COVER SHEET

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Title: **Computationally Efficient Solution of the High-Fidelity Generalized Method of Cells Micromechanics Relations**

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ABSTRACT

The High-Fidelity Generalized Method of Cells (HFGMC) is a powerful technique for simulating composite materials and is based on Aboudi's method of cells micromechanics theories. Unlike the original generalized method of cells, the HFGMC uses a higher order approximation for the subcell displacement field. Although this allows for a more accurate determination of the subcell stress/ strain fields, the solution to the simultaneous set of equations can become computationally burdensome. In order to overcome expensive computational costs associated with solving large systems of equations, order-reduction techniques have been developed to approximate the solution with an acceptable error. These techniques are widely used in the computational fluid dynamics community and are increasingly being implemented for solving solid mechanics problems involving the finite element method. In this study, the HFGMC global system of equations for doubly-periodic RUCs was reduced in size through the use of Proper Orthogonal Decomposition (POD) with Galerkin projection. Order-reduced models were then implemented within an ABAQUS UMAT and used to perform multiscale analyses. A number of cases were presented that show the computational feasibility of using order-reduction techniques to solve the HFGMC set of simultaneous equations. By simulating composite materials in a more computationally efficient manner, a pathway forward is presented for performing multiscale analyses of composite structures consistent with the Airframe Digital Twin concept.

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INTRODUCTION

Current computational limitations at both the microscale and macroscale inhibit the implementation of high-fidelity multiscale models within existing commercial finite element (FE) software. Such limitations must be overcome if concepts such as the Airframe Digital Twin [1] are to be realized. Computational savings at the microscale can be achieved by improving the efficiency of lower length scale calculations. The High-Fidelity Generalized Method of Cells (HFGMC) is a powerful technique for simulating composite materials [2]. However, the solution to the set of simultaneous equations can become computationally burdensome. In order to overcome expensive computational costs associated with solving large systems of equations, order-reduction techniques have been developed to approximate the solution with an acceptable error.

Order-reduction concepts are widely used in the computational fluid dynamics community [3-5] to enhance the computational efficiency of large, complex systems. However, these techniques are increasingly being considered for structural applications and have been readily applied to structural problems involving nonlinear FEs [6-9]. A significant portion of the literature involves the use of Proper Orthogonal Decomposition (POD) [10, 11] to generate a reduced model. The goal of POD is to generate a set of basis functions that can be used to reduce the dimensionality of a large system (*e.g.*, set simultaneous of equations) by optimally determining any dominant components. This is often accomplished by performing a singular value decomposition (SVD) of a "snapshot" matrix [12]. In this work, the HFGMC global system of equations for doubly-periodic RUCs is reduced in size through the use of POD with Galerkin projection. The order-reduced HFGMC model is then be coupled to the ABAQUS FE software and used to assess the accuracy and computational efficiency of order-reduced models.

HIGH-FIDELITY GENERALIZED METHOD OF CELLS (HFGMC)

The HFGMC is a technique used for modeling composites based on Aboudi's method of cells micromechanics theories [2]. Using the HFGMC, a doubly or triply periodic repeating unit cell (RUC) is discretized into an arbitrary number of subcells. Each subcell is then assigned material properties and a constitutive law to describe the local material behavior. Continuity of displacements and tractions are enforced along the subcell boundaries in an average sense, and all field quantities are evaluated at the subcell centroids. An illustration of this scheme for a unidirectional composite is shown in Figure 1. Using the GMC, a doubly-periodic RUC may be defined in the x_2-x_3 plane and is discretized into N_β and N_γ subcells along the x_2-direction (height) and the x_3-direction (width), respectively, while the fibers extend in the x_1-direction (length). Damage can then be allowed to initiate within individual subcells (*e.g.*, fiber failure, matrix cracking) or at subcell interfaces (*e.g.*, fiber/ matrix debonding).

