Multiscale failure analysis with coarse-grained micro cracks and damage

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\begin{abstract}
A multiscale aggregating discontinuities method for treating unit cells which undergo material failure is further described; the method can also be used when the material response predicted by the unit cell loses rank-one stability. Its notable features are the decomposition of the unit cell response into a continuous and a discontinuous response, and the extraction of the equivalent discontinuities by coarse-graining procedures. In this study, the method is further combined with the extended finite element method for macro model and the cracking nodes method for micro model so that arbitrary discontinuities in the macro and the micro models can be treated free from the initial mesh topologies. The examples that are studied include a composite with circular inclusions and a micro cracking solid with an emerging macro failure.
\end{abstract}

\section{1. Introduction}

Computational multiscale analysis for predicting failure of materials is of great importance in evaluating and designing mechanical products. Physical processes such as micro cracking and material damaging, which govern the material failure of these systems generally, occur on too small of a scale to be considered in standard engineering analysis. The ability to simulate failure without extensive experimental testing hinges on the development of methods that can incorporate these physical processes into the description of the standard engineering analysis. Computational modeling and reliable prediction of failure for various materials remain highly problematic and are some of the biggest challenges in computational mechanics. Several classes of multiscale methods have been proposed; the taxonomy of the multiscale methods can be found in Belytschko and Song\cite{1}. However, most of the conventional multiscale methods such as those described in Zohdi and Wriggers\cite{2}, and Nemat-Nasser and Hori\cite{3} are limited to the computation of effective material properties, i.e. homogenized material constitutive laws, or the prediction of the macro scale behaviors before failure regime. When failure progresses beyond a critical point at the micro scale, the tangent stiffness of the unit cell loses its positive definiteness. As a consequence, the corresponding material models at the macro scale lose rank-one stability, and unless some modifications are made to the classical continuum formulation, the problem, broadly speaking, is no longer well-posed.

In this study, we attempt to circumvent these difficulties with multiscale aggregating discontinuities (MAD) method\cite{1,4,5,6} in conjunction with the extended finite element method (XFEM)\cite{7,8} to model the equivalent discontinuities at the macro scale and the cracking node method\cite{9} to model material failure behaviors at the micro scale.

The MAD approach we are taking is closely related to the FE\textsuperscript{2} approach of Feyel and Chaboche\cite{10} and Feyel\cite{11}. The micro scale model is not a representative volume element at a scale much smaller than the macro model as is common in homogenization theories. Instead, the micro model can only be one scale smaller than the scale of the macro model and must be the same scale as the elements in the macro model. However, the notable feature of the MAD method is the decomposition of the deformation of fractured unit cells into an equivalent discontinuity and a homogenous deformation. Three key concepts are fundamental to the this method: the perforated unit cell, coarse-graining an equivalent discontinuity at the macro scale, and coupling of the hourglass mode displacement to the unit cell.

In this paper, we describe a method wherein failure in the micro model, as predicted by a unit cell, is treated by an injected discontinuity and an implicitly passed cohesive law at the macro scale. The transformation of micro cracks is accomplished via a coarse graining procedure of the discontinuities of unit cells. The methodology is particularly useful for situations where many micro cracks nucleate and grow in the unit cells. The method then aggregates the cracks (discontinuities) into a single discontinuity at the macro...
scale; therefore, we call the method multiscale aggregating discontinuities method. The effectiveness of this method is demonstrated with several examples by comparing the multiscale analysis results with direct numerical simulations.

2. Overview of the multiscale aggregating discontinuity method

In the multiscale aggregating discontinuities (MAD) method, the coarse scale model is linked to unit cells with fine scale details. Generally, these unit cells are only needed for "hot spots", i.e. where a preliminary computer simulation indicates that material failure is likely. During the computation, the effect of an arbitrary number of crack growths at the micro unit cell model is aggregated into an element-wise equivalent discontinuity in the macro finite element as shown in Fig. 1.

