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**MESOSCALE MODELS CHARACTERIZING MATERIAL PROPERTY FIELDS USED
AS A BASIS FOR PREDICTING FRACTURE PATTERNS IN QUASI-BRITTLE
MATERIALS**

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ABSTRACT

To accurately predict fracture patterns in quasi-brittle materials, it is necessary to accurately characterize heterogeneity in the properties of a material microstructure. This heterogeneity influences crack propagation at weaker points. Also, inherent randomness in localized material properties creates variability in crack propagation in a population of nominally identical material samples. In order to account for heterogeneity in the strength properties of a material at a small scale (or “microscale”), a mesoscale model is developed at an intermediate scale, smaller than the size of the overall structure. A central challenge of characterizing material behavior at a scale below the representative volume element (RVE), is that the stress/strain relationship is dependent upon boundary conditions imposed. To mitigate error associated with boundary condition effects, statistical volume elements (SVE) are characterized using a Voronoi tessellation based partitioning method. A moving window approach is used in which partitioned Voronoi SVE are analysed using finite element analysis (FEA) to determine a limiting stress criterion for each window. Results are obtained for hydrostatic, pure and

simple shear uniform strain conditions. A method is developed to use superposition of results obtained to approximate SVE behavior under other loading conditions. These results are used to determine a set of strength parameters for mesoscale material property fields. These random fields are then used as a basis for input in to a fracture model to predict fracture patterns in quasi-brittle materials.

INTRODUCTION

Material inhomogeneities at the microstructural scale greatly influence fracture response. Failure initiates locally where stress concentrations are induced in large part by local heterogeneity. Therefore, fracture models that ignore microstructural inhomogeneity, or employ Representative Volume Elements (RVE) to homogenize material properties, may not accurately capture fracture response. The high sensitivity of brittle fracture to material microstructure not only contributes to the form of failure patterns, but also size effects [1–3] and high response variability for samples with identical geometry and loading specifications [4–6].

In previous work, the Spacetime Discontinuous Galerkin

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(SDG) Finite Element Method (FEM) [7] has been employed for the solution of elastodynamic problems. The SDG method has high accuracy from the direct discretization of space and time, and is also efficient in characterizing the local solution properties critical for simulation of fracture in quasi-brittle materials by using adaptive operations in spacetime that control discretization errors [8] and track propagating cracks [9].

In this work, a mesoscale modeling technique will be used to characterize mesoscale material property behavior; the model outputs can be used in SDG fracture simulation. The mesoscale model characterizes behavior of Statistical Volume Elements (SVE) that are below the scale of the RVE. These elements retain a degree of local descriptiveness, which is missing in an RVE-based analysis. Previous work has focused on the use of mesoscale modeling techniques to model composite material behavior [10–15]. A main advantage of the approach is that it can ultimately be used to create random field representations of local composite properties. This type of mesoscale material characterization can be used as a basis for stochastic simulation, or as a statistical basis for models predicting damage and failure, which is the focus of the current work.

MESOSCALE MATERIAL MODELING

A Voronoi tessellation based partitioning scheme is used to model the SVE, in place of a more commonly used square partitioning approach. Voronoi tessellations have been shown to provide closer approximations of material properties because stress concentrations are reduced when inclusions are not allowed to intersect inclusion boundaries [16]. The collection of SVE that partition an RVE are tested using Finite Element Analysis (FEA) to determine material behavior under hydrostatic, pure and simple shear displacement based loading. An SVE failure criterion is defined and superposition is used to determine the approximate failure stress of the SVE when loaded in any direction.

CONSTRUCTION AND LOADING OF SVE

An RVE with randomly placed inclusions is initially partitioned into Voronoi cells using Delaunay triangulation based on center points of inclusions. The cells are grouped into similarly sized SVE by calculating the location of each Voronoi cell centroid with respect to a square grid imposed on the RVE. If a Voronoi cell centroid lies within a given square grid area, the cell is assigned to that SVE grouping. For small sizes of SVE, there may be regions in which no Voronoi cell centroid lies, limiting the number of SVE that may be generated. In this work, the RVE is generated with a volume fraction of approximately 10% inclusions; each inclusion diameter has a unit value, the RVE has equal side lengths 100 times the size of the inclusion. Results are given for a material with inclusion to matrix contrast ratio 100 : 1.