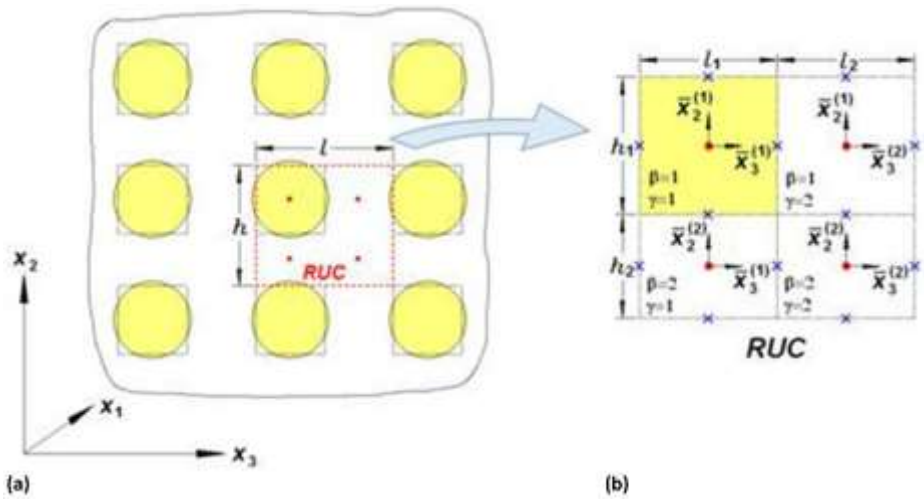


Figure 1. a) Representation of a unidirectional composite with fibers aligned in the x_1-direction and b) RUC representation of the unidirectional composite. Figure from [2].

For the HFGMC, a second-order asymptotic expansion of the subcell displacement field is performed. By imposing the subcell equilibrium conditions, interfacial continuity conditions and periodic boundary conditions, a linear system of equations can be derived by relating the average surface tractions to the unknown microvariables (coefficients in the expansion of the subcell displacement field) [2]. Bansal and Pindera [13] and Arnold *et al*. [14] reformulated the HFGMC equations in order to reduce the number of unknowns by expressing the surface-averaged tractions as a function of surface-averaged displacements. These surface-averaged displacements are then related to the microvariables [2]. As previously mentioned, each subcell can be assigned a unique constitutive relationship that accounts for material moduli, and the total, inelastic, and thermal strains. For perfectly bonded constituents, the reformulated HFGMC relationships can be expressed as a square system of $n = 6N_\beta N_\gamma+3(N_\beta+N_\gamma)$ equations of the form:

$$Ku = f + g \tag{1}$$

where K is a sparse, unsymmetric matrix that is a function of subcell properties and geometry, f is a vector containing the thermomechanical properties, the applied average strains, and the temperature change, and g is an vector containing any inelastic effects. The vector u represents the unknown surface averaged displacements for each subcell. After solving this linear set of equations, the subcell stresses and strains can be determined. It should be noted that $3(N_\beta+N_\gamma)$ equations have been included for programming convenience (see discussion in Ref. [2]).

Unlike the generalized method of cells [2], a higher accuracy in the subcell stress/ strain fields is obtained at the cost of computational efficiency by employing a higher-order subcell displacement field. As a result, the HFGMC has been scarcely used to perform multiscale analyses of composite laminates and structures. A central goal of this work will be to enhance the computational efficiency of the HFGMC in multiscale analyses using order-reduction techniques.

ORDER-REDUCTION CONCEPTS APPLIED TO THE HFGMC

Consider the HFGMC system of equations given by Eq. 1 (referred to herein as the "exact" solution). The complete solution space can be spanned by a set of *n* orthonormal basis vectors. However, the solution could be likely attracted to a particular subspace comprised of only *k* of the *n* orthonormal basis vectors where hopefully $k << n$. By collecting this set of *k* orthonormal basis vectors into a matrix, V_k, the solution of Eq. 1 can be approximated using Galerkin projection by $u = V_k \tilde{u}$ where $\tilde{u}$ can be referred to as the reduced solution vector. A reduced set of *k*x*k* equations can then be given by:

$$V_k^T K V_k \tilde{u} = V_k^T f + V_k^T g \tag{2}$$

It should be noted that in order to set up the reduced set of equations, the matrix *K* and vectors *f* and *g* must be evaluated. However, for RUCs containing only linear elastic materials, the *K* matrix is constant and *g* is the null vector. Additionally, *K* can be pre-computed and stored. The reduced solution vector can therefore be directly determined without the need to use a numerical equation solver:

$$\tilde{u} = (V_k^T K V_k)^{-1} V_k^T f \tag{3}$$

To minimize the usage of computer memory, the matrix $(V_k^T K V_k)^{-1}$ can be precomputed and then multiplied by $V_k^T f$. Different strategies relating to the computer implementation of Eq. 3 are discussed for a similar development by Krysl *et al*. [8].

