Combining Metamodels with Rational Function Representations of Discretization Error for Uncertainty Quantification

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Abstract

A new method is presented for extending metamodeling techniques to include the effects of finite element model mesh discretization errors. The method employs a rational function representation of the discretization error rather than the power series representation used by methods such as Richardson extrapolation. Examples dealing with simple function estimation and estimation of the vibrational frequency of a one dimensional bar showed that when extrapolated to the continuum, the rational function model gave more accurate estimates using fewer terms than the Richardson extrapolation technique. This is an important consideration for computational reliability assessment of high consequence systems, as small biases in solutions can significantly affect the accuracy of small magnitude probability estimates. In general, the rational function form of the discretization error produces a nonlinear model requiring an iterative nonlinear least-squares solution technique. However, all the examples studied in this work proved to be close-to-linear, meaning that the linear least-squares estimate of the model coefficients could not be improved. In subsequent nondeterministic analyses, the rational function based metamodel also produced more accurate estimates of failure probabilities using fewer terms than the Richardson extrapolation method under very severe extrapolation conditions. Rational function representations of discretization error offer greater flexibility by allowing a user to accurately extrapolate to a continuum representation from numerical experiments performed outside the asymptotic region where the usual power series representation is not converging. This allows the use of coarser meshes in the numerical experiments, saving a significant amount of time and effort.

1 . Introduction

Numerical simulations of system response are used throughout the research and industrial communities to help make critical system design and performance decisions. These simulations contain errors due to known simplifications, variabilities due to random inputs with known statistics, and uncertainties due to lack of knowledge [1]. In order to make proper decisions, it is important to understand how all three of these types of deviations propagate through simulations into computed results. A particularly important source of error, variability, and uncertainty is the analytical model of the system being simulated.

Model parameter variability has received the most attention in the literature. Assuming that the variabilities in model parameters follow known probability distributions, the ultimate goal of the quantification of their effects is to determine the corresponding probability distributions of the simulation outputs of interest. Accurate prediction of these distributions requires Monte Carlo analysis incorporating hundreds of thousands of simulation runs. In most cases, the computational cost is prohibitive. In many situations, the computational effort can be greatly reduced by generating what is commonly referred to as a *Response Surface* or *Metamodel*. An appropriate functional form is assumed for the simulation response of interest and then fit to the output produced by the simulation of a set of carefully selected numerical experiments. The functional form is usually taken as a quadratic polynomial in the input variables.

In contrast with the full numerical simulation, evaluation of the metamodel is very fast. Assuming that the underlying system is itself deterministic, the prediction of the response can be decoupled from the probabilistic Monte Carlo sampling using the metamodel. This technique has been referred to as "decoupled" Monte Carlo analysis [2]. The metamodel approach has long been used in the biological, physical, and sociological sciences [3], but has more recently received attention from the structural dynamics community. Applications include structural optimization [4, 5] and probabilistic design [6-8]. Response surfaces based on finite element / lattice sampling have been investigated by Romero and Bankston [2].

While most of the work mentioned has focused on the effects of model parameter variability, Alvin [9] recently incorporated mesh discretization error into the metamodel formulation in an effort to quantify its effect on nondeterministic analysis. The approach is based upon the classical Richardson extrapolation [10] technique used in finite element modeling to quantify the error due to spatial discretization inherent in a mesh. Discretization error is modeled as a polynomial in parameter h, which could, for example, represent a characteristic element length. The method strongly resembles the metamodel approach itself, making it very attractive to combine the two into a single formulation. In general, a metamodel is used to predict desired responses by interpolating among selected experiment design points. In contrast, the idea behind including the discretization parameter is to eventually extrapolate to the value of $h = 0$, obtaining a metamodel representing the continuous system. The discretization error is then theoretically removed from the subsequent decoupled Monte Carlo analysis. In this way, the effects of bias error due to discretization on the nondeterministic analysis can be quantified. Alvin demonstrated the efficacy of this approach for a simple bar example using three different mesh refinements [9]. One conclusion drawn from Alvin's work is that small failure probability estimates, which are typical in high consequence systems such as nuclear reactors, can be very sensitive to small bias errors in computational solutions. Hence, estimating the potential effects of discretization error is important in computational reliability analysis.

In order for Richardson extrapolation to produce accurate results, the numerical experiments must be performed within the asymptotic region of the power series being used to model the discretization error. This simply means that the term or terms retained from the power series dominate the terms that are omitted. The implication is that even the coarse meshes used in the numerical experiments must be sufficiently refined. The work presented in this paper considers an alternative representation of the discretization error in the form of a rational function or ratio of polynomials in the parameter h. In general, rational functions are much more flexible than polynomials for approximating mathematical functions. They are capable of representing a wide variety of ascending and descending curves, including curves with minima and maxima, and curves that approach asymptotes. Due to this greater flexibility, it has been found that the use of rational functions in general response surface analysis can produce metamodels that are more accurate and require fewer coefficients than the corresponding polynomial representations [11]. Minimizing the number of coefficients is important to avoid systematic error. The increased flexibility of rational functions over power series is also reflected in the observed superiority of rational functions in extrapolation applications [12]. A rational function approximation of an analytic function can remain accurate even after all the terms in a power series representation in h have similar magnitudes making the idea of "method order" meaningless [13]. It is believed that this attribute will allow the use of coarser meshes in the numerical experiments, which would save a significant amount of time and effort.

