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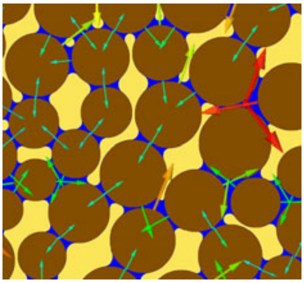
A numerical toolkit to understand the mechanics of partially saturated granular materials



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The mechanisms by which a wetting, non-saturating liquid bestows macroscopic cohesion and strength to a granular material are usually not accessible to micromechanical investigations for saturations exceeding the pendular regime of isolated menisci, easily studied by discrete element models (DEM). The paper by Delenne *et al.* (*J. Fluid Mech.*, 2015, vol. 762, R5) exploiting a multiphase lattice Boltzmann approach, pioneers the simulation of the micromorphology and of the mechanical effects on grains of an interstitial liquid, in equilibrium with its vapour, for the whole saturation range. Interestingly, in accordance with some experiments and phenomenological models, the results suggest that the mechanical effect of capillary forces is maximized for some intermediate saturation level (near 40 % in the model), well beyond the pendular range. In general, the proposed simulation technique opens the way to many studies of partially saturated granular assemblies, for different saturation or imbibition processes and histories.

Key words: complex fluids, granular media

1. Introduction

Mixtures of granular materials with some amount of interstitial liquid (Mitarai & Nori 2006) are ubiquitous in our everyday environment and activities as well as in engineering applications (Mitchell & Soga 2005) and industrial processes (Litster & Ennis 2004). The quasi-static, solid-like behaviour of wet granular materials is considerably influenced by the capillary pressure $p_c = p_a - p_w$, the difference between liquid pressure p_w and the (larger) gas pressure, p_a, entailing additional forces on the solid grains, compared to the dry (or gas-saturated) case, and endowing such materials with cohesion and strength. In general, capillary pressure p_c decreases for growing saturation S, defined as as the ratio of the wetting liquid volume to the total interstitial volume, although p_c–S curves are not uniquely defined, but depend on

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saturation history and process. Pressure uniformity within continuous liquid domains requires complex-shaped, constant-curvature liquid–vapour interfaces, as Scheel *et al.* (2008) visualized by X-ray microtomography.

A recurring issue in the literature on macroscopic modelling of partially saturated granular media, mostly motivated by soil mechanics applications (Mitchell & Soga 2005; Lu, Godt & Wu 2010), is the possibility of dealing with capillary effects in terms of 'effective stresses', or corrected stresses that, if applied to the sole granular skeleton, would produce the same mechanical behaviour. In a saturated medium, such an effective stress tensor $\boldsymbol{\sigma}'$ is very successfully defined by the celebrated Terzaghi formula $\sigma'_{ij} = \sigma_{ij} - p\delta_{ij}$, in terms of total applied stress $\boldsymbol{\sigma}$ and interstitial fluid pressure p (compressive stresses are counted positive here and we use Krmecker's delta). The simplest proposed generalization to non-saturated cases, which is

$$\sigma'_{ij} = \sigma_{ij} - p_a\delta_{ij} + Sp_c\delta_{ij}, \tag{1.1}$$

coinciding with the Terzaghi formula with a volume-averaged interstitial pressure, is, at best, satisfactory as a rough approximation (Lu *et al.* 2010). Appropriate macroscopic modelling of capillary effects, through the effective stress concept or by other means, is still actively debated.

Discrete element modelling (DEM) provides useful insights into the microscopic origins of macroscopic granular material mechanics, but relies on models for intergranular forces, ignoring the continuous interstitial fluid. Its use to model partially saturated grain packs (Richefeu, El Youssoufi & Radjai 2006) is limited to the so-called pendular regime of small saturations, for which the wetting liquid is confined within isolated bridges joining neighbouring grains. Such pairs are attracted by a capillary force $F_0 = \pi\gamma d$ for two spheres of diameter d joined by a small meniscus of a perfectly wetting liquid with surface tension γ, and those tensile forces (which have little dependence on meniscus volume) simply shift the values of normal contact forces in the granular skeleton. Beyond the pendular regime, though (above $S \simeq 5\,\%$ for nearly equal-sized spherical grains according to Scheel *et al.* 2008), the determination of the morphology adopted by the liquid phase and of the mechanical effects of capillary forces escapes simple DEM approaches.

The contribution by Delenne, Richefeu & Radjaï (2015), relying on a two-phase lattice Boltzmann method (LBM) able to provide a complete description of the spatial distribution of the liquid phase throughout the complete saturation range $0 \leqslant S \leqslant 1$, offers a way to overcome this limitation, and shows that coupled LBM–DEM studies are a particularly promising tool to explore the micromechanics of partially saturated granular materials, and discuss the foundations of macroscopic modelling schemes.

2. Overview

Specifically, the study carried out by Delenne *et al.* (2015) uses a two-dimensional (2D) model of an isotropically compressed model granular assembly (care being taken nevertheless to allow for pore-space phase percolation despite the continuous contact network). While the vapour pressure stays fixed below the saturating value, a gradual increase of the liquid content is enforced, resulting in a steady decrease of capillary pressure (as p_w increases). The liquid distribution adapts itself as saturation grows, approximately satisfying equilibrium requirement, which involves motions and rearrangements of liquid nuclei, first in intergranular menisci, then in more extended liquid clusters as those menisci merge, as shown in figure 1. Compared to previous LBM studies of fluid mixtures within porous media (Sukop & Or 2003;

