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Method for Treating Discretization Error in Nondeterministic Analysis

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A response surface methodology-based technique is presented for treating discretization error in nondeterministic analysis. The response surface, or metamodel, is estimated from computer experiments that vary both uncertain physical parameters and the fidelity of the computational mesh. The resultant metamodel is then used to propagate the variabilities in the continuous input parameters, while the mesh size is taken to zero, its asymptotic limit. With respect to mesh size, the metamodel is equivalent to Richardson extrapolation, in which solutions on coarser and finer meshes are used to estimate discretization error. The method is demonstrated on a one-dimensional prismatic bar, in which uncertainty in the third vibration frequency is estimated by propagating variations in material modulus, density, and bar length. The results demonstrate the efficiency of the method for combining nondeterministic analysis with error estimation to obtain estimates of total simulation uncertainty. The results also show the relative sensitivity of failure estimates to solution bias errors in a reliability analysis, particularly when the physical variability of the system is low.

I. Introduction

NONDETERMINISTIC analysis methods are applied to simulations of physical systems to quantify the effects of random variations in system parameters and inputs on the predicted output of the simulation. Typically, nondeterministic methods are used to propagate probability or frequency distributions of continuous physical variables through a deterministic mapping, such as the discretized numerical solution of a system of partial differential equations (PDEs), plus boundary and initial conditions and auxiliary submodels. In this case, it is important to have a verified and validated model structure through which to propagate these continuous variabilities. However, all finite discretized models possess some degree of discretization error, and often little or no attempt is made to estimate the magnitude of discretization error in the model. Furthermore, even when some error estimate is available, it is unclear how to apply that estimate to the ensemble of results computed during a nondeterministic analysis. Thus, the effect of discretization error in nondeterministic analysis is rarely treated at the present time.

There has, however, been a significant amount of attention devoted to the problem of estimating errors in numerical methods for solving deterministic PDEs. Among these methods are a posteriori error estimators,[1,2] as well as such classical methods as Richardson extrapolation.[3–5] Of particular interest in this study is Richardson extrapolation, in which discretization errors are estimated from the numerical solution. Richardson extrapolation is extremely general in that it can be applied to any output of the model, as well as functionals of the solution. Its primary drawback is that it depends on knowledge of the formal convergence rate of the numerical method and requires that the mesh size used is fine enough that the higher-order terms of the error are negligible compared to the lowest-order term. For this reason, it often requires more that two mesh spacings on the same model to verify the convergence order and, thus, establish the validity of the extrapolation.

A conservative approach to accounting for discretization error in a nondeterministic analysis (which relies on the numerical solution of PDEs) would be to use Richardson extrapolation (or some other error estimator) for every combination of input values to the model. For example, we might perform a structural dynamics simulation in which the elastic modulus of some material in the design model has some inherent variability. Then, for each particular value of that parameter we could compute the response on two or more spatial discretizations and use these results in some to-be-determined way in our nondeterministic analysis. This approach would then increase the number of analyses to be performed by a factor of two to three. On the other hand, we might consider performing error estimation for only one particular value of the variable parameter (such as its mean value) and then apply that error estimate in a relative or absolute sense to the analyses performed for other values of the input. This approach would require only a modest increase in computational cost compared to the cost of the nondeterministic analysis itself, but cannot account for the dependence of the error estimate on the values of the parameters of the model. Note that the investment in generating multiple discrete models with different mesh spacings might be much more significant than the cost of computing solutions on each of the meshes.

In the present study, an alternative approach is considered in which solutions are computed on different mesh sizes, but not for every parameter value in the nondeterministic analysis. Instead, both mesh size and parameter values are varied for the purpose of building a surrogate model, or metamodel, for interpolation. Once solutions are computed to build the metamodel, a regression is performed to obtain the coefficients of the metamodel. The metamodel can then be used in the nondeterministic analysis in place of the complex full-order model. For example, frequency distributions on input variables can be easily propagated through the metamodel via Monte Carlo analysis because the cost of computing a response based on the metamodel is negligible. The treatment of discretization error is accomplished by extending traditional response surface methods (RSMs) for determining metamodels to include mesh size as a variable input parameter. Then the nondeterministic analysis can be performed for a mesh size of zero, which conforms to a higher-order accurate solution of the governing PDEs.

