Parameterization of Large Variability using the Hyper-Dual Meta-Model

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Abstract. One major problem in the design of aerospace components is the nonlinear changes in the response due to a change in the geometry and material properties. Many of these components have small nominal values and any change can lead to a large variability. In order to characterize this large variability, traditional methods require either many simulation runs or the calculations of many higher order derivatives. Each of these paths requires a large amount of computational power to evaluate the response curve. In order to perform uncertainty quantification analysis, even more simulation runs are required. The hyper-dual meta-model is introduced and used to characterize the response curve with the use of basis functions. The information of the response is generated with the utilization of the hyper-dual step to determine the sensitivities at a few number of simulation runs to greatly enrich the response space. This paper shows the accuracy of this method for two different systems with parameterizations at different stages in the design analysis.

Key words. Hyper-Dual, HDM, PROM, Parameter Uncertainty, Surrogate Model

AMS subject classifications. 68-02, 68Q05, 68U07, 68U20

1. Motivation.

During the design phase of a product cycle, there are many engineering decisions that must be made. One of the most important decisions is the physical characteristics of the product, such as physical dimensions and materials. Some of these decisions are based on previous designs, available materials and equipment, and if the component will be combined with other products. Since these criteria can be a rough estimate on the design, the actual model can experience a large amount of variability. Another important consideration is the nominal values of the design and the other modeling choices, such as linear or nonlinear finite elements. For products used for the aerospace field, the typical nominal values, such as skin thickness, can be relatively small, which implies that any small change can have a large effect in the response.

In order to characterize this variability, typically a Taylor series expansion of the response is used with sensitivities determined using the finite difference approach. When the variability becomes larger, more derivatives are required to get an accurate representation. This requires more simulation evaluations and can result in high computational costs.

Once the response is clearly mapped, an uncertainty quantification (UQ) analysis is typically performed to determine the margin of safety or other reliability information due to the tolerances of the input parameters. This is normally performed with a Monte-Carlo (MC) propagation method. A MC analysis is performed by taking a random sample from the input distribution, such as physical distance or material property, and perform the simulation at that random input. These multiple simulation results produce a distribution on the output that can be analyzed based on statistics. A typically MC analysis uses on the order of $10,000$ random samples to produce an accurate distribution [25, 29].

As can be expected, this is a large computational cost. There are many methods available to reduce the computational burden of this design process. One commonly used reduction technique is to characterize the response due to an uncertain input by using a surrogate model or reduced order model (ROM). Typically, a surrogate model is a mathematical expression of the response and a ROM uses some physics of the system to reduce the size of the model. An example of a surrogate model is to use a Taylor series expression to characterize the response then to use the Taylor series in the MC analysis. The most commonly used ROM for structural dynamics is the Craig-Bampton ROM [7, 8, 20]. This ROM uses the modal information and the superposition of modes to reduce the system. Another commonly used reduction technique is to use a reduced sampling method such as latin hypercube sampling [18, 24, 26] that separates the distribution into equally probable sections and takes a single point from each section. This can be used independently

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or combined with the ROM/surrogate model to reduce the total computational time.

This paper presents a new method to characterize the response of the system due to a large variability in the input parameters, the Hyper-Dual Meta-Model (HDM). The main advantage that this method presents, compared to more traditional approaches, is the accuracy range for large variations by using the extra information of the derivatives, typically generated with the use of the hyper-dual (HD) step.

This paper is setup as follows: Section 2 describes several methods for determining the sensitivity of the output due to a change in the input including the HD step. In Section 3, the definition of the HDM in a general sense that uses very few simulation runs with the sensitivities at each simulation run is presented. Section 4 describes a couple methods of how to characterize the response by using different basis functions. Numerical examples are presented in Section 5. These examples include two different systems that are parameterized at different levels with varying complexity. Section 6 gives a discussion about the required future work to make this method more usable for a larger user set. Finally, some concluding remarks are presented in Section 7.

2. Determining Parameter Sensitivity.

The evaluation of the parameter sensitivity can be calculated via multiple methods. Each method has its own advantages and disadvantages. As can be informed by the naming of this method, HDM, the preferred method is the HD step. This allows for exact calculations where as the other methods are approximations. The methods explained in this section are not an exhaustive study of the techniques, but does give a general overview of the basic and most commonly used methods.

2.1. Finite Difference.

The simplest and most commonly used method for determining gradients is the finite difference approach. This is based on the Taylor series expansion about a design point. The Taylor series can be written as

$$f(x+h) = f(x) + hf'(x) + \frac{h^2 f''(x)}{2!} + \cdots + \frac{h^n f^{(n)}(x)}{n!} + \dots \tag{1}$$

where x is the design point, h is a perturbation from the design point, $f(.)$ is the functional such as a polynomial or finite element code, and $f^{(n)}(.)$ is the n^{th} derivative of the function. This infinite series can be truncated to give an approximation, but this introduces truncation error. The magnitude of this error varies based on the size of the perturbation and the order of the truncation.

The finite difference scheme uses this expansion at multiple perturbation points to estimate values of the derivatives. This assumes that the perturbation is small such that the series can be truncated. These multiple evaluations are then combined in a linear combination to eliminate the undesirable components of Equation 1. The linear combination of the evaluations introduces subtractive errors when the perturbation is small. Subtractive error is the error associated with the bit resolution of the computer. Since the computer can only store a set number of digits, for any two numbers that are very close in value, the computer interprets the numbers as the same and can result in a zero difference.

For a set number of function evaluations, the central difference methods tend to have the best accuracy. The first derivative using two function evaluations can be determined by

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + \mathcal{O}(h^2). \tag{2}$$

In Equation 2, the Taylor series is truncated to the second derivative. The notation of $\mathcal{O}(h^2)$ represents that the infinite series is truncated for terms that contain higher orders of the step size. Any term that contains h^3 or higher in Equation 1 is assumed to be small and is neglected. This determination only requires two function evaluations at $(x+h)$ and $(x-h)$. If more function evaluations are used, the truncation error can decrease. Since the derivative requires taking the difference of two different function evaluations, subtractive error is introduced when the step size becomes small. There is a trade-off between decreasing the truncation error and the subtractive error. This trend can be seen later in the comparison section.

Higher order derivatives can also be found with similar methods. By using higher order derivatives, larger steps in an optimization routine can be used and thus account for larger variability on the design parameters. A second order central difference for the second derivative can be calculated as

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + \mathcal{O}(h^2). \tag{3}$$

Using the HDM typically only uses up to the first two derivatives at each design point. Determining the coefficients for any arbitrary derivative with arbitrary order of truncation error can be calculated with the algorithm developed in [15]. This gives both the algorithm and the solution of the algorithm for the first four derivatives at several orders of truncation error for both central difference and directional difference.

This technique is straight forward and requires no special solver to determine the gradient of a functional. Current finite element codes, such as Ansys and Nastran, use this formulation to perform sensitivity analysis. While this method does not give the most accurate solution, it is a robust method that is simple to implement in current commercial finite element code.

2.2. Complex and Multi-Complex Step.

One way to eliminate the subtractive error that the finite difference approach introduces is to determine the gradient by using a single function evaluation. This can be accomplished by using a perturbation step in the non-real direction [22, 23]. By using an imaginary step, Equation 1 can be rewritten as

$$f(x+ih) = f(x) + ihf'(x) - \frac{h^2 f''(x)}{2!} + \cdots + \frac{(ih)^n f^n(x)}{n!} + \ldots \tag{4}$$

where i is the imaginary number defined as $i^2 = -1$. The determination of the first derivative can be calculated with a single function evaluation thus eliminating the subtractive error. There is still an induced error due to the truncation of the Taylor series. The first derivative can be calculated as

$$f'(x) = \frac{Imag[f(x+ih)]}{h} + \mathcal{O}(h^2). \tag{5}$$

The second derivative using the complex step introduces a subtractive error. This is due to the fact that the real component of the expansion contains both the nominal function value and the second derivative. In order to determine the second derivative without subtractive error, a more complicated expression is needed. With two function evaluations, the second derivative can be calculated as

$$f''(x) = \frac{2(f(x) - Real[f(x+ih)])}{h^2} + \mathcal{O}(h^2). \tag{6}$$

The multi-dimensional expansion of this complex step requires the use of multiple non-real components. This multi-dimensional expansion logically uses imaginary numbers, called quaternions. These quaternions can be characterized by three imaginary numbers: i, j, k. The imaginary numbers are defined by $i^2 = j^2 = k^2 = ijk = -1$. One important consideration is the relationship between these imaginary numbers. These are defined by two independent directions and a third dependent direction that is perpendicular to these imaginary directions and the real direction. The relationships between these are similar to unit vectors on a Cartesian coordinate system. This is one of the major problems with the use of quaternions. The multiplication of the imaginary numbers is not commutative. One realization of this problem is in the calculation of the second derivative. Due to this non commutative property, the second derivative is contained in the real part similarly to the complex step.

