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A calibration procedure for two-dimensional laboratory-scale hybrid finite–discrete element simulations

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ABSTRACT

In recent years, Bonded-Discrete element methods (Bonded-DEM) and hybrid finite–discrete element methods (FDEM) have become widely employed to model brittle fracturing processing in geomaterials. These approaches possess the ability to explicitly simulate fracture and fragmentation, but necessitate a large number of input parameters to be specified. Many of these parameters cannot be directly measured or characterized via laboratory tests and therefore must be estimated via calibration procedures to attain reliable results. In this work, a prescriptive procedure to arrive at a combination of input parameters for the newly developed Y-Geo FDEM code is developed. The proposed procedure is applicable for laboratory-scale simulations where some laboratory testing data for the material to be simulated is available. It uses a combination of the known elastic parameters, uniaxial compressive strength, and Brazilian disc strength of a material as calibration targets and limits the over-determined nature of the calibration problem by considering the similitude of the resulting fracture patterns. The development of this procedure represents a major step forward in obtaining reliable and consistent results using an FDEM approach.

1. Introduction

Numerical models can serve as a useful tool to gain an understanding of the expected mechanical behaviour of rock and other brittle geomaterials and aid in the decision making process for rock engineering problems. Conventionally, numerical approaches can be classified into two categories, namely, those based on continuum formulations and those based on discontinuous or discrete formulations. In general, continuum methods (e.g., finite element methods (FEM), finite difference methods (FDM), and boundary element methods (BEM)) are applicable when deformations are small and the medium is either free of fractures or contains numerous uniformly distributed fractures. Conversely, discontinuous approaches (e.g., discrete element method (DEM) and discontinuous deformation analysis (DDA)) are suitable for mediums that are moderately fractured and where individual blocks are subject to large translations and rotations [1,2].

A common limitation of each of these conventional approaches is the inability to capture the emergence of new discontinuities generated by brittle fracturing processes. Over the last two decades, attempts to ameliorate this limitation have blurred the division between conventional continuum and discontinuous techniques [3]. Although several continuum-based approaches that incorporate emergent discontinuities have been developed (e.g., [4–6]), approaches based on "bonded" discrete element methods have arguably become the most popular. In particular, bonded particle models (BPMs) within PFC2D/3D [7,8] as well as bonded assemblages of triangular and Voronoi elements within UDEC [9] have been widely used to simulate brittle fracturing in rock and other geomaterials ([10–18], among many others). In addition to bonded-DEM approaches, the hybrid combined finite–discrete element method (FDEM) pioneered by Munjiza et al. [19,20], and implemented in the ELFEN [21], Virtual Geoscience Workbench [22], Y-Geo [23], and V-FDEM [24] codes, has emerged as a promising technique to explicitly simulate particle interaction, fracture, and fragmentation processes in brittle geomaterials (e.g., [25–30]).

A key benefit of both the bonded-DEM and FDEM approaches is that failure evolution laws do not need to be prescribed. Instead, the macroscopic behaviour of the material develops as a result of the evolution of micro-scale damage [11–13,31]. Nevertheless, this ability to capture more complex processes is directly linked with an increase in number of input parameters which must be correctly specified. Unfortunately, many of these parameters, even those based directly on fracture mechanics principles, cannot be measured in the laboratory. Instead, these parameters must be established through some calibration procedure. Generally the calibration of

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such models involves adjusting the micro-parameters via trial and error until the macroscopic response of Unconfined Compressive Strength (UCS) and Brazilian Disc (BD) strength models correspond to the macroscopic response observed in the laboratory [11–13,30].

The characterization of micro-mechanical parameters via laboratory techniques represents a challenging task [32]. Many micro-parameters cannot be easily measured and, at the same time, the number of parameters makes calibration an over-determined problem. As a result, the validity of such modelling techniques is often rightly questioned. To improve the confidence in the results of such models, more prescriptive calibration procedures must be devised to obtain suitable input parameters [33,34,15,16]. The purpose of this paper is to develop and present a prescriptive calibration procedure for laboratory-scale models in the 2D Y-Geo FDEM code developed by Mahabadi et al. [23]. To do so, the fundamental principles of the FDEM approach are first reviewed to ensure that the physical meaning of all the required input parameters is clear. Subsequently, the proposed calibration procedure, which involves performing several UCS, BD, and Biaxial simulations, is outlined. As the steps of the procedure are described, the sensitivity of the results to the various input parameters is thoroughly examined. In demonstrating each step of the procedure, the mechanical properties of a high strength micro-fine sulphate cement mortar are considered. Thus, by the end of the paper the Y-Geo input parameters to correctly simulate the mortar, that can be used as a synthetic rock in laboratory studies (e.g., [35]), are established. Although the calibration procedure is demonstrated by considering the properties of a synthetic rock herein, it can be employed for the simulation any brittle geomaterial.

