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DRAFT: FULLY PARAMETERIZED REDUCED ORDER MODELS USING HYPER-DUAL NUMBERS AND COMPONENT MODE SYNTHESIS

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ABSTRACT

The uncertainty of a system is usually quantified with the use of sampling methods such as Monte-Carlo or Latin hypercube sampling. These sampling methods require many computations of the model and may include re-meshing. The re-solving of the model is a very large computational burden. One way to greatly reduce this computational burden is to use a parameterized reduced order model. This is a model that contains the sensitives of the desired results with respect to changing parameters such as Young's modulus. The typical method of computing these sensitives is the use of finite difference technique which gives an approximation that is subject to truncation error and subtractive cancellation due to the precision of the computer. One way of eliminating this error is to use Hyper-Dual numbers, which are able to generate exact sensitives that are not subject to the precision of the computer. This paper uses the concept of Hyper-Dual numbers to parameterize a system that is composed of two substructures in the form of Craig-Bampton substructure representations, and combine them using component mode synthesis. The synthesis transformations using other techniques require the use of a nominal transformation while this approach allows for exact transformations when a perturbation is applied. This paper presents this technique for a planar motion frame and compares the use and accuracy of the approach against the true full system. This is the preliminary work in performing a component mode synthesis using Hyper-Dual numbers.

1 Introduction

In order for designers to overcome the variability in a design due to manufacturing tolerances and unknown loads, the uncertainty and sensitivity of the design must be evaluated. The sensitivity analysis is typically the preliminary step in an uncertainty quantification analysis. There are multiple ways to get the sensitivity of the system that is used: predominately finite difference and complex step [1]. Both of these methods have some major drawbacks which will be discussed along with an expected solution to each of these drawbacks by the use of Hyper-Dual numbers.

One problem that all sensitivity and uncertainty quantification analyzes experience is the curse of dimensionality. As computers and super-computers get faster and better every year, the finite element (FE) models are becoming more complex with higher fidelity. This causes many troubles for the transfer of information along with different techniques such as sub-structuring which require multiple models combined together. One way to reduce the dimensionality of the model is to use a reduced order model (ROM) such as a Craig-Bampton representation. This representation contains modal degrees of freedom (DOF) for the interior of the model and physical DOF for the interface where the model is expected to be connected to another model [2]. This can greatly reduce the size of a model due to the independence of the modal DOF in the system which can be truncated based of expected load range or experimental resolution.

While ROMs are good at reducing the size of the model, this can still produce a problem for the uncertainty quantification

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analysis. This ROM does not contain any information about how the model will change due to a change in a parameter. This brings about the use of parameterized reduced order models (PROMs) which contain the information about the sensitives [3]. These PROMs can allow the uncertainty quantification to be performed at a much lower computational cost since the entire model is no longer required and small variations can be accounted for with perturbation theory.

This paper is structured as follows: Section 2 explains how to determine the sensitives using multiple methods while presenting the use of Hyper-Dual numbers to get exact sensitives with only a single computational evaluation. Section 3 describes the Craig-Bampton substructure representation used to generate the PROM. Section 4 shows an example of a planar frame with an appendage that is separated into two substructures and then resynthesized and compared to the true solution. This section also includes a preliminary sensitivity analysis by using PROMs and comparing to the true perturbed solution. Section 5 summarizes the results and describes the planned future work in this field of research.

2 Determining Sensitivities

The most common way to determine the sensitivity of the system to a parameter is to use a finite difference approach. The finite difference method requires multiple calculations of the system's FE model. As the size of the models increase to produce more accurate results, the time required for a single calculation becomes very large and multiple calculations can take an impractical amount of time and computational effort. Along with the computational effort, the accuracy of the results must also be taken into account. The order of the finite difference method used determines the accuracy of the solution, which will never be exact. For the first derivative, a 1^{st} order scheme requires 2 evaluations of the FE model and a 2^{nd} order scheme requires 3 evaluations.