Figure 1 shows a typical SVE, with grid spacing set to 5 times the inclusion diameter, under the three load cases considered in this work. Displacement conditions on the boundary $\mathbf{u}|_{\partial\Omega}$ are given by:

$$\mathbf{u}|_{\partial\Omega} = \mathcal{E} \cdot \mathbf{x} \rightarrow \langle \varepsilon \rangle_{\Omega} = \mathcal{E} \quad (1)$$

where hydrostatic, pure shear, and simple shear loading conditions are generated using the three values of \mathcal{E} shown below, respectively.

$$\begin{aligned} \mathcal{E} &= e^H \cdot \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \\ &e^P \cdot \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \\ &e^S \cdot \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \end{aligned} \quad (2)$$

Scale factors e^H , e^P and e^S correspond to each of the three cases. Using a superposition approach, any displacement boundary condition can be obtained by linear combination of these three load cases for a planar problem. A stiffness matrix is generated based on the results of these three loading conditions, such that displacement boundary conditions can be related to average nodal stresses on the boundary of the SVE.

FAILURE CRITERION

The mesoscale approach is fully elastic, with failure assumed when a threshold value of stress occurs in the matrix. In particular, stresses are calculated at the matrix/inclusion interface, within the matrix material only, in the direction normal to the inclusion boundary. The “path” function in the finite element program ABAQUS is used to determine the stresses in the matrix surrounding the inclusion, as shown in Fig. 2.

A uniaxial tensile, or simple shear loading direction may be assumed. By superposition, the stress at a position \mathbf{x} on the boundary of any inclusion, in the direction normal to the inclusion as shown in Fig. 3, is given by:

$$\sigma_N(\mathbf{x}) = e^H \sigma_N^H(\mathbf{x}) + e^P \sigma_N^P(\mathbf{x}) + e^S \sigma_N^S(\mathbf{x}) \quad (3)$$

where each of the three load cases (hydrostatic, pure shear and simple shear) are denoted by superscripts (H, P and S, respectively).

Using the stiffness matrix developed as described in the previous section, scale factors e^H , e^P and e^S are determined such that superposition of H, P, and S strain loadings generate far field

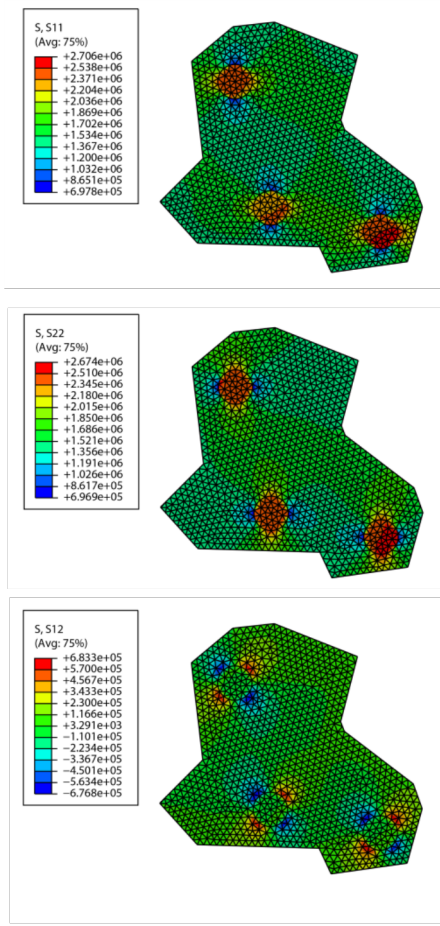


FIGURE 1. LOADING OF VORONOI TESSELLATION BASED SVE BY (A) HYDROSTATIC (B) PURE SHEAR AND (C) SIMPLE SHEAR DISPLACEMENT BOUNDARY CONDITIONS

(SVE averaged) stress loading $\Sigma_{nm}, \Sigma_{nt}, \Sigma_{tt}$, cf. Fig. 3. The unit magnitude normal and tangential stress loading at an angle θ are realized by having the only nonzero stress components of $\Sigma_{nm} = 1$ and $\Sigma_{nt} = 1$, for normal and shear modes respectively.