After solving this set of equations for $\tilde{u}$, the exact solution can be recovered by using the relationship $u \approx V_k \tilde{u}$. In effect, the original set of $n = 6N_\beta N_\gamma + 3(N_\beta + N_\gamma)$ equations can be converted into a hopefully much smaller set of *k* equations. Of course, by only including *k* of the *n* orthonormal basis vectors, an approximation error is introduced. The goal of an order-reduction technique in this context is then to determine the smallest system of equations while minimizing the approximation error.

In order to determine the set of *k* orthonormal basis vectors and hence the size of the reduced set of equations, a proper orthogonal decomposition procedure can be performed using the method of snapshots [12]. Suppose that the solution to Eq. 6 (*i.e.*, an *n* x 1 vector) for an RUC under a particular set of applied strains is known. This "snapshot" can be used to form the first column of a new matrix, *M*. If the set of applied strains is varied, other snapshots can be determined and used to populate *M*. By performing a singular value decomposition of the snapshot matrix, *M* can be expressed as:

$$M = V \Sigma U^T \tag{4}$$

where *V* and *U* are the left- and right-singular vectors, respectively, and Σ is a diagonal matrix of singular values arranged in descending order. The first *k* columns of *V* correspond to the *k* dominant singular values and can be used to populate the matrix V_k. Providing that the variation in applied strains (or other input parameters) spans a sufficient space, an accurate reduced model can likely be generated. Since any nonlinearity tends to increase the size of the reduced system (*i.e.*, reduce computational savings), other techniques have been developed to approximate the nonlinear contributions. For example, the nonlinear contribution to the system of equations, *g*,

could be approximated using the Discrete Empirical Interpolation Method (DEIM) [15, 16]. Effectively, the DEIM determines only the dominant terms of the nonlinear contribution for the full system and finds the remaining components through interpolation.

For illustration purposes, Figure 2 shows an RUC of a fiber/ matrix composite with N_β = 118 and N_γ = 117 for a total of 13,806 subcells. Both the fiber and matrix were considered isotropic, and linearly elastic materials. The fiber was assumed to have a Young's modulus of 72.7 *GPa* and Poisson's ratio of 0.2 while the matrix had a Young's modulus of 4.25 *GPa* and Poisson's ratio of 0.35. For this RUC, at every strain increment applied, a sparse system of 83,541 equations must be solved. As a result, an RUC of this fidelity is currently impractical to be employed in multiscale analyses. However, higher-fidelity RUCs are needed to accurately simulate realistic composite microstructures. Since both materials are linear elastic, each of the six components of applied strain were varied independently and used to form the snapshot matrix from these six solutions of Eq. 1 [9]. Individual strain increments were not stored in the snapshot matrix, but will likely be stored if nonlinear materials or elastic materials with damage are considered. As a result of the doubly-periodic HFGMC formulation, only five dominant basis vectors are required to generate the reduced model for linear elastic materials. A reduced model was generated from the snapshot matrix and compared to the existing exact model for each of 1000 validation load cases. These validation cases were generated by varying each strain component randomly in the interval [-0.1, 0.1]. Effectively, the reduced model solved a dense set of k = 5 equations while the exact model solved a highly sparse (99.988%) set of n = 83,541 equations. The maximum error between the exact solution (u_E) and the order-reduced solution (u_R) across all applied strain increments (N_{inc}) was determined using the following relationship for each of the validation load cases:

$$Err = max\left(\left\|u_{E_1} - u_{R_1}\right\|_2, \left\|u_{E_2} - u_{R_2}\right\|_2, \ldots, \left\|u_{E_{Ninc}} - u_{R_{Ninc}}\right\|_2\right) \quad (5)$$