While the finite difference methods can take multiple computations, the complex step method was developed in order to determine sensitivities with only a single calculation [4]. This calculation now involves performing complex calculations that takes longer per calculation but overall requires much less computational time compared to the finite difference methods. The complex step method however is only a second order approximation since it truncates the Taylor series at the second derivative [4]. This method eliminates the rounding error due to the computer bit size, but no matter the step size, the complex step is still an approximation since the Taylor series is truncated. A way to eliminate this approximation is with the use of a generalized complex number, the dual number.

The dual number is a non-real number that is in a perpendicular direction than the real axis, much like a complex number. The main difference comes in how the square is defined. For a complex number, the complex variable, i, is defined as $i^2 = -1$, while for a dual number, the complex variable, e, is defined as $e^2 = 0$ but $e \neq 0$. This is useful, for example, when considering a first order Taylor series expansion. All of the higher order terms contain at least e^2 and are therefor zero. This shows that using a dual number step instead of a regular complex step will give the solution along with the exact sensitivity with only a single calculation [1].

A dual number is only able to extract a single first order sensitivity of the solution. In order to produce multiple sensitivities, a multi-dimensional generalization is used, which is called a Hyper-Dual number [1]. This higher dimensional dual numbers is similar to the higher dimensional complex numbers, which are called quaternions [1]. Each step is thought of as a movement in a mutually perpendicular direction with respect to the other steps and the real domain. The Hyper-Dual numbers that are used in this paper contain two independent directions and a cross direction which are represented by the variables e_1, e_2, and e_{12} respectably. For a more detailed presentation on how to perform these calculations both analytically and numerically, the reader is referred to [1] while a short review is given below. For the most part, Hyper-Dual numbers act mathematically similar to complex variables with some added simplifications. For example, the commutative property $e_1 \times e_2 = e_2 \times e_1 = e_{12}$. This property is not shared with quaternions, which makes the use of Hyper-Dual numbers simple since the order of multiplication does not affect the sign of the result. The main advantage of Hyper-Dual numbers is based on a Taylor series expansion. A n^{th} order Taylor series for a single parameter x close to a nominal value a is given by Eq. 1.

$$f(x) = f(a) + f'(a)(x-a) + \frac{1}{2!}f''(a)(x-a)^2 + \cdots + \frac{1}{n!}f^n(a)(x-a)^n \tag{1}$$

This series is subject to truncation and subtractive cancellation errors since the Taylor series is an infinite series. The use of Hyper-Dual numbers eliminates these errors. If the variable x is designated a Hyper-Dual number of the form of Eq. 2, then the Taylor series expansion becomes of the form in Eq. 3.

$$x = a + h_1 e_1 + h_2 e_2 + 0 e_{12} \tag{2}$$

$$f(x) = f(a) + h_1 f'(a) e_1 + h_2 f'(a) e_2 + h_1 h_2 f''(a) e_{12} \tag{3}$$

By the definition of Hyper-Dual numbers, all the higher order terms are zero. The first derivative of the function at point a can be determined exactly by taking the coefficient of e_1 then

dividing by h_1. With a similar computation, the second derivative can be determined exactly by dividing the e_{12} coefficient by $h_1 h_2$. This can be generalized for multiple parameters. The first derivative can be determined by Eq. 4

$$\frac{\partial f(\mathbf{x})}{\partial x_i} = \frac{e_1 part(f(\mathbf{x} + he_1\mathbf{e_i} + ge_2\mathbf{e_j} + 0e_{12}\mathbf{e_{ij}}))}{h} \tag{4}$$

where f is the output functional such as the natural frequency or mode shape, $\mathbf{x}$ is a vector of nominal parameter values, $\mathbf{e_i}$ is a unit vector in non-real space that is spanned by the perturbed parameter. The cross derivative or the second derivative can be found in a similar way. This can be calculated based on Eq. 5. Any higher order derivatives can be determined in a similar way but with additional non-real variables, such as e_3.