In this study, it has been found that including mesh size in the metamodel can be an efficient way to estimate discretization error while performing nondeterministic analysis. For example, a traditional metamodel with 3 continuous input variables might require 13 evaluations of the complex simulation with different parameter values to determine the coefficients of the metamodel. If we wished to minimize discretization error, we would perform those 13 evaluations on a fine mesh, that is, with small element edge lengths. By extending that model to include element edge length as an input variable of the metamodel, we must now perform 25 evaluations of the complex simulation. However, only six of those evaluations are performed on the fine mesh model, whereas the other evaluations are performed on coarser meshes, which require much less time to solve. Therefore, it is possible to determine the extended metamodel with less overall computational effort. Furthermore, the

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extended metamodel can be used to estimate the converged continuum solution, whereas the traditional metamodel determined strictly from evaluations of the fine mesh model still suffers some overall unquantified error due to the discretization.

The remainder of the study is organized as follows. First, the theory for estimating the effect of discretization error in the numerical solution of differential equations is reviewed. Second, the technique for using RSM for nondeterministic analysis is presented. Then, this methodology is extended to include the dependence of the simulation on mesh size. Finally, results are presented for linear dynamics of a prismatic bar with three uncertain input parameters. The results demonstrate the importance of treating discretization error when estimating system reliability measures such as probability of failure. In the example, discretization error on the order of 1% of the response quantity results in a probability of failure estimate that is more than one order of magnitude smaller than the exact solution, an error of more than 90%. Thus, the bias caused by small discretization errors can result in a significant overprediction of reliability. The technique developed herein yielded an accurate estimate of the error in the probability of failure measure due to the discretization.

II. Discretization Error Models and Extrapolation-Based Error Estimation

Quantifying the effects of approximations on the numerical solutions of ordinary and partial differential equations has been a focus of research and analysis ever since numerical solution procedures were first developed. In Richardson's classic paper from 1910 on a finite difference solution to the PDEs associated with stresses in a dam structure,[3] he introduces a very general extrapolation procedure that estimates the leading error term from multiple solutions using different differencing steps. This procedure, since referred to as Richardson extrapolation, does not exactly estimate the desired continuum solution but rather, by eliminating the leading error term, increases the order of convergence of the numerical method. Richardson extrapolation is still used extensively as both an error estimation technique and as a verification tool for numerical solution methods.[5] The error estimate is simply taken as the difference between the basic numerical solution and the higher-order solution developed from multiple meshes and has the same order of accuracy as the higher-order solution. It is, therefore, a reliable estimate as long as the leading error term is the primary source of error. One of its strengths is that it estimates the total discretization error, including both the local and global effects of discrete approximations (including finite element approximations) throughout the entire problem domain and boundary conditions. Furthermore, it can also estimate errors not only on the solution field variables but also on many linear functionals of the solution field. Its drawback is that it requires uniform mesh refinement with at least three mesh spacings. Such a requirement may be difficult to meet for some complex problems.

With the advent of the finite element method (FEM), other approaches to discretization error estimation have been developed. Most of these procedures are broadly classed as a posteriori error estimation methods[1,2] because they locally postprocess the numerical solution to estimate certain norms of the solution error. These methods, which were developed primarily as indicators for adaptive mesh refinement procedures, are usually based on multiple local mesh refinement problems using such techniques as superconvergent patch recovery to estimate local higher-order accurate estimates of solution gradients. These estimates can be compared the recovered solution gradients from the normal finite element interpolation functions and the differences used to estimate local or global solution error measures. The relative localized contributors to the error measure help identify mesh regions that require more refinement, whereas the global norm measure is used in some sense as a stopping criterion for mesh refinement. One drawback of a posteriori error estimation for global error, however, is that because it relies on local computations it cannot account for so-called pollution error, that is, the propagation of local errors through the global domain of the problem. These errors cannot be detected and, if significant, will reduce the reliability of the error estimate.

Note that the underlying polynomial model for global discretization error is the same regardless of the error estimation procedure and has been developed repeatedly in the various texts on FEMs and finite difference methods.[6–10] It is written as

$$y_D = y + \alpha h^q + \mathcal{O}(h^{q+1}) \tag{1}$$

where y is the solution to the given differential equation defined on a continuous domain in space and/or time, y_D is the approximate numerical solution on a mesh with characteristic size h, q is the order of accuracy for the numerical method, and α is a sensitivity parameter of the solution that is independent of h. The order of accuracy q is a characteristic of the numerical method that reflects the quality of the interpolation functions for the solution quantity of interest. For example, typical low-order finite elements for structural mechanics with linear shape functions lead to displacement solutions that are second-order accurate, whereas the corresponding stress solutions based on the gradient of the displacement interpolation functions are first-order accurate. The order of accuracy of the numerical method is independent of the specific problem only to the extent that we acknowledge the existence of higher-order terms in h. The magnitude of these higher-order terms are very much problem dependent and determining their importance is a necessary consideration in error estimation. This error model is also independent of the dimensionality of the problem; it is equally valid for one-dimensional and three-dimensional calculations, although it is not equally easy to estimate errors for one-dimensional and three-dimensional problems. That is, for a uniform doubling of the mesh fidelity, the number of algebraic equations for the one-dimensional problem would approximately double, whereas the size of the three-dimensional problem would increase by a factor of eight (because the mesh would double in each of the three spatial directions).

