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Mechanics of granular and polycrystalline solids

Microstructural self-organization in granular materials during failure

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ABSTRACT

The present paper is concerned with the analysis of microstructural instabilities in granular materials and with their relation to both macroscopic localized and diffuse failure modes. A discrete-element (DEM) computer simulation of deformations in an idealized two-dimensional frictional particle assembly subject to various biaxial loadings—notably drained compression and proportional strain paths—is proposed as a prototype model to investigate the underlying physics of material failure. Based on the transfer of the second-order work criterion to the microscopic level, we seek for contacts tagged as c^- within the granular assembly that undergo instabilities during loading history. The DEM computations yield a description of failure as a microstructural self-organization process by which c^- contacts aggregate into clusters which can either grow or breakdown as the network of contacts adjusts itself to externally applied loads during deformation history. It is proposed here that there is a close relation between the clustering of c^- contacts and the resulting failure mode based on cluster size and spatial distribution. Localized deformations are found to correlate well with sustained growth of the above clusters, while diffuse failure has more to do with smaller clusters experiencing suppressed development. A comprehensive statistical analysis on the clusters lends support to this conclusion.

1. Introduction

Granular materials undoubtedly continue to fascinate researchers, even though some key constitutive properties are today well understood. In effect, much effort has been devoted to the study of segregation mechanisms during shear flow. According to numerical studies [1–4], deformation processes in a granular assembly reveal the co-existence of two separate phases: a strong phase representing quasi-linear patterns of contacting grains—the so-called force chains—that transmit the stronger normal forces within the system, and a weaker phase encompassing the remaining grains, which provides lateral stabilization to the force chains. In fact, the constitutive richness of granular material behaviour stems from the very essence of their microstructural constitution, which can be viewed as a disordered assembly of particles interacting through a simple contact law, if long-range forces are to be excluded. It would be expected generally that such a simplified description of the underlying physics would preclude any self-organization of the system. However, rich organized microstructural patterns are observed, even if the complexity of the particle shape such as surface irregularity and concavity are ignored and replaced with spherical particles. Given that granular materials are inherently disordered, they certainly find multiple

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Table 1
Physical and mechanical parameters used for the discrete element model.

Particles diameter (mm)	Density (ρ) (kg/m^3)	k_n/D* (MPa)	k_t/k_n	Friction angle (φ) (deg)
6–18	3000	356	0.42	35

* D denotes the mean diameter between two particles in contact.

ways to rearrange, build and adapt their fabrics in response to an external loading [5]. Here, fabric refers to the topological construct of the contacts between particles. Thus, in the absence of disorder as in quasi-crystalline materials, most of the above salient constitutive features would disappear.

During the past several decades, there has been a great interest in the occurrence of various classes of failure in granular materials [6–11]. While soils can be regarded to some extent as a granular material, this interest was partly justified by the crucial need to better predict and describe gravity-driven phenomena such as rockfalls and landslides. In the middle of the last century, since the pioneering contribution of Hill (1958) [12], many studies have treated failure based on different approaches. In particular, the following basic questions were raised: (i) which class of failure (localized versus diffuse) should occur, (ii) can failure be properly described as a bifurcation problem, and (iii) what are the microstructural origins of failure?

Even though much effort has been expended to address these questions, they remain widely open and require further inquiry. Hence, the purpose of this paper is to probe deeper into the above-mentioned questions following a micromechanical approach. It is shown that various features of failure can be formally checked numerically using an appropriate discrete element code. Just as well confirmed by laboratory experimental tests [13], different modes of failure appear according to the loading path considered. In some cases, the computed strain field presents a chaotic pattern, with no visible sign of structuring. In other cases, localized deformations develop clearly into a shear band [14,15]. As another goal of this paper, we wish to investigate what are the microstructural ingredients that could explain why the deformation of the material localizes or not. For this purpose, material failure is described as a bifurcation process within the general framework of the second-order work theory [9,11]. According to the load-control program, the constitutive response of the material can bifurcate from a quasi-static regime towards a dynamical one [11,16]. This approach was shown to be a powerful mechanical framework that describes most of the failure modes observed before the conventional plastic limit is reached. Furthermore, taking advantage of a micromechanical approach, a microscopic formulation of the second-order work can be proposed [17] to bridge the macroscopic scale to relevant local scales. In particular, the formulation enables us to identify specific contacts associated with a negative local second-order work. These contacts are thought to play a basic role in the development of a failure mode within the material. As such, in this work, we investigate how these particular contacts emerge and evolve within the granular assembly, following a self-organization process, to eventually cluster into mesoscopic structures, the size of which determines the occurrence and the nature of failure [18].

Throughout the paper, both δ and Δ notations stand for time derivatives. They are used, according to the context, to denote infinitesimal and numerical incremental variations respectively.

2. Discrete element modelling

In this numerical study, a two-dimensional discrete element [19] model of a granular packing was considered in order to examine the link between the macro- and micro-scales in terms of instability and the ensuing mode of failure, namely diffuse or localized. The discrete element open source code ‘Yade’ [20] was used to perform the numerical simulations presented in this paper.

The granular packing was initially generated as a cloud of non-touching particles enclosed within four rigid frictionless walls. Then the granular assembly was subjected to a confining pressure $\sigma_2 = 300$ kPa by moving the walls towards the center at a constant rate until the isotropic state is reached. A cohesionless contact law was used to describe the interaction between the particles. It is based on three mechanical parameters: a normal contact stiffness (k_n), a tangential contact stiffness (k_t) and a friction angle (φ) introduced at the contact level through the Coulomb friction law governing the sliding between particles. The damping coefficient λ^a accounting for Cundall’s non-viscous damping [21] was set to 0.05 for all simulations. The mechanical parameters of the granular packing are outlined in Table 1.

It is well recognized that the emergence of either localized or diffuse modes of failure in a granular assembly is related to the loading path followed during the test. For instance, dense sands are more likely to undergo localized failure in the form of one or more shear bands around the limit stress state during a drained compression as demonstrated through several studies [22–25]. On the other hand, diffuse failure can also be observed for the same dense sand along dilatant proportional strain or mixed (stress–strain) paths as long as the material stress response path is strictly inside the Mohr–Coulomb limit.

In the above, a dilatant proportional loading involves a constant parameter $R < 1$ constraining the lateral strain to evolve proportionally to the axial strain such that $\varepsilon_2 = -\varepsilon_1/R$. However, for a dense sand, an exceedingly low R must be chosen in order to avoid the material stress response path reaching the plastic limit condition, which would readily lead to localization. Thus, to explore the characteristics of both localized and diffuse modes within the context of the above-mentioned cases, we adopt two grain assemblies G_1 and G_2 subjected to two different loading paths in the subsequent discrete element modelling. Specimen G_1 represents a ‘dense’ sand ($e = 0.174$) subjected to a drained compression, while G_2 refers to a