$$\frac{\partial^2 f(\mathbf{x})}{\partial x_i \partial x_j} = \frac{e_{12} part(f(\mathbf{x} + he_1\mathbf{e_i} + ge_2\mathbf{e_j} + 0e_{12}\mathbf{e_{ij}}))}{hg} \tag{5}$$

The use of Hyper-Dual numbers can be implemented at several different levels of a calculation. This example uses Hyper-Dual numbers at the very beginning of the problem, the creation of the mass and stiffness matrices from the FE model. A non-real perturbation is applied to a model parameter and the rest of the calculations are performed with the perturbation already built into the system. Using this method produces all values in terms of Hyper-Dual numbers. This process however takes some extra computational effort using functions such as an eigenvector solver and taking the inverse of a matrix of Hyper-Dual numbers. For this example, a class is created in Matlab which performs all the special operations automatically. Once this is done, the same functions that perform the sub-structuring analysis with real numbers are used and requires only minor changes. This is helpful if functions that are going to be used are already created and verified. Using Hyper-Dual numbers does not affect the results of these functions with the added benefit of be able to produce extra information. The real part of the Hyper-Dual number is the same as if the calculation is performed with only real numbers. Besides applying a non-real step at the generation of the system, the Hyper-Dual number can be formulated analytically with just using real numbers and by determining the sensitivities analytically based on the specific FE or result. This can be done for simple cases but can become impossible with any small complexity in the model.

With the information about the sensitives, an uncertainty quantification analysis or an optimization analysis can be performed. This paper addresses uncertainty quantification by using Hyper-Dual numbers. Other research is taking place on the use of Hyper-Dual numbers in an optimization. For more information about using Hyper-Dual numbers in an optimization, the reader is referred to [5]. Hyper-Dual numbers can require less computational time to perform either of these analyzes compared to other methods.

3 Reduced Order Model Representation

In order to produce a PROM, a ROM must be selected. For this paper, the Craig-Bampton substructure representation is used. The Craig-Bampton substructure representation uses a mixed coordinate system that uses physical interface DOF and modal interior DOF which can be truncated due to the independence of the modes [2]. The transformation from physical substructure coordinates to Craig-Bampton coordinates is shown in Eq. 6

$$\begin{bmatrix} u_i \\ u_j \end{bmatrix} = \begin{bmatrix} \Phi_k & \Psi \\ 0 & I \end{bmatrix} \begin{bmatrix} \eta \\ u_j \end{bmatrix} \tag{6}$$

where u is the physical displacement vector, subscript i refers to the interior partition of the DOF, subscript j refers to the interface partition of the DOF, Φ_k is the fixed-interface mode matrix truncated to the desired range based on frequency or importance, 0 is a zero matrix, I is an identity matrix, Ψ is a matrix of constraint modes describing the deflection of the substructure interior due to a unit deflection in the interface, and η represent the modal DOF of the fixed-interface substructure. The constraint modes are determined using the partitioned stiffness matrix as shown in Eq. 7

$$\Psi = -K_{ii}^{-1} K_{ij} \tag{7}$$

where K_{ii} is the partition of the stiffness matrix corresponding to the interior DOF and K_{ij} is the partition of the stiffness matrix corresponding to the coupling of the interface and interior DOF. This process is performed for each substructure. The substructures are then combined to determine the system matrices. This recombination can be seen in Eq. 8

$$\begin{bmatrix} \eta^\alpha \\ u_j^\alpha \\ \eta^\beta \\ u_j^\beta \end{bmatrix} = \begin{bmatrix} I & 0 & 0 \\ 0 & 0 & I \\ 0 & I & 0 \\ 0 & 0 & I \end{bmatrix} \begin{bmatrix} \eta^\alpha \\ \eta^\beta \\ u_j \end{bmatrix} \tag{8}$$

where the superscript α corresponds to the first substructure and the superscript β corresponds to the second substructure. This synthesis enforces equal displacements at the interface, $u_j^\alpha = u_j^\beta$.