Another method of determining the higher order derivatives with complex numbers is with the use of multi-complex numbers. These are slightly different than quaternions and are able to produce higher derivatives will less error. The methodology was first introduced in [21] explaining the mathematics. Millwater has introduced this mathematics into a complex step analysis in [16] and into a time integrator in [17]. These multi-complex numbers are similar to HD in several aspects. They introduce independent imaginary numbers. While this is the same as quaternions, these are communicative such that $i_1 i_2 = i_2 i_1$. This simple difference allows for calculation of the second derivative to be calculated with a single code evaluation, which is impossible with quaternions. Using multi-complex numbers eliminates the subtractive error in the determination of the higher-order derivatives, but it still is subject to truncation error. Typically a step of 10^{-16} is used, but is still problem dependent and thus needs to be verified that truncation error is small. Using multi-complex numbers, it is possible to expand these into multiple dimension. The methodology is the same for both HD and multi-complex step; this is explained in the next section.

The use of the complex step allows for evaluation of the first derivative with a single function evaluation. This method, however, requires multiple function evaluations for the second derivative. With the single evaluation, the model solver must be able to handle complex numbers and the arithmetic associated with this. This may be difficult with some commercial software but is fairly simple with programs such as Matlab. The complex step still introduces truncation error and sometimes subtractive error. In order to calculate higher order derivatives with a single code evaluations, multi-complex numbers can be used. Multi-complex numbers are very similar to HD in the implementation, but are less accurate since there is still truncation error.

2.3. Hyper-Dual. The study of HD numbers originated in 2011 in [12]. It is used for optimization techniques in [11, 14] and further developed in [13]. The use in terms of finite elements along with substructuring is analyzed in [2, 5]. HD numbers are not specified to a certain number of non-real parts, but it is discussed similarly to the quaternions with two independent directions and one dependent direction. There is a clear possibility for expanding the method to more independent direction, but the programming is not as straight forward.

With the use of HD numbers, the Taylor series in Equation 1 becomes

$$f(x + h_1\epsilon_1 + h_2\epsilon_2 + 0\epsilon_{12}) = f(x) + h_1 f'(x)\epsilon_1 + h_2 f'(x)\epsilon_2 + h_1 h_2 f''(x)\epsilon_{12}, \tag{7}$$

where ϵ_k is an independent dual number and ϵ_{kl} is the dependent dual number with $\epsilon_k^2 = \epsilon_{kl}^2 = 0$. One main advantage of using HD numbers is the commutative property of these numbers. This property can be expressed as $\epsilon_1\epsilon_2 = \epsilon_2\epsilon_1 = \epsilon_{12}$. Using HD numbers for a single uncertain parameter allows for the determination of higher order derivatives. The first two derivatives can be determined as

$$f'(x) = \frac{\epsilon_1 Part[f(x + h_1\epsilon_1 + h_2\epsilon_2 + 0\epsilon_{12})]}{h_1} \tag{8}$$

$$f''(x) = \frac{\epsilon_{12} Part[f(x + h_1\epsilon_1 + h_2\epsilon_2 + 0\epsilon_{12})]}{h_1 h_2}. \tag{9}$$

These derivatives are by definition exact. There is no truncation error of the Taylor series and is not subject to subtractive error. One interesting aspect is that the accuracy of the derivative is not dependent on the step size due to the lack of truncation and subtractive errors.

With multiple uncertain inputs, the mathematics does not change within the simulation but does change what each component represents. For example, the ϵ_1 direction and ϵ_2 correspond to two different inputs and the ϵ_{12} direction corresponds to the correlation between the two inputs. The first derivatives of the two different inputs can be calculated with an input vector $\boldsymbol{x}$ as

$$\frac{\partial f(\boldsymbol{x})}{\partial x_i} = \frac{\epsilon_1 Part[f(\boldsymbol{x} + h_1\epsilon_1\boldsymbol{e_i} + h_2\epsilon_2\boldsymbol{e_j} + \boldsymbol{0}\epsilon_{12})]}{h_1} \tag{10}$$

$$\frac{\partial f(\boldsymbol{x})}{\partial x_j} = \frac{\epsilon_2 Part[f(\boldsymbol{x} + h_1\epsilon_1\boldsymbol{e_i} + h_2\epsilon_2\boldsymbol{e_j} + \boldsymbol{0}\epsilon_{12})]}{h_2} \tag{11}$$

where $\boldsymbol{e_i}$ is a vector of zeros with unity at the i^{th} input. This calculation is also able to determine the cross derivative as

$$\frac{\partial^2 f(\boldsymbol{x})}{\partial x_i \partial x_j} = \frac{\epsilon_{12} Part[f(\boldsymbol{x} + h_1\epsilon_1\boldsymbol{e_i} + h_2\epsilon_2\boldsymbol{e_j} + \boldsymbol{0}\epsilon_{12})]}{h_1 h_2}. \tag{12}$$

In order to calculate the second derivative with respect to a single uncertain parameter, the unit vector is set as $i = j$. Doing this transforms the cross derivative into the second derivative with respect to the input parameter. Extending this concept to more dimensions is not theoretically complex. This would only involve including more non-real dimensions, such as ϵ_3. Including this also involves programming the cross directions, ϵ_{13},ϵ_{23}, and ϵ_{123}. These extra directions increase the computational time and storage requirements to perform the calculations. The current programming is classified as either two or three independent dual numbers. Current research is being conducted to program an arbitrary number of independent dual numbers.

2.4. Comparison of Methods. Three different methods are explained in the section: finite difference, complex step, and HD step. Each of these methods has its own advantages and disadvantages. To compare these methods, the accuracy of the first derivative is analyzed. One of the main considerations of using any of these methods is the step size. For two of the methods, the Taylor series is truncated based on step size. This implies that the accuracy of the truncation is highly dependent on the magnitude of the step size.

To examine the error on the derivatives, a polynomial function is used. This choice allows for quick calculations and a known true value of the derivative. The polynomial is not a commonly used output function, but does show the trend and is able to show the trade-off between the truncation and subtractive errors along with the relative errors between the three methods. A normalized error is used and the error on the first derivative can be seen in Figure 1.

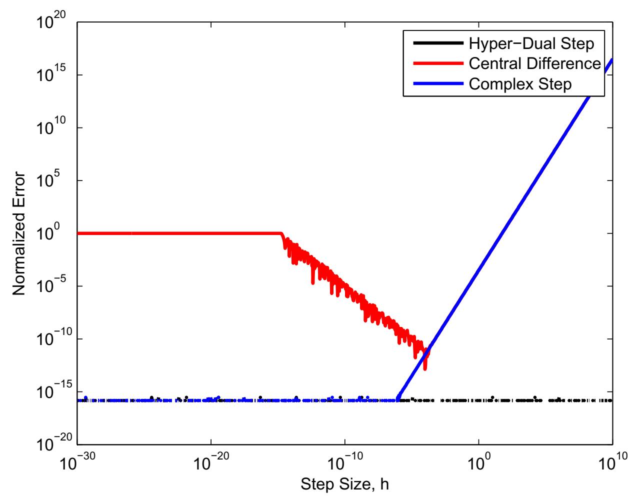

Figure 1: First Derivative Error as a Function of Step Size

The first trend is for step sizes of 10^{-4} or larger, the complex step and the central finite difference have the same errors that are predominantly caused by the truncation of the Taylor series. One important comparison is the accuracy of the HD step. The error is considered a numerical zero. Since the HD step is not subject to truncation error or subtractive error, the total error does not depend on step size and is numerically zero for every step size tested. Another important trend that is noticed is on the central finite difference. For large step sizes, the main error is the truncation error, but as the step size decreases, the main error is the subtractive error. If the step size is smaller than around 10^{-15}, the difference between the function evaluations are zero due to the bit resolution.

3. Hyper-Dual Meta-Model Formulation. The main motivation for this research is to create an accurate and inexpensive representation for the response of a system that undergoes a large change in the input parameters to be further used in sampling techniques such as MC or latin hypercube. One of the main uncertain inputs that causes a very nonlinear change in the response is a geometric variation, in particular for values that are small, such as in aerospace components. Typically, each change in geometric variation requires a re-computation of the finite element mesh. This requires a large amount of man-hours and computational power for each simulation run. Due to this, a numerical sampling method becomes computationally prohibitive.

