

Calculation of capillary forces in a mesoscale assembly of grains

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Résumé :

On propose ici une méthode d'évaluation des forces capillaires dans des assemblages de grains, par minimisation de l'énergie de surface de l'eau à l'aide du logiciel Surface Evolver. La méthode est évaluée dans le cas simple d'un doublet capillaire entre deux grains. Elle est ensuite testée dans le cas de la coalescence de deux ponts dans un assemblage de trois grains. A terme, ces résultats permettront de calculer les forces capillaires dans un assemblage plus complexe afin d'enrichir un modèle multi-échelle de sol.

Abstract :

We present in this work a methodology for calculating capillary forces in grains assembly by minimizing the surface energy of water with the software Surface Evolver. The methodology is first validated on a capillary bridge between two grains. Then we compare numerical and experimental results in the case of the coalescence of bridges in an assembly of three grains. This method will permit to evaluate the capillary forces in a more complex assembly of grains, in order to improve a multi-scale model of soil.

Mots clefs : capillary bridge, cluster, coalescence, surface minimization

1 Introduction

Multiscale models are a powerful alternative approach to continuous and discrete models in the numerical study of granular materials. By embedding a mesoscale, they take into account most of the important physical mechanisms occurring in granular materials. For instance, the 3D H-model developed in [18] and [17] constitutes an analytical incremental constitutive relationship for soil, initially developed in dry conditions.

In many cases, however, granular materials are in partially saturated states. The suction effect resulting from capillary bridges and liquid clusters strongly affects their mechanical behavior. The inclusion of water in model for soils in pendular regime has already been treated in several works as [14] and [13]. Indeed, at the microscale, determination of accurate features for capillary bridges between grains stand

as a subject widely studied both experimentally, for example in [9], and theoretically, by solving Laplace-Young equation with either a toroidal approximation in [8], a cylindrical approximation in [11] and [3] or numerically in [4].

However, for higher degrees of saturation, capillary bridges tend to merge and form more complex clusters that have been far less analyzed. One can, however, mention experimental studies [5] and [7] and theoretical results [15], [16] and [6] regarding the coalescence of bridges. In particular, the incremental evolution of the capillary force at the coalescence of three bridges has been investigated analytically in [6] for a particular three grains configuration.

In the present work, a numerical approach was used to determine the geometry of the liquid phase in contact with spherical particles which minimizes the surface energy for a given volume of water, for different grains configurations. We first consider simple configurations with two or three grains in pendular or funicular regime. Then we infer some preliminary results with ten-grains assemblies, in coherence with the previously mentioned H-model.

2 Calculation of capillary forces with Surface Evolver

Surface energies in wet granular assemblies are calculated with the energy minimizer software Surface Evolver [1]. The capillary forces are deduced from surface energies from the virtual work principle. Spherical grains with the same radius r were used in this approach.

The surface energy of water can be expressed as :

$$E_s = \gamma_w A^{lg} + \sum_{i=1}^N \gamma_i^{sl} A_i^{sl} + \sum_{i=1}^N \gamma_i^{sg} A_i^{sg} \quad (1)$$

with $\gamma_w = 0.073 \text{ N.m}^{-1}$ the surface tension of air/water interface, A^{lg} the area of the liquid/gas interface, N the number of grains in contact with the volume of water, γ_i^{sl} and A_i^{sl} the surface tension and the area of the interface between the grain i and water, and γ_i^{sg} and A_i^{sg} the surface tension and the area of the interface between the grain i and the gas.

The surface tension of the interfaces are related by the Young-Dupré equation :

$$\gamma_i^{sl} - \gamma_i^{sg} = -\cos \theta_i \gamma_w \quad (2)$$

where θ_i is the wetting angle of water on grain i .

Thus, the surface energy of the system can be expressed by :

$$E_s = \gamma_w A^{lg} - \gamma_w \sum_{i=1}^N \cos \theta_i A_i^{sl} + C \quad (3)$$

where C is a constant.

Energy minimization is based on an alternative use of remeshing steps and iterative gradient descent steps.

Initially, a basic geometry is defined (Figure 1 left). During the computational process, the triple lines are represented by edges located at the surface of the grains. The solid/liquid interfaces are represented by

facets geometrically constrained on the grains, with a surface tension γ^{sl} as defined by Eq. (2). Similarly, the liquid/gas interface is made up of facets with a surface tension γ_w .

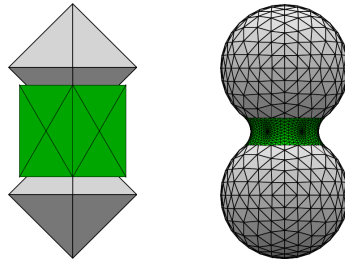


FIGURE 1 – Geometry of a capillary bridge between two grains as initially defined and after meshing and minimization of the surface energy with Surface Evolver.