Extrapolation-based estimation of discretization error proceeds as follows. Calculations are performed on at least three meshes, where the finer meshes are uniformly refined with respect to the coarser meshes. Then, the error on the finest mesh is given as the difference between that solution and the extrapolated solution:

$$e = y_{\text{fine}} - y_{\text{extrap}} = \alpha h_{\text{fine}}^q \tag{2}$$

where α is estimated from the difference between the nominal and fine mesh solutions, namely,

$$\alpha = \frac{y_{\text{fine}} - y_{\text{nominal}}}{h_{\text{fine}}^q - h_{\text{nominal}}^q} \tag{3}$$

At least three mesh solutions are required to verify the order of accuracy of the method, q, that is assumed in the earlier equations. This is verified by estimating q, which for mesh doubling is given by

$$q = \log\left(\frac{y_{\text{nominal}} - y_{\text{coarse}}}{y_{\text{fine}} - y_{\text{nominal}}}\right) \Big/ \log 2 \tag{4}$$

Verifying the assumed value of q is equivalent to showing that the higher-order terms in the error model are negligible compared to the leading q-order term. One might also seek to estimate two error terms using more than three mesh solutions to either improve the error estimate or enable it to be computed on a coarser set of meshes.

III. RSM for Nondeterministic Analysis

Montgomery[11] notes the following:

> Response surface methodology, or RSM, is a collection of mathematical and statistical techniques that are useful for the modeling and analysis of problems in which a response of interest is influenced by several variables and the objective is to optimize the response. . . .
>
> The process yield is a function of the levels. . . , say
>
> $$y = f(x_1, x_2) + e$$
>
> where e represents the noise observed in the response y. If we denote the expected response by $E[y] = f(x_1, x_2) = h$, then the surface represented by
>
> $$h = f(x_1, x_2)$$
>
> is called the response surface.

In the present context, we will use RSM as a surrogate or metamodel for the complex physics model of interest, and we will estimate the coefficients of the response surface by performing a limited number of analyses of the complex model. Our goal is to use the response surface to propagate uncertainties in the variables to determine a distribution of the response quantity. From this distribution we can make estimates of failure probability or other statistics of interest.

The use of RSM is logically coupled to design of experiments (DOE). To apply RSM we must determine a selection of input vectors for the complex simulation. Designing the input vectors for the suite of simulations to be run is the objective of experiment design. A logical goal of DOE is to minimize the variance of the error between the response surface and the discrete responses of the complex model. It is important, however, to also consider the frequency distributions of the input parameters, as well as the type of statistic to be computed from the distribution of the output. Finally, as noted by Sacks et al.,[12] there are fundamental differences between physical experiments and computer experiments that influence the issue of experiment design.

In this study, we focus on a simple global surface model that includes second-order terms in the parameters. The model response is given by

$$y = \beta_0 + \sum_i \beta_i p_i + \sum_i \sum_j \beta_{ij} p_i p_j \tag{5}$$

where β_0, β_i, and β_{ij} are coefficients of the metamodel to be estimated from analyses performed on the complex model. Note that this metamodel form is just one possibility; other functions could be considered, as well as the finite element lattice sampling approach of Romero and Bankston.[13] In addition, a metamodel could be constructed using solution derivatives obtained from the analysis code, although to obtain quadratic term coefficients it would also be necessary to compute the second-order derivatives.

To this standard metamodel form we will apply the well-known Box–Behnken experiment design,[14] which dictates a set of input vectors for which the parameters p_i take on nominal, high, or low values. It is suggested that these levels be taken as the mean and the mean plus or minus one to two standard deviations, respectively. Furthermore, the number of simulation runs is somewhat greater than the number of coefficients being estimated, so that a least-squares estimate for the metamodel coefficients is obtained. The Box–Behnken designs for three and four input variables are given in Tables 1 and 2, where 0, +1, and −1 represent the nominal, high, and low values, respectively. Other possible designs are Central composite and suboptimal iterate selection algorithms such as Effective Independence[15] and Subset selection.[16] Once an experiment design has been determined and the computer experiments are performed, the coefficients β_{ij} of the metamodel are estimated, typically using a least-squares method.