The HDM uses the finite element code at a few selected values of the input variable. Along with the desired output, the information about the sensitivity of the output to the varied input is also needed. This sensitivity can be generated via many different methods. An in-depth discussion of the numerical derivatives is presented in Section 2. The main development is based on methods that determine the output and the sensitivities with a single code evaluation, such as the HD step [5]. For the analytical example that is presented in this section, the analytical derivatives are known via beam theory.

Once the output and the sensitivities are known, the HDM characterizes this data with the use of basis functions. These functions can be any function that matches the output and derivatives at all of the code evaluations. Some of the possible basis functions are discussed in Section 4. This selection can be based on a known relationship or as a simple mathematic function such as a polynomial. For the analytical example, a simple matrix polynomial is used.

Another important engineering decision is where to parameterize the model within the simulation. This is an important decision and is based on how the simulations are performed. If the geometry is complex and the analysis is simple, this parameterization is more effective at the system level, such as the mass and stiffness matrices. One important check when performing the parameterization at the system level, particularly for geometric variations, is to ensure that the degrees of freedom (DOF) are the same for each evaluation. This introduces a requirement that any geometric change does not change the number of nodes in the system and to enforce the same ordering of DOF within the matrix. The analytical example is parameterized at the stiffness matrix level. Another possible level of parameterization is at the output level. One major advantage of this parameterization is that the mesh for each simulation run can contain different number of DOFs depending on the output. This is important for large geometric variations that can change the system. One example is if a hole within the material that expands larger than the mesh size such that entire elements are removed from the model. A disadvantage of this is that the solver must be able to calculate the derivative. All solvers are able to calculate derivatives with a finite difference approach, but if a more accurate result is required, the solver must be able to perform in either multi-complex math or HD math. This parameterization is expected to be more accurate, but typically require special solvers. An independent analysis of this parameterization level was performed in [5]. The trends found from this analysis and the one in [5] are very similar.

3.1. Analytical Example. In order to show the core concept of this method, a simple analytical example of a cantilever beam is presented. This system can be seen in Figure 2. The variability expressed in this system is the total length of the beam and the desired result is the tip deflection due to a constant load P applied at the tip.

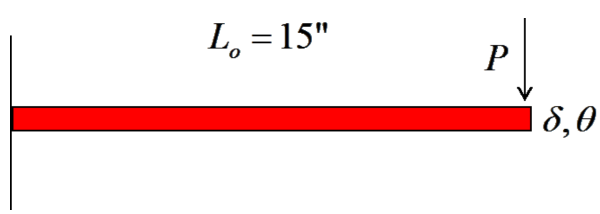

Figure 2: Example Cantilever System

Due to the simplicity of this system, an analytical expression for the tip displacement and rotation for a linear isotropic material is used. The tip deflection can be determined by

$$EI_x \begin{bmatrix} 12/L^3 & 6/L^2 \\ 6/L^2 & 4/L \end{bmatrix} \begin{pmatrix} \delta \\ \theta \end{pmatrix} = \begin{pmatrix} P \\ 0 \end{pmatrix}, \tag{13}$$

where E is the Young's modulus, I_x is the area moment of inertia, L is the length of the beam, δ is the tip deflection, and θ is the slope at the tip. This is thought of as a classic linear system of $KX = F$. Since the tip deflection is known analytically, the derivative with respect to the changing length is also known analytically.

This system contains an uncertain length of the beam. For this example, the beam length is described by the interval of $[10, 20]in$. Since the response is very nonlinear with respect to the length of the beam, along with the large variability, the traditional Taylor series expansion requires many higher order derivatives to be accurate. This leads to the implementation of the HDM. For this example, the stiffness matrix is evaluated at three different lengths, $10, 15, \&20in$, and the first derivatives are also calculated at each of those lengths. This information is used to determine the HDM using a polynomial fit that matches the stiffness matrix and the derivative at each length. The stiffness matrix is expressed as

$$K = K_0 + K_1\gamma + K_2\gamma^2 + K_3\gamma^3 + K_4\gamma^4 + K_5\gamma^5, \tag{14}$$

where K_i are matrix coefficients and γ is a non-dimensional length. This is defined as $\gamma = \frac{L-L_0}{5}$ for this system, such that the maximum and minimum have values of unity and negative unity respectively. The reason for this is for numerical conditioning used in order to determine the matrix coefficients. These are determined by solving the linear equation of

$$\begin{bmatrix} I & -I & I & -I & I & -I \\ I & 0 & 0 & 0 & 0 & 0 \\ I & I & I & I & I & I \\ 0 & I & -2I & 3I & -4I & 5I \\ 0 & I & 0 & 0 & 0 & 0 \\ 0 & I & 2I & 3I & 4I & 5I \end{bmatrix} \begin{bmatrix} K_0 \\ K_1 \\ K_2 \\ K_3 \\ K_4 \\ K_5 \end{bmatrix} = \begin{bmatrix} K(L_{-1}) \\ K(L_0) \\ K(L_1) \\ K'(L_{-1}) \\ K'(L_0) \\ K'(L_1) \end{bmatrix}, \tag{15}$$

with I being the identity matrix, K' being the derivative of the stiffness matrix with respect to the non-dimensional length γ, and L_γ is the length associated with the non-dimensional length γ.

The linear system in Equation 15 can then be solved for the unknown matrix coefficients. Those coefficients are used in Equation 14 for the stiffness matrix then used to determine the tip deflection and rotation at any given length. This method is compared to a traditional Taylor series with the first two derivatives used at the nominal length. The results are shown in Figure 3. This shows that the HDM very closely matches the truth data while the Taylor series is accurate close to the nominal length but becomes very inaccurate for large changes in length.

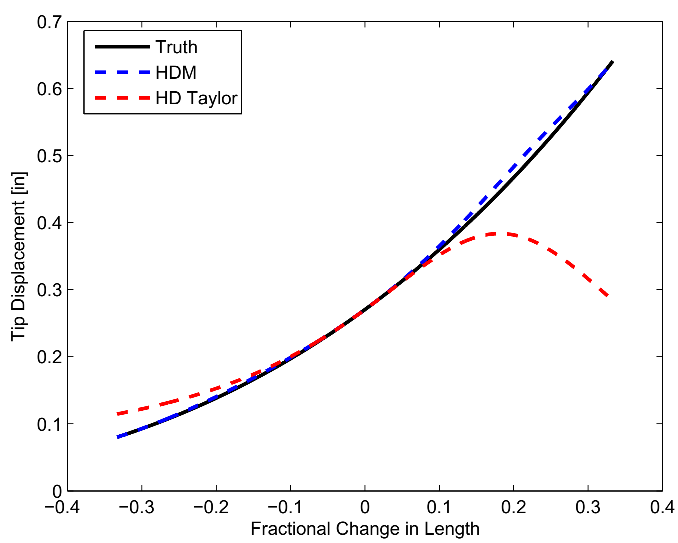

Figure 3: Tip Deflection as a Function of Length

4. Selection of Basis Function. One of major decision when using the HDM is what basis function(s) to use in the model. While there are many candidate functions, some are discussed here and two are implemented. The first basis function is the use of a polynomial function. This is a classic function that is simple to generate and evaluate. The current use of this polynomial is to match the data from the full simulation runs exactly. This forces the surrogate model to match both the nominal value and derivatives at each data point. Using this type of formulation increases the accuracy of the surrogate, but can require many unknown matrix coefficients. One simple example of how to use this polynomial is shown in Section 3 within the analytical example. Another interesting aspect of this example is the use a dimensionless parameter γ. The main reason for this is the numerical conditioning of the equations used to determine the matrix coefficients. If the uncertain parameter has a nominal value that is small, some numerical issues arise during the inversion of a large matrix when determining the coefficients.

The HDM presented in this paper uses the information from the high-fidelity model to generated a determined system, where the number of unknown coefficients and data is the same. This was performed to incorporate the information and be able to reproduce the results from the high-fidelity model exactly. One alternative to this approach is to utilize the higher order derivatives in a least squares sense, thus creating an overdetermined system. While this is possible, it is not currently implemented in the work presented in this paper. One advantage that using an overdetermined system provides is a much greater history of methods to determine the accuracy of the meta-model, such as regression metrics and maximum residuals.

While this formulation of a polynomial is simple, there are other possible basis functions to use. Another possible basis function is the use of orthogonal polynomials. There are many possible orthogonal polynomials, such as Legrange, Hermite, or Jacobi. This is similar to the formulation of polynomial chaos [30]. These would utilize a matrix coefficient for each polynomial to generate the HDM. Computationally, this would require more time for a single evaluation compared to previous use of polynomials, but can be more accurate. This formulation has not previously been implemented.