4 Applied Example Problem

The use of Hyper-Dual numbers in sub-structuring is investigated using an example that shows some complexity while being simple enough that a truth model can be used as a verification. This example is a frame with an appendage. The frame is constrained to planar motion. The full system can be seen in Fig. 1. The full system is split into two substructures with repeated nodes that are identified by the red nodes in Fig. 1.

This system has some unique characteristics that adds a level of complexity to the system. One complexity is that the cross-sectional area of the frame is not constant. The cross-section of the left substructure is a $1.0\ in^2$ square while the substructure on the right has a cross-section of a $0.75\ in^2$ rectangle with the same width as the left section. Since the cross-sections are different, this frame can be unbalanced if this structure were to be experimented upon.

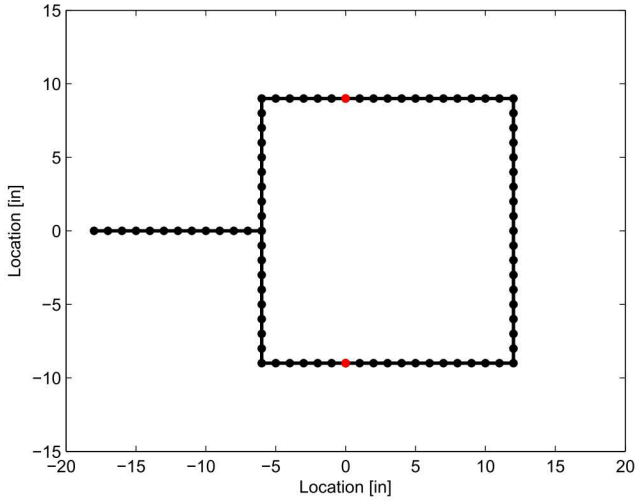

FIGURE 1. Example system finite element model

For each substructure, the red nodes are defined as the interface nodes, each possessing two translations and one rotation, totaling six interface DOF due to constrained planar motion. Finite elements are represented by Euler beams. The interior physical DOF are transformed into fixed-interface modal DOF. This example keeps all substructure modes up to 500 Hz. This results in nine modes for each sub-structure that include three rigid-body modes, which produces a dramatic reduction from 129 DOF to 15 DOF. Since this is a simple example, there is not much computational effort required to analyze the full system, but this example shows the usefulness of the technique.

The mass and stiffness matrices for each substructure are generated as Hyper-Dual numbers. In order to do this, uncertain model parameters must be defined. For this example, two different parameters are used: Young's modulus and mass density. Due to the implementation within Matlab, a single evaluation of the FE code can only produce a single second derivative, so the code is evaluated twice, once for Young's modulus and another for the mass density. The 2^{nd} order perturbation analysis requires the second derivative which can be determined based on the e_{12} term of the Hyper-Dual number. For a 1^{st} oder perturbation analysis, only the e_1 or the e_2 value of the Hyper-Dual number depending on how each one of those is defined. In order to do this, a non-real step is taken. For the evaluation of the Young's modulus, the Young's modulus is defined as in Eq. 9

$$E = E_o + 1e_1 + 1e_2 + 0e_{12} \tag{9}$$

where E is the Young's modulus and E_o is the nominal value of the Young's modulus. With this redefinition, the substructure model matrices are determined. By using Hyper-Dual numbers, the mass matrix takes the form of Eq. 10

$$[M] = [M_o] + \frac{\partial [M_o]}{\partial E} e_1 + \frac{\partial [M_o]}{\partial E} e_2 + \frac{\partial^2 [M_o]}{\partial E^2} e_{12} \tag{10}$$

where $[M]$ is the mass matrix and $[M_0]$ is the nominal mass matrix. This is the same form that the stiffness and damping matrices take. Since the non-real step was a value of 1, then no extra calculations are required to determine the sensitivities. These matrices are then transformed into a Craig-Bampton substructure representation and then synthesized together. This synthesized system is then compared to the system as fully constructed in the FE code.

