | 40s | 1.1% |
| **SFEM,** $N_1 = N_2 = 3$ | 104s | 1.1% |
| **Direct Calculation** | 480s | 0% |

## *5* CONCLUSIONS

We have defined a stochastic finite-element method for the perturbation analysis of the eigenvalue and eigenvector of a problem with stochastic parameter dependence. For small examples, we have shown that the method is more accurate (by virtue of providing global, rather than local answers) than a sensitivity approach and is faster than a simulation method.

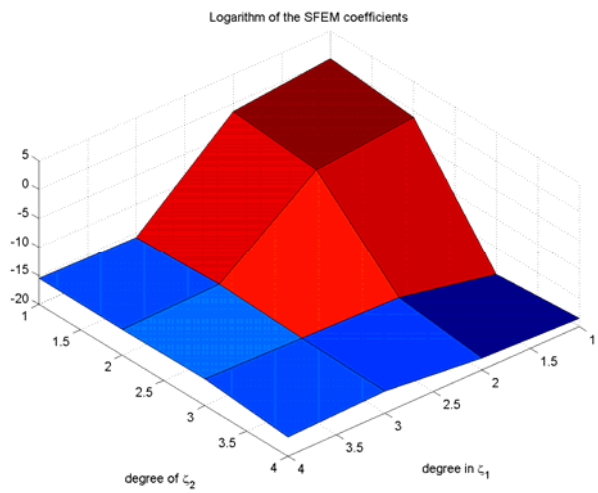


**Figure 3: Logarithm of the spectral coefficients, by degree of tensor basis component.**

## ACKNOWLEDGEMENTS

Mihai Anitescu and Monika Neda were supported in part by the Mathematical, Information, and Computational Sciences Division subprogram of the Office of Advanced Scientific Computing Research, Office of Science, U.S. Dept. of Energy, under Contract DE-AC02-06CH11357.

## 6 REFERENCES

1. M. Anitescu, "Constrained optimization formulation of stochastic finite element methods for minimum eigenvalue problems", Preprint ANL/MCS-P1302-0906 (2006)
2. R.G. Ghanem and P. Spanos, *Stochastic Finite Elements: A Spectral Approach*, Springer, New York , USA (1991).

The submitted manuscript has been created by UChicago Argonne, LLC, Operator of Argonne National Laboratory ("Argonne"). Argonne, a U.S. Department of Energy Office of Science laboratory, is operated under Contract No. DE-AC02-06CH11357. The U.S. Government retains for itself, and others acting on its behalf, a paid-up, nonexclusive, irrevocable worldwide license in said article to reproduce, prepare derivative works, distribute copies to the public, and perform publicly and display publicly, by or on behalf of the Government.