At each linked macro element, the macro model passes a measure of deformation to the linked unit cell; for the measure of the deformation and the stress, the deformation gradient, $F$, and the second Piola-Kirchhoff stress, $P$, are respectively used so that the method is applicable to large deformations and material nonlinearities. The boundary condition of the unit cell is then prescribed by

$$u_m(X) = (F^M - I) \cdot X + q^{MXY}(X) \quad X \in I^m$$

where $u^m$ is the displacement field for the micro model boundary, $I$ is the second order identity tensor, $q^{MXY}$ is the hourglass mode displacement field to represent crack opening in the micro model and $C_m$ is the boundary of the unit cell. Note that we used a superscript $m$ and $M$ to denote variables associated with the micro and the macro model, respectively.

The MAD method is mainly based on three key concepts:

1. The perforated unit cell; all subdomains of the unit cell which have lost material stability are excluded from the definition of the average stress and strain.

2. The equivalent discontinuity; a coarse-grained discontinuity, i.e. an equivalent discontinuity, is extracted from the difference between the deformation of a macro element and its associated unit cell; note that this coarse-graining procedure is accomplished by using a form of Hill's theorem.

3. The hourglass mode displacement; the hourglass mode displacement field is superimposed along the unit cell boundary to properly account for the bilinear motion of the unit cell boundary due to crack opening.

2.1. The perforated unit cell

For the illustration of the perforated unit cell, let us consider a unit cell such as that shown in Fig. 2(a). The unit cell contains a discontinuity $\Gamma_D^m$ and a damage localization band $\Gamma_L^m$; it is assumed that the width of the localization band is small compared to the dimensions of the unit cell.

In the perforated unit cell, all subdomains which have lost material stability, i.e. cracks and damage localization bands, are excluded as shown in Fig. 2(b); i.e. $\Omega_m^0 = \Omega_m^0 \setminus (\Gamma_D^m \cup \Omega_L^m)$, and then the averaging operation for any given function $f(X)$ is defined by

$$\langle f(X) \rangle = \frac{1}{\| \Omega_m^0 \|} \int_{\Omega_m^0} f(X) d\Omega$$

where $\| \cdot \|$ denotes the measure of the domain, which is the area in two dimensions and the volume in three dimensions. Note that in contrast to conventional multiscale analysis methods, the averaging operation is performed over the perforated unit cell domain $\Omega_m^0$.

In terms of the averaging operator defined in Eq. (2), the average bulk strain in the micro model is given by

$$\langle F^m \rangle = \frac{1}{\| \Omega_m^0 \|} \int_{\Omega_m^0} F^m d\Omega$$

We define the bulk strain in the macro model to be the average strain of the linked micro model.
Similarly, the stress in the macro model is also defined in terms of the average stress of the micro model, so

\[
P_m = \frac{1}{\|\Omega_q\|} \int_{\Omega_q} P^\text{m} \, d\Omega
\]  

where \( P \) is the second Piola–Kirchhoff stress.

Note that in Belytschko et al. [4], we have already proven that the relation between bulk strain and stress as defined by Eqs. (3)–(5) are rank-one stable, if the material in the perforated unit cell is rank-one stable. In other words, we have shown that if we restrict the perforated unit cell to material that is strictly elliptic, then we assure the rank-one stability of the governing partial differential equation of the macro model.

2.2. The equivalent discontinuity

Another crucial feature of the MAD method is the coarse-graining of the micro cracks and material damage emanating from the response of the unit cell. The objective of this approach is to segregate the bulk strain from the strain associated with unstable material behavior; the unstable behavior is contained entirely in the discontinuity which is passed to the macro model.

Since the magnitude of the displacement jump and the traction are both passed to the macro model, in effect, a cohesive law across

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**Fig. 4.** Representation of crack opening mode in terms of constant \( F \) mode and hourglass modes.