2. Theory

In metamodel analyses, parsimony is usually preferred over generality, therefore, quadratic metamodels are assumed in the form of simple polynomials in the input variables. This same approach is used here, but the formulation can be easily generalized to higher order surfaces and more sophisticated basis functions if there is a need. Assuming a single output y for the simulation, such as a peak displacement or stress, the general form of the quadratic metamodel is given by

$$y(x,\beta) = \beta_0 + \sum_{i=1}^{l} \beta_i x_i + \sum_{i=1}^{l} \sum_{j=i}^{l} \beta_{ij} x_i x_j \tag{1}$$

in which x_i are usually quantitative input variables, like mass, spring stiffness, elastic modulus, etc., and β_i are constant coefficients to be determined. Quantitative variables are usually coded such that they vary continuously between -1.0 and 1.0 using the relation

$$x_i = \frac{X_i - X_{io}}{\Delta_i} \qquad \Delta_i = \tfrac{1}{2}\left(X_{i\max} - X_{i\min}\right) \tag{2}$$

where x_i is the *i*th coded input, X_i is the corresponding uncoded input, X_{io} is the nominal value of the *i*th input, and $X_{i\,min}$ and $X_{i\,max}$ represent the lower and upper bounds on the range of the *i*th uncoded input. The nominal value of the coded input variable always corresponds to 0.0. Coding is performed to offset large possible differences in units between various model inputs, which can cause numerical error during fitting of the metamodel.

Spatial discretization error is fundamental to all finite element models as well as other types of analytical model representations [14]. Richardson extrapolation is a technique that attempts to account for this by modeling the error as a low order polynomial in the discretization parameter *h* of the form

$$y_h = y + \alpha h^q + O\left(h^{q+1}\right) \tag{3}$$

where y_h is the numerical solution for the current value of *h*, *y* is the continuum solution, α is an unknown coefficient, and *q* is defined as the formal order of the method. In its classic application, *h* is assumed to be sufficiently small, i.e. in the asymptotic range, such that the leading term in Eq. (3) will dominate and the higher order terms can be omitted. More general polynomial extrapolation methods often use an even asymptotic expansion in *h* for the error

$$y_h - y = \alpha_1 h^2 + \alpha_0 h^4 + \cdots \alpha_m h^{2m} \tag{4}$$

It can be shown that for the same number of terms, an even powered asymptotic expansion will converge twice as quickly in extrapolation applications as a series with powers increasing by one [12].

2.1 Combined Metamodel Forms

Assuming a multiplicative discretization effect, the metamodel for the continuum approximation, given by Eq. (1), can be combined with the asymptotic expansion of Eq. (4) to produce an extended metamodel that explicitly includes the effects of discretization in the form

$$y_h = y(x,\beta)\left[1+\alpha_1 h^2 + \alpha_2 h^4 + \cdots \alpha_m h^{2m}\right] \tag{5}$$

This form allows coupling between the discretization parameter *h* and the continuum form of the metamodel $y(x,\beta)$ and is analogous to that used by Alvin [9]. It is believed that improved convergence properties can be obtained by alternatively using a rational function approximation for the discretization error, producing the metamodel form

$$y_h = y(x,\beta)\frac{1+N(\alpha_i,h)}{1+D(\gamma_i,h)} = y(x,\beta)\frac{\left[1+\alpha_1 h^2 + \alpha_2 h^4 + \cdots \alpha_m h^{2m}\right]}{\left[1+\gamma_1 h^2 + \gamma_2 h^4 + \cdots \gamma_n h^{2n}\right]} \tag{6}$$

where, in general, $m \le n$. The corresponding rational function (RF) representation of the discretization error, $y_h - y$, is given by

$$\varepsilon_{hRF} = y(x,\beta)\frac{N(\alpha_i,h) - D(\alpha_i,h)}{1+D(\gamma_i,h)} \tag{7}$$

A specific example can be considered in order to clarify and compare the two discretization error model forms. Three quantitative inputs are considered, x_1, x_2, and x_3. The fourth model input is the discretization parameter *h*. The truncated metamodel considered for this application containing the polynomial form of the discretization error is given by

$$y_{hRE} = y(x,\beta)\left[1+\alpha_1 h^2 + \alpha_2 h^4\right] \tag{8}$$

Retaining only the linear coupling between the quantitative variables x_i and h^2, the expanded form becomes

$$\begin{aligned} y_{hRE} = {} & \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{33} x_3^2 + \\ & \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \alpha_1 h^2 + \alpha_{11} x_1 h^2 + \alpha_{12} x_2 h^2 + \\ & \alpha_{13} x_3 h^2 + \alpha_2 h^4 \end{aligned} \tag{9}$$

Additional terms from the general form in Eq. (5) can be easily included in the analysis. Equation (9) will be called the Richardson extrapolation (RE) metamodel in the sequel. In order to calculate the metamodel coefficients in Eq. (9), a sequence of simulations, or numerical experiments, is performed using predetermined settings for the input variables. The data for the complete set of experiments is then combined into the matrix equation

$$X\theta = Y \tag{10}$$

in which X is the experiment design matrix, θ is a column vector containing the model coefficients, and Y is a column vector containing the responses from the numerical experiments. An estimate of the model coefficients is generated using linear least-squares (LS)

$$\hat{\theta} = \left[X^T X\right]^{-1} X^T Y \tag{11}$$

There are many criteria that can be used to optimally design numerical experiments [15]. For example, the well-known Box-Behnken experiment design [8] for the case of four model inputs is presented in Table 1. The coded values of the three quantitative inputs x_i are –1, 0, and 1, representing low, nominal, and high levels, respectively. The nominal value of the inputs corresponds to their expected values, while the high and low levels represent plus and minus two standard deviations. In the case of a finite element analysis, the values –1, 0, and 1 corresponding to the discretization variable h represent coarse, nominal, and fine meshes.