Table 1 Box–Behnken design for three input variables

Runs	$p(1)$	$p(2)$	$p(3)$
1–4	±1	±1	0
5–8	0	±1	±1
9–12	±1	0	±1
13	0	0	0

Table 2 Box–Behnken design for four input variables

Runs	$p(1)$	$p(2)$	$p(3)$	$p(4)$
1–4	±1	±1	0	0
5–8	0	±1	±1	0
9–12	0	0	±1	±1
13–16	±1	0	±1	0
17–20	0	±1	0	±1
21–24	±1	0	0	±1
25	0	0	0	0

IV. Extension of RSM to Include Mesh Size

From Sec. II, the model for spatial discretization error is given as

$$y(h) = y_{\text{exact}} + \alpha h^q + \mathcal{O}(h^{q+1}) \tag{6}$$

where h is the characteristic mesh spacing or element length, $y(h)$ is the numerical solution resulting from the mesh, y_{exact} is the exact solution of the corresponding continuum model, q is the formal order of the method, and α is some unknown factor. Assuming knowledge of method order q, we could easily construct a metamodel from a small number of simulation runs with different values of h. Because the only unknowns are α and y_{exact}, we require only two different mesh spacings. With three different mesh spacings, we could also confirm the method order q. This approach of estimating the terms of the error model using the results from different mesh spacings is in fact just the classical Richardson extrapolation method.

Thus, given the similarity between RSM and Richardson extrapolation, it is reasonable to combine the two methods into a larger metamodel form to treat discretization error within the context of nondeterministic analysis. The form of the extended metamodel is taken to be

$$y(\boldsymbol{p}, h) = \beta_0 + \sum_i \beta_i p_i + \sum_i \sum_j \beta_{ij} p_i p_j + \alpha_0 h^q + \sum_i \alpha_i p_i h^q \tag{7}$$

which allows for the metamodel to account for the coupling between the constant and linear terms of the nominal metamodel and the discretization error, but neglects the terms of $\mathcal{O}(p^2 h^q)$ and above.

A. Experiment Design for Extended Metamodel

For experiment design purposes, we will again use the Box–Behnken design, where the number of input variables is increased by one for input value h. This requires that we develop discretized models with three different mesh spacings. As with Richardson extrapolation, it is usually desirable to perform mesh doubling. The values −1, 0, and +1 with respect to h are strictly qualitative and correspond to coarse, nominal, and fine mesh models, respectively. For example, reinterpreting Table 2 for the case of three input parameters plus variation in mesh fidelity, we have the experiment design given in Table 3. The value h/h_{nom} implicitly assumes the use of mesh doubling, but this is not specifically required.

The efficiency of the present method can be seen in examining Tables 1 and 3. When the metamodel is extended by one input variable in order to include the mesh size parameter h, the total number of analyses increases, but the number performed with a fine mesh is only a small fraction of the total and less than the total number of runs of the nonextended metamodel. Thus, a traditional response surface (without h) estimated by analyses performed using the fine mesh can actually be less efficient than extending the model to include h inasmuch as the total computational effort is dictated by the number of fine mesh analyses performed. This comparison is summarized in Table 4 for different numbers of continuous input variables. Note that as the number of input parameters increase, the efficiency gains become dramatic.

B. Verification of the Assumed Order of Accuracy

In a real sense, the nominal mesh model, together with the coarse mesh model, is being used to infer or interpolate the effects of the

Table 3 Box–Behnken design for three input variables plus mesh fidelity variation

Runs	$p(1)$	$p(2)$	$p(3)$	Mesh	h/h_{nom}
1–4	±1	±1	0	Nominal	1.0
5–8	0	±1	±1	Nominal	1.0
9–10	0	0	±1	Coarse	2.0
11–12	0	0	±1	Fine	0.5
13–16	±1	0	±1	Nominal	1.0
17–18	0	±1	0	Coarse	2.0
19–20	0	±1	0	Fine	0.5
21–22	±1	0	0	Coarse	2.0
23–24	±1	0	0	Fine	0.5
25	0	0	0	Nominal	1.0

Table 4 Efficiency gains by using extended metamodel with mesh parameter and Box–Behnken experiment design

Number of metamodel inputs (not including h)	Efficiency[a]
3	2.2
4	3.1
5	6.7
6	8.3

[a] $\left[\frac{\text{no. fine mesh runs in extended model}}{\text{total no. runs in nonextended model}}\right]^{-1}$.

parameter variations that would be seen at the fine mesh level. The mechanism for performing this inference is the form of the response surface that is grounded in the error model equation (6). This error model is valid, however, only in the asymptotic range and, thus, imposes a restriction on the fidelity of the meshes considered. In a sobering demonstration of the limitations of Richardson's method, Oberkampf and Blottner[17] showed that for a particular system of nonlinear equations with large local gradients, reaching the asymptotic range for Richardson's method required very fine grids with relative errors on the order of 0.1%. Therefore, computational meshes that simply meet an analyst's subjective criteria for goodness cannot be immediately assumed to meet the asymptotic range requirements of Richardson's method and the present extended response surface technique. It is important to assess the convergence characteristics for the range of meshes considered and to demonstrate the formal convergence of the method before proceeding with extrapolative procedures.