**Fig. 5.** Schematic of typical bilinear hourglass modes: (a) \( x \)-direction bilinear hourglass mode and (b) \( y \)-direction bilinear hourglass mode.

**Fig. 6.** Schematic of a typical arrangement of cracked nodes: hollow and solid circles denote regular and cracked nodes, respectively, and the dashed line represents the actual crack path.

**Fig. 7.** Schematic of crack opening at cracked node \( I \) and its enriched finite element nodal shape function: \( n_i \) is the normal to crack surface and \( q_i \) denote extra degrees of freedom which determine the crack opening.

**Fig. 8.** Schematic of the onset point of material instability in a softening material for the small strain case in uniaxial strain.

**Fig. 9.** Initial setups for cell failure mode testings.

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**Fig. 10.** Representation of crack opening mode in terms of constant \( F \) mode and hourglass modes.
the discontinuity is passed to the coarse model so that the unstable material behavior is reflected in the cohesive law, whereas the bulk response of macro model remains stable.

A coarse-grained equivalent macro crack can be established from the difference between the effective strain at the macro model, $\varepsilon^M$, and the average strain at the micro model, $\varepsilon^m$ which corresponds to the bulk strain at macro model:

$$U^M \otimes N^M = \varepsilon^M - \varepsilon^m$$

(6)

where $N^M$ and $U^M$ is the coarse-grained crack normal and non-dimensional displacement jump at the macro model, respectively; see Fig. 3.

In general, we cannot directly compute $U^M$ and $N^M$ with Eq. (6) since the left hand side of Eq. (6) is a rank-one tensor whereas the right hand side is usually a rank-three tensor. Therefore, we find $U^M$ and $N^M$ by minimizing the following quadratic form to achieve a single discontinuity for each macro element:

$$\begin{align*}
(U^M, N^M) = \arg \min_{U, N} & \quad U^M \otimes N^M - \varepsilon^M + (\varepsilon^m)^2 \\
\text{subject to} & \quad \|U\| = 0.3 \text{mm} \\
\end{align*}$$

(7)

This coarse-grained discontinuity is then injected into the macro model in elementwise manner through the XFEM approach [7,8]; note that in this study for the actual implementation of the XFEM, we employed the phantom node method [12–16] which is a variant of the conventional XFEM approach. A key advantage of these methods is that no remeshing is needed to treat the growth and evolution of these discontinuities at the macro model; this provides a significant advantage in practical computations.

2.3. The hourglass mode

The boundary motion of unit cells during the failure process, i.e. crack opening and growing, cannot be solely driven by the deformation gradient tensor passed from the macro model, because the deformation gradient tensor only can represent constant deformation fields, whereas important motions of the unit cell for crack opening are bilinear motions; see Fig. 4. To circumvent this difficulty, we described the motion of the unit cell boundary by superimposing constant and bilinear motions as in Eq. (1).

Here, we will briefly describe a numerical scheme which allows us to extract the bilinear motion, i.e. the hourglass mode, from the macro model that is discretized with 4-node quadrilateral ele-
ments [17,18]; the typical hourglass modes for a 4-node quadrilateral element are shown in Fig. 5.

Based on Flanagan and Belytschko [17], the displacement field of the hourglass mode at the center of a 4-node quadrilateral element can be computed by

$$
\tilde{\epsilon}_i = \sum_j u_{ij}
$$

(8)

$$
\gamma_i = \frac{1}{4} \left\{ h_i - \left( \sum_j h_j x_j \right) b_{ij} - \left( \sum_j h_j y_j \right) b_{ij} \right\}
$$

(9)

where $x_i$ is the current nodal coordinates of the finite element, and $h$ and $b$ are defined respectively as

$$
\begin{bmatrix}
  h_i \\
  b_{x_i} \\
  b_{y_i}
\end{bmatrix} = \begin{bmatrix}
  \frac{\partial N_i(0)}{\partial x} \\
  \frac{\partial N_i(0)}{\partial y}
\end{bmatrix}
$$

(10)

where $u_{ij}$ and $\gamma_i$ are the nodal displacements and the gamma projection operator of the macro element associated with the unit cell, respectively. Note that to prescribe the computed hourglass mode along the unit cell boundary, we used a normalized bilinear field; i.e. $\epsilon_i = \frac{u_{ij}}{b_{iy_i}}$ since $u_{ij}b_{iy_i}$ is the hourglass displacement vector at the center of the macro element and does not have a field.