The first result for this example is a perturbation of the Young's modulus. The first system elastic natural frequency as a function of the change in the Young's modulus is shown in Fig. 2. This shows three different curves, the black curve is the truth data, the red curve is for a 1^{st} order Taylor series expansion that only uses the first derivative, and the blue curve is for a 2^{nd} order Taylor series expansion. It is easy to see that the second order approximation is accurate for a larger region compared to the first order approximation. The percentage error of Fig. 2 is calculated and shown in Fig. 3. The figures for the rest of the paper are generated with the same resolution. The resolution is 0.1% change in the parameter. The parameter is swept from -75% to 75%.

For a 5% tolerance range, the first order approximation is valid for a fractional change of greater than -40% while the second order approximation is valid for a fractional change of greater than -65%. This range would roughly be the same if a finite difference calculation was performed, but would require

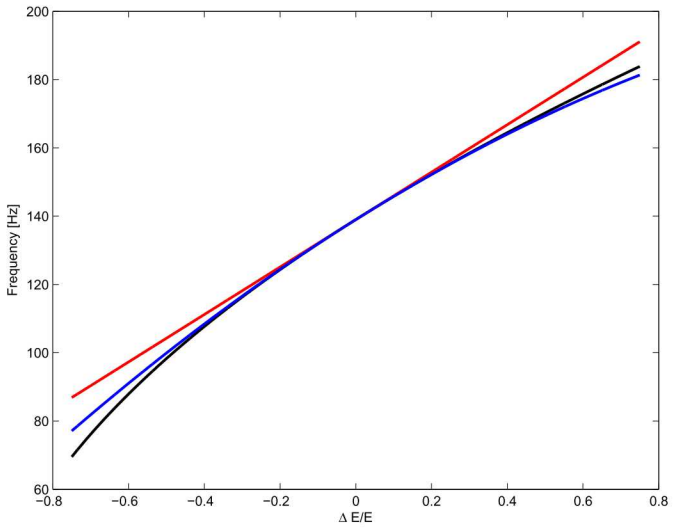

FIGURE 2. 1^{st} System elastic natural frequency as a function of fractional change of Young's modulus with the black line as the true data, the red line as the 1^{st} order perturbation, and the blue line as the 2^{nd} order perturbation

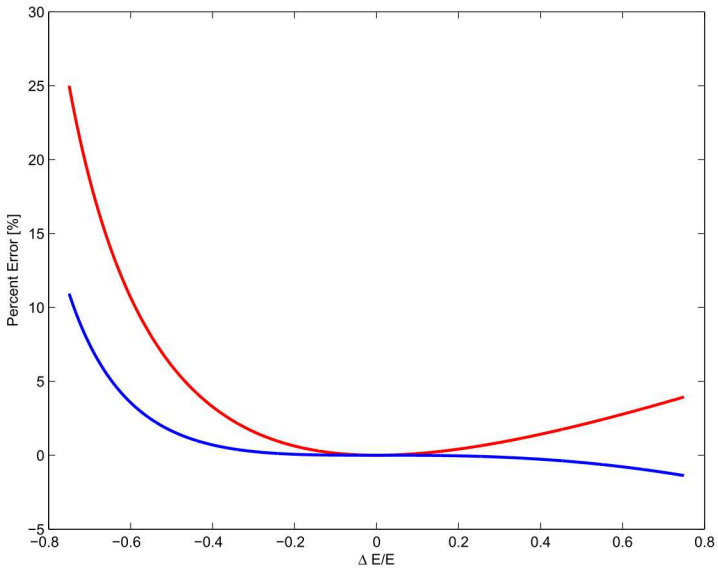

FIGURE 3. Percentage error as a function of fractional change in Young's modulus with the red line as the 1^{st} order perturbation and the blue line as the 2^{nd} order perturbation

more computational effort. This calculation however is more accurate since the sensitivities are exact compared to an approximation. The computational effort for this calculation is less than that for a finite difference, which requires at least three computational runs in order to get the sensitivities while using Hyper-Dual numbers only requires one computational run. The exact difference in computational time and accuracy between a Hyper-Dual step and finite difference is not computed but is expected to be computed in future work.