The truncated metamodel containing the rational function form of the discretization error considered in this paper is given by

$$y_{hRF} = y(x,\beta)\left[\frac{1+\alpha_1 h^2}{1+\gamma_1 h^2+\gamma_2 h^4}\right] \tag{12}$$

or in its expanded form

$$\begin{aligned} y_{hRF} = [&\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{33} x_3^2 + \\ &\beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \alpha_1 h^2 + \alpha_{11} x_1 h^2 + \alpha_{12} x_2 h^2 + \\ &\alpha_{13} x_3 h^2]\left[\frac{1}{1+\gamma_1 h^2+\gamma_2 h^4}\right] \end{aligned} \tag{13}$$

Only quadratic terms in h have been retained in the numerator of the discretization error model, while a quartic term is included in the denominator. As in the case of the RE metamodel, only linear coupling between the quantitative variables x_i and h^2 is retained. Additional terms in the numerator and denominator can be easily included if required. The metamodel represented in Eqs. (12) or (13) is nonlinear in the coefficients γ_1 and γ_2, meaning that an iterative nonlinear least-squares technique, such as the Marquardt method [16], must be used to estimate the coefficients. In the case of a linear model, such as Eq. (9), if the errors are assumed to be independent and normally distributed, with zero mean and constant variance, LS produces estimates of the model parameters which are unbiased, normally distributed, and minimum variance. In practice, least-squares produces the best available estimates. Other desirable properties of linear models include ease of obtaining the LS estimates, i.e. no iteration, straightforward statistical interpretation of the estimates, and the predicted values of the response variable y will be unbiased. In contrast, LS estimates for a nonlinear model achieve these properties only asymptotically. However, if the LS estimator for the parameters of a nonlinear model is only slightly biased, with a distribution that is close to normal, and has variance close to the minimum, the model can be considered as close-to-linear [17].

Fortunately, the nonlinear model form in Eq. (12) is found to be close-to-linear. It is important to understand that this does not mean that the coefficients that appear nonlinearly, γ_0 and γ_1, are necessarily small, but rather that the rational form will have properties close to those discussed for a linear model. An iterative technique for nonlinear LS requires an initial guess for the model coefficients θ. A good initial guess is provided by the linear LS estimate, where the nonlinear estimation problem associated with the RF metamodel is cast in a linear form

$$X_{RF}\theta_{RF} = Y \tag{14}$$

by multiplying through Eq. (13) by the denominator of the discretization error term and then subtracting $Y\gamma_1 h^2 + Y\gamma_2 h^4$ from both sides of the resulting expression. The jth row of the corresponding experiment design matrix is given by

$$\begin{aligned} X_{RFj} = [1 \quad & x_1 \quad x_2 \quad x_3 \quad x_1^2 \quad x_2^2 \quad x_3^2 \quad x_1x_2 \quad x_1x_3 \quad x_2x_3 \\ & h^2 \quad x_1h^2 \quad x_2h^2 \quad x_3h^2 \quad -Y_jh^2 \quad -Y_jh^4] \end{aligned} \tag{15}$$

where the inputs and the response Y_j are evaluated at the jth experiment in Table 1. The corresponding coefficient vector is given by

$$\begin{aligned} \theta_{RF} = \{\beta_0 \quad & \beta_1 \quad \beta_2 \quad \beta_3 \quad \beta_{11} \quad \beta_{22} \quad \beta_{33} \quad \beta_{12} \quad \beta_{13} \quad \beta_{23} \\ & \alpha_1 \quad \alpha_{11} \quad \alpha_{12} \quad \alpha_{13} \quad \gamma_1 \quad \gamma_2\}^T \end{aligned} \tag{16}$$

If the RF metamodel described by Eq. (12) behaves as though it is close-to-linear, the optimization scheme used by the nonlinear LS method will find the minimum of the sum of squared errors function in one step. In all of the examples considered during this work, when the linear LS estimate was used as a starting point, convergence took just one step and the optimum estimate essentially coincided with the original starting point. This indicates that the RF metamodel behaves linearly and the best estimate is produced by linear LS. In general, every example should be checked for linearity when using RF metamodels.

2.2 Error Analysis

When working with finite sequences to approximate functions, it is desirable to be able to compute a rate of convergence. For a truncated sequence of simple polynomials, the rate of convergence is straightforward to estimate. In the case of the general RE metamodel

$$y_{hRE}^{m} = y(x,\beta)\left[1+\alpha_1 h^2 + \alpha_2 h^4 + \cdots \alpha_m h^{2m}\right] \tag{17}$$

the rate would be $O\left(h^{2(m+1)}\right)$ or at least as fast as the term $h^{2(m+1)}$ for small h. In the case of a RF metamodel, the truncated sequence is a little more difficult to identify. Due to the nonzero polynomial in the denominator, Eq. (6) is equivalent to a sum of infinite sequences of simple polynomials given by

$$y_{hRF}^{n} = y(x,\beta)\left[1+N(\alpha_i,h)\right]\sum_{i=1}^{n} S_i \tag{18}$$

where

$$S_1 = 1 + \delta_{11}h^2 + \delta_{12}h^4 + \delta_{13}h^6 + \cdots$$

$$S_i = \delta_{ii}h^{2i} + \delta_{ii+1}h^{2(i+1)} + \delta_{ii+2}h^{2(i+2)} + \cdots \qquad , \quad i > 1$$

The order of convergence can be estimated by computing the difference between a rational function representation containing an infinite number of terms in the denominator, y_{hRF}^{∞}, and the truncated expression in Eq. (6) containing terms through order h^{2n}. Equation (18) produces the result

$$y_{hRF}^{\infty} - y_{hRF}^{n} = y(x,\beta)\left[1+N(\alpha_i,h)\right]\left[S_{n+1} + S_{n+2} + \cdots\right] \tag{19}$$

Therefore, assuming $n > m$, the representation y_{hRF}^{n} converges at least as fast as $h^{2(n+1)}$.