3. Representation of micro cracks

For the predictions of micro cracking behaviors in unit cells, the cracking nodes method [9] is employed. The cracking nodes method [9] is based on the XFEM [7,8,12]. The major difference between the XFEM and the cracking nodes method is that in the cracking nodes method, the growth of the actual crack is tracked and approximated with contiguous discrete crack segments that lie on finite element nodes so that fracture behavior beginning from arbitrary crack nucleations to macroscopic crack propagation is seamlessly modeled.

A typical arrangement of the cracked nodes is shown in Fig. 6 along with the actual crack path that is approximated. It can be seen that the cracking nodes method approximates the actual crack path by injecting discrete crack segments. This feature
enables the method to avoid the complexity of tracking crack geometry due to micro structural details. Note that as shown in Fig. 6, near the material interface, the crack segments are injected so that the crack segments are aligned with material interfaces.

3.1. Overview of the cracking nodes method

During failure analysis in micro model, a crack segment is injected at a finite element node when the finite element node satisfies the loss of material stability criterion which will be discussed subsequently. In the cracking node method, the displacement field is defined based on the XFEM approach [8] with small modifications:

\[
\mathbf{u}(\mathbf{X}, t) = \mathbf{u}^{\text{cont}}(\mathbf{X}, t) + \mathbf{u}^{\text{disc}}(\mathbf{X}, t) = \sum_{i \in \mathcal{S}} N_i(\mathbf{X}) \mathbf{u}_i(t) + \sum_{j \in \mathcal{S}_c} N_j(\mathbf{X}) H\left(\frac{n^0_j \cdot (\mathbf{X} - \mathbf{X}_j)}{|\mathbf{X} - \mathbf{X}_j|}\right) \mathbf{q}_j(t)
\]

(13)

where \( \mathcal{S} \) is the set of all finite element nodes and \( \mathcal{S}_c \) is the set of cracked nodes, i.e. \( \mathcal{S}_c \subseteq \mathcal{S} \) and \( \mathcal{S}_c \cap \mathcal{S}_c = \mathcal{S}_c \), and \( H(\cdot) \) is the step function defined by:

\[
H(x) = \begin{cases} 
1 & \forall x \geq 0 \\
0 & \forall x < 0
\end{cases}
\]

(14)

Note that in Eq. (13), \( n^0 \) is the normal to the crack surface in the reference configuration \( \Omega_0 \). In general, \( n^0 \) can be computed by pulling back the computed crack normal in the current configuration at time \( t_{cr} \), i.e. \( n^0_{t_{cr}} \), to the reference configuration \( \Omega_0 \) in terms of Nanson’s law:

\[
n^0_i = J^{-1} n^0_{t_{cr}} \cdot F(X_i, t_{cr})
\]

(15)

where \( F(X_i, t_{cr}) \) is the deformation gradient tensor at the material point \( X \) at time \( t_{cr} \) and \( J \) is the determinant of the deformation gradient tensor.

The crack opening of each discrete crack segment is a wedge function as shown in Fig. 7. This implies that the change in angle between the normal and the crack surface due to large shear strains cannot be considered; note that this is not the limitation of the cracking nodes method since this can easily be corrected by defining the crack surface in terms of the material or element coordinates.
3.2. Fracture Law: the loss of material stability

The micro cracks are injected when the material loses stability. For the small strains in uniaxial loading, loss of material stability occurs when the material tangential modulus becomes negative as shown in Fig. 8; this is called strain softening. In a rate-independent material, loss of stability coincides with loss of hyperbolicity for the dynamic system, and the conditions are well known [19].