2. Fundamental principles of FDEM

The combined finite–discrete element method (FDEM), a numerical method initially developed by Munjiza et al. [19], permits the dynamic simulation of multiple interacting bodies. A simulation can begin with a single intact domain or a collection of discrete intact bodies. As the simulation progresses, these bodies can deform elastically, translate, rotate, interact, and fracture upon satisfying some fracture criterion, thus producing new discrete bodies. The newly generated bodies can then undergo further movement, interaction, deformation, and fracture. The approach employs a combination of FEM techniques to assess the deformation and evaluate the failure criterion for fracturing and DEM concepts for detecting new contacts and dealing with the translation, rotation, and interaction of discrete bodies.

The calibration procedure developed herein is applicable to the 2D FDEM code, known as Y-Geo [32]. This code represents an extension of the original Y2D code of Munjiza [20,22] that continues to undergo development at the University of Toronto for geomechanical applications. In the following subsections, the fundamental principles of FDEM as implemented in the Y-Geo code are outlined. In describing each of the key processes, including contact detection and interaction, and damage and fracture, the governing parameters which are later determined according to the proposed calibration procedure are introduced and defined.

2.1. Governing equation

In FDEM, each intact body is discretized with a mesh composed of 3-noded triangular elements. An explicit second-order forward finite-difference integration scheme is employed to solve the equations of motion for the discretized system and update the nodal coordinates at each simulation time step. The generalized governing equation can be expressed as [19]

$$\mathbf{M}\frac{\partial^2\mathbf{x}}{\partial t^2}+\mathbf{C}\frac{\partial\mathbf{x}}{\partial t}=\mathbf{F}, \tag{1}$$

where $\mathbf{M}$ and $\mathbf{C}$ are the lumped system mass and damping diagonal matrices, respectively; $\mathbf{x}$ is the vector of nodal displacements; and $\mathbf{F}$ is the nodal force vector, which accounts for forces related to external loading, the interaction of discrete bodies, the elastic deformation of triangular elements, and the deformation of crack elements.

The introduction of numerical viscous damping is required to account for energy dissipation due to non-linear material behaviour and model quasi-static phenomena by dynamic relaxation [20]. The matrix $\mathbf{C}$ is equal to

$$\mathbf{C}=\mu\mathbf{I}, \tag{2}$$

where μ is a constant viscous damping coefficient and $\mathbf{I}$ is the identity matrix.

2.2. Contact detection and interaction

An FDEM simulation can involve a large number of interacting discrete elements. To correctly capture this behaviour, contacting couples (i.e., pairs of contacting discrete elements) must first be detected. Detection is accomplished in Y-Geo using the No Binary Search (NBS) method [36].

Subsequently, the interaction forces resulting from the detected contacts can be defined. Contact interaction forces are calculated between all pairs of elements that overlap in space. In the normal direction, repulsive forces are applied to enforce a body impenetrability condition, while in the tangential direction, frictional forces are applied.

2.2.1. Repulsive forces

The repulsive forces between contacting elements (i.e., couples) are calculated using a distributed contact force penalty function method [37]. According to this method, it is assumed that pairs of contacting couples penetrate into each other and thereby generate contact forces that depend on the size and shape of the resulting overlapping area.

Denoting two contacting discrete bodies as the target, E_t, and contactor, E_c, the overlapping area is $S=E_t\bigcap E_c$, which is bounded by $\Gamma_{E_t\cap E_c}$ (Fig. 1a). The infinitesimal repulsive interaction force, $\mathrm{d}\mathbf{f}$, due to the infinitesimal overlapping area, $\mathrm{d}A$, is given by the difference in the gradients of the potential functions of the elements, φ_c and φ_t, at the points P_t and P_c (which define $\mathrm{d}A$) as

$$\mathrm{d}\mathbf{f}=\left[\mathrm{grad}\,\varphi_c(P_c)-\mathrm{grad}\,\varphi_t(P_t)\right]\mathrm{d}A. \tag{3}$$

The total repulsive interaction force, $\mathbf{f}_c$ on element E_c, is then obtained by integrating the difference of the gradients of the potential functions over the total overlapping area S as

$$\mathbf{f}_c=\int_{S=E_t\cap E_c}(\mathrm{grad}\,\varphi_c(P_c)-\mathrm{grad}\,\varphi_t(P_t))\,\mathrm{d}A. \tag{4}$$

With each of the discrete elements E_t and E_c discretized into n and m finite elements, respectively (e.g., Fig. 1b), the potential functions φ_c and φ_t can be expressed as a summation of the potentials for the constituent finite elements as

$$\varphi_t=\sum_{i=1}^{n}\varphi_{ti} \tag{5}$$

$$\varphi_c=\sum_{j=1}^{m}\varphi_{cj} \tag{6}$$

and the total repulsive force, $\mathbf{f}_c$, can be expressed as a summation over the finite elements:

$$\mathbf{f}_c=\sum_{i=1}^{n}\sum_{j=1}^{m}\int_{E_t\cap E_c}(\mathrm{grad}\,\varphi_{cj}(P_c)-\mathrm{grad}\,\varphi_{ti}(P_t))\,\mathrm{d}A. \tag{7}$$