Injecting particle scale physics into continuum models of granular materials for large-scale applications.

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Abstract

Models of granular materials that incorporate grain scale behaviour can be developed using a "bottom-up" approach known as micromechanics. Typically these models are derived from laws introduced to represent inter-particle contact behaviour. Here models based on two separate contact laws are compared. The first law is based on a binary contact interaction governed by spring-slider systems similar to those used in discrete element methods. In the second model, an effective contact law is introduced that is based on the observed behaviour of particle clusters.

While the model based on the binary contact law can reproduce some aspects of granular behaviour, it is not capable of predicting both strain softening and dilatant behaviour under biaxial compression. In contrast, the effective contact law is able to reproduce not only the correct stress-strain response, but also the observed microstructural evolution in the two cases examined: uniform deformation and strain localisation.

It has the additional advantage that it is able to simulate granular assemblies where the numbers of particles involved would make discrete element methods impractical. To demonstrate this ability results from a finite element simulation of an assembly consisting of over half a million particles are presented. These results suggest that the contact laws used in micromechanical models must account for physical mechanisms occurring in at least two length scales: at the contacts and within particle clusters.

Micromechanical Models

Discrete element methods have proven tremendously successful because of their ability to reproduce observed behaviour of granular assemblies over multiple length scales. However, these models provide descriptive, rather than predictive, information on the assembly's macroscopic behaviour. In particular, they do not provide an explicit link between the particle scale physics and the macroscopic response of the granular assembly. This is problematic, for example, if the task is to design, or, determine the composition of, a granular material based on a given set of macroscopic rheological properties. Moreover, large-scale applications remain beyond the scope of discrete element simulations. At present, even discrete element simulations of granular assemblies undertaken on supercomputers are limited to a few million particles (a mere handful of sand particles!), while use of oversized particles to solve prototype scale problems leads to scaling errors in the solution (Peters and Horner, 2002; Horner et al., 2001). Thus, to date, continuum methods remain the only practical means of modelling large-scale engineering problems.

Predictive continuum models of granular media that incorporate grain scale behaviour can be developed using a “bottom-up” approach known as micromechanics. The key challenge for micromechanical continuum theory lies in the development of constitutive models that can capture the governing physical mechanisms and material structure at multiple length scales, while still retaining efficiency in their computational implementation. In this context, a granular material may be viewed in hierarchical terms, where the relevant length scales range from the particle scale (microscale), particle clusters (mesoscale), to bulk engineering scale (macroscale).

The great majority of micromechanical constitutive models are conceived from consideration of particle-particle contact behaviour. This contact behaviour is usually described by contact laws governing isolated binary contact systems (Chang and Hicher 2005). However, our studies indicate that physics of particle interactions in at least two different length scales must be introduced for the resulting continuum model to capture observed behaviour (e.g. strain-softening under dilatation). Specifically, our results suggest that physical mechanisms at both the contact scale (e.g. interparticle friction) and meso-scale (e.g. force chains or long-range forces spanning several particles typically found in jammed or interlocked clusters) must be accounted for. The latter requires knowledge of multi-body contact interactions: a multi-body contact law that is the solution to a multi-body contact problem. Although some headway has been made in solving this problem for static granular assemblies (see, for example, the work of Edwards and Grinev (2003) which is based on a 3-body contact problem), a general contact law governing an n-body contact system has yet to be found.

In the absence of an explicit formula governing n-body contact systems, two different approaches are pursued. In the first, a contact law for an isolated binary contact system, i.e. a simple spring-slider model similar to those used in many discrete element models, is adopted. In the second, an effective contact interaction law is derived for a large cluster of particles using discrete element simulations.