The previous basis functions are candidate functions that do not consider any information about the physics of the system. These can be used for any variable on any system. If some information about how the response changes with the uncertain input, this can be used to increase the accuracy of the model. One example of how this can be used is the interpolation function used by Epureanu in [19] for the stiffness matrix. This basis function can be used on the stiffness matrix for the case of geometric variation. The function used is based on a 8-node brick finite element, but the procedure can be used for other element types with a slightly different function. This function can be expressed as

$$K(p_0+\delta p)=\frac{K_0+K_1\delta p+K_2\delta p^2+K_3\delta p^3+K_4\delta p^4}{D(\delta p)}, \tag{16}$$

where K_i are unknown matrix coefficients, p is the unknown parameter, and $D(\delta p)$ can be expressed as

$$D(\delta p)=(1+\frac{\delta p}{p_0})(1+\frac{\delta p}{2p_0})(1+\frac{\delta p}{3p_0}). \tag{17}$$

This implementation uses five unknown matrix coefficients and requires at least five data points. The work done in [19] only applies this basis function for the stiffness matrix and a classic polynomial for the mass matrix. Useful incite into the physics of the system is able to give a much more accurate surrogate model. Even at a possible increase in computational requirement, the computational time is significantly less than that of the full system due to the possible re-meshing and new models to be generated at each desired thickness.

The functions discussed in this section are only a selected few candidate functions that are simple to use. These are by no means an extensive survey of functions, but show a couple examples of polynomial type of basis functions. Other possible classes of functions can be used. One example of this would be similar to a Fourier transform, where the response is described with the use of sine functions. Another class of functions would be that of splines or exponentials. These different classes of functions are not implemented but are feasible.

5. Numerical Examples. In order to evaluate this new surrogate model, two different systems are evaluated. Each system contains a different type of uncertain parameter. The study utilizes the results from a high-fidelity code named SIERRA SD [10, 28]. This is a code that is focused on parallel computing and has been implemented in select versions to be able to evaluate structural dynamics problems using HD numbers. The implementation of HD numbers into SIERRA is done at an object overload level. This replaces the simple arithmetic within the code to accommodate HD numbers. An alternative method to implement HD numbers in commercial code is to use a matrix notation for the HD number as a new element type. This notation has been partially implemented into Ansys by Millwater for multi-complex numbers [16]. The high-fidelity code simulations used in this paper were performed by Jeff Fike at Sandia National Labs.

The first system that this method is tested on is the Brake-Reuß beam [3, 6]. This system is a simple beam that contains a lap joint and can be seen in Figure 4. Another use of this system is to study a simple joint as a test bed specimen. For this analysis, the uncertain parameter is the Young's modulus, E, of the aluminum material. While the response follows an expected trend, a simple polynomial is used for the basis function. In this system, the natural frequencies are used for the interpolation. This study was originally used in [1] as a comparison of different parameterized ROMs.

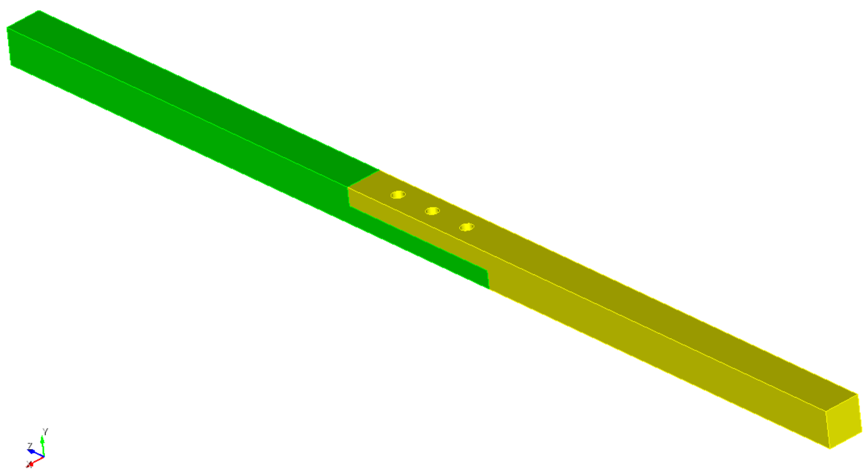

Figure 4: Brake-Reuß Beam Schematic

The second system is slightly more complicated, but contains a much more difficult uncertainty. Figure 5 shows the geometry of the plate for one of the used meshes. The height of the "bumps" is the uncertain parameter in this system. Due to known applications of similar type of panels, the height of this bump is bounded between 0 and $6mm$, but is not expected to experience this large of a design range.

Due to the geometric variations, some special considerations must be taken into account within the mesh. With the increase in volume, two possible options are available: increase element size, or increase the number of elements. Since the data for all possible heights are compared directly, the size of the elements at the bump is chosen to increase. The thickness of the panel is comprised of two brick elements. For the bump, one of those elements is fixed then the other is increased in size by moving the surface nodes. In this system, the sensitivities of the output to the height of the bump is computed with a HD step. Since the uncertain parameter is a geometric variable, the implementation of the HD step is not straight foreword. One method would be to write a program to recreate the geometry and mesh for each value of the geometric parameter. This is impracticable since the geometry generation is not typically simple. The current implementation generates the geometric location of the node points, then the HD step is implemented into the XYZ location of the changing nodes.

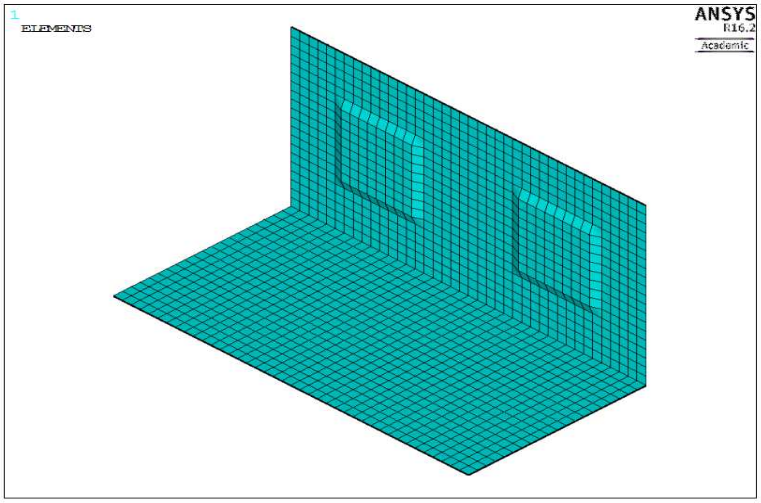

Figure 5: Paneling Schematic

5.1. Brake-Reuß, Beam. For this system, two different ranges of variability were used: one for small variability $E \in [60, 80]GPa$, and one for large variability $E \in [50, 300]GPa$. For both of these ranges, three code evaluations are used with up to the first three derivatives. Since this is the first practical application of the HDM, many engineering choices are explored. The two main choices that are explored are: location of evaluation points within the sample space, and the number of derivatives to use. These results are compared to a Taylor series expansion using the derivatives generated from the nominal HD step.

In order to evaluate the accuracy and cost savings of each range, a parameter sweep is performed. During this sweep, two main criteria are used: root-mean-squared (RMS) accuracy, and the computational time to perform the evaluation sweep. This type of validation check is important for new models, but it is not the only use of surrogate models. Another important use of this model is for a probability distribution propagation. With a specified distribution on the input parameters, either from experimental data or engineering knowledge, the output distribution is desired. This is particularly useful when attempting to determine a failure criteria, such as a natural frequency approaching the driving frequency, or the tensile stress reaching the yield or ultimate strength. In order to test the HDM against other surrogate models, this distribution propagation is performed on the large variability scenario.

5.1.1. Small Parameter Sweep. The first result is the small variability parameter sweep. This sweep is performed on the range of $E \in [60, 80]GPa$. The determination of this range was due to a believed Young's modulus of $70GPa$. This was proven incorrect as investigation of the Brake-ReußBeam continued, but does show interesting characteristics for poor choice of evaluation points and number of derivatives. One important thing to note about these points is that they do not span the sample space well. They are clustered about the expected value very closely.

In order to compare the HDM to typical surrogate models, another surrogate model and a truth curve are used. The truth curve is generated with the high-fidelity finite element code at increments in the modulus of $0.1GPa$; this process was automated for convenience. A surrogate model used as a comparison is based off of the Taylor series expansion. This model uses the information about the derivatives at the nominal point to setup the basis for the expansion. The model uses the HD step to calculate the derivatives at the nominal value. These derivatives are exact and therefore more accurate than a typical finite difference approach. The curves are presented in Figure 6 for the first natural frequency using only the first derivative information; these curves are shown as a difference between the surrogate models and the truth data. The vertical dotted lines represent where the code evaluations are used in the sample space to generate the HDM. This shows that the use of the HDM provides a larger range of accuracy compared to the traditional Taylor series.