There are two approaches to verifying the convergence order using the experiment design procedure discussed. Examining Table 3 for the particular case of three metamodel input parameters, there are six points in the design space where solutions are computed using both the coarse and fine meshes of the model. Two mesh sizes are not sufficient, however, to independently estimate both the mesh error and the convergence order q. To independently estimate q we also require a solution at these design points for the nominal mesh. These can be obtained by performing additional computer experiments using the nominal mesh at these design points (corresponding to extreme values of each parameter). Alternatively, we could use the results from the runs on the nominal mesh to build a traditional metamodel with respect to the input parameters conditioned on the nominal mesh, and then use that metamodel to interpolate the response for the nominal mesh at the design points where coarse and fine mesh runs have been performed.

V. Nondeterministic Analysis with Extended Metamodel

The final stage of the nondeterministic analysis involves the use of the metamodel to propagate the parametric uncertainties through to the simulation output. From the distribution of the output, probabilistic or statistical quantities such as probability of failure, expected output value and variance can be estimated. One straightforward approach is what Romero and Bankston[13] term decoupled Monte Carlo (DMC) analysis. Decoupled refers to that the building of the response surface from complex simulation runs and the Monte Carlo analysis using the response surface are separate activities. For the Monte Carlo analysis, we would generate a very large number of samples from the joint distribution function of the uncertain variables and compute the metamodel response for each sample to build the output distribution. The only modification required for the extended metamodel is determining how to sample the mesh spacing parameter h.

Of course, as a solution method parameter, h is not a physical variable and has no associated distribution. Instead, we will use variations in h to estimate bias error in the nondeterministic solution. The nominal or fine mesh-based nondeterministic solution is obtained by holding h fixed at h_{nominal} or h_{fine}, respectively. Then an extrapolated nondeterministic solution is obtained by holding h fixed at zero. Finally, the biases in the nominal or fine mesh-based nondeterministic solutions are given by the differences between these solutions and the extrapolated ($h = 0$) solution. Whereas this procedure involves extrapolation of the metamodel, which is a practice normally avoided in such use of function approximations, the potential problems related to extrapolation are mitigated in two ways. First, by the verification of accuracy order q, which specifically addresses the validity of the error model form for use in extrapolation, and second, by the use of the extrapolation strictly as a means to estimate solution error, rather than as a means to obtain a more exact solution.

VI. Example: One-Dimensional Prismatic Bar

The first example is a uniform prismatic bar with fixed–free boundary conditions as shown in Fig. 1. The objective of the analysis is to estimate the probability of failure of the bar, where failure is defined by the condition $f_3 < 16{,}000$ Hz, where f_3 is the frequency of the third mode of vibration. The physical parameters defining the system are given in Table 5, where the coefficient of variation is equal to the standard deviation of the distribution divided by the mean. The mesh chosen for the nominal model is also shown in Fig. 1. Note that the mesh was chosen to be nonuniform. There are two reasons for this. First, in most complex problems it is difficult or impossible to achieve a uniform grid, and often the mesh is refined in some areas to enhance accuracy for some output of the model. Second, it is understood that numerical methods tend to behave better in a theoretical sense on uniform grids; thus, the nonuniform grid in this problem is intended to make a very simple problem somewhat more difficult. From the fixed end to the free end, the element lengths are four elements at 1.25 in., four elements at 1.00 in., four elements at 0.75 in., four elements at 0.50 in., and four elements at 0.25 in. Thus, there is a total of 20 elements and 20 degrees of freedom (DOF) in the nominal model. The coarse and fine meshes for this problem are related to the nominal mesh by doubling and halving the element lengths, respectively. Therefore, the coarse mesh has 10 DOF and the fine mesh has 40 DOF.