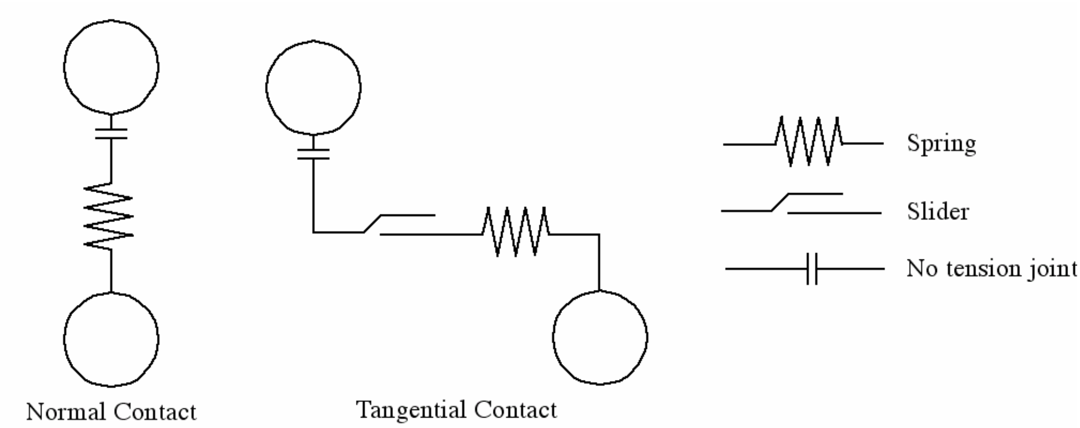

Figure 1: The spring slider model of particle contact governing the binary contact law.

Model based on a binary contact law

The contact law governing the first model is based on a system of interparticle springs, frictional-sliders and no-tension joins similar to that employed in discrete element simulations (e.g. Oda and Iwashita 2000, Peters et al. 2005). In particular, the force normal to each contact is governed by an interparticle spring in series with a no-tension joint; the tangential contact force is governed by a second spring in series with a frictional slider (Figure 1).

The model derived from this contact law is able to reproduce some phenomena characteristic of granular materials. It predicts dilatancy and a preferred direction of contact consistent with those seen in real assemblies. However, the model does not provide enough energy dissipation to exhibit the observed peak stress and subsequent strain-softening behaviour of dense granular assemblies (Figure 2).

Model based on an effective contact law

The model based on the binary contact law fails to reproduce the observed softening behaviour. Specifically, it predicts a monotonic increase in the normal contact forces aligned with the direction of compression. However, experimental studies clearly show that normal contact forces do not increase without bound (Geng and Behringer 2005). In photoelastic disk experiments, the relatively large contact forces developed in the so-called force chains experience a sudden drop once the chain collapses. The effective contact law was developed to capture this behaviour that is characterized by a coordinated release of the normal contact force over several particles (Walsh et. al. 2005). In this law, a plastic component is introduced to reproduce the observed reduction in the normal contact forces that is attributed to the buckling or collapse of force chains. Unlike the previous model, the model based on

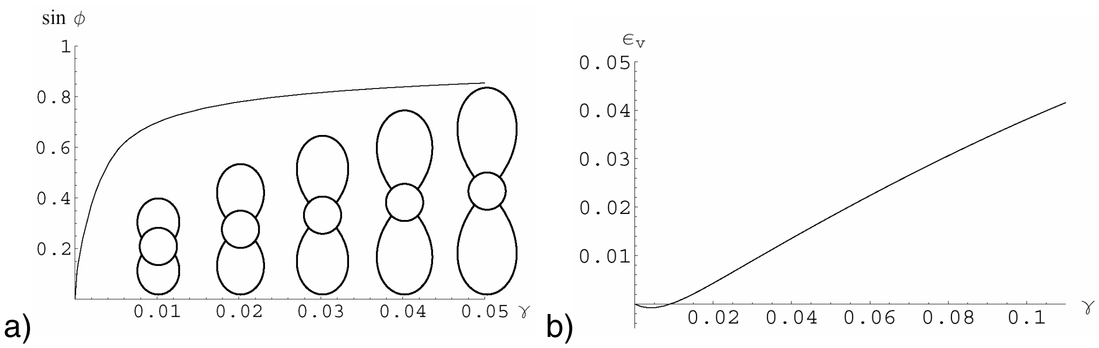

Figure 2: Graphs of a) the sine of the mobilised friction angle vs. the deviatoric strain and b) the volumetric strain vs. the deviatoric strain for the binary contact model under biaxial compression. The inset figures in a) show the evolution of the normal contact force distribution.

the effective contact law accurately reproduces the contact force behaviour in the biaxial compression test (Figure 3).