Macroscopic failure threshold of SVE is associated with far field stress loadings that makes the maximum of interfacial stress over all points, $\max_{\mathbf{x}}(\sigma_N(\mathbf{x}))$, equal to a predetermined debonding threshold σ^{TH} . Accordingly, normal $\tilde{s}_n(\theta)$ and tangential $\tilde{s}_t(\theta)$ strengths for far field loadings at angle θ are equal to load factors s ,

$$s = \frac{\sigma^{TH}}{\max_{\mathbf{x}}(\sigma_N(\mathbf{x}))} \quad (4)$$

that scale unit magnitude normal and tangential far field loadings and cause matrix stress at the inclusion boundary, normal to the inclusion, to reach the threshold value σ^{TH} . While

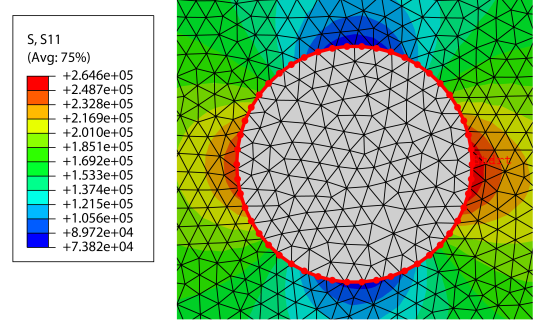


FIGURE 2. CIRCULAR PATH AROUND THE INCLUSION, LOCATION WHERE MATRIX MATERIAL STRESSES ARE DETERMINED

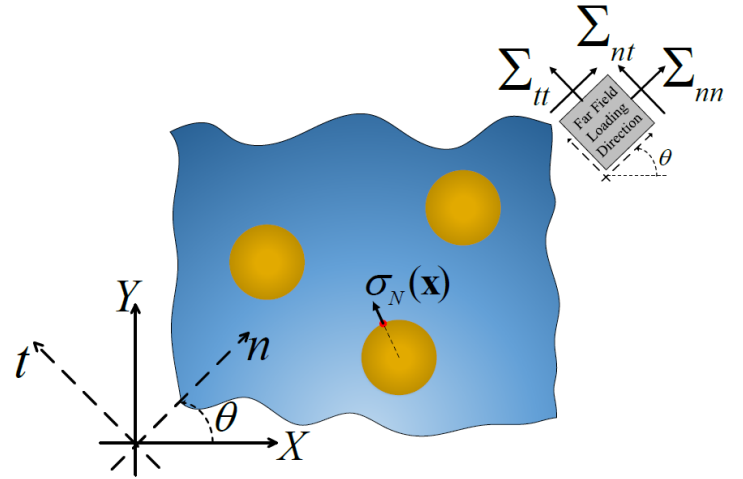


FIGURE 3. SCHEMATIC OF AN SVE AND THE n, t AXES FOR FAR-FIELD LOADING RELATIVE TO GLOBAL X, Y AXES.

$\tilde{s}_n(\theta)$ and $\tilde{s}_t(\theta)$ correspond to stress values, at angle θ , for which the SVE response starts to significantly deviate from linear elasticity they are very close to the ultimate stress, *i.e.*, strength, of the SVE for quasi-brittle materials. The proximity of linear elasticity stress limit and strength is demonstrated in various works, see for example [3, 17], and is due to the lack of significant bulk energy dissipative mechanisms for quasi-brittle materials.

RESULTS

Results given in Fig. 4 and 5 show the strength of a given SVE as a function of the angle of the applied load for uniaxial tensile load \tilde{s}_n and simple shear load \tilde{s}_t , respectively, where a threshold value of failure in the matrix is normalized to a

unit value. These results show the SVE reaching failure significantly below this threshold value, for most loading directions, because of the effects of stress concentrations around the inclusion boundaries. Results are given in Fig. 4 and 5 for a single SVE, with dimensions approximately 5 times the inclusion diameter, taken from a set of approximately 400 SVE that partition an RVE with side length approximately 100 times the inclusion diameter.