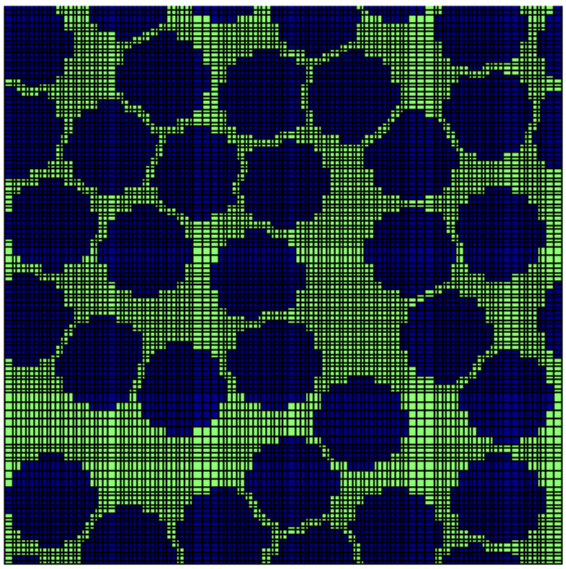


Figure 2. RUC where blue indicates a fiber subcell and green indicates a matrix subcell.

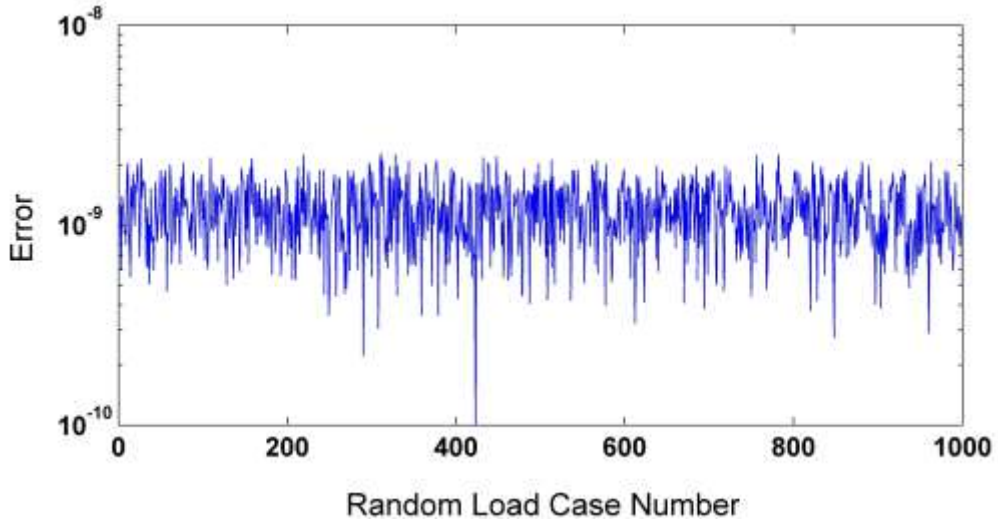


Figure 3. Error between the exact model and reduced model for each validation load case.

Three separate order-reduced models were generated in this study in order to test the computational implementation of the reduced system of equations. Method 1 was implemented by solving Eq. 2 using a linear equation solver. Similar to Krysl *et al*. [8], Methods 2 and 3 were developed by solving Eq. 3 and precomputing the matrices $(V_k^T K V_k)^{-1}$ and $(V_k^T K V_k)^{-1} V_k^T$, respectively. It should be noted that while Method 3 involves less matrix multiplications each loading increment than Method 2, the memory requirements are larger as the size of the reduced system of equations is increased [8]. Note that the error is negligible (~10^{-9}) for each of the 1000 validation cases when the exact model was compared to the reduced Method 2. Similar error estimates were obtained for the other two reduced methods. Since this estimate of error is based on a vector norm, any individual differences in the solution vector would tend to get smeared out. Other estimates of error based on local fields are also possible. For example, the maximum difference in subcell stress components was found to be <<1%. Additional estimates of error are currently being explored.