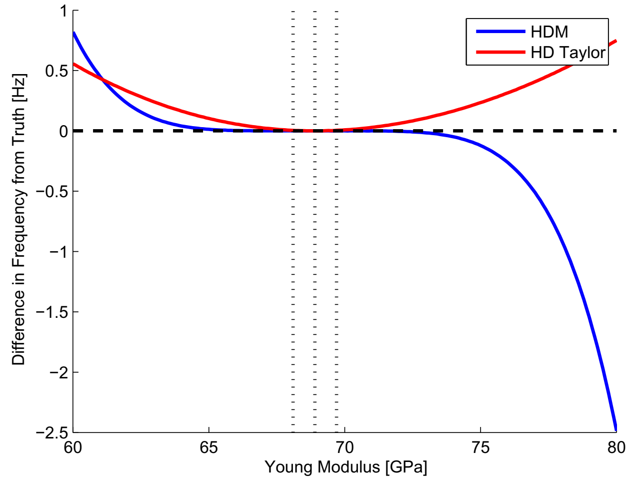

Figure 6: First Natural Frequency for Small Sweep with 1st Order Models

One of most interesting results for this small sweep comes when higher order models are used. The same first natural frequency can be seen in Figure 7. For the range where the modulus is outside the evaluation points used to determine the HDM, large extrapolation errors occur. This is primarily thought to be due to the order on the polynomial used for the basis function. As more data is used in the HDM generation, more coefficients are used and requires higher order polynomials. This can be classified as over-fitting of the data.

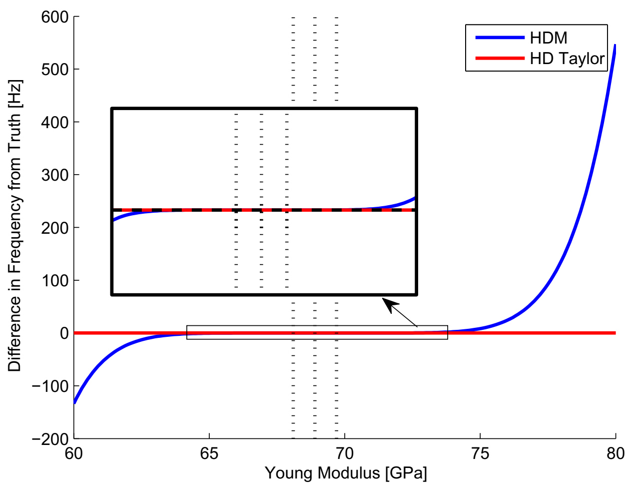

Figure 7: First Natural Frequency for Small Sweep with 2nd Order Models

While the qualitative results comparing the models and the truth data is useful, quantitative results are very useful to demonstrates which model is better over the entire range to the casual observer. This data is available in Table 1. The RMS errors takes into account each value of the Young's modulus for each of the first fourteen frequencies. Time is measured as the time to generate the parameter sweep curve after the model is generated. The time to generate the models are not measured, but the HDM takes more time to generate due to the matrix inversion and multiple code evaluations. This is thought of as a one time cost since the model can be used for both a parameter sweep to check the accuracy and to perform a MC analysis.

Table 1: Numerical Results of Accuracy and Speed

Order	RMS Error (HDM) [%]	RMS Error (HD) [%]	Time (HDM) [s]	Time (HD) [s]
1	0.73	0.12	0.90	14.97
2	3727.8	7.53E-2	0.65	11.56
3	Large	6.44E-4	0.64	11.77

While the actual equations used for both the HDM and the HD Taylor series are similar, there is a large time difference. There are a couple possible reasons for this difference. One possible explanation is the use of the factorial command used in the Taylor series that is not in the algorithm for the HDM. Another possible difference is how the information is stored and retrieved. The HD Taylor model stores both the natural frequencies and model shapes, including the derivatives. For the HDM, the mode shapes were not calculated since the required matrix inversion was too computationally expensive. There are approximately $63,000$ DOF in the model and thus would require the inversion of at least a $400,000$ by $400,000$ matrix for the first order HDM. This is believed to be the main difference by looking at the size of the file and the time to load in the file. When the information relating to the mode shapes is removed, the load in times are approximately the same.

This example is a good case where a method is used inappropriately. The HDM is a proposed interpolation type surrogate model. Therefore the evaluation points for the model should span a majority of the sample space. The Taylor series surrogate model is an extrapolation type model since it is based off of a single point. So to correctly compare these two methods, a new parameter sweep is performed.

5.1.2. Large Parameter Sweep. This new parameter sweep is performed on the range of $E \in [50, 300]$ GPa. One main difference between this sweep and the previous one is the location of the code evaluation. These new locations are close to edges of the sweep. This allows for an accurate comparison between the two surrogate models. After more investigation into the material of the beam, the nominal value of the Young's modulus is changed to $150GPa$ since the beam is physically made of aluminum. The values of simulation runs for the HDM is selected to be $[70, 150, 230]$ GPa. This is selected more on the lower end of the range but is centered about the nominal value and the HD Taylor series is selected at the nominal value. The first comparison for this sweep is the first natural frequency. This can be seen in Figure 8 along with the truth data. The HDM almost matches the truth data exactly except for at the large end of the range.

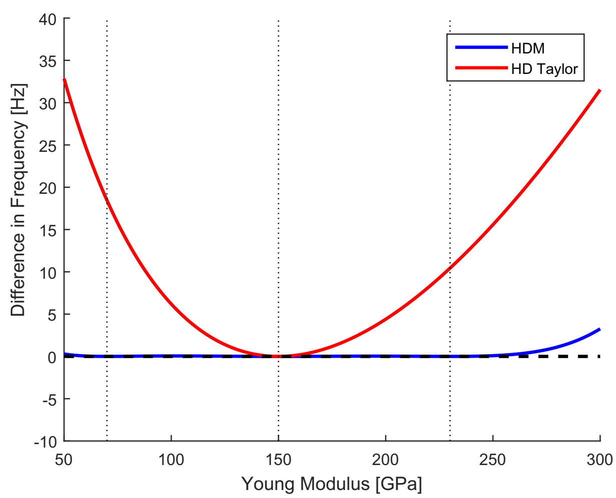

Figure 8: First Natural Frequency for Large Sweep with 1st Order Models

The same trend can be seen for higher order models and other natural frequencies and therefore not shown. Figure 8 also shows the location of the function evaluations. Since these are farther out to sample the entire space, the accuracy of the HDM has greatly increased compared to the small sweep. The accuracy is quantitatively given in Table 2. This shows that the second order model is the most accurate for the HDM. The over-fitting of the data for the higher order model creates a reduction in the model accuracy since there is some extrapolation of the model compared to the simulation runs.

Table 2: Numerical Results of Accuracy and Speed for Parameter Sweep

Order	RMS Error (HDM) [%]	RMS Error (HD) [%]	Time (HDM) [s]	Time (HD) [s]
1	0.1274	4.3038	0.26	32.07
2	0.0524	1.4877	0.20	33.94
3	0.2681	0.6712	0.21	36.31

These results, compared to the small sweep, show that the HDM is more accurate and requires less time to compute. This also shows that an intelligent selection of the evaluation points is required for the HDM to be the most effective.

5.1.3. Distribution Propagation. A parameter sweep, typically, is a preliminary analysis for validation and model calibration. Once the model is calibrated, the sensitivity to the calibration is desired, typically done by assigning a distribution to the input parameters and propagating those distributions to the output. This tells the design engineer an idea on the tolerances that need to be specified when production begins. Along with tolerances, this information can also be useful for failure analysis.

For this analysis, a simple MC sampling analysis is used. For convergence and accuracy, $100,000$ samples are selected. Along with the number of samples, the distributions can be determined either from experimental data or from engineering judgment. For this system, the Young's modulus is chosen to be a log-normal distribution. The main reason for this is that the log-normal distribution spans the same range as the Young's modulus. This distribution has a support of $(0, \infty)$ and can never reach zero. For the log-normal distribution, two parameters are required, the mean and the coefficient of variation. The mean is chosen to be $150GPa$ and the coefficient of variation is chosen to be 14%. This variability is chosen to fully test the range of the HDM that was shown to be accurate from the range of $[50, 300]GPa$.

One of the main choices in this type of analysis is what the output quantity is along with how to quantify the distribution of the output. For this section, the fundamental frequency is selected. Similar results can be seen for any of the first fourteen frequencies since the HDM and HD Taylor models are generated for each frequency independently, the performance of the model does not depend heavily on which natural frequency is selected since the parameterization occurs at the output level. If the HDM is applied at the system matrix level, this would not be the case.

