International Journal of Solids and Structures 63 (2015) 82-98

Contents lists available at ScienceDirect



International Journal of Solids and Structures

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



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Gradient-based adaptive discontinuity layout optimization for the prediction of strength properties in matrix–inclusion materials

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ARTICLE INFO

Article history: Received 18 December 2012 Received in revised form 7 November 2014 Available online 21 March 2015

Keywords: Discontinuity layout optimization Limit-analysis Gradient method Adaptivity Material strength Multiscale modeling

ABSTRACT

The prediction of strength properties of engineering materials, which in general are time dependent due to chemical and deterioration processes, plays an important role during manufacturing and construction as well as with regard to durability aspects of materials and structures. On the one hand, the speed of production processes and the quality of products may be significantly increased by improved material performance at early ages. On the other hand, the life time of materials and structures can be enlarged and means of repair and maintenance can be optimized.

For determination of strength properties of materials, an extension of the discontinuity layout optimization (DLO) towards an iterative adaptation of the underlying mode of discretization (nodes and discontinuities) is proposed in this paper. This technique yields an improved representation of the underlying failure mechanism (thus, avoiding interlocking in consequence of the chosen discontinuity layout) at reduced computational costs. The performance of the proposed DLO method is assessed by the re-analysis of problems with available analytical solution and finally applied to upscaling of strength properties considering, in a first step, two-phase material systems representing matrix-inclusion morphologies.

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1. Introduction

Within the framework of multiscale modeling, effective material properties are determined by means of upscaling information from finer scales of observation towards the macroscale. For this purpose, depending on the considered type of material behavior, analytical and/or numerical techniques were proposed in the open literature. E.g. as regards upscaling of stiffness properties, continuum micromechanics is commonly employed with applications to e.g. cement-based materials (Bernard et al., 2003; Pichler et al., 2008), bone (Hellmich et al., 2003), hydroxyapatite biomaterials (Fritsch et al., 2010), wood (Hofstetter et al., 2005; Stürzenbecher et al., 2010), and woven composite fabrics (Chung and Tamma, 1999). More recently, continuum micromechanics was extended towards upscaling of viscoelastic material behavior (Aigner et al., 2009; Pichler and Lackner, 2009; Pichler et al., 2011; Lackner et al., 2006), transport properties (Eitelberger and Hofstetter, 2011; Eitelberger and Hofstetter, 2011), shrinkage

deformation (Pichler et al., 2007), and heat transfer in heterogeneous solids (Özdemir et al., 2008). As regards upscaling of strength properties, continuum micromechanics was applied to concrete (Pichler et al., 2008) and hydroxyapatite biomaterials (Fritsch et al., 2007, 2010). In contrast to analytical methods, numerical methods allow for the solution of complex problems, considering distribution and shape of inclusions as well as complex behavior of the material phases. E.g. the finite element method was successfully applied in Mercatori and Massart (2011) for determination of strength properties of masonry. Limit analysis, on the other hand, was employed for predicting strength properties of cohesive-frictional materials (Ganneau et al., 2006) and upscaling of strength properties of porous (Cariou et al., 2008) and twophase materials (Füssl et al., 2008; Lackner et al., 2006). Hereby, two different approaches of numerical limit analysis were developed on the one hand, the considered domain is divided into elements (Sloan, 1988; Sloan, 1989; Lyamin and Sloan, 2002; Bonet et al., 2008), employing nodes and finite elements for the spatial description of the material system under consideration offering the possibility to represent the microstructure of heterogeneous materials in an appropriate manner. Problems associated with the use of the FEM such as the dependency of the results on the

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underlying discretization and unsatisfactory modeling of the interface behavior between inclusions and the matrix material were reported in Wriggers and Moftah (2006). On the other hand, the approach proposed in Smith and Gilbert (2007, 2008) is exclusively based on discontinuities building up the potential failure mechanism. As regards the latter, no spatial discretization is required. In this work, the aforementioned discontinuity-based approach present in Smith and Gilbert (2007, 2008) for numerical limit analysis considering discontinuity layout optimization (DLO) (Smith and Gilbert, 2007) is combined with adaptive schemes successfully developed in recent years e.g. for the finite-element method, aiming at a numerically efficient and robust method for application of limit analysis to complex material systems.