Since it is computationally intensive to write individual subcell level information to data files, the efficiency of the exact and order-reduced models was determined by suppressing all local subcell output. Effectively, only the system of equations represented by Eqs. 1-3 was solved and used to determine the local subcell fields and homogenized stresses. Both the total solution time and solution time for each increment were determined when each of the 1000 validation load cases was applied over 25 increments. The average runtimes for each of the models are shown in Table I. For each increment, the HFGMC relations were solved approximately three times faster using order-reduction techniques. The average total runtimes for the reduced models were between 5.5 and 7.2 times less than the exact model. This significant difference between the incremental and total runtimes was primarily due to assembling the left-hand side of Eq. 1 for the exact model at the first increment. Hence, an added benefit of using order-reduction techniques is that the equation assembly procedure can be significantly made

Table I. Computational runtimes associated with the exact and reduced models.

		Increment Runtime (s)	Increment Speedup	Total Runtime (s)	Total Speedup
Exact		5.25E-02	1.0	5.46	1.0
Reduced	**Method 1**	1.84E-02	2.9	0.79	6.9
	Method 2	1.74E-02	3.0	0.76	7.2
	Method 3	1.81E-02	2.9	0.99	5.5

more efficient. It is envisioned that the computational savings associated with an order-reduced model will further increase when nonlinear materials are considered.

These preliminary results demonstrate that order-reduction concepts can be successfully applied to the HFGMC relationships resulting in significant computational cost savings. Order-reduced HFGMC models are expected to have a profoundly beneficial impact when embedded in a multiscale analysis and can potentially make high-fidelity multiscale analyses of composites more computationally feasible without losing accuracy. Additionally, order-reduction could allow for a tractable means of incorporating more realistic doubly or triply-periodic RUCs into a multiscale analysis; this is an idea that is currently seldom considered due to computational costs.

MULTISCALE ORDER-REDUCED HFGMC

In order to assess the computational efficiency of order-reduced micromechanical models in a multiscale analysis, multiple multiscale analyses were performed of unidirectional open-hole tensile composite specimen. The same materials were used for the fiber and matrix as done in the previous analyses. A simple 3,848 FE mesh was used for illustration purposes and is shown in Figure 4. In practice, a much finer mesh (particularly near the hole) would be considered. Multiscale analyses were performed where RUCs of increasing complexity were implemented at every FE integration point within the model. Four different RUCs comprised of 16, 64, 256, and 1024 subcells, respectively, were considered and are shown in Figure 5. Local HFGMC analyses were performed for both the exact model and the order-reduced model based on Method 2 (the most computationally efficient). A longitudinal displacement was applied over 50 increments at one end of the specimen while the other end was fixed. Separate reduced models were generated for each of the RUC architectures considered in a manner similar to the previous analyses. Note that since only elastic materials without damage were considered, this implies that regardless of the size of the RUC, the reduced system of equations will always result in a system of five equations. All calculations were performed on a workstation class, personal desktop computer.

A comparison of the longitudinal stress field in the vicinity of the hole is shown for the exact and reduced local models in Figure 6 where a 1024 subcell RUC was implemented at the microscale. The stress fields are virtually identical (<<1% difference). Similar results were obtained for multiscale analyses involving other RUC architectures. A more rigorous characterization of error for multiscale analyses is currently being explored. Table II shows the computational runtimes for multiscale analyses where exact and order-reduced models were implemented at the microscale. No subcell level information was stored at each integration point. For a 16 subcell RUC,

the order-reduced model is only slightly more efficient than the exact. However as the number of subcells increases, the order-reduced models become increasingly more computationally efficient (up to 3.4 times faster) since the size of reduced system of equations is constant. Additionally, the memory requirements for the order-reduced models is less than the exact model. This implies that order-reduced models can have the biggest impact for larger RUCs. It should be noted that if subcell level data was stored, a smaller improvement in computational efficiency (up to 2.2 times for the 1024 RUC) was observed for the order-reduced model. Nevertheless, significant computational savings can be obtained in multiscale analyses where order-reduction techniques are employed.