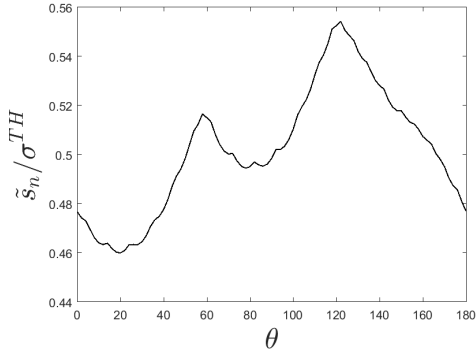


FIGURE 4. TENSILE STRENGTH OF AN SVE AS A FUNCTION OF BOUNDARY CONDITION LOADING DIRECTION θ .

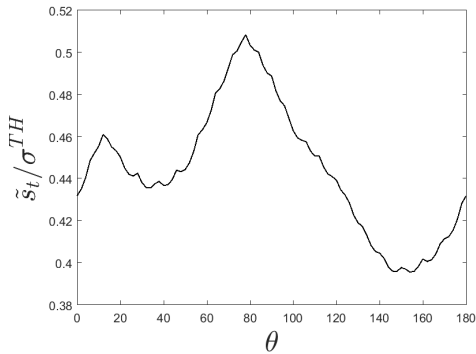


FIGURE 5. SHEAR STRENGTH OF AN SVE AS A FUNCTION OF BOUNDARY CONDITION LOADING DIRECTION θ .

To visualize the variability among the population of SVE that partition the RVE, Fig. 6 shows the minimum strength value under tensile loading at any load angle for a set of approximately 400 SVE. Based on this data, the probability density function (PDF) in Fig. 7 is generated.

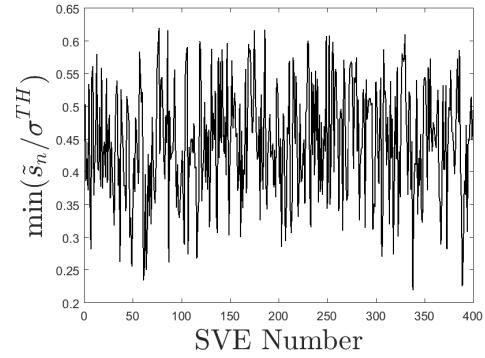


FIGURE 6. MINIMUM STRENGTH VALUE AT ANY LOADING DIRECTION FOR A SET OF SVE.

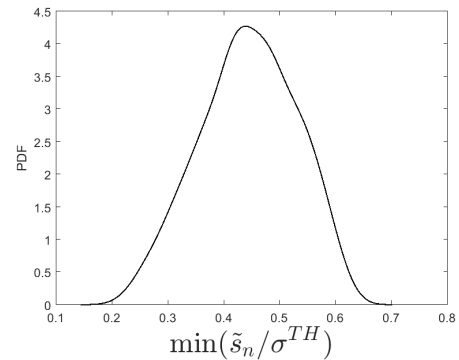


FIGURE 7. PDF OF MINIMUM STRENGTH VALUE BASED ON SVE DATA SET.

Another way to approach the data is to determine the mean value of strength of a given SVE under loadings at all angles (e.g., averaging the results shown in Fig. 4). Calculating the average value of tensile strength for the set of all SVE produces the PDF shown in Fig. 8.

Finally, the maximum value of strength of a given SVE under loading at all angles may be calculated; the PDF showing these results for tensile strength is given in Fig. 9.

The PDF of minimum values of \tilde{s}_n from Fig. 7 and the spatial covariance function, computed by the moving window approach [18], are used in the Karhunen-Loève (KL) method [19] to generate random field realizations for \tilde{s}_n . The random field realization shown in Fig. 10, normalized by σ^{TH} , is subsequently used for the fracture analysis of the domain under a spatially uniform (before any crack generation) and temporally increasing stress field. Figure 11 shows the final fracture pattern, where as expected fractures have mostly occurred in low failure strength regions. The details of generation of random field for $\tilde{\sigma}_n$ by the

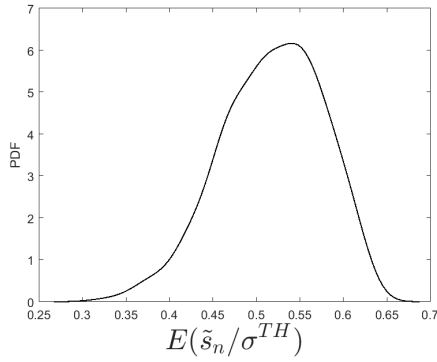


FIGURE 8. PDF OF MEAN STRENGTH VALUE BASED ON SVE DATA SET.