Fig. 16. The comparison of load–deflection curves for the two different loading cases: (a) the MAD method without the hourglass mode, and (b) the MAD method with the hourglass mode.

Fig. 17. The initial setups for the failure analysis of a ceramic ring with: (a) the DNS and (b) the MAD methods.
a measure of the material stability, we define the material stability indicator \( S \) as
\[
S(A) = \min_{h_1, h_2} h_1 \otimes h_2 : A : h_1 \otimes h_2 \quad \forall \ h_1 \text{ and } h_2
\]
where \( h_1 \) is the polarization direction, \( h_2 \) is the direction of the wave propagation, and \( A \) relates the rate of stress to the rate of strain; i.e. the tangential modulus tensor.

At the point that there exist any arbitrary set of \( h_1 \) and \( h_2 \), such that
\[
S(A) \leq 0 \quad \forall \ h_1 \text{ and } h_2
\]
a discontinuity is introduced so that the crack normal is coincident with \( h_1 \).

In this study, material softening is modeled by a continuum damage model [20]; in this damage model, a scalar damage parameter \( D \) was introduced to represent the extent of material damage. The constitutive relation is then given as:
\[
\sigma_{ij} = A_{ijkl} e_{kl}
\]
\[
A_{ijkl} = (1 - D)C_{ijkl} - \frac{\partial D}{\partial e_{ij}} C_{ijkl} e_{pq}
\]
where \( \sigma \) and \( \epsilon \) is the rate of stress and the rate of strain, respectively, \( D \in [0, 1] \) is the damage parameter, \( C_{ijkl} \) is the elastic modulus of the undamaged material; an increase in damage parameter \( D \) leads to a material softening behavior, i.e. the loss of material stability.

4. Numerical examples

4.1. Computation of the coarse-grained equivalent discontinuity

We will initially illustrate the application of the coarse-graining procedure to a unit cell with micro cracks. We consider a specimen as shown in Fig. 9. A boron particle and aluminum matrix is considered at the center of the specimen. The bottom of the specimen is clamped and the top of the specimen is pulled with a constant velocity, \( \dot{v} = 10 \text{ m/s} \).

As can be seen from the right column of Fig. 10, contiguous discrete micro cracks are nucleated around the boron particle at the beginning of the failure process, and then complete percolation of the unit cell has occurred at the end of the failure process. The computed orientations of the coarse-grained cracks along with their crack opening magnitudes are represented in the right column of Fig. 10; the orientations of the coarse-grained cracks are quite well aligned with the emerged micro cracks.

4.2. Boundary motion of the fractured unit cells

We will further demonstrate the advantages of the hourglass mode to unit cell boundary conditions by considering two different failure modes. For the clear demonstration, we consider a set of specimens as shown in Fig. 11. A boron particle and aluminum matrix is considered again at the center of each specimen, and

The damage evolution law is given by
\[
D(\epsilon) = 1 - (1 - A)\epsilon_{th} \epsilon^{-1} - Ae^{-B(\epsilon - \epsilon_{th})}
\]
where \( \epsilon \) is the effective strain, \( A \) and \( B \) are characteristic parameters of the material, and \( \epsilon_{th} \) is the initial damage threshold strain. The effective strain \( \epsilon \) is defined as
\[
\epsilon = \sqrt{H(e_{i}^{p}) e_{i}^{p} e_{i}^{p}}
\]
where \( e_{i}^{p} \) is the ith principal strain; it should be noted in Eq. (21) that compressive strain components are filtered out and therefore do not contribute to the damage evolution. When the tangential stiffness matrix \( A \) in Eq. (19) undergoes loss of stability as defined by Eqs. (16) and (17), the crack segments are injected into the unit cell in terms of the cracking node method.
the bottom of each specimen is clamped. At the top of the specimen, we applied two different constant velocity boundary conditions so that those boundary conditions derive two different boundary motions of the fractured unit cells; i.e. linear and bilinear boundary motions.