An iteration of the gradient descent method consists in finding a new geometry for water with a smaller surface energy under the constraint of a fixed volume V . For each vertex x_i , the gradients of the volume constraint $C(x_i) = V(x_i) - V$ and of the energy $E(x_i)$ are calculated. Under the constraint $C(x_i) = 0$, the vertex is moved in the plane orthogonal to $\nabla C(x_i)$. The displacement of the vertex is then given by the orthogonal projection of $\nabla E(x_i)$ on this plane, multiplied by an adequate scale factor [1]. Once a new geometric configuration of smaller energy is reached after some iterations, a remeshing of both the spheres and water surfaces is performed to better account for the real shape of the bodies at stake. Remeshing introduces additional geometric degrees of freedom and new iterative gradient steps are performed.

The main difficulty of the shape optimization process consists in finding the optimal number of remeshings and iterations of the gradient descent method to avoid being trapped in a local energy minimum. For instance, after the coalescence of two bridges, five remeshings of the surface are shown to be sufficient to have a convergence of the capillary force values, with a variation under 0.1% between two remeshings. For a number of gradient descent iterations between 12 and 25, the standard deviation of the value of the capillary force is under 1%. In the present study, all the computations were performed with 20 iterations between two successive remeshings.

Capillary forces are next determined from surface energy following the virtual work principle between two close geometric configurations. A small virtual displacement $\pm\delta d$ is imposed to one particle in the direction of the capillary force, and the force is deduced from the difference in surface energies between the two configurations :

$$F_{cap} = \frac{E_S(\delta d) - E_S(-\delta d)}{2\delta d} \quad (4)$$

For a unique capillary bridge, for instance, the capillary force is equivalent to an additional contact force between the two grains due to the presence of water. In this case, an axial displacement of one of the grains is imposed.

For an assembly of three grains, the force taken into account is the vertical resulting force due to water. In this case a vertical displacement of the upper grain relatively to the others is imposed.

3 Validation for two and three grains systems

Before calculating the capillary forces in complex grain assemblies, the methodology has been checked from simple configurations, such as a capillary bridge between two grains and on a system of three grains with two capillary bridges that coalesce when the volume of water increases.

3.1 Validation for a capillary bridge

As capillary bridges between two grains have been widely discussed in the literature, we can compare our results obtained with Surface Evolver to several other methods. The comparison is carried out on the dimensionless axial capillary force between two grains $F^* = \frac{F}{\gamma_w r}$ expressed as a function of the dimensionless interparticle distance $d^* = \frac{d}{r}$ for an increasing dimensionless water volume $V^* = \frac{V}{r^3}$.

The results obtained with Surface Evolver [2] are compared in Figure 2 with those reported in the literature :

- by numerically solving Laplace-Young equation [4]
- by an experimental fitting [12] :

$$F^* = \cos \theta \exp\left(-\frac{dr}{0.9\sqrt{V}}\right) \quad (5)$$

- by solving Laplace-Young equation with a cylindrical approximation of the bridge [11] :

$$F^* = \cos \theta \left(1 - \frac{1}{\sqrt{1 + \frac{2V^*}{\pi d^{*2}}}}\right) \quad (6)$$

- by measuring experimentally the capillary forces [10]

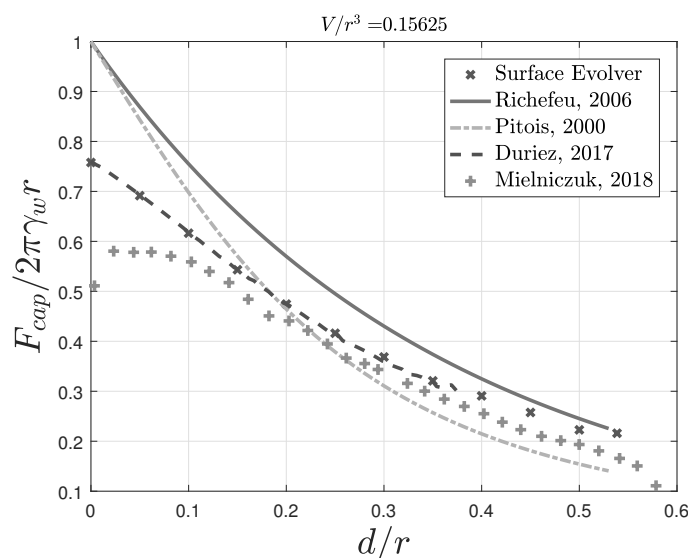


FIGURE 2 – Dimensionless capillary force as a function of the dimensionless interparticle distance in a capillary bridge with $V^* = 0.156$, calculated with Surface Evolver (cross) , by solving Laplace-Young equation [4] (dashed line), with the equation proposed by [12] (solid line) and [11] (dash-dot line) and experimentally measured in [10] (plus).