This paper is organized as follows: The underlying formulation of the methodology of the DLO is reviewed and its extension towards adaptive techniques are presented in the following section. In Section 3, the performance of the proposed adaptive DLO (ADLO) method is assessed by the re-analysis of problems with available analytical solution. Finally, ADLO is applied for the determination of strength properties of matrix–inclusion materials. The obtained results are compared with analytical and/or numerical solutions of benchmark problems, leading to concluding remarks given in Section 4.

2. Methodology

DLO is a limit-analysis methodology for the determination of the collapse load of structures. Recently, this method was applied to geotechnical-engineering problems (Smith and Gilbert, 2007, 2011), and masonry structures (Gilbert et al., 2010). Within the domain of the considered structure, DLO requires the generation of *n* nodes which are connected by *m* discontinuities, of which every one may be a potential failure discontinuity and, thus, contribute to the failure mode. Discontinuities are geometrically generated by connecting nodes. By assigning material properties to every discontinuity (Mohr–Coulomb-type material) and defining boundary conditions, the discontinuities contributing to the failure mechanism are determined aiming at minimization of the internal energy. This leads to an upper-bound (UB) formulation with the following linear programming (LP) problem (for details, see Smith and Gilbert (2007)):

min $\lambda \mathbf{f}_{I}^{T}\mathbf{d} = -\mathbf{f}_{D}^{T}\mathbf{d} + \mathbf{g}^{T}\mathbf{p},$

subject to



where \mathbf{f}_L [N] and \mathbf{f}_D [N] are (2*m*) vectors containing the shear and normal component for live and dead load, respectively, and λ is the failure load factor, \mathbf{g} [N] is the (2*m*) vector containing the product of length ℓ [m] and cohesive shear strength *c* [N/m] of the discontinuities, \mathbf{B} [-] is a (2*n* × 2*m*) compatibility matrix, and \mathbf{N} [-] is a (2*m* × 2*m*) plastic-flow matrix. In Eq. (1), \mathbf{d} and \mathbf{p} represent the unknowns of the LP problem, where \mathbf{d} [m] is a (2*m*) vector of discontinuity displacements, and \mathbf{p} [m] is a (2*m*) vector of plastic multipliers. In Fig. 1, discontinuity *i* is shown, connecting Nodes A and B (Smith and Gilbert, 2007). The assembly of the corresponding compatibility matrix \mathbf{B}_i for the following example is given in the Appendix A. The compatibility requires that the shear and normal displacement of all discontinuities connected to node *j* sum to zero, yielding $\mathbf{Bd} = \mathbf{0}$ as given in Eq. (1). Fig. 2 contains the shear and normal displacements of discontinuities contributing to the failure



Fig. 1. Discontinuity *i* connecting Nodes A and B (notation according to Smith and Gilbert (2007)).



Fig. 2. Failure mode of DLO: Thick lines indicate discontinuities contributing to the failure mode.



Fig. 3. Illustration of the two possible modes of displacement of discontinuity *i*: (a) positive shear and dilation and (c) negative shear and dilation.

mode of the considered example subjected to compressive loading. Hereby, the bottom boundary was fixed with a force acting at the top boundary and free boundaries on the side were chosen. For discontinuities located on unconstrained boundaries (top and side boundaries) s_i and n_i are considered as independent variables. For the other discontinuities, the normal displacement n_i is related to the shear displacement s_i according to the Mohr–Coulomb failure criteria, reading for the case of an associated flow rule $n_i = s_i \tan \phi_i$, where ϕ_i represents the angle of friction. Introducing the plastic multipliers p_i^+ and p_i^- for the *i*th discontinuity, the shear displacement is either in or opposite to the positive shear direction indicated in Fig. 1, giving for the shear displacement in the positive

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