In order to have confidence in the accuracy of extrapolated results using either the RE or RF error representations, consistency checks must be computed. For conciseness, only first and second order models in h^2 will be considered, but the following consistency checks can be generalized to models of any order. Let ε_h^1 and ε_h^2 represent the discretization error produced by truncating either the RE or RF representations to first and second order in h^2, respectively. In the case of RE representations, Malkus and Webster [18] proposed a check of the relative contributions at first and second order given by the measure

$$r_1 = \frac{\varepsilon_h^2 - \varepsilon_h^1}{\varepsilon_h^1} \tag{20}$$

For the RE models proposed in Eqs. (4) and (5), the measure has the form

$$r_{1RE} = \frac{\alpha_2 h^2}{\alpha_1} \tag{21}$$

In the case of RF models of the form given in Eq. (12), ε_h^1 and ε_h^2 are given by

$$\varepsilon_{hRF}^1 = y\frac{(\alpha_1 - \gamma_1)h^2}{1+\gamma_1 h^2} \tag{22}$$

$$\varepsilon_{hRF}^2 = y\frac{\left[(\alpha_1 - \gamma_1)h^2 - \gamma_2 h^4\right]}{1+\gamma_1 h^2 + \gamma_2 h^4} \tag{23}$$

which produces

$$r_{1RF} = \frac{-\gamma_2 h^2\left(1+\alpha_1 h^2\right)}{(\alpha_1 - \gamma_1)\left[1+\gamma_1 h^2 + \gamma_2 h^4\right]} \tag{24}$$

A second measure, proposed by Conte and de Boor [19], estimates the dominance of that portion of the series retained in the discretization error model over that portion discarded. Assuming that the desired output value is available at three different discretizations, the measure is computed using the relation

$$r_2 = \frac{y_1 - y_2}{y_2 - y_3} \tag{25}$$

in which y_i denotes the value produced at a discretization parameter value h_i. In a finite element analysis, h_i would correspond to three different mesh refinements. In the following analysis, it is assumed that h_1 corresponds to the coarsest discretization, with $h_2 = h_1/q_2$ and $h_3 = h_1/q_3$ in which q_2 and q_3 are integers. Assuming a second order RE metamodel in the form of Eq. (8), an estimate of measure r_2 can be computed by substituting into Eq. (25)

$$\hat{r}^2_{2RE} = \frac{\alpha_1\left(1-\frac{1}{q_2^2}\right)+\alpha_2 h_1^2\left(1-\frac{1}{q_2^4}\right)}{\alpha_1\left(\frac{1}{q_2^2}-\frac{1}{q_3^2}\right)+\alpha_2 h_1^2\left(\frac{1}{q_2^4}-\frac{1}{q_3^4}\right)} \tag{26}$$

The corresponding measure for a first order model, $\hat{r}^1_{2RE}$, can be found by setting α_2 equal to zero. For the second order RF metamodel in Eq. (12), the corresponding estimate is given by

$$\hat{r}^2_{2RF} = \frac{\left[\gamma_1\left(1-\frac{1}{q_2^2}\right)+\gamma_2 h_1^2\left(1-\frac{1}{q_2^4}\right)\right]\left(1+\gamma_1\frac{1}{q_3^2}h_1^2+\gamma_2\frac{1}{q_3^4}h_1^4\right)}{\left[\gamma_1\left(\frac{1}{q_2^2}-\frac{1}{q_3^2}\right)+\gamma_2 h_1^2\left(\frac{1}{q_2^4}-\frac{1}{q_3^4}\right)\right]\left(1+\gamma_1 h_1^2+\gamma_2 h_1^4\right)} \tag{27}$$

Setting γ_2 equal to zero produces the measure for the corresponding first order RF model, $\hat{r}^1_{2RF}$.

These consistency measures can be used in a fashion analogous to that proposed by Malkus and Webster [18]. It will be considered strong evidence that either of the methods is first order in h^2 and in its asymptotic range if r_1 is small with respect to 1 and $\hat{r}^1_2 \approx r_2$. Conversely, if r_1 is large and $\hat{r}^2_2 \approx r_2$, it will be considered strong evidence that the method is second order in h^2 and in its asymptotic range. Otherwise, it will be concluded that the analysis is indeterminate, meaning that the methods are not in the asymptotic range or possibly of higher order.

3. Numerical Examples

Several numerical examples are considered in this paper. Initially, a very simple problem is presented to illustrate the superior convergence properties of the rational function representation of the discretization error model. The second example deals with the prediction of the natural frequency of the third axial mode of vibration of a one dimensional prismatic bar which is constrained at one end.

3.1 Convergence Study for Simple Example

The function

$$y_h = 3 \cdot \left(\cos \frac{\pi}{2} x \right) e^{h^2} \tag{28}$$

will be considered as a simple representation of the possible effects of discretization on a system response. This might represent the solution produced by a finite element analysis. The extended metamodel formulations discussed in the previous section will be applied to estimate y_h and then extrapolated to their continuum estimates at $h = 0$. Quantitative variable x varies between –1 and 1 while the discretization variable h will take on three different values in the numerical experiments representing different mesh sizes. Thirty numerical experiments were generated by randomly varying x according to a modified Latin Hypercube centered at zero. The corresponding value of h was randomly selected from the three possible values used for the analysis.