The Young's modulus is not the only model parameter for the FE code, the mass density is also an important parameter since the density of a material can also change based on environmental factors such as humidity and temperature. For this reason, the same calculations are also performed for a perturbation in the mass density. The first system elastic natural frequency is shown in Fig. 4 where the black line is the truth data, the red line is the 1^{st} order Taylor series expansion, and the blue line is the 2^{nd} order Taylor series expansion. Compared to the change in Young's modulus, the mass density is much more non-linear. This is emphasized in the percentage error which can be seen in Fig. 5.

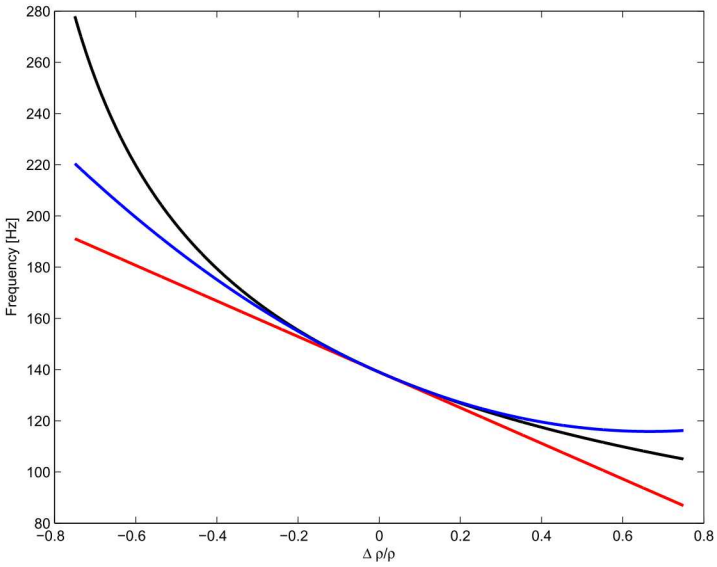

FIGURE 4. 1^{st} System elastic natural frequency as a function of fractional change of mass density with the black line as the true data, the red line as the 1^{st} order perturbation, and the blue line as the 2^{nd} order perturbation

For a 5% tolerance range, the first order approximation can be treated as accurate for a percentage change in mass density on the range of -40% to 40% and the second order approximation can be treated as accurate on the range of -55% to 60%. The time required to perform this calculation was compared to assembling the entire system for each value of mass density or Young's modulus. For this particular example, using Hyper-Dual numbers along with a perturbation analysis was significantly faster. On the computer used by the authors, which is a fairly standard