In Figure 2, it appears that the forces deduced from surface energy minimisation perfectly correspond to

those obtained by solving Laplace-Young equation, except for the rupture distance, which is significantly smaller in [4]. Even through all the models give similar results for $d^* > 0.2$, it should be noted that the results obtained with Surface Evolver are closer to the experimental forces than when using other models (except [4]).

3.2 Validation for an assembly of three grains

As the modelling of capillary forces with Surface Evolver has proven a good accuracy with other models in the case of a capillary bridge, more complex configurations have to be considered. In this section, we compare our numerical results with Surface Evolver to experiments with an assembly of three grains in [5].

The experimental set-up used in [5] consists of three identical spherical glass beads with a radius $r = 4$ mm. The base of the assembly is constituted of two grains, the centers of which are separated by a distance $D_2 = 8.3$ mm. The third grain is placed above at a distance $D_1 = 8.7$ mm from the centers of the other grains (Figure 3). The vertical capillary force is measured by differential weighing between the total mass (beads and water) and the apparent mass of the system. In our simulations, the vertical capillary force is deduced from the virtual work principle as detailed in section 2.

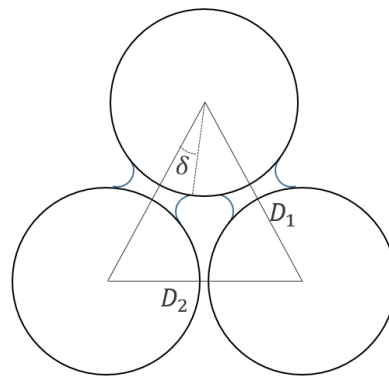


FIGURE 3 – Configuration of the triplet of grains and definition of the filling angle.

For small water volumes, two capillary bridges are created between the upper grain and the two lower ones. Then, for a sufficiently high volume, the water bridges coalesce and form a liquid cluster in between the three grains. As coalescence of bridges is not explicitly accounted for in the software, we consider that the topological change of the water is thought to occur when the triple lines on the upper grain mutually intersect (see Figure 3).

In pendular regime, the computation of the resulting vertical force is obtained by projecting the two capillary forces in the vertical direction :

$$F_{c,total}(V) = 2F_{c,bridge}(V, d = D_1 - 2r) \frac{\sqrt{D_1^2 - (D_2/2)^2}}{D_1} \quad (7)$$

For each volume, the filling angle δ as defined in Figure 3 is measured in order to detect when the two liquid bridges intersect on the upper grain. It happens for a volume of coalescence V_c when

$$\sin \delta = \sin \delta_{max} = \frac{D_2}{2D_1} \quad (8)$$

For $V \geq V_c$, the system reaches the funicular regime with a unique volume of water in contact with the three grains, as illustrated in Figure 4.

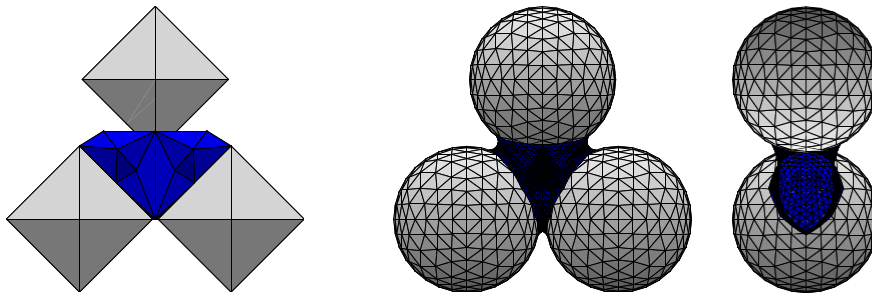


FIGURE 4 – Geometry of a triplet of spherical grains in funicular regime as initially defined and after meshing and minimization of the surface energy with Surface Evolver.

The forces obtained successively in the pendular and funicular regime have been plotted as a function of the volume in Figure 5, together with the experimental results from [5]. It appears that the forces calculated with Surface Evolver are significantly higher than the ones measured in the experiment. However, qualitatively speaking, the evolution of the capillary force is rather similar, with a relatively fast increase in the pendular regime. The coalescence of the bridges occurs for a volume $16 \mu\text{l} < V_c \leq 17 \mu\text{l}$ in our modeling, in good agreement with $16 \mu\text{l} < V_{c,exp} \leq 20 \mu\text{l}$ in the experiment. At the coalescence, the force slightly decreases in our calculations whereas it should significantly increase, according to [5] and [6]. In funicular regime, our method predicts a slight force increase, while it reaches a nearly steady regime in the experiment.