The reduction in the normal forces is captured in discrete element simulations even though no explicit dissipative mechanism is associated with the normal contact direction. However, a microstructural explanation can be given for this behaviour by considering the way in which forces are transmitted within the assembly. When an assembly undergoes biaxial compression, particle contacts are lost in the direction of extension and chains of particles bearing the majority of the load (i.e. force chains) emerge parallel to the direction of compression. However, these force chains require secondary contacts to provide lateral stability (Radjai et al 1998). As the assembly continues to deform, continuing loss of contacts in the direction of extension results in the eventual collapse of these force chains.

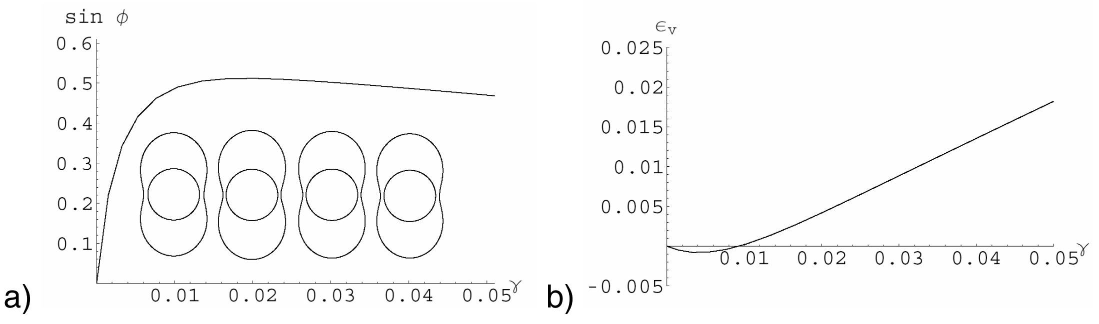

Figure 3: Graphs of a) the sine of the mobilised friction angle vs. the deviatoric strain and b) the volumetric strain vs. the deviatoric for the binary contact model under biaxial compression. The inset figures in a) show the evolution of the normal contact force distribution.

Figure 4 shows the formation and collapse of a force chain, as predicted by a discrete element simulation. When the force chain looses its structural integrity, energy is dissipated by relative tangential motion at the particle contacts. However, the energy lost is that originally stored in the normal contact forces. Thus the collapse of a force-chain results in the coordinated reduction of normal contact forces over several particles even though the contact law used in the simulation has no explicit dissipative mechanism associated with the relative normal contact displacement. These results indicate that micromechanical models developed within the confines of continuum mechanics must take into account these long-range forces developed within particle clusters.

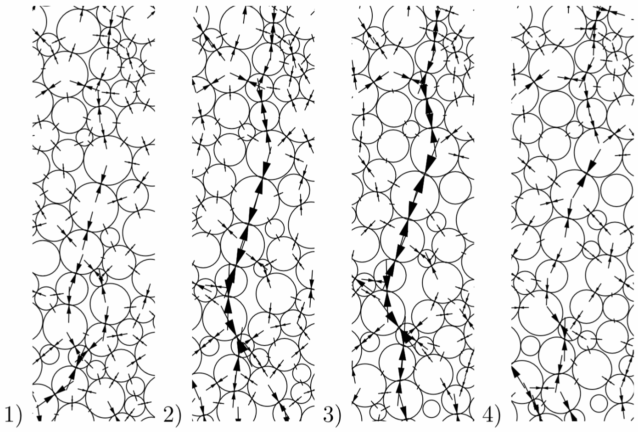

Figure 4: The formation and collapse of a typical force chain

Large scale applications

Materials that experience strain-softening have the potential to undergo strain localisation, in which continued deformation becomes concentrated within a small region of the material. Strain localisation is typically observed in biaxial compression tests in the form of shear bands. The model based on the effective contact law was capable of reproducing shear bands over the range of widths observed in real materials. Moreover, the model was able to predict the correct microstructural evolution within the band, in particular, the bucking of particle columns observed by Oda and Kazama (1998) (see Figure 5) .