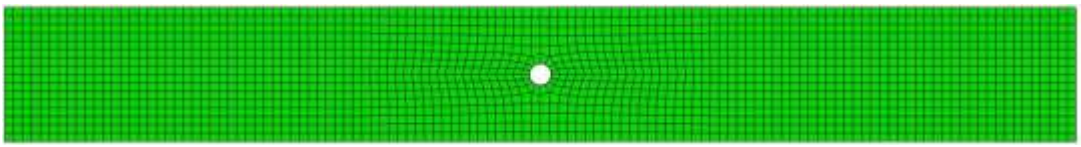


Figure 4. FE mesh of a unidirectional open-hole tensile composite specimen.

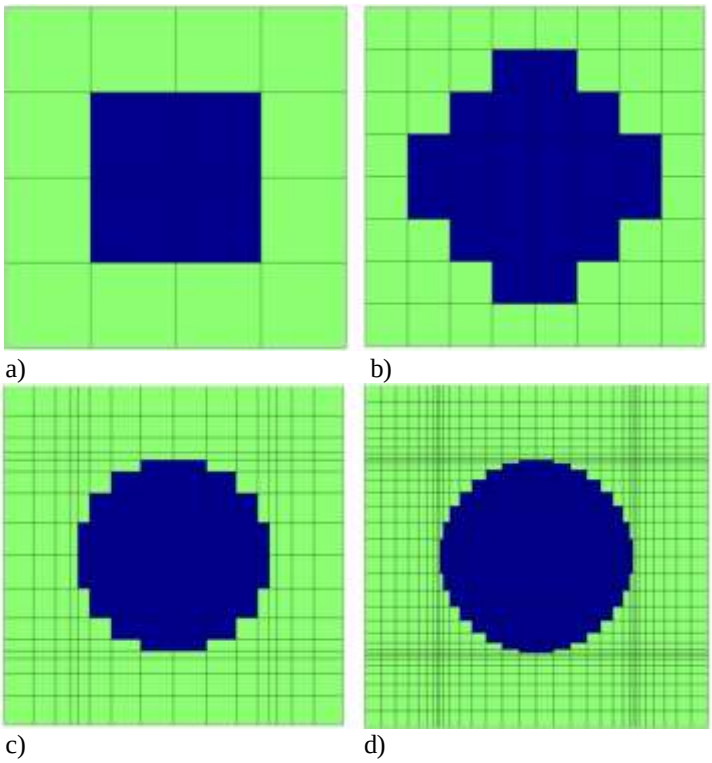


Figure 5. Four different RUC architectures comprised of a) 16, b) 64, c)256 and d) 1024 subcells used in multiscale analyses where blue indicates a fiber subcell and green indicates a matrix subcell.