In order to quantify the accuracy, two methods are reported: qualitative distribution, and quantitative information on the statistical moments. The qualitative distribution can be seen in Figure 9. The truth distribution is generated from a linear interpolation of the results from the parameter sweep using the same input samples as the other methods. By looking at the Figure 9, there is only a slight difference between the distributions. Since the difference is difficult to see, a point-by-point difference between the methods and the truth distribution can be seen in Figure 10.

The main take away from Figure 10 is that the HDM is almost perfect while the HD Taylor model varies from the truth data more in the lower frequency range. While the qualitative results are good for a visual interpretation, numerical results are very helpful. For this numerical result, the first four statistical moments are determined from the distribution and the RMS of those first four moments of the first fourteen natural frequencies is computed. These results can be seen in Table 3. This shows that the HDM provides nearly perfect results while only requiring about 1% of the time as compared to the HD Taylor model.

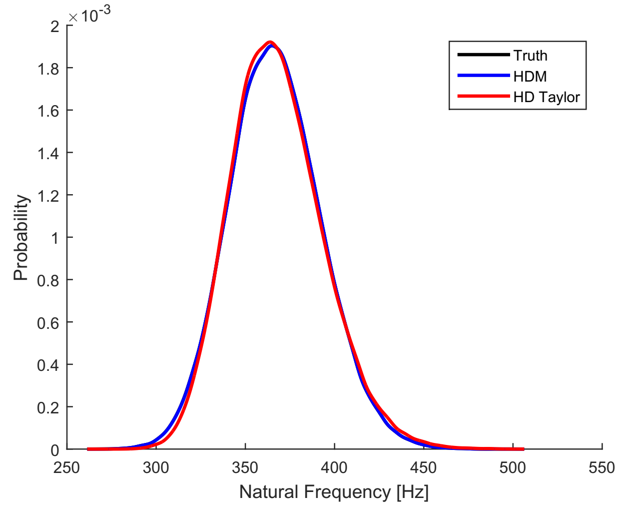

Figure 9: Distribution of the Fundamental Frequency

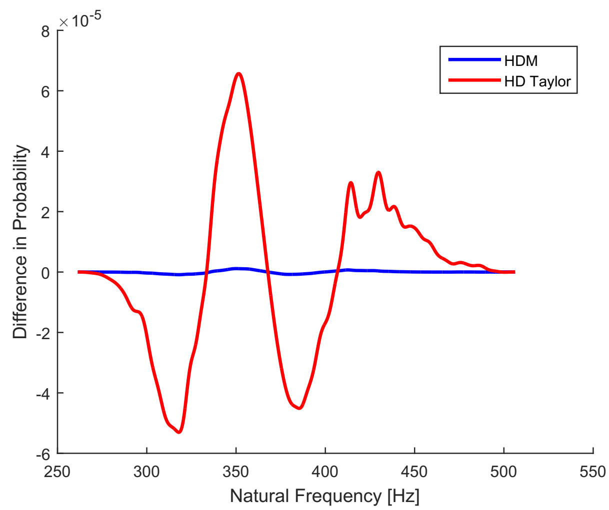

Figure 10: Point-by-Point Difference in PDF of the Fundamental Frequency

5.2. Paneling with Bump. The results of using the HDM for a material variation shows that the accuracy range of the surrogate model is much larger than that of the Taylor series approximation. Along with the increase in accuracy, a decrease in computational time is also seen for both a parameter sweep and a distribution propagation using MC methods. While a material variation is common, the output behaves in a predictable manner. In order to test the usability and robustness of this surrogate model, a geometric variation is desired.

In order to test this, the paneling is selected since it uses a large geometric variation with industrial applications. This system is shown in Figure 5 and the bump is expected to be anywhere between $0-6$mm in height. The bump is thought of as an extra deposit of material, such as from additive manufacturing. In order to model this, the HD step is implemented for the location of only the surface nodes. The change on element height affects both the stiffness and mass of the system.

The implementation of the HDM is tested with two different basis functions. These basis functions are: a simple polynomial and the interpolation function described in Section 4, which is denoted in this paper as 'NX'. Along with the two basis functions, the HDM is also implemented at both the system matrix and

Table 3: Numerical Results of Accuracy and Speed for Distribution Moments

Order	RMS Error (HDM) [%]	RMS Error (HD) [%]	Time (HDM) [s]	Time (HD) [s]
1	0.0089	0.6952	30.4	3697
2	0.0003	0.0318	30.9	3721
3	0.0003	0.0149	30.7	3765

the eigenvalue level. Since the NX basis function is designed for the stiffness matrix, it is only used for the system matrix level implementation.

In order to test out the design choices of using the HDM, two different evaluation sets are discussed: far point selection and near point selection. These sets are based on the assumption that the nominal value of the height of the bump is 3mm. For the far point selection, three data points are used at $[0, 3, 6]$mm. The near point selection uses data points at heights of $[1.5, 3, 4.5]$mm. This smaller variability will show a greater accuracy of the HDM.

When using the NX basis function, five pieces of information are required in order to determine the matrix coefficients. Since this is a physics based function, the data used should not affect the basis function. This was tested out using multiple combinations of data points and derivatives. While the results are not shown, all the combinations give the same results. Besides the stiffness matrix in the NX basis function, the mass matrix uses a simple polynomial.

In order to show the accuracy, two main outputs are selected to report. The first output is one element of the stiffness matrix. This is selected as a diagonal DOF that is effected by the change in the bump. To measure this accuracy, the system matrices are generated at many different values for the height of the bump and used as truth data. These are clustered around a small value in height since that has the most nonlinear behavior. This output is primarily used to show the accuracy of the polynomial fit along with the NX basis function. The second output is the fundamental frequency of the system. This frequency in around 175 Hz and is a bending mode of the system. Since this system is fixed along one edge, no extra treatment is needed for rigid body modes. This output primarily is used to visualize the difference between the parameterization levels. Looking at this data will show that, if applicable, the HDM should be applied as late in the analysis as possible. This is however not always possible since the HD numbers must be able to be used in the desired solvers. Simple solvers, such as eigenvalue/eigenvector, can easily be programmed with HD numbers, but this is more difficult for nonlinear vibration analysis and stress determination analysis.

5.2.1. Far Point Selection. The first analysis to report is the far point selection showing a diagonal term of the stiffness matrix. This result can be seen in Figure 11. The first thing to note is that using a polynomial fit for the stiffness matrix does not give a very accurate answer for this large of variability/ distance between data points. Along with this inaccuracy, the higher order polynomial also shows an over-fitting of the data.

There are five different plot in Figure 11. The red lines represent a simple polynomial basis function and the different dashing on it represent how many derivatives are used at each data point. The solid line represents using the nominal value and the first derivative at each data point, the dotted line represents using the nominal value and the first two derivatives, and the dashed line represents using the nominal value and the first three derivatives at each point. This shows an over-fitting of the data with the higher order polynomials, since the third order HDM has the largest error with height values that are far away from the data points used in the generation.

The other two lines represents when using the NX interpolation function. The green line represents when it is applied to the HDM, thus using three nominal values and two derivatives requiring only three simulation evaluations. Theoretically, the same information can be generated by a single code evaluation with the first four derivatives calculated, but not tested. Not shown here is a study of the selection of data points for the generation of the NX interpolation function. This study showed that the selection

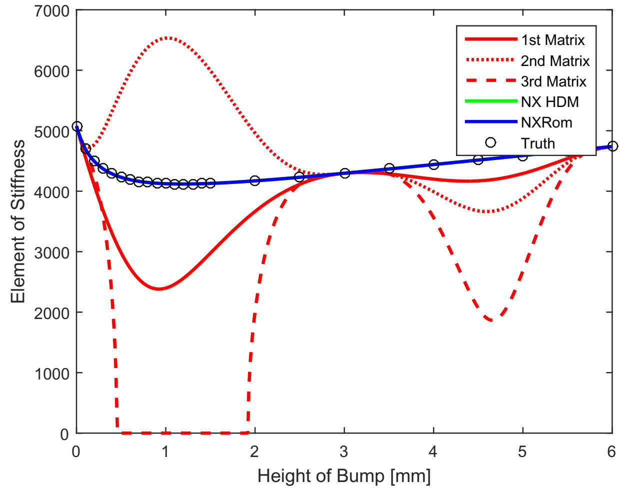

Figure 11: Diagonal Term of Stiffness Matrix

of the data points produced nearly identical matrix coefficients for the stiffness matrix. The blue line represents when you use five nominal value simulations. This requires more time since a total of five code evaluations are required where the green line only requires three. On this plot, there is no difference between these two models, but future plots will show some slight differences. The black dots represent the truth data generated from the full finite element model. Each of these simulations required several man-hours to remake the node locations at the variable portions while maintaining the same number of DOF and indexing of the node numbers.