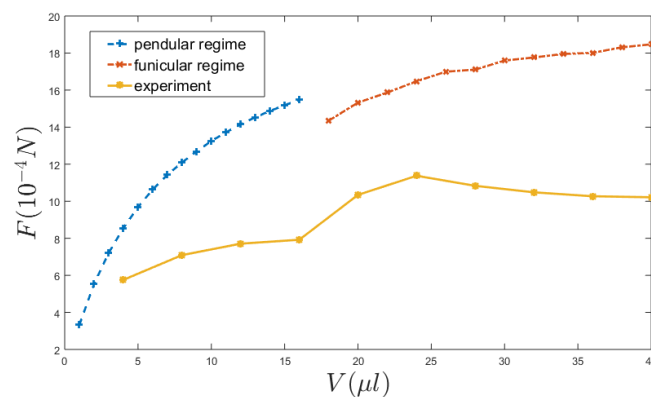


FIGURE 5 – Vertical capillary force in a triplet of spheres as a function of the volume of water, calculated with Surface Evolver and compared to experimental results from [5].

Even if our first results are quite acceptable in terms of qualitative behavior, the quantitative discrepancy with the experimental results is around a factor 2. This difference in the pendular regime is quite surprising, considering that the proposed modeling applied to one capillary bridge matches well with other model and experimental results, as shown in figure 2. A possible explanation for this could arise the quantitative value of surface tension that is not specified in the experiment. Due to its polarity, water captures the impurities from immediate environment, inducing a significant reduction of its actual surface tension. Undergoing experimental measures of surface tension shows that for pure water, it can decrease really fast and could reasonably be divided by two during experiments. Considering that capillary forces

are directly proportional to the surface tension, this reduction would provide a better adequacy with the experiment, at least in pendular regime.

Concerning the evolution of the force at the coalescence of the bridges, it should be noticed that in [6], the coalescence of three bridges is studied, instead of two in the present configuration. The horizontal bridge does not contribute to the vertical capillary force in the pendular regime, but it induces an additional 50% of water volume just after coalescence. As a result, the substantial increase in the force at the coalescence might be dependent on the particular geometric configuration of interest.

Note that an alternative or complementary explanation could also be related to a variation of the wetting angle when the volume increases in the bridges and the cluster. This latter hypothesis tends to be confirmed by some photographs taken during the experiment in [5]. Eventually, the effect of the gravity can also be evoked. Indeed, for the volumes of water and for the interparticle distances considered here, the intensity of gravity forces corresponds approximately to 20 % of the capillary forces, while gravity is absolutely not taken into account in this computations.

4 Conclusion and further works

The computation methodology of capillary forces presented in this work has been tested for a simple capillary bridge between two spherical grains and during coalescence of bridges in a three-grains assembly. The results calculated with Surface Evolver match well with those obtained from other theoretical model or from experiments in the case of one capillary bridge between two grains.

In the case of the coalescence of bridges, our results seem less accurate, with higher forces than expected, and a small decrease in the force when the bridges merge. The difference may be due to the uncertainty in the surface tension in the experiments and to other reasons as variation of the wetting angle or gravity effect.

The validation of this method will make it possible to evaluate the capillary forces in the ten-grains cell of the 3D H-model [18], for different volumes of water and for different geometries of the unit cell, as parametrized by the so called opening angle. This work on the coalescence of water volume constitutes a solid ground to further determine the different capillary regimes of the cell. Such a work is currently in progress and preliminary results are illustrated in Figure 6.

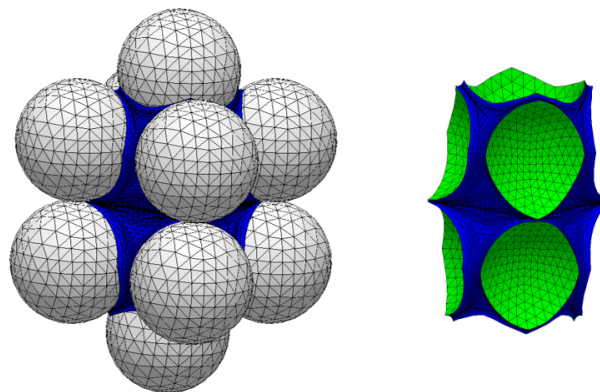


FIGURE 6 – Ten-grains cell in capillary regime with an opening angle $\alpha = 55^\circ$.

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