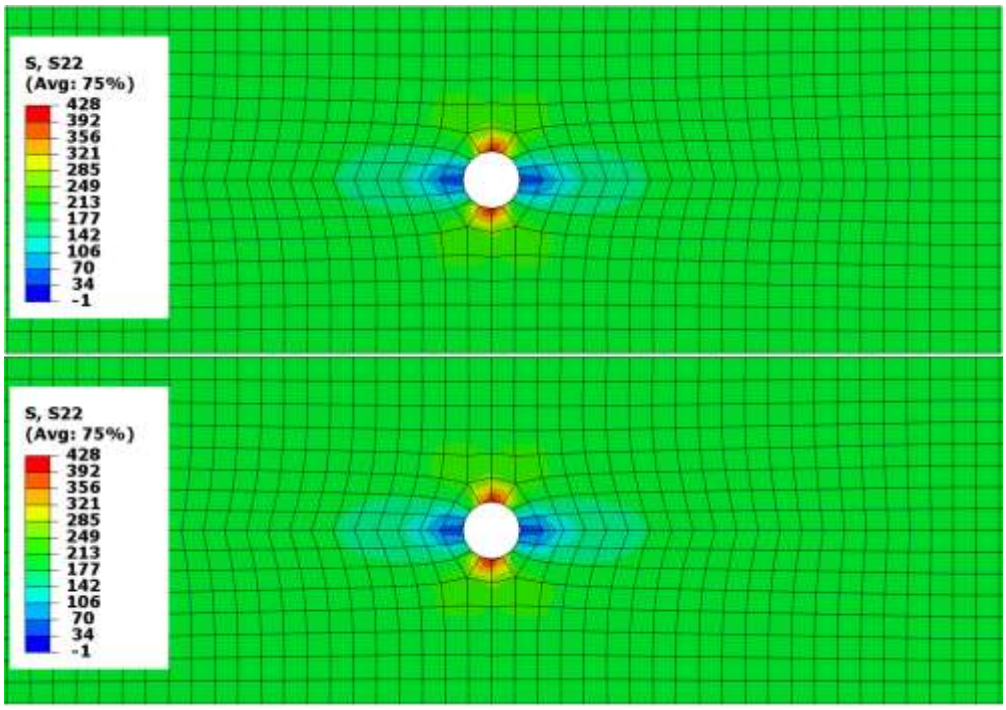


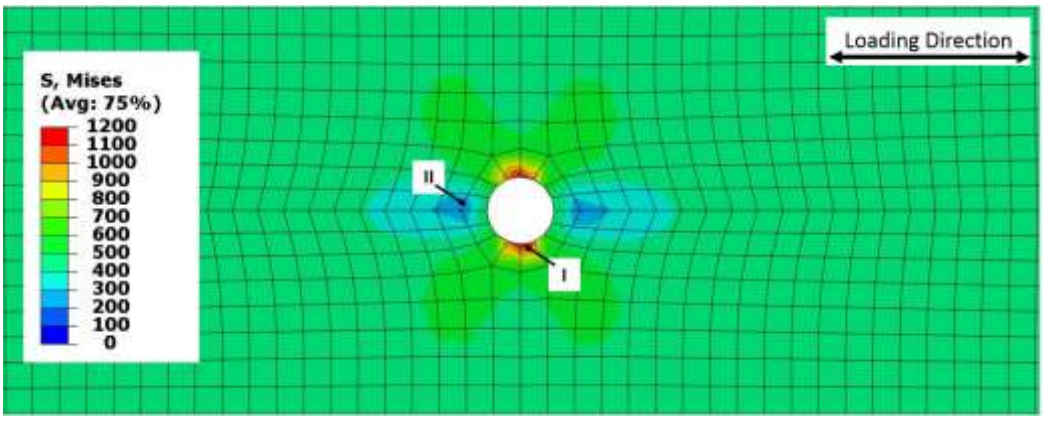
Figure 6. Comparison of the stress field in the direction of the applied loading in the vicinity of the hole where the exact (top) and order-reduced (bottom) HFGMC relationships were implemented at the microscale for a 1024 subcell RUC. All stresses are reported in units of *MPa*.

Table II. Computational runtimes for multiscale analyses

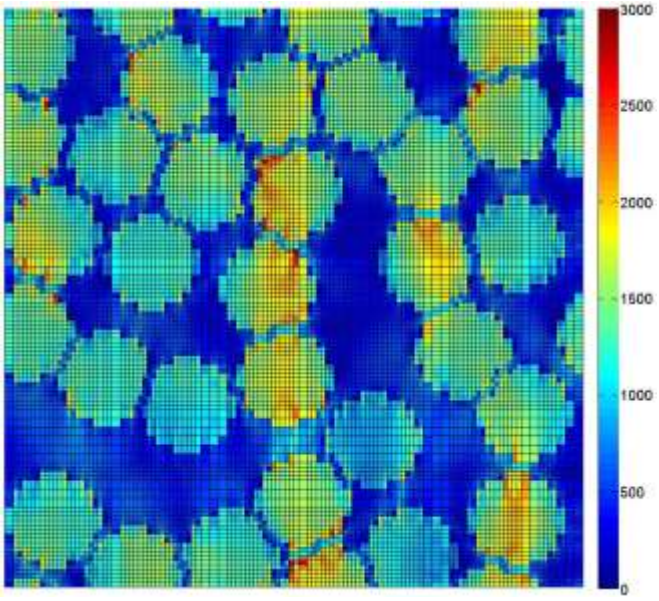
RUC Number of Subcells	Runtime (s)		Speedup
	Exact	Reduced	
16	111	97	1.1
64	344	228	1.5
256	1607	753	2.1
1024	9487	2802	3.4