The main desired output is how the fundamental frequency changes with the geometric variation. For the first result, the Eigen level parameterization is shown in Figure 12. This shows a similar analysis as performed on the Brake-Reuß beam in Section 5.1. The HDM is applied using the information at the output level since the Eigen analysis has theoretical derivatives that can be calculated using HD numbers. The result of the HDM gives almost exact results for the entire range. The dotted line represents using the first two derivatives at each evaluation point and gives a more accurate result than using just the first derivative.

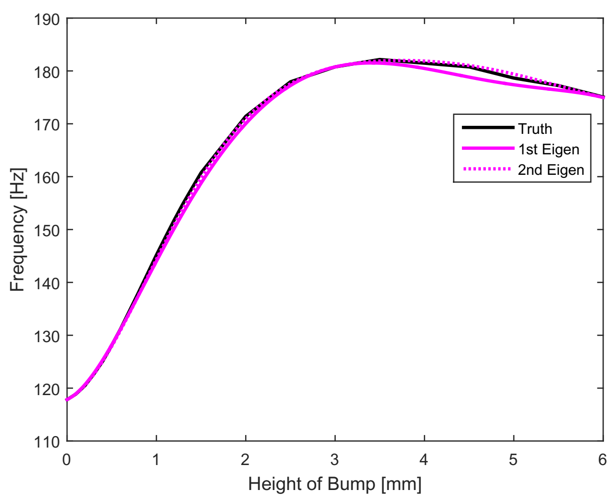

Figure 12: Fundamental Frequency with Far Point Selection with Eigen Parameterization

If parameterization is possible at the final result level, the HDM has shown to have very accurate results, but this is not always feasible. When parameterization must happen earlier in the analysis, the accuracy can decrease, and this result is shown in Figure 13. The first thing to notice is that using the matrix parameterization does not produce as accurate result as the Eigen parameterization. This can easily be seen by the difference between the red and black curves. One interesting aspect is that the fundamental frequency is exact for the evaluation points. This is due to how the HDM is derived, the stiffness and mass matrix are exact at each of those evaluation points. Due to this, the frequencies are also exact. When the height of the bump is not near an evaluation point however, the accuracy is very poor. This is believed to be caused by the distance between the evaluation points being too large for accurate results. Due to this realization, the near point evaluation is used to test this belief.

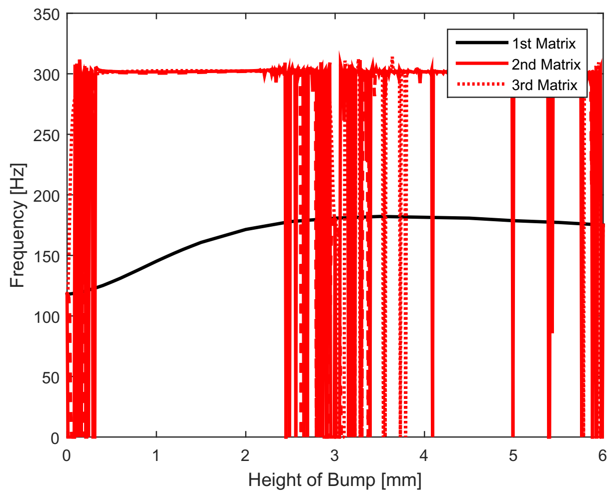

Figure 13: Fundamental Frequency with Far Point Selection with Matrix Parameterization

Along with the polynomial, the NX interpolation function is shown in Figure 14. This shows the best polynomial fit, the NX interpolation function in the HDM, and using the NX-PROM as it is originally derived. One of the most interesting aspects is that the NX-PROM and the NX HDM show different results. This is unique since the interpolation function is the same for both in terms of the stiffness and mass matrices. Another interesting aspect is the comparison between the polynomial fit and the NX HDM. While the NX HDM is not perfectly accurate, it is much more accurate compared to the polynomial fit. This leads to the thought that using a more realistic basis function allows for a larger variability compared to a generic polynomial fit.

For a large variability of a system, any selection of a PROM is a difficult choice. The most accurate solution for this large variability is to parameterize at the result level. This shows that the HDM is very accurate for the output parameterization. When the parameterization is performed at the system matrix level, the accuracy decreases due to the large change. Using a more physics based basis function can greatly increase the accuracy of these matrices for a given large range. The variability of $0-6$mm of the height of the bump is very large and is expected to be larger than the expected range. In order to more accurately test the expected range, the difference between the data points used to generate the HDM is reduced.

5.2.2. Near Point Selection. For the variability of $0-6$mm, the Eigen parameterization is accurate while the matrix parameterization is less accurate. Using a more physics based basis function gives a more accurate results as compared to a simple polynomial. In order to test the limit of variability when using a matrix parameterization, the variability is reduced to $1.5-4.5$mm. This range assumes that there is an expected bump, either by design or some malfunction.

For the far point selection, the design space was fully enclosed within the evaluation data points. When the variability is reduced, the simulations still use the full range of $0-6$mm. This shows how the HDM

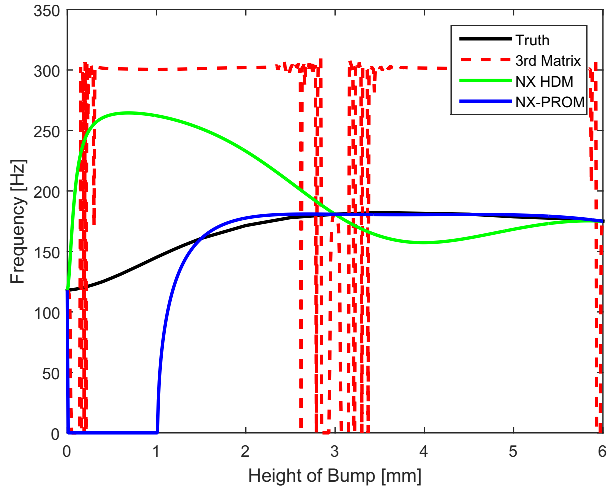

Figure 14: Fundamental Frequency with Far Point Selection with Matrix Parameterization with NX

predicts an extrapolation past the evaluation points. In Figure 15, the Eigen parameterization is shown. The accuracy within the evaluation points is almost perfect and the extrapolation is accurate when the second derivatives are used, and slightly less accurate when only using the first derivative.

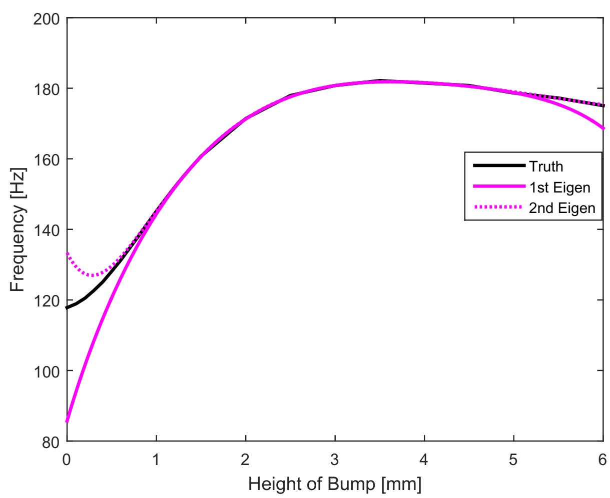

Figure 15: Fundamental Frequency with Near Point Selection with Eigen Parameterization

The far point selection showed that the Eigen parameterization is accurate for large variability. When the parameterization is performed at the system matrix level, the accuracy is much less for that large variability. Figure 16 shows the parameterization for the reduced variability at the matrix level. When using only the first derivatives, the HDM is not very accurate. However in this variability level, when the higher order derivatives are used, the accuracy becomes reasonable. This can especially be seen when the first three derivatives are used. For almost every point within the evaluation data points, the 3^{rd} order HDM produces very accurate results. The extrapolation however is not very accurate. This is due to the higher order polynomial used in the basis functions.