The metamodel forms applied in this example are given by

$$\begin{aligned} y_{hRE} &= y(x,\beta)\left[1 + \alpha_1 h^2 + \alpha_2 h^4\right] \\ y_{hRF} &= y(x,\beta)\left[\frac{1}{1 + \gamma_1 h^2 + \gamma_2 h^4}\right] \end{aligned} \tag{29}$$

Note that the RF metamodel has no polynomial present in its numerator. This form was selected such that both of the metamodels in (29) have the same number of unknown coefficients in the discretization error, allowing direct comparison of the models. This form of the RF model is sometimes referred to as an Inverse Polynomial [20]. When expanded, the metamodels in Eq. (29) have the forms

$$\begin{aligned} y_{hRE} &= \beta_0 + \beta_1 x + \beta_2 x^2 + \alpha_1 h^2 + \alpha_{11} x h^2 + \alpha_{12} x^2 h^2 + \alpha_2 h^4 \\ y_{hRF} &= \beta_0 + \beta_1 x + \beta_2 x^2 - \gamma_1 y_h h^2 - \gamma_2 y_h h^4 \end{aligned} \tag{30}$$

Note that both models are second order in h^2, but the RE model possesses two more unknown coefficients than the RF metamodel due to the explicit coupling between the quantitative variable x and h^2. In contrast, the RF model form in Eq. (29) possesses this type of coupling without explicitly introducing new coefficients.

Two cases are considered for this example. In the first, the values of the discretization parameter are selected as $h_1 = 1.2$, $h_2 = 0.6$, $h_3 = 0.3$. This corresponds to the usual practice of doubling the mesh size between refinement analyses. Values of h were selected such that the numerical experiments were not performed in what would be expected as the asymptotic region.

Parameters q_2 and q_3 have values 2 and 4, respectively. Both first and second order metamodels in h^2 are considered. The first order models are derived from Eq. (29) by simply omitting terms proportional to h^4. Linear LS was used to estimate the RF and RE model coefficients. The estimate of the leading coefficient β_0, corresponding to the response at nominal *x* and zero mesh size, serves as a measure of the ability of the associated metamodel to accurately extrapolate to the continuum value of 3.0 at $h = 0$. Analysis results are presented in Table 2.

A first order RF model produces the extrapolated result $\hat{\beta}_0 = 3.23$ possessing an error of 7.67%. In general, the true value of 3.00 is not known, therefore, the consistency measures r_1 and r_2 must be applied to validate the accuracy of the extrapolated results. Note that r_1 cannot be computed until a second order metamodel is generated. However, r_2 can be immediately calculated using Eq. (25) resulting in the value 8.22. An estimate, $\hat{r}_2 = 14.59$, can be computed from the first order RF metamodel using Eq. (27). A lack of agreement between r_2 and its estimate, indicates that the result extrapolated from the first order RF model cannot be assumed to be accurate. A first order RE metamodel produced the extrapolated result $\hat{\beta}_0 = 2.33$ having an error of -22.33%. Equation (26) gives the corresponding estimate $\hat{r}_2 = 4.00$. Measure r_2 indicates that the extrapolated result cannot be accepted as an accurate estimate, which is consistent with the large amount of error that is actually present.

Second order metamodels were then investigated. The RF model produces the estimate $\hat{\beta}_0 = 2.96$. Measure r_1 can now be computed using Eq. (24) resulting in a value of -1.82, which indicates that the additional second order term is almost twice as large in magnitude as the first order term. Measure r_2 now has the value 7.95 compared with the value of 8.22 computed from the actual response data. Due to the facts that r_1 is not small and $\hat{r}_2 \approx r_2$, it can be assumed that the RF method is second order and in its asymptotic range, meaning that the extrapolated results can be accepted as accurate. This is consistent with the actual amount of error, -1.33%, present in the estimate. The RE model produced an estimate of $\hat{\beta}_0 = 2.77$ with $r_1 = 0.74$ and $\hat{r}_2 = 6.26$. The -23.86% error in $\hat{r}_2$ coupled with the relatively large value of r_1 indicates that the RE method is not second order and not in its asymptotic range. The estimate of $\hat{\beta}_0$ cannot be accepted as accurate, even though the actual error level of -7.67% might be accurate enough for some applications. Note that bad values of r_1 and $\hat{r}_2$ are necessary, but not sufficient, to conclude that the extrapolated result is inaccurate. Further details can be found in Ref. [18].

The second case considered for this simple example puts even greater demands on the extrapolation capabilities of the methods. The values of the discretization parameter are increased to $h_1 = 2.0$, $h_2 = 1.0$, $h_3 = 0.5$. Only second order models were considered. Table 2 shows a 2.00% error in the estimate of β_0 for the RF model, while there is a -283.67% errors in the corresponding RE estimate. The values listed for r_1 and $\hat{r}_2$ indicate that there is strong evidence that the RF method is second order and in its asymptotic range, while there is no such evidence for the RE method. This is consistent with the actual error levels and illustrates the superior extrapolation capability of the RF representation. In all of the cases listed, the RF discretization error model clearly outperforms the RE model in extrapolating to the continuum at $h = 0$. Note that the nonlinear Marquardt LS method was unable to improve on the initial linear LS estimate of the RF model coefficients, indicating that the RF model is close-to-linear in this region of parameter space.