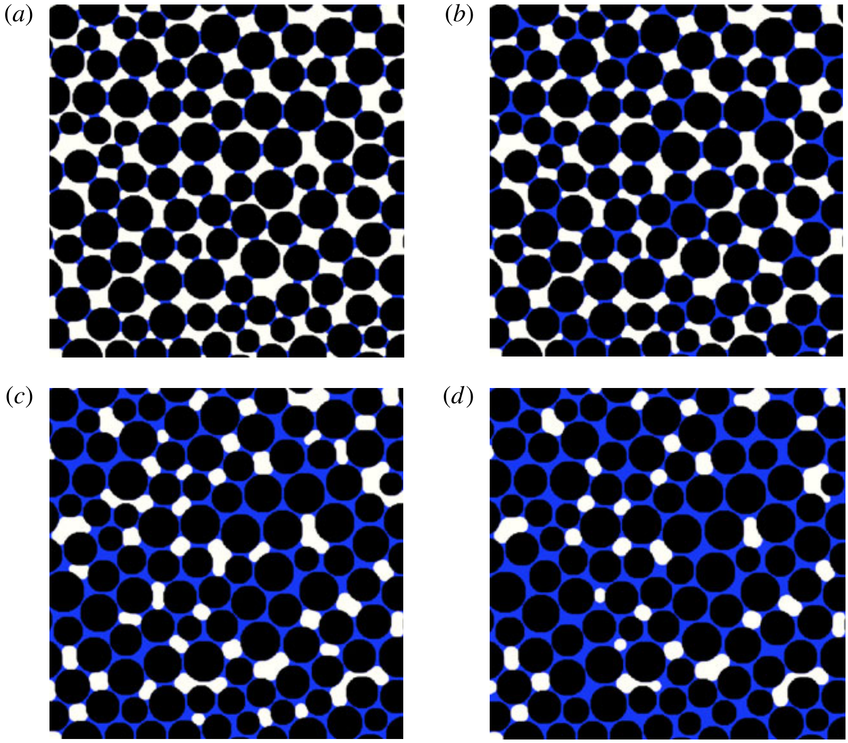

FIGURE 1. Aspects of liquid distribution at growing saturation S.

Huang & Lu 2009), the choice of the condensation route to saturation enables the study of more representative homogeneous states, with no gradient effect on the liquid phase distribution and morphology. After the pendular regime ends ($S=0.15$), menisci are observed to merge into a set of liquid clusters with varying sizes. Those clusters, in turn, gradually coalesce, the percolation threshold of the liquid domain occurring near $S=0.6$. Those phenomena should be qualitatively unchanged between 2D and three-dimensional (3D) models (save for the possibility of both fluid phases simultaneously percolating in 3D).

One major original contribution of the study is the evaluation of Laplace pressures as exerted on grains for varying S. More precisely, Delenne *et al.* (2015) actually evaluate the average pressure increase or decrease within the solid grain phase, with respect to the situation at vanishing liquid saturation, with constant interstitial vapour pressure p_a. Upon investigating the capillary effects on the mechanics of the granular skeleton, this latter value may be fixed to zero, for simplicity. As the grains are kept fixed in this study, a direct measurement of the strength (say, the resistance to shear) of the granular skeleton is not possible. Yet, an effective stress approach to the effect of interstitial fluids on the granular skeleton may be attempted; this amounts to a re-evaluation of the third term of the right-hand side of (1.1). For given total stress transmitted through the medium, $\boldsymbol{\sigma}$, a negative contribution to the pressure in the grains will tend, by compensation, to increase the average contact pressure stabilizing the contact network – the isotropic part of tensor $\boldsymbol{\sigma}'$. The negative capillary contribution to the pressure in the grains, due to the capillary pressure pulling on their surface in contact with the liquid phase, denoted as p_p^-, can be directly calculated in the LBM approach, from the grain perimeter length (in this 2D case) wetted by the liquid. These pressure terms, which are equal to the product of the fast decreasing capillary pressure $p_c(S)$ with either S itself or with a wet perimeter fraction growing with S, reach a maximum for some intermediate saturation (near 0.4 for Sp_c, near 0.6 for $-p_p^-$). A direct application of the effective stress concept would imply, in a grain pack with internal friction coefficient μ^*, a positive capillary contribution to shear strength equal to $-\mu^* p_p^-$. However, the effective stress principle is not expected to apply in such a naive form, as the net capillary effects for intermediate saturations will produce a disordered force field acting on the grains in various directions, as is apparent in the figure by the title, which shows the net capillary forces on the grains, as calculated separately in each wetted region of their perimeters. The effects on contact network stability should differ from those of a global pressure change. Anyway, one should bear in mind that the use of (1.1), or variants thereof, is reported to be qualitatively correct in predicting a maximum capillary contribution to shear strength for some saturation level well above the upper limit of the pendular regime. Qualitatively, the strong capillary pressure decrease as a function of S is compensated by the increase of the grain surface in contact with the wetting liquid.

3. Future

The simplest immediate developments of this work would explore, in a fixed grain pack, the effects of varying solid fraction, coordination number and network anisotropy, on the suction curve $p_c(S)$ and its hysteresis. But the most promising continuation of this work should involve a full-fledged LBM–DEM coupled model, in which the granular network is allowed to readjust to capillary effect. Much awaited direct investigations of cohesion and strength of model unsaturated granular materials should ensue, probably confirming the optimal effect on strength of saturations in the 0.4–0.6 range. The authors are also planning to develop a 3D model, which should eventually enable a critical review of effective stress concepts for partially saturated materials. As the LBM approach is naturally capable of dealing with fluid flow, a whole range of poromechanical phenomena in partially saturated granular materials will become available for numerical studies at the microscopic scale, as well as processes combining imbibition and mixing.

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