While the third order HDM is accurate, it requires a large amount of data collection, mainly the determination of 24 matrix coefficients (12 for stiffness and 12 for mass). One method to reduce the number of matrix coefficients is with a more accurate basis function. The accuracy comparison between

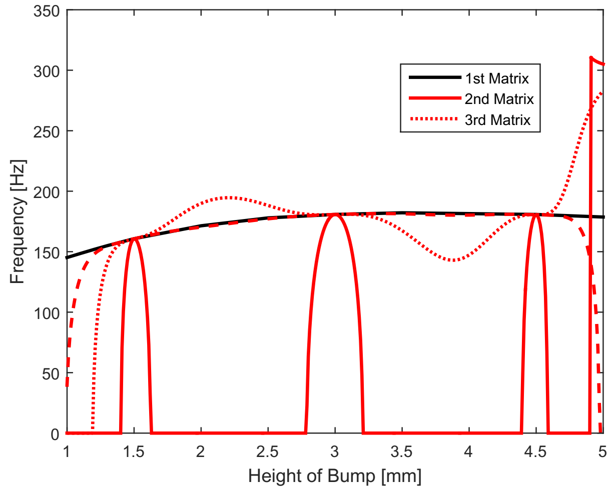

Figure 16: Fundamental Frequency with Near Point Selection with Matrix Parameterization

the polynomial basis and NX basis is shown in Figure 17 along with the same NX-PROM as presented in the previous section. When looking within the evaluation data points, the NX HDM and the third order HDM have nearly identical accuracy with the NX HDM only using 8 matrix coefficients (5 for stiffness and 3 for mass). Another major advantage is the extrapolation of the NX HDM since it remains accurate for a much larger range compared to the polynomial basis function. This is particularly true for larger bumps since the NX basis function is more accurate for larger deviations.

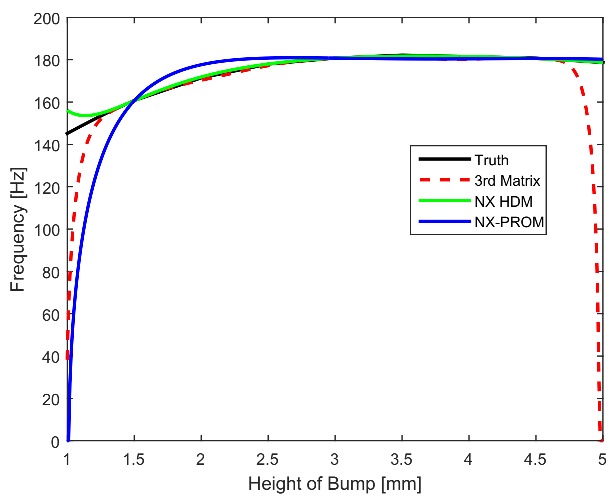

Figure 17: Fundamental Frequency with Near Point Selection with Matrix Parameterization with NX

The variability shown in this section is approximately the limit to the variability of the matrix parameterization. Using a simple polynomial required the use of the first three derivatives at each data point while the NX basis function only required the three nominal values and two first order derivatives with approximately the same accuracy. It is expected that a smaller range would require less information to be accurate. Further investigation is needed to find a general rule-of-thumb for the variability range for a given accuracy requirement.

6. Future Work.

As this is the preliminary utilization of the HDM, the authors have acknowledged three main aspects of future work to extend this method for the use of a larger user set: commercial implementation, completeness measure, and multi-dimension expansion. One of the major obstacles is the implementation of the HD step in large scale finite element programs, such as Ansys or Nastran. Currently, the HD step is primarily available in Matlab and Fortran. One large scale code that it is implemented in is the finite element code at Sandia National Laboratories. This implementation is limited to Eigen type problems. The code is also able to produce the mass and stiffness matrices of the system for further processing in Matlab. For ease of use, these matrices only contain displacement degrees of freedom with all the rotations statically reduced out.

In order to add the HD step into commercial codes, two possible implementations are possible. The first implementation is to create a new element type and perform calculation using a matrix representation of the HD step. This type of implementation has been performed for multi-complex numbers within Ansys by Millwater [27]. Using the multi-complex step maintains the symmetry of the matrices. For the HD step, the matrix representation is no longer symmetric. An advantage is that the matrix is lower triangular, so a forward substitution algorithm can be implemented. One unknown issue that might occur is for the matrix representation of a geometric variation. Current use of this matrix representation uses a parameter variation, such as a material property. An alternative methodology is to write new solvers that handle HD numbers. This requires the changing of the basic mathematics to HD evaluations [12]. These new solvers would be simpler to utilize in a program similar to Nastran or any non-GUI based codes. This would only require a simple change to the solver card. The implementation must be able to evaluate the algorithm based on the simple mathematics, such as multiply and add.

A discussion on possible methods to evaluate the convergence of the model is presented in Section 6.1. The discussion of the expansion to multiple uncertain parameters is in Section 6.2.

6.1. Data Point Selection.

One of the most important questions when performing a response surface method, such as HDM, is the completeness of the model. "Should the model include another data point or an extra derivative?" This questions is difficult to answer and typically requires expert engineering judgment. Some initial thoughts into showing the completeness of the model are discussed. The first idea of convergence is similar to an adaptive time step for numerical integration. One particular example of this is implemented in the IMEX time integrator [4]. This compares the result from a forth order and fifth order time step as in [9]. The results from each order is compared and if the difference between the two results is small, then that time step is stable. This can be modified for the HDM by removing one data point from the generation and recompute the desired results. Comparing these two results can give a good measure of the convergence of the model.

Another possible method to check for convergence is dependent of the basis function used. If a polynomial basis function is used, then comparing the matrix coefficients can give some insight into the convergence. The coefficient on the highest order polynomial gives a piece of information about the convergence. Some special consideration must be used since there is a unit mismatch, but can be normalized based on the nominal value of the parameter. An alternative approach would be to evaluate the model with neglecting the final term. Comparing these results is a simpler approach than trying to compare the different matrices since a scalar or a vector can used.

6.2. Expansion into Multiple Uncertain Variables.

The systems and examples shown in this paper only contain a single uncertain variable, either a material property or a geometric value. As a preliminary analysis, a single uncertain variable can show the usefulness of the new model. Expected applications of the HDM could involve multiple parameters, such as topology optimization. Due to this possible use of the HDM, this section discusses some of the expected difficulties and solutions due to this expansion.

The main consideration is the selection of data points. This selection is based on the dependence of the uncertain variables. If the input is independent, then the data points can be selected to vary each variable individually while keeping the other inputs at the nominal values. With this assumption, the basis function can be written as a superposition of the contribution of each input. For two independent variables, x and

y, the HDM can be written as

$$f(x, y) = f_o + g(x) + h(y), \tag{18}$$

where $f(x, y)$ is the parameterization, $g(x)$ is the basis function for the variable x, and $h(y)$ is the basis function for the variable y. Another advantage of independent inputs is that the cross derivatives do not have to be calculated. This simplifies the calculations and allows for less computational time in the model generation.

When the inputs are not independent, more consideration must be considered in both the data points and for the basis function(s). Depending on the order of the HDM, the information about the cross derivatives can be utilized. The implementation of this cross derivative information is dependent on the basis function(s) that are used. One possible solution is to treat the HDM as a product of individual basis functions. This is thought of as

$$f(x, y) = g(x) * h(y). \tag{19}$$

The selection of the data points for these dependent inputs is very complicated and can become computationally expensive. For a single variable, typically three data points are selected with first or second derivative information available at each data point. In a first order HDM, six pieces of information are used. An equivalent analysis for two uncertain parameters would require five data points and three pieces of information at each data point, totaling 15 pieces of information, and thus 15 unknown coefficients. If the cross derivative is incorporated, this implies 20 unknown coefficients.

Expansion of the HDM into multiple variables is conceptually possible. Doing this will require more engineering judgments and intuition. One of the main judgment is the location of the data points along with the basis function. These choices have a large effect on the computational requirements to determine the unknown coefficients and also the accuracy of the analysis.

7. Conclusions. In the design process, there can be a large variation due to optimization routines and tolerance propagation. One issue in this large variability is that a single reduced order model is not sufficient for accurate results. In order to increase this accuracy, the Hyper-Dual Meta-Model is introduced and demonstrated for a variety of situations. The HDM uses the exact derivatives from a code evaluation through the use of hyper-dual numbers, which is a multi-dimensional expansion of a generalized complex number. Using the HDM is useful for a system with large variability and size since it only requires a small amount of code evaluations to generate.

The HDM is introduced with an analytical example and demonstrated on two different finite element systems. For the first system, the material properties are varied to demonstrate a model calibration example. The second system contains a geometric variation that is much more nonlinear analysis. For the geometric variation, multiple ranges, basis functions, and parameterization levels are investigated. The most accurate HDM is the parameterization at the desired output values. This may not possible since the analysis solver needs to be able to calculate the result with HD numbers. When this is not possible, the parameterization at the system matrices can still produce an accurate result, but has a smaller range of accuracy. Using a more physics based basis function allows for a large accuracy range without the risk of over-fitting the data, which can be seen with the use of a simple polynomial.

The HDM is a novel surrogate model that greatly expands the accuracy range of the Taylor series with the increased accuracy of using the HD step as compared to the finite difference. This is a great reduction for geometric variations since only a limited number of meshes need to be generated, where traditional methods can require a large amount of man-hours to generate a large amount of meshes, thus making the analysis infeasible. The HDM produces more accurate results for a fraction of the computational cost for large geometric variation.

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