The experiment design given in Table 3 was used for estimating the extended metamodel, with the interpolation function given by Eq. (7) and $q = 2$ as the formal order of the method. Then the DMC analysis was performed with 100,000 samples of the joint density function of E, ρ, and L. All samples were evaluated at $h = 0$. For comparison, a direct Monte Carlo analysis was performed using the exact continuum solution[18]:

$$f_3 = 5\sqrt{E/\rho}/4L \tag{8}$$

Also, for comparison, two approximate solutions are treated. First, a direct Monte Carlo analysis was performed using the nominal mesh model. Second, a DMC analysis was performed for the fine mesh model, where the response surface was estimated with respect to the three physical variables E, ρ, and L, using Eq. (5) and the experiment design given in Table 1. Finally, histograms of each of the four Monte Carlo analyses were computed using 1000 bins, and the results input to a kernel density estimator to arrive at

Table 5 Parameter information for one-dimensional bar

Parameter	Distribution	Mean value	COV, %
Elastic modulus E	Normal	10×10^6 psi	1.0
Mass density r	Normal	0.000259 lb-s^2/in.^{2}	1.0
Total length L	Normal	15.0 in.	1.0

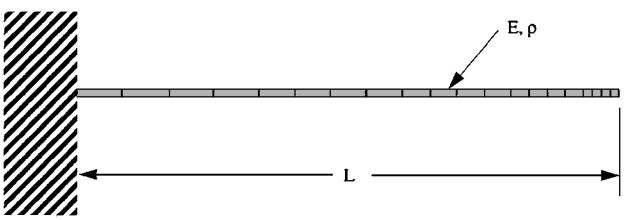

Fig. 1 One-dimensional prismatic bar model with nominal mesh.

estimates of the output probability density functions. These final results are shown in Fig. 2.

VII. Discussion of Results

The results from this example are summarized in Tables 6 and 7. In Table 6, for each of the approaches, the total number of finite element analyses is given, as well as the number of analyses using the fine resolution grid. This is important because the computational effort is primarily associated with the number of finite element analyses performed on the most refined grid. Then the total number of computations required for the nondeterministic analysis are given in million floating-point operations (MFLOPs) (10^6 FLOPs). Finally, the error in the estimated mean of the distribution is given, as well as the estimated probability of failure, which is the statistic of interest in the problem. The extended metamodel result given is the estimated solution at $h = 0$ obtained via extrapolation using the extended RSM (ERSM). Note, first, that the continuum solution is the exact result, subject to Monte Carlo sampling errors (which are small because of the number of samples). The rest of the methods are given in Table 6 in order of their accuracy.

The ERSM method is not only the most accurate approximation, but is also the most efficient. There is some remaining bias in this solution because extrapolation does not calculate the exact solution, but rather a high-order accurate estimate of the exact solution. This bias could be further reduced by either refining the set of meshes considered or by performing additional mesh variations and using the results to estimate higher-order error terms. The extrapolated solution is sufficiently accurate, however, for the purpose of error estimation. The more traditional RSM based on the fine mesh is still a reasonable result, although it requires more computations and is somewhat less accurate than the ERSM. Finally, the direct Monte Carlo method based on the nominal mesh is not only very inefficient, but also leads to a significant error in the probability of failure estimate. Noted that all of the results have negligible sampling errors, and the errors introduced by the limitations of the metamodel forms were also small. The errors shown on both the estimated mean and failure probabilities are primarily due to the biases in the finite element solutions caused by the fidelity of the discretizations.

In Table 7, the results are presented in terms of estimating the bias error on the nondeterministic solution using the extended metamodel. The first result given for the fine mesh is obtained from the extended metamodel by fixing h at h_{fine}. The estimated bias on this solution is then obtained by comparison to the extrapolated solution using the extended metamodel. The true bias is given by comparison to the continuum solution. The second result given for the fine mesh is that obtained by estimating a traditional response surface

Table 7 Bias error estimation for nondeterministic analysis

Mesh	Estimated bias error in mean (f_3), %	Actual bias error in mean (f_3), %	Estimated bias error in P_{failure}, %	Actual bias error in P_{failure}, %
Fine (using ERSM)	0.27	0.27	−41.3	−42.5
Fine (using RSM)	Unknown	0.27	Unknown	−41.5
Nominal (using ERSM)	1.07	1.08	−91.6	−91.7
Nominal (using DMCS)	Unknown	1.09	Unknown	−91.6

Table 6 Nondeterministic analysis results for one-dimensional bar example

Method	Total number of FEM analyses	Number of fine grid FEM analyses	Number of computations (MFLOPs)	% Error in mean (f_3), %	Estimate of P_{failure}, %[a]
Continuum solution	n/a	n/a	n/a	n/a	2.75
ERSM (with $h = 0$)	25	6	59	0.01	2.69
RSM on fine mesh	13	13	94	0.27	1.61
Direct Monte Carlo on nominal mesh	100,000	0	90,000 (est)	1.09	0.23

[a] $P_{\text{failure}} = P(f_3 < 16{,}000\,\text{Hz})$.