The ability to capture both bulk and microstructural behaviours makes these types of micromechanical continuum models invaluable for investigating granular assemblies – especially in applications beyond the reach of current discrete element simulations. This ability is demonstrated by considering the indentation of a two dimensional granular assembly by a rigid flat punch. The width of the assembly is 10 times the width of the punch, while the depth is 5 times the punch width. The punch itself is 100 times the average particle diameter, giving an assembly with over half a million particles. Although this number of particles is outside the capabilities of most discrete element simulations, the finite element simulation of the assembly can be

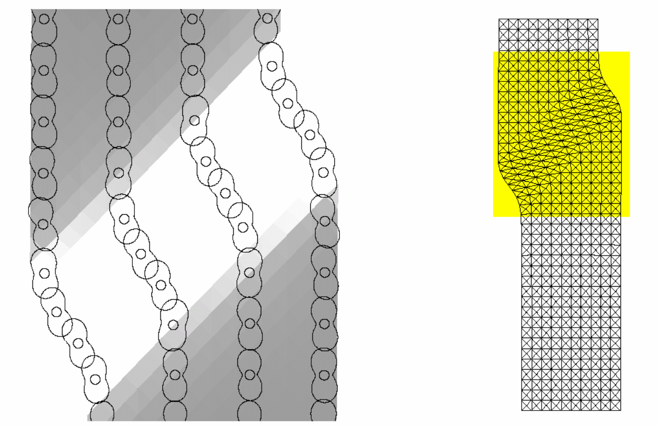

Figure 5: The normal contact force distribution within a shear band predicted by the model based on the effective contact law.

run on a single processor in under 10 hours. Moreover, this particular micromechanical model can predict material behaviour down to the scale of a particle and its first ring of neighbours. Consistent with experiments, Figure 6 shows the predicted rotation fields for the two contact conditions at the granular-punch interface: (a) full-stick contact and (b) frictionless contact. In all cases examined, the rotations are confined to the localization regions. For the case of full-stick contact, the deformation pattern exhibits the characteristic triangular wedge beneath the punch: as shown in Figure 6(a), this solid-like region moves with the punch in rigid body motion and is so-called “dead-zone” in soil mechanics. In contrast, the case of frictionless contact does not lead to any moving solid-like regions within the material. Moreover, the localization zones meet at the centre of the punch surface (as opposed to a point within the material, directly below the punch centreline in Figure 6(a)). The deformation patterns predicted by the model are reminiscent of the classical slip-line field solutions for a granular material at the point of incipient failure, specifically, Prandtl’s solution for full-stick contact and Hill’s solution for frictionless contact (Shield 1953).

Conclusion:

Micromechanics offers a means of incorporating material behaviour across multiple length scales into constitutive laws. This paper has discussed the behaviour of two micromechanical continuum models based on different contact laws. The first model is based on a binary contact law similar to those employed in discrete element simulations was adopted, while the second model is based on an effective contact law derived from observed contact behaviour of groups of particles.

While the first model is able to capture dilatant behaviour, it fails to reproduce the observed peak in the moblilized friction angle. In contrast, the second model which incorporates behaviour at both the microscale (at the level of contacts) and mesoscale (long-range interactions spanning several particles) is able to predict both dilatant behaviour and strain-softening. Moreover, the second model correctly predicts