To further demonstrate the feasibility of using the order-reduced HFGMC relations in a multiscale analysis, another multiscale analysis was performed where a 13,806 RUC (*cf*., Figure 2) was implemented at the microscale. This RUC was only used over one-third of the model domain (near the hole) to reduced memory storage requirements. Effective properties based on the same RUC were used elsewhere. Multiscale analyses with an RUC of this complexity are seldom considered due to the computational resources required. A multiscale analysis based on the exact model cannot be reasonably performed in this case on a personal desktop computer. However, recall that the order-reduced model based on this RUC was shown match the exact model without incurring any significant error across a wide spectrum of applied loading conditions (*cf*., Figure 3). This issue highlights one of the key advantages of order-reduced HFGMC modeling: significantly more complex RUCs can be implemented within a multiscale framework than have been previously considered. The von Mises stress distribution near the hole is shown in Figure 7a. Local subcell fields are plotted at two locations near the hole in

Figures. 7b-c. The von Mises stress was plotted purely for illustration purposes, and any other subcell level data (e.g., stress/ strain components, damage parameters) could be plotted if desired. By having access to local subcell level information, critical locations and failure initiation mechanisms can be investigated. For example, note that although the maximum stress at the macroscale is approximately 1200 *MPa*, local fields can far exceed that value (3000 *MPa* maximum observed within an RUC at Location I, Figure 7a). An in-depth study of these local fields can then be used to guide the design process to resist failure initiation. Parametric studies can also be performed to explore how non-uniform stress/ strain fields at the macroscale affect the microscale fields. If extended to account for damage and material nonlinearity, order-reduction concepts hold promise to potentially enable faster development/ certification of composite structures and to provide a viable pathway toward Airframe Digital Twin models for full aerospace vehicles.



a)



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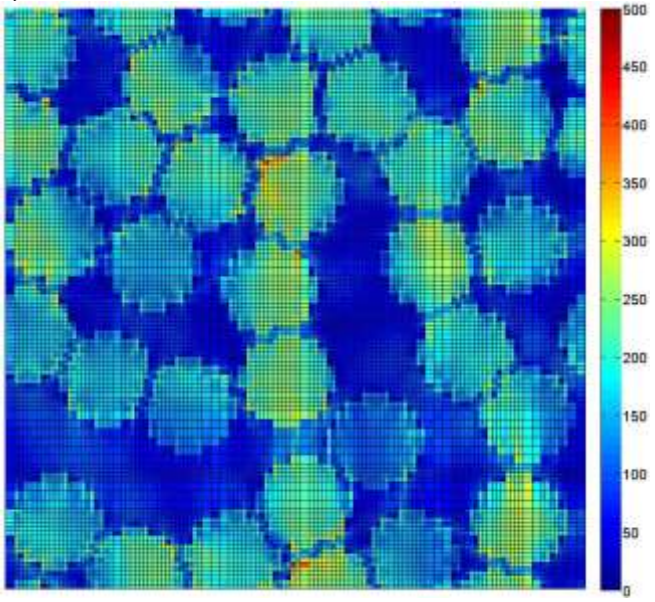

c)

Figure 7. a) Stress distribution near the hole for a multiscale analysis where a 13,806 subcell RUC was implemented at the microscale and the resulting microscale stress distribution at b) Location I and c) Location II. All stresses are reported in units of *MPa*.

CONCLUSIONS

In this study, the HFGMC global system of equations for doubly-periodic RUCs was reduced in size through the use of a POD technique with Galerkin projection. The reduced system of equations was compared to the unmodified HFGMC equations for standalone micromechanics models as well as multiscale analyses. Multiscale analyses were performed by implementing order-reduced models within an ABAQUS UMAT. A variety of RUC architectures ranging from 16 to 13,806 subcells was considered. Simulations involving only elastic materials showed that significant computational savings can be obtained when using order-reduction techniques without incurring any significant error in subcell fields. Furthermore, multiscale simulations based on lower length scale order-reduced models allowed much larger RUCs to be simulated at the microscale than what is traditionally implemented. Ongoing work is aimed at extending these concepts to capture the response of damaged, elastic/ nonlinear composites. By accurately simulating composites in a more computationally efficient manner, a possible method was developed for performing multiscale analyses of composite structures consistent with the Airframe Digital Twin concept.

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