3.2 Finite Element Bar Example

The proposed methods are now applied to a more realistic example. The natural frequency of the third axial mode of a one dimensional continuous prismatic bar, constrained at one end, is to be predicted using results based on finite element models. This example is based on the problem studied by Alvin [9]. The exact continuum solution in Hertz is given by the expression

$$y = \frac{5\sqrt{E/\rho}}{4L} \tag{31}$$

Three quantitative inputs are considered, including elastic modulus (x_1), mass density (x_2), and length of the bar (x_3). Numerical experiments using finite element models of the beam were generated using the Box-Behnken design in Table 1. The standard deviations of the quantitative inputs are taken as 1.0% of their mean values. The coded values of –1, 0, and 1 for the three quantitative inputs in Table 1 represent low, nominal, and high levels, respectively. The nominal value of the inputs corresponds to their expected values, while the high and low levels represent plus and minus two standard deviations. In the following computations, the nominal values of the quantitative inputs *E*, _, and *L*, correspond to 10^7 psi, 0.10 lb/in^3/g, and 16.0 in, respectively.

The fourth model input is the discretization parameter *h*. In general, *h* can be expressed as

$$h = \frac{1}{N^{1/p}} \tag{32}$$

where *N* is the number of elements in the finite element mesh and *p* is the spatial order of the elements [14]. In this example, elements are one dimensional, therefore, *h* is just the inverse of the number of elements in the mesh. In the case of the discretization variable *h*, values –1, 0, and 1 correspond to coarse, nominal, and fine meshes. The actual values of *h* given by Eq. (32) are used in the design matrix instead of the coded values listed in Table 1. In each of the following cases, a consistent mass distribution was used and the meshes were uniform for simplicity. It is believed that analogous results would be obtained for nonuniform meshes as considered by Alvin [9].

3.2.1 Case 1

The first case investigated uses a nominal mesh with 20 elements, h_2 =1/20. Employing the usual convention of halving and doubling the number of elements, the coarse and fine meshes have 10 and 40 elements with discretization parameter values of h_1 =1/10 and h_3 =1/40, respectively. This particular case is comparable to the one considered by Alvin [9]. Linear LS was used to fit both the RE model in Eq. (9) and the RF model in Eq. (13) to the response data obtained from the numerical experiments. The estimated model coefficients were tested for statistical significance at the 95% confidence level using the t-Test statistic [3]. All 15 coefficients in the RE model were found to be statistically significant while the four h dependent terms in the numerator of the RF representation were insignificant resulting in the reduced RF metamodel

$$y_{hRF} = [\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{33} x_3^2 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3]\left[\frac{1}{1+\gamma_0 h^2 + \gamma_1 h^4}\right] \quad (33)$$

This form of the discretization error is identical to the inverse polynomial form used in the simple convergence example of Section 3.1 in which α_1 was assumed to be zero.

Two measures of goodness for extrapolation capability are considered. The first is the estimate of the zero-intercept coefficient β_0 which represents the frequency corresponding to the nominal continuum model, 15,351.12 Hz. The results presented in Table 3 show that both the RE and RF metamodels are essentially exact in their predictions. In both cases, measure r_1 is small and $\hat{r}_2 \approx r_2$ indicating there is strong evidence that each of the methods is first order and in its asymptotic range.

One of the main goals of this work is to accurately extrapolate the discrete metamodel form to the continuum metamodel such that an accurate decoupled Monte Carlo analysis can be performed. Therefore, all the h-independent coefficients must be accurately estimated, not just β_0. One hundred random experiments were selected within the initial design region and applied to the exact relation given in Eq. (31). The estimated RE and RF metamodels were extrapolated to h = 0 and applied to the same 100 experiments. The second measure of goodness considered is the maximum percentage residual error for the 100 experiments. Table 3 indicates that the RF model is slightly better, but both models give very accurate estimates within the design region. However, it is important to remember that the RF model is able to achieve this level of accuracy using three less terms than the RE representation. As suggested earlier, simplicity is desired over generality in response surface analysis.

3.2.2 Case 2

The extrapolation capabilities of the RE and RF metamodels were then tested by using coarser meshes. In Case 2, the nominal mesh has only 6 elements, h_2 = 1/6, while the coarse and fine meshes correspond to

y insignificant, resulting in 13 terms in the RE metamodel. All the *h* dependent terms were retained. Linear LS was also applied to the RF model form. As in Case 1, all the *h* dependent terms in the numerator of the discretization error model were found to be statistically insignificant producing a reduced RF metamodel with 12 terms. The extrapolation performed in Case 1 was repeated with the results presented in Table 3. Percentage-wise, both metamodels accurately predict the nominal frequency for the continuum, but the RF metamodel is twice as accurate as the RE representation. With respect to the 100 random experiments within the design space, the RF model produced a residual error, 0.11%, that was less than half that of the RE model. In both cases, measure r_1 is not small and $\hat{r}_2 \approx r_2$ indicating there is strong evidence that each of the methods is second order and in its asymptotic range.

