Theoretical and Applied Fracture Mechanics 72 (2014) 100-109

Contents lists available at ScienceDirect

Theoretical and Applied Fracture Mechanics

journal homepage: www.elsevier.com/locate/tafmec

Multiscale failure analysis with coarse-grained micro cracks and damage

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ARTICLE INFO

Article history: Available online 9 May 2014

Keywords: Multiscale method Failure analysis Extended finite element method Cracking node method

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.

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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 [1]. However, most of the conventional multiscale methods such as those described in Zohdi and Wriggers [2], and Nemat-Nasser and Hori [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 [1,4–6] in conjunction with the extended finite element method (XFEM) [7,8] to model the equivalent discontinuities at the macro scale and the cracking node method [9] to model material failure behaviors at the micro scale.

The MAD approach we are taking is closely related to the FE^2 approach of Feyel and Chaboche [10] and Feyel [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







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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, and then receives stress from the unit cell; for the measure of the deformation and the stress, the deformation gradient, *F*, and the second Piola-Kirchoff 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

$$\boldsymbol{u}^{m}(\boldsymbol{X}) = (\boldsymbol{F}^{M} - \bar{\boldsymbol{I}}) \cdot \boldsymbol{X} + \boldsymbol{q}^{M} \boldsymbol{X} \boldsymbol{Y}(\boldsymbol{X}) \quad \boldsymbol{X} \in \boldsymbol{\Gamma}^{m}$$
(1)

where \mathbf{u}^m is the displacement field for the micro model boundary, $\bar{\mathbf{I}}$ is the second order identity tensor, $\mathbf{q}^M XY$ is the hourglass mode displacement field to represent crack opening in the micro model and Γ^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.



Fig. 1. Schematic of the multiscale linkage between macro and micro models.

(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 Γ_0^D and a damage localization band Ω_0^L ; 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. $\tilde{\Omega}_0^m = \Omega_0^m \setminus (\Gamma_0^D \cup \Omega_0^L)$, and then the averaging operation for any given function $f(\mathbf{X})$ is defined by

$$\langle f(\boldsymbol{X}) \rangle = \frac{1}{\|\tilde{\Omega}_0^m\|} \int_{\tilde{\Omega}_0^m} f(\boldsymbol{X}) \mathrm{d}\Omega$$
⁽²⁾

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 $\tilde{\Omega}_0^m$.

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

$$\langle \boldsymbol{F}^{m} \rangle = \frac{1}{\|\tilde{\Omega}_{0}^{m}\|} \int_{\tilde{\Omega}_{0}^{m}} \boldsymbol{F}^{m} \, \mathrm{d}\Omega \tag{3}$$

We define the bulk strain in the macro model to be the average strain of the linked micro model:



Fig. 2. Schematic of: (a) a typical micro model with material failure and (b) its corresponding perforated unit cell domain.



Fig. 3. Schematic of: (a) a typical failure pattern in the micro model and (b) its coarse-grained equivalent discontinuity in the macro finite element.

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