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Monte Carlo simulation of complex cohesive fracture in random heterogeneous quasi-brittle materials

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ABSTRACT

A numerical method is developed to simulate complex two-dimensional crack propagation in quasi-brittle materials considering random heterogeneous fracture properties. Potential cracks are represented by pre-inserted cohesive elements with tension and shear softening constitutive laws modelled by spatially-varying Weibull random fields. Monte Carlo simulations of a concrete specimen under uni-axial tension were carried out with extensive investigation of the effects of important numerical algorithms and material properties on numerical efficiency and stability, crack propagation processes and load-carrying capacities. It was found that the homogeneous model led to incorrect crack patterns and load–displacement curves with strong mesh-dependence, whereas the heterogeneous model predicted realistic, complicated fracture processes and load-carrying capacity of little mesh-dependence. Increasing the variance of the tensile strength random fields with increased heterogeneity led to reduction in the mean peak load and increase in the standard deviation. The developed method provides a simple but effective tool for assessment of structural reliability and calculation of characteristic material strength for structural design.

1. Introduction

Quasi-brittle multiphase materials, such as concrete, fibre-reinforced polymer composites and toughened alloys, are widely used in engineering structures and systems in many industries. Many of them have intrinsic heterogeneous and nonlinear mechanical properties due to random distribution of multiple phases from nano-, micro-, meso- to macro-scales. Their underlying mechanical properties, dependent on their compositions, microstructures, and loading history, in turn directly determine the performance and reliability of structural systems. Therefore, a better understanding of their mechanical properties including damage and fracture by experiments and computer modelling has become one of the most critical and challenging engineering and scientific problems (Oden et al., 2003; Kassner et al., 2005). This paper is focused on finite element modelling of nonlinear fracture in these materials.

1.1. Numerical characterisation of random heterogeneity of materials

There are basically two approaches in characterising the random heterogeneity in materials numerically: the direct approach and the indirect approach. In the direct approach, the different phases in a material such as the matrix, inclusions and interfaces are explicitly modelled by finite elements and their material properties are directly assigned to the elements. The randomness in the spatial distribution of different phases is realised by randomised positions and shapes of inclusions (e.g., fibres, grains and aggregates). In the indirect approach, the material properties such as the tensile strength and the fracture energy are modelled as spatially-varying random fields with given correlation structures in the domain of interest, so different phases are implicitly modelled. To the best knowledge of the authors, there is no report available on comparing which method is superior in terms of computational efficiency and effectiveness to date.

Both the direct approach and the indirect approach have been widely employed but mostly for two-dimensional (2D) problems. As examples of the direct approach, Teng et al. (2004), Zhu et al. (2004) and Lopez et al. (2008a,b) explicitly modelled the matrix, coarse aggregates of random shapes and sizes and interfaces in concrete specimens under 2D tension and compression. Realistic and complex crack patterns were successfully simulated. Using the similar approach, Caballero et al. (2006) modelled 3D meso-scale fracture in a 80 mm concrete cube with 14 and 64 aggregates explicitly embedded in the matrix. This appears to be the only journal publication on 3D fracture of concrete using the direct approach. Trias et al. (2006) explicitly modelled fibres as plane circles in a representative volume element (RVE) of carbon fibre

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reinforced polymers. Al-Ostaz et al. (2007) carried out a similar study using Voronoi cells and Delaunay triangulation to characterise random distribution of fibres in the polymer matrix. Sfantos and Aliabadi (2007) also utilised a Voronoi tessellation method for generating artificial microstructures with randomly distributed and orientated grains to simulate the inter-granular micro-fracture evolution in polycrystalline brittle materials. No attempt has been made to obtain the statistical information of the responses using the Monte Carlo simulation (MCS) method, probably due to the high computational cost associated with generating a large number of finite element meshes and the high nonlinearity involved in the cohesive fracture process.

In the indirect approach, many new methods have been developed for generating realistic random fields of material properties (e.g., Koutsourelakis and Deodatis, 2006; Xu and Graham-Brady, 2005; Graham-Brady and Xu, 2008), but most of them have not been used in damage and fracture modelling. By modelling material properties as non-Gaussian random fields (typically Weibull distribution for concrete), Yang and Xu (2008), Bruggi et al. (2008) and Most (2005) modelled discrete crack propagation in concrete beams. All these studies used MCS to assess the structural reliability, probably thanks to the ease in generating random fields. No 3D simulation of fracture using the indirect modelling approach has been reported to the best knowledge of the authors. It is worth noting that as an indirect approach, the Weibull integral method proposed by Bazant and Planas (1998) is able to take into account the random heterogeneity of material strength but it does not require a large number of random samples. It was recently generalised to model structures with non-uniform stress fields (Bazant et al., 2007) and applied to size effect investigation (Vorechovsky and Sadílek, 2008). Although being simple and efficient, this method has limitations. For example, it can neither consider spatial correlation of local strengths nor explicitly model crack initiation and growth processes.