3.2.3 Case 3

Case 3 represents the most extreme case of extrapolation possible for the chosen example. The nominal mesh contains only 4 elements, while the coarse and fine meshes only contain 3 and 5 elements, respectively. In this case, the usual convention of halving and doubling the mesh is not followed. In an extreme case, this could be considered a perturbation of the nominal mesh. Linear LS was used to estimate each model and the same terms were found to be significant. The extrapolation results listed in Table 3 indicate that the RF representation is again more than twice as accurate as the RE model. As in Case 2, measure r_1 is not small and $\hat{r}_2 \approx r_2$ indicating strong evidence that each of the methods is second order and in its asymptotic range. An error of –1.57% in the prediction of the nominal continuum frequency and a residual error of 1.57% indicates that, even in this extreme case, the RF metamodel is an accurate predictor on the experiment design space for the continuum. The error measures are consistent with this observation. In an actual application, the estimate of coefficient β_0 can be used to estimate the discretization error present in a finite element mesh. For the refined mesh, the finite element model with nominal inputs predicts the frequency of 16,927.04 Hz. Using the RF estimate of β_0, the mesh error can be estimated as 12.04%. Note that in all three cases discussed, the Marquardt nonlinear LS method could not improve on the linear LS solution.

3.3 Decoupled Monte Carlo Analysis

The ultimate goal of the extended metamodel approaches presented in this report is to eliminate or at least quantify the effect of mesh discretization error on the results of nondeterministic analyses. Assuming each of the inputs satisfies a normal probability distribution, a Monte Carlo analysis was performed using the exact relation for the continuum frequency given by Eq. (31). The inputs were randomly sampled 100,000 times and the results used to compute the probability of failure, defined as the vibrational frequency being less than 15,000 Hz. In each of the cases discussed, the metamodels were extrapolated to the continuum approximation at $h = 0$ and applied to the 100,000 samples used in the exact formulation.

In Case 1, which used the most refined meshes, both the RE and RF metamodels accurately predict the mean frequency value and the probability of failure as listed in Table 4. The benefit of the RF model is that it uses 3 less terms. Case 2 uses coarser meshes and begins to exercise the extrapolation capabilities of each of the metamodel forms. The results presented in Table 4 indicate that the RF model is more than twice as accurate as the RE representation. But, while the mean frequency value is very accurately estimated, the percentage error in the estimated probability of failure is large, at 21.24%. This result agrees with Alvin's bar example observations that the accuracy of the estimate of the mean value must be extreme to be able to accurately estimate small magnitude failure probabilities. The accuracy of the extrapolated metamodels in Case 2 is illustrated in Fig. 1 in which the percentage error in the probability of failure estimate is plotted against the number of standard deviations that the failure criterion is away from the mean frequency. The RF metamodel is clearly superior as the failure criterion deviates below the mean. Above the mean value, both methods approach zero error. Case 3 uses the most coarse meshes possible (3, 4, and 5 elements) for metamodel estimation. Even in this extreme case, the RF model produced small residual errors over all 100,000 experiments and an accurate estimate of the mean frequency at –1.57% error as listed in Table 4. The RF model, once again, is better than twice as accurate as the RE representation, but the RF probability of failure estimate is very inaccurate, while the RE prediction is grossly in error for this extreme case of extrapolation.

4. Conclusions

A new method has been presented for extending response surface techniques to include the effects of finite element model mesh discretization errors. The method employs a rational function representation of the discretization error in parameter h rather than the power series representation used by the straightforward Richardson extrapolation technique. Consistency measures were introduced to test the method order and whether the method is in its asymptotic range. Examples dealing with simple function estimation and the estimation of the third axial vibration frequency of a one dimensional bar showed that the rational function representation gave more accurate extrapolated estimates using fewer terms than the Richardson extrapolation technique. In subsequent nondeterministic analyses used to estimate failure probabilities, the rational function based metamodel also produced more accurate estimates than Richardson extrapolation under severe extrapolation conditions. However, it was also shown that accurate estimates of small magnitude failure probabilities are difficult to obtain in cases of extreme extrapolation. Future work will address this problem.

While the rational function form of the discretization error produces a nonlinear model, requiring an iterative nonlinear least-squares solution technique, all the examples studied in this work proved to be close-to-linear, meaning that the linear least-squares estimate of the model coefficients could not be improved. It is believed that the rational function representation of the discretization error offers greater flexibility by allowing a user to accurately extrapolate to a continuum representation from numerical experiments performed outside of the asymptotic region where the usual power series representation is not converging. This allows the use of coarser meshes in the numerical experiments, saving a significant amount of time and effort.

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Table 1. Box-Behnken design for four input variables.

Runs	x1	x2	x3	x4
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

Table 2. Metamodel extrapolation results for simple function example.

Case 1. $h_1 = 1.2$, $h_2 = 0.6$, $h_3 = 0.3$

RF	$\hat{\beta}_0$	% Error	r_1	$\hat{r}_2$	r_2	% Error
First Order	3.23	7.67	----	14.59	8.22	77.49
Second Order	2.96	-1.33	-1.82	7.95	8.22	-3.28
RE						
First Order	2.33	-22.33	----	4.00	8.22	-51.34
Second Order	2.77	-7.67	0.74	6.26	8.22	-23.84

Case 2. $h_1 = 2.0$, $h_2 = 1.0$, $h_3 = 0.5$

RF						
Second Order	3.06	2.00	-35.19	35.17	36.17	-2.76
RE						
Second Order	-5.51	-283.67	3.79	10.51	36.17	-70.94

Table 3. Simple beam extrapolation results.