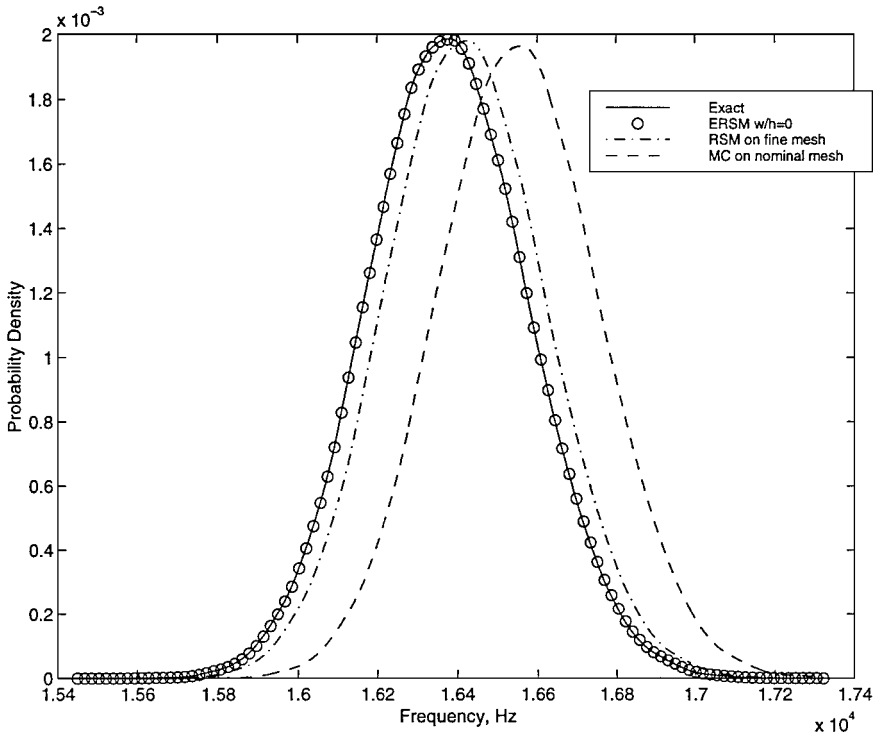

Fig. 2 Results from nondeterministic analysis of one-dimensional bar.

Table 8 Order of accuracy estimates from experiments used to estimate extended metamodel

Reference runs	$p(1)$	$p(2)$	$p(3)$	q
9,11	0	0	+1	1.9816
10,12	0	0	−1	1.9813
17,19	0	+1	0	1.9817
18,20	0	−1	0	1.9811
21,23	+1	0	0	1.9810
22,24	−1	0	0	1.9819

without the mesh size parameter. For this approach, there is no estimate of the bias error due to discretization because there are no other mesh solutions considered. The true bias is again obtained by comparison to the continuum solution. Note that the fine mesh solutions obtained from both response surface models are essentially identical, but, referring back to Table 6, the solution obtained using the extended metamodel not only required fewer finite element computations on the fine mesh, but also allowed for the estimation of the discretization bias error on the solution. The last two rows of Table 7 give similar results for the nominal mesh size. Again, the accuracy of the extended metamodel is seen by its similarity to the direct Monte Carlo results for the nominal mesh, that is, with no function approximation employed.

Finally, estimates for the order of accuracy of the set of discretizations is given in Table 8. These estimates were obtained by fitting an independent response surface model to the nominal mesh experiments and then using this model to interpolate the nominal mesh results to the experiments performed on the coarse and fine meshes. Then the three different mesh solutions for each of six points in the continuous parameter space were used with Eq. (4) to estimate q, the exponent of the characteristic mesh size h in the discretization error model. These results verify that the set of discretizations is within the sphere of convergence of the numerical method, for which $q = 2$.

Apart from the comparison of methods, one of the most interesting aspects of these results is the effect the prediction error, as measured by the error in the estimated mean of the distribution, has on the relative error in the probability of failure estimate. In the case of the direct Monte Carlo analysis based on the nominal mesh, the discretization error results in a prediction error of about 1% of the exact solution. This would normally be considered more than adequate for engineering purposes. However, this error leads to a probability of failure estimate that is over one order of magnitude smaller than the exact solution. Thus, the reliability of the system might be judged to be more than 10 times higher than its actual reliability. The heightened sensitivity is a function of the probability of failure magnitude we are trying to estimate, as well as the coefficient of variation (the ratio of the standard deviation of the distribution to the mean value) of the simulation output used in the failure calculation.