An initial crack is located at the right side of each unit cell edge, and then make it propagates toward the left side edge. For fracture, we used the material stability criterion along with the fracture energy \( G_f = 6.0 \times 10^4 \) N/m. The discretized fine scale model is shown in Fig. 11(a); its solution is henceforth referred to the direct numerical simulation (DNS) result. The coarse scale model and its linked unit cell model for the MAD method are shown in Fig. 11(b); the finite element denoted by the dashed line is semi-concurrently linked with the unit cell in terms of the MAD method.

The results for the prescribed uniform constant velocity boundary condition are shown in Fig. 12; note that Fig. 12(b) and (c) shows the results for the MAD method with and without the hourglass mode, respectively. As can be seen from Fig. 12(a), the displacement field of the DNS is close to a constant \( F \) mode, and the MAD method can reproduce the displacement field regardless of the hourglass modes. In this case, as shown in Fig. 13, the peak load of the DNS and the MAD method are identical for all cases.

However, once a bilinear mode starts to derive the unit cell motion, the role of the hourglass mode becomes crucial. The results for the prescribed linearly varying constant velocity boundary condition are shown in Fig. 14; Fig. 14(a) shows the results for the DNS, and Fig. 14(b) and (c) shows the results for the MAD method with and without the hourglass mode, respectively. As can be seen form Fig. 14(a), the displacement field of the DNS shows bilinear deformation, i.e. the hourglass mode, and such bilinear mode is only reproduced at the unit cell when the hourglass mode is considered; see Fig. 14(b). Whereas, as shown in Fig. 14(c), the MAD method without the hourglass mode cannot correctly reproduce bilinear deformation in the unit cell and as a consequence, the MAD method quite over predicts the peak load; see Fig. 15.

Fig. 20. The comparison of the DNS and the MAD results for the deflection histories at three different points: (a) point A (b) point B and (c) point C.
The effects of the hourglass mode are more clearly observed from Fig. 16. As shown in Fig. 16(a), when the hourglass mode is not considered in prescribing the boundary condition of the unit cell, the behavior of the unit cell for the constant and bilinear motions are identical and the MAD method predicts the same peak load regardless of the actual deformation of the linked macro finite element. However, as shown in Fig. 16(b), if the hourglass mode is used to prescribe the boundary condition of the unit cell, the behavior of the unit cell with those two different motions are distinguished and the method could correctly predict the peak load.

4.3. Failure of quasi-brittle ring under impulsive loading

To further test the adequacy of the MAD method, we considered a multiple crack growth problem in a ceramic ring which is loaded impulsively. Fig. 17(a) and (b) illustrate the two fold symmetry models for the DNS and the MAD analysis, respectively. A vertical discontinuity at the macro scale, including both the direction and the hourglass mode from the linked macro finite element. By prescribing the boundary motion of the unit cell displacements with the coarse-graining of an equivalent discontinuity, and the coupling of the boundary motion of the unit cell displacements with the hourglass mode from the linked macro finite element. By means of these concepts, it is possible to compute an equivalent discontinuity at the macro scale, including both the direction and the magnitude of the discontinuity, and then link it to the macro scale model along with the computed stress from the unit cell that are computed over the perforated unit cell domain. The presented multiscale method is further combined with the extended finite element method for the coarse scale model and the cracking nodes method for the fine scale model so that arbitrary discontinuities at both scales can be accurately modeled.

The effectiveness of the presented multiscale method has been demonstrated with manufactured problems by comparing the results for the method with direct numerical simulations of full fine-scale models. It is quite clear that the predicted peak loads and final failure patterns from the method agree quite well with those from the direct numerical simulations.

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