Case 1. $h_1 = 1/10,\ h_2 = 1/20,\ h_3 = 1/40$

	$\hat{\beta}_0$	% Error	r_1	$\hat{r}_2$	r_2	Max. Residual % Error
RF	15351.15	2.00e-4	-1.98e-2	4.02	4.02	6.00e-4
RE	15351.13	6.50e-5	5.97e-3	4.00	4.02	7.40e-4

Case 2. $h_1 = 1/3,\ h_2 = 1/6,\ h_3 = 1/12$

	$\hat{\beta}_0$	% Error	r_1	$\hat{r}_2$	r_2	Max. Residual % Error
RF	15334.93	-0.11	-0.55	2.38	2.38	0.11
RE	15319.67	-0.20	-0.38	2.38	2.38	0.27

Case 3. $h_1 = 1/3,\ h_2 = 1/4,\ h_3 = 1/5$

	$\hat{\beta}_0$	% Error	r_1	$\hat{r}_2$	r_2	Max. Residual % Error
RF	15110.19	-1.57	-0.62	0.92	0.92	1.57
RE	14841.28	-3.32	-0.49	0.92	0.92	3.63

Table 4. Nondeterministic beam analysis results.

Case 1. $h_1 = 1/10,\ h_2 = 1/20,\ h_3 = 1/40$

Method	Max. Residual % Error	Mean Value	% Error	% Probability of Failure	% Error
Continuum	0.00	15352.40	0.00	2.93	0.00
RF	8.2e-3	15352.43	2.0e-4	2.94	0.48
RE	1.0e-2	15352.43	2.0e-4	2.94	0.48

Case 2. $h_1 = 1/3,\ h_2 = 1/6,\ h_3 = 1/12$

Method	Max. Residual % Error	Mean Value	% Error	% Probability of Failure	% Error
Continuum	0.00	15354.22	0.00	2.84	0.00
RF	0.11	15338.04	-0.11	3.45	21.24
RE	0.31	15323.46	-0.20	4.44	56.11

Case 3. $h_1 = 1/3,\ h_2 = 1/4,\ h_3 = 1/5$

Method	Max. Residual % Error	Mean Value	% Error	% Probability of Failure	% Error
Continuum	0.00	15353.51	0.00	2.86	0.00
RF	1.58	15112.55	-1.57	27.36	856.30
RE	3.84	14844.51	-3.32	78.16	4886.10

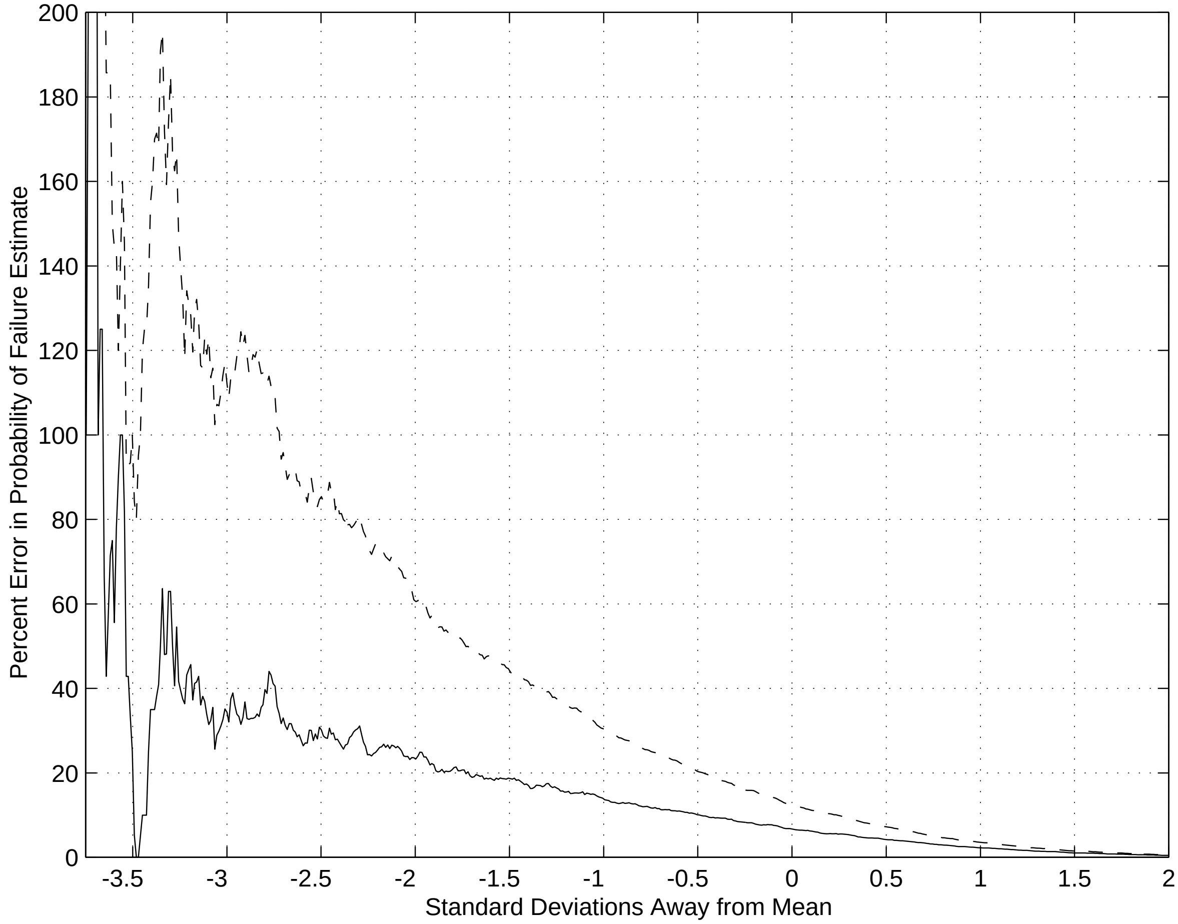

Figure 1. Case 2 probability of failure estimate errors. ----- RE metamodel, -------- RF metamodel