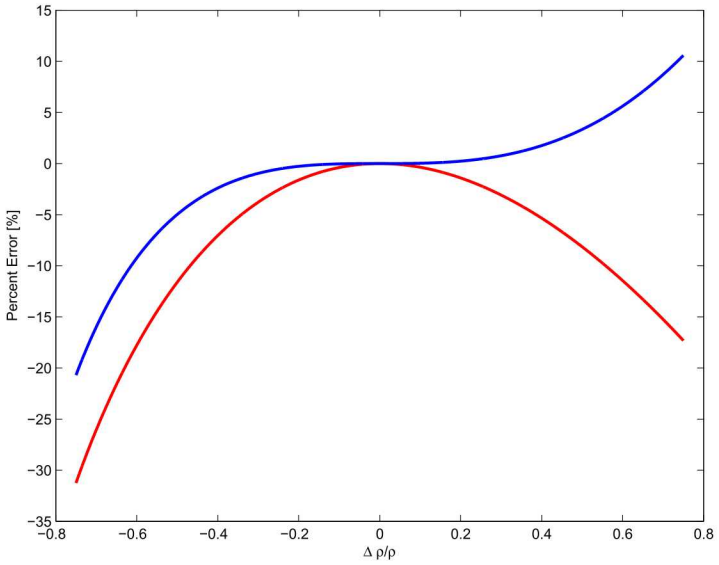

FIGURE 5. Percentage error as a function of fractional change in mass density with the red line as the 1^{st} order perturbation and the blue line as the 2^{nd} order perturbation

desktop, constructing the full system takes about 175 times more computational time than using the Hyper-Dual numbers. This time was measured for the full construction of the FE model for the full system at all of the perturbations. For the Hyper-Dual number system, the time measured the construction of the substructures, synthesis of the full system, and then matrix perturbation based on a Taylor expansion.

5 Conclusions and Future Work

This technique of using Hyper-Dual numbers for sensitivity and uncertainty quantification is a new technique that is very powerful. This paper is a preliminary assessment of using Hyper-Dual numbers for a sensitivity analysis on a relatively simple example. The use of Hyper-Dual numbers on a system is an exact method for determining sensitives. These sensitivities are determined without the use of multiple computational evaluations of the FE code or subject to truncation error due to the Taylor series expansion to determine the sensitives. The Hyper-Dual number is a multi-dimensional expansion of a generalized complex number, the dual number. The use of the dual number allows for the Taylor series expansion to produce a finite series compared to the expected infinite series which then is truncated. This technique is applied to a substructure representation in order to produce a parameterized reduced order model which can be combine with other PROMs in order to produce a full system representation. The approach was applied to two Craig-Bampton substructure representations on a example of a planar frame with an appendage. The accuracy of the method is compared to the full system that is constructed at each perturbation value to determine the true solution. Hyper-Dual numbers allow analysts to overcome the weaknesses of approximating the sensitivity of a model that are present in the use of finite difference and the complex step approaches.

There are many possible future paths that this research can lead. One of the expected future work options is to do a direct comparison to the finite difference and complex step analysis. This would include both an accuracy analysis along with a computational time requirement analysis. Another expected topic of future work is to use the sensitivities to perform an uncertainty quantification analysis such as covariance propagation. Along with a traditional uncertainty quantification analysis, the authors are particularly interested in the quantification of epistemic uncertainty, specifically uncertainty due to the model form. These techniques are currently being derived and evaluated. While the topics described are interested in the system after the synthesis, different forms of ROMs are available besides the Craig-Bampton substructure representation. Another topic of future work is the use of different substructure ROMs to produce a PROM. This can be done with purely numerical data such as the example that is presented in this paper or with experimental data gathered in the laboratory.

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REFERENCES

[1] J.A. Fike, J. J. A., 2011. "The development of hyper-dual numbers for exact second-derivative calculations". In AIAA paper 2011-886, 49th AIAA Aerospace Sciences Meeting.

[2] R.R. Craig, M. B., 1968. "Coupling of substructures for dynamic analysis". *AIAA Journal 6*, pp. 1313–1319.

[3] M.R.W. Brake, J.A. Fike, S. T. "Parameterized reduced order models from a single mesh using hyper-dual numbers".

[4] R. Abreu, D. Stich, J. M. "On the generalization of the complex step method". *Journal of Computational and Applied Mathemeatics,* ***241***, pp. 84–102.

[5] J.A. Fike, S. Jongsma, J. J. A., and van der Weide, E., 2011. "Optimization with gradient and Hessian information calculated using hyper-dual numbers". In AIAA paper 2011-3807, 29th AIAA Applied Aerodynamics Conference.