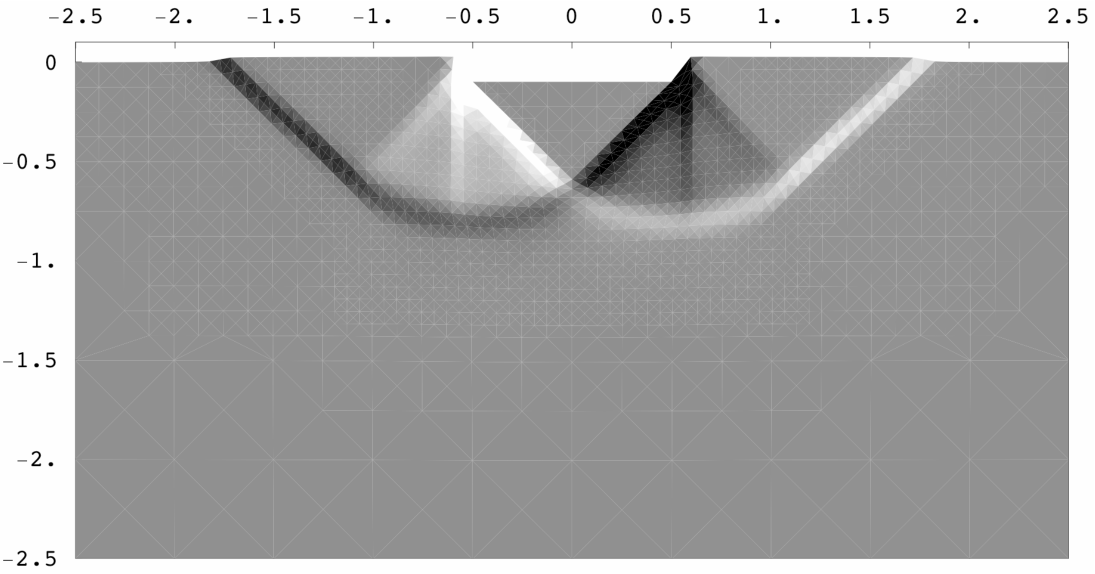

Figure 6a: Particle rotations in strain localisation zones beneath a rigid flat punch (full stick contact). Regions of localisation are similar to Prandtl's slip-line solution.

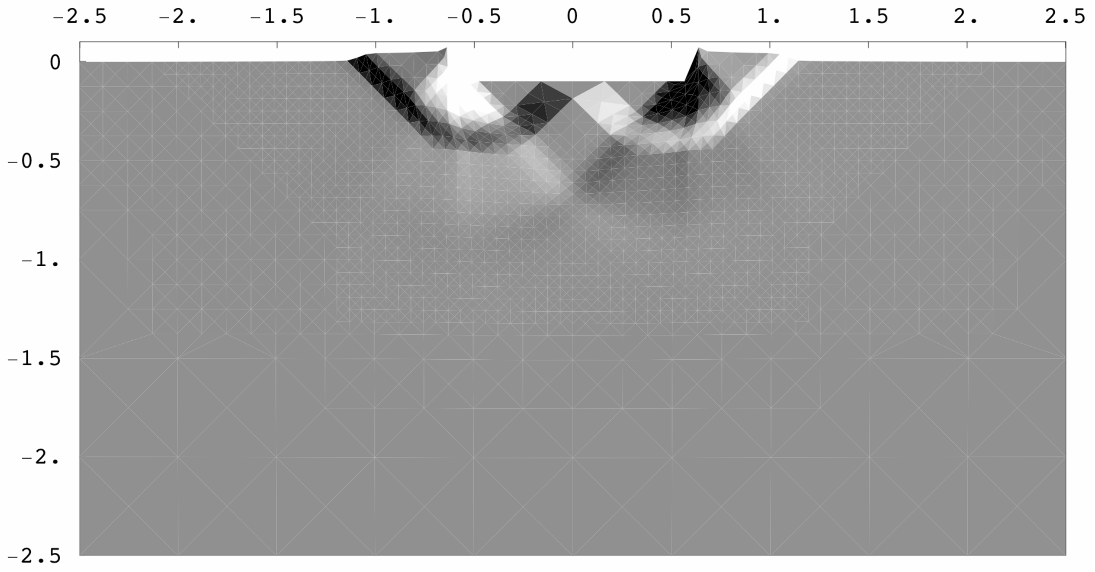

Figure 6b: Particle rotations in strain localisation zones beneath a rigid flat punch (full slip contact). Regions of localisation are similar to Hill's slip-line solution.

microtructural evolution in specimens undergoing strain-localization. These results suggest that the contact law used in the construction of micromechanical models must account for the influence of group behaviour in particulate clusters.

Micromechanical continuum models of this kind offer a reasonably high level of predictive performance for relatively small computational cost of implementation. However, the challenge for the future remains the development of homogenisation schemes that provide an explicit link between material behaviour at multiple length scales – from the particle level to the continuum.

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