This can be seen by considering the effect of a relative bias error on the value of a standard normal random variable z at the point of failure, namely,

$$z = (y_F - \mu)/\sigma \tag{9}$$

where μ is the mean of the distribution of the response y, σ is the standard deviation of the distribution of y, and y_F is the value of the response that defines the failure boundary. If the computational prediction of y is given by y_c and suffers a relative bias error ε, we have

$$y_c = y(1+\varepsilon), \qquad \mu_c = \mu(1+\varepsilon), \qquad \sigma_c = \sigma(1+\varepsilon) \tag{10}$$

Substitution into Eq. (9) yields

$$z_c = \frac{y_F - \mu}{\sigma} = \frac{z - (\varepsilon/\mathrm{COV})}{1+\varepsilon} \approx z - \frac{\varepsilon}{\mathrm{COV}} \tag{11}$$

for small ε, where $\mathrm{COV} = \sigma/\mu$ is the coefficient of variation (COV) of the distribution y. Using this result, we can estimate the relative error in the probability of failure due to the computational bias. Using a first-order Taylor series expansion of the cumulative distribution function, we have

$$\Phi(z_c) = \Phi\left(z - \frac{\varepsilon}{\mathrm{COV}}\right) \approx \Phi(z) - \left(\frac{\varepsilon}{\mathrm{COV}}\right)\frac{\mathrm{d}\Phi(z)}{\mathrm{d}z}$$

$$\therefore \Phi(z_c) \approx \Phi(z)\left(1 - \frac{\varepsilon}{\mathrm{COV}}\left(\frac{\phi(z)}{\Phi(z)}\right)\right) \tag{12}$$

Thus, the relative error in the failure probability is

$$\frac{\Delta\Phi(z)}{\Phi(z)} \approx -\left(\frac{\varepsilon}{\mathrm{COV}}\right)\left(\frac{\phi(z)}{\Phi(z)}\right) \approx \frac{\varepsilon}{\mathrm{COV}} z \tag{13}$$

where $\phi(z)/\Phi(z) \approx -z$ is a reasonably good approximation for $z < -3$ and a lower bound for all $z < 0$. This approximation to the relative error in the probability of failure clearly demonstrates that the sensitivity of the probability of failure to bias error is exacerbated by two factors: a small coefficient of variation (or one which is of similar magnitude to the bias error ε) and a small failure probability for the exact solution. For the sample problem on the fine mesh, with $\mathrm{COV} = 1.22\%$, $\varepsilon = 0.27\%$, and $z = -1.92$, the relative error in the probability of failure approximated by Eq. (13) is -42.5%, which is equivalent to the results in Table 7.

Although the example problem is relatively simple, there are no issues that limit the present procedure to one-dimensional problems or to few parameters. Richardson extrapolation has been used extensively in two- and three-dimensional computational fluid dynamics, both for verification of codes and calculations.[5] Furthermore, as noted earlier and in Table 4, there is a potential for improvement in efficiency by utilizing multiple meshes over a large dimensional parameter space, rather than limiting a probabilistic analysis to function evaluations on fine meshes alone. Note that not every potential response quantity will use the same error model; stress and displacement, for example, differ in their order of accuracy and require different coefficients for h in the error models. However, the basic approach is the same, given an understanding of the formal order of accuracy of the numerical methods employed in the computational analysis.

VIII. Conclusions

A technique has been presented for treating discretization error in nondeterministic analysis. The technique involves the use of RSM, in which a metamodel representation of a complex simulation model is estimated from a limited number of computer experiments on the complex model. The metamodel is then extended to include the characteristic element edge length as an model input parameter. The extended metamodel is used to propagate the variabilities in the continuous input parameters, whereas the effect of discretization error is estimated by taking the mesh size to zero, its asymptotic limit. The technique is demonstrated on a one-dimensional prismatic bar, in which the uncertainty in the frequency of the third mode of vibration is estimated by propagating variations in the elastic modulus and mass density of the material, together with variation in the total length of the bar. Results are compared to the closed-form solution, a direct Monte Carlo analysis using a nominal mesh size, and a traditional response surface without a mesh size parameter built from computer experiments using a fine mesh size. The results demonstrate the importance of treating discretization error when estimating system reliability measures, such as probability of failure, and the efficiency of the present technique for combining nondeterministic analysis with error estimation to obtain more accurate estimates of total simulation uncertainty.

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