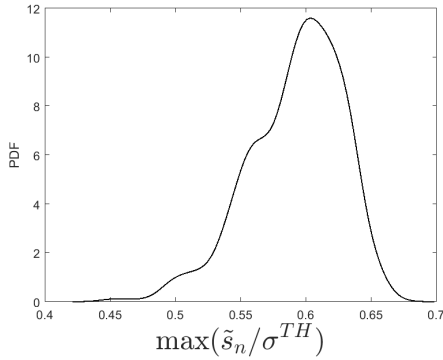


FIGURE 9. PDF OF MAXIMUM STRENGTH VALUE BASED ON SVE DATA SET.

KL method and the SDG method used for the fracture simulation can be found in [9, 20].

CONCLUSIONS

Based on this work, a method to capture variability in microstructural material strength has been demonstrated. This characterization includes minimum, mean and maximum values of strength as a function of the angle of loading of a given SVE. It is then possible to generate PDFs of the minimum, mean, and maximum strength values of the population of SVE that partition an RVE. The use of a Voronoi tessellation based partitioning method increases the accuracy of the predicted SVE response by eliminating spurious stress concentrations that arise when inclusions intersect RVE boundaries. The use of a superposition approach when loading each individual SVE allows for determination of SVE behavior at any loading angle based on combination of a set of hydrostatic, pure and simple shear loading conditions.

This work provides a method for generating realistic

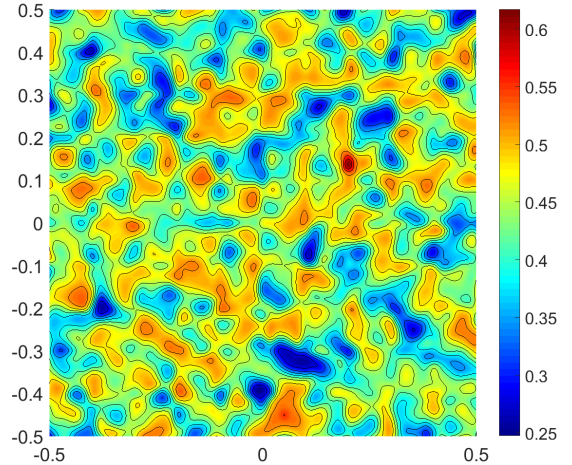


FIGURE 10. A REALIZATION OF RANDOM FIELD FOR \tilde{s}_n USING THE KARHUNEN-LOÈVE METHOD.

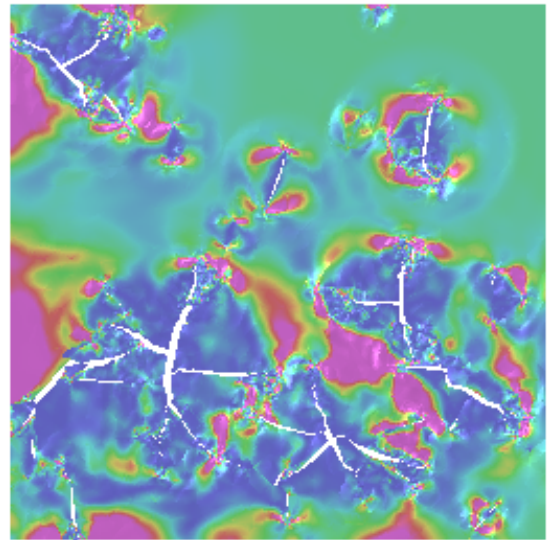


FIGURE 11. FRACTURE SIMULATION OF A DOMAIN WITH NONUNIFORM \tilde{s}_n BY THE SDG METHOD.

stochastic fields and as shown it can be used as a basis for fracture modeling. It is critical to accurately model material heterogeneity at the mesoscale to identify the influence of weaker points in the initiation and propagation of cracking. Future work will investigate the influence of microstructure on statistical properties of fracture strength and subsequently their effect on macroscopic fracture patterns.

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