1.2. Numerical models for crack propagation

The continuum smeared crack models have been used to study heterogeneous and stochastic aspects of local failure since 1994 (Carmeliet and Hens, 1994; Gutierrez and De Borst, 1999; Vorechovsky, 2007). It is difficult however for existing smeared crack models to simulate macroscopic discrete cracks and particularly to calculate crack widths which are needed in serviceability design of materials and structures. It appears that more heterogeneous and stochastic models now employ the discrete crack approach, which is mostly based on the cohesive crack model (Espinosa and Zavattieri, 2003a,b; Zhou and Molinari, 2004; Tomar and Zhou, 2005; Most, 2005; Pearce and Kaczmarczyk, 2008) where cohesive interface elements are pre- or dynamically inserted into existing elemental edges. For problems with crack paths unknown a priori, fine meshes are needed to minimise the dependence of crack paths on the initial FE mesh. This often leads to large-scale nonlinear equation systems, of which the computational costs often become prohibitively expensive when uncertainties are further taken into account by using MCS method or non-MCS stochastic methods. To overcome this difficulty, Yang and Xu (2008) developed a heterogeneous cohesive rack model based on Weibull random fields of fracture properties and remeshing with a new crack growth direction criterion. The model was able to predict more realistic tortuous crack paths and assess the structural reliability using the MCS. Compared with models with pre-inserted cohesive interface elements (CIEs), this remeshing-based model has much higher computational efficiency as it employs relatively coarse meshes with far fewer nonlinear CIEs without compromising the accuracy. However, this model becomes cumbersome when modelling complex crack patterns. Other non-classical models, such as lattice model (Blair and Cook, 1998; Cusatis et al., 2003a,b) have also been developed in fracture modelling of heterogeneous materials.

Clearly only 2D fracture has been modelled in the limited existing studies which considered heterogeneity and randomness. Statistical analysis using MCS has been rarely conducted due to its high computational cost. The mesh-objectivity of results in stochastic fracture modelling remains a challenging problem in all crack models, due to unresolved puzzles on crack resolution or fractals (Carpinteri et al., 2006).

1.3. Methods of extracting statistical responses

To date, the most general and robust method for processing and estimating the uncertainty or reliability of structural performances is still the Monte Carlo simulation method. Compared to other methods such as stochastic finite element method which requires the variability of random parameters be small (Altus and Givli, 2004), the MCS method is applicable to any problems for which the deterministic problem can be solved, as long as the sample number is sufficiently large. For random heterogeneous multiphase materials involving high nonlinearity and fracture, the MCS method seems the best option. In fact, all the very limited 2D studies with statistical analysis used this method (Most, 2005; Vorechovsky, 2007; Yang and Xu, 2008; Bruggi et al., 2008). It may be noted that a 3D study (Papadrakakis et al., 2008) treats concrete as a homogeneous materials although the MCS method is used to generate response statistics from simulations with different material properties.

The biggest disadvantage of the MCS is that it requires a considerable number of samples from the same number of nonlinear analysis. Nonlinear modelling of multiple crack propagation in multiphase materials is very time consuming, even for small specimens as RVEs. This makes supercomputers a necessity when it is used if a large number of random variables are considered. To overcome the bottleneck of computation cost, a variety of exciting new techniques are emerging to reduce the required sample number (e.g., Webster, 2007; Ganapathysubramanian and Zabaras, 2007; Au and Beck, 2001). However, none of these new techniques has been applied to fracture modelling of complex multiphase materials.

1.4. Scope of this study

This study develops a numerical method to simulate the complex 2D fracture process in quasi-brittle materials considering random heterogeneous fracture properties, in a view to critically assess their performance and structural reliability under external loadings. In this method, all the finite elemental edges in the domain of interest are regarded as potential cracks, modelled by pre-inserted cohesive interface elements with tension and shear softening laws. The special features of this study are: (i) the cracks are modelled by a special type of "cohesive elements" (COH2D4) in the general-purposed finite element analysis package ABAQUS (2007). The cohesive elements, only available in Abaqus Version 6.5 or higher, are designed to model bonded interfaces. Their effectiveness in modelling cracks has hardly been validated. Another intention of this study is to fully exploit the powerful pre/post-processing modules and standard/explicit solvers of Abaqus in modelling complex fracture problems; (ii) the softening laws of the cohesive elements are modelled as spatially-varying Weibull random fields, i.e., an indirect approach is used to model the random heterogeneity of fracture properties; (iii) the statistical information of structural responses is obtained by extensive Monte Carlo simulations for a range of heterogeneity levels, which have rarely been conducted before; (iv) a concrete specimen under uniaxial tension is modelled as a benchmark problem with extensive parametric studies and investigation of the effectiveness and efficiency of rel-