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Marie Miot, Guillaume Veylon, Antoine Wautier, Pierre Philippe, François Nicot, et al.. Numerical analysis of capillary bridges and coalescence in a triplet of spheres. *Granular Matter*, 2021, 23 (3), 10.1007/s10035-021-01127-0 . hal-03462432

HAL Id: hal-03462432

<https://hal.inrae.fr/hal-03462432>

Submitted on 1 Dec 2021

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Numerical analysis of capillary bridges and coalescence in a triplet of spheres.

Marie Miot · Guillaume Veylon · Antoine
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Received: date / Accepted: date

Abstract The behavior of a natural soil is known to change substantially in presence of water under unsaturated conditions, due to additional capillary forces. Water can be absorbed by hygroscopic soil particles (such as clay), or remains at the surface of solid grains (sand, silt) and forms either a discontinuous (pendular regime) or a continuous phase (funicular regime), depending on the water content of the soil. Capillary bridges exist solely between pairs of grains at small water contents, giving rise to simple capillary force expressions and straightforward subsequent modeling. For larger water contents, these generic capillary bridges

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progressively merge into more complex coalesced bridges involving several grains (i.e. at least three) and whose description remains little known. In the present study, a numerical approach based on surface energy minimization is proposed to compute capillary forces for assemblies of two or three grains. The methodology is first validated for a standard capillary bridge between two grains by comparison both with previous experiments and with other alternative theoretical and numerical approaches. The method is next extended to a triplet of grains within a wide range of water content (or equivalently reduced water volume) during imbibition, to switch from uncoalesced to coalesced bridges. Eventually, the influence of contact angle, surface tension and gravity on the capillary force, the volume of coalescence and the morphology of the bridge as well is investigated. The present study paves the way for the implementation of capillary effects in micromechanical models relying on mesostructures composed of a few grains.

Keywords Capillary forces · Coalescence · Surface energy · Unsaturated conditions · Granular materials

1 Introduction

Granular material is involved in a great variety of phenomena and processes from natural hazards to industrial applications. Although intensively modeled for the sake of simplicity as dry grains interacting solely through frictional forces at contacts, a large class of granular materials exhibits substantial capillary effects depending on both the size of the constitutive particles and the water content. A famous example in everyday life is the sand castle on the beach, whose mechanical stability relies on an optimal water content [1, 2]. In the field of civil engineering, the mechanical behavior of unsaturated granular materials is of particular interest when considering earthen dykes or dams, where different regimes of water saturation can coexist. A fully saturated material is mainly equivalent to a dry material, owing that effective stresses σ' are introduced using Terzaghi's relationship [3]: $\underline{\underline{\sigma}}' = \underline{\underline{\sigma}} - u_w \underline{\underline{I}}$, with u_w the pore water pressure. In the case of partially saturated media, capillary effects give rise to internal stresses (often referred to as suction) within the material, inducing significant changes in its mechanical behavior [4] and [Terzaghi's relationship does not hold anymore](#). The complexity of unsaturated

granular materials stems from the existence of different capillary regimes [5–7], depending on the degree of saturation, the pore geometry and the wettability.

Apart from the specific case of hygroscopic materials, such as clay, where water is adsorbed by the outer surface of the porous particles (so-called hygroscopic regime), the capillary regimes in a material made up of solid particles are commonly described as follows. For small enough water contents, water spontaneously forms bridges connecting two or more grains but with overall water phase remaining discontinuous. This corresponds to the pendular regime. When water content increases, the progressive coalescence of all bridges results in a continuous liquid phase and the material is said to be in the funicular regime [5]. This regime remains challenging to be modeled numerically at the sample scale: in DEM, only the pendular regime has been implemented [8,9], and the Lattice Boltzmann Method, that can essentially model any capillary regime, is computationally expensive [10–12]: for instance, modeling of water drainage in a 40-grains packing takes more than 100 days. Funicular regime is mostly studied experimentally, for example in triaxial tests in Bishop *et al.* [13] and in shear tests in Cuomo *et al.* [14].

Many previous studies have focused at the local scale on capillary bridges between a few grains in the pendular regime. The shape of an axisymmetric capillary bridge between a pair of grains and the resulting axial capillary force have been studied experimentally [15–17], and theoretically, using Laplace-Young equation, with either cylindrical [18], toroidal [19–21], or elliptic [22] approximations of the bridge profile. A mixed methodology is presented in [23–25], coupling experiments, through accurate measurements of the bridge geometry, and numerical resolution of Laplace-Young equation in order to evaluate capillary pressure and force. At the macroscale, for small degrees of saturation (typically less than 10%), capillary forces can be accounted for with a discrete element method, both in static [9,26–29] and dynamic situations [30–32], considering solely liquid bridges between pairs of grains.

Hysteresis effects on the capillary forces and on the shape of water bridge at microscale have been measured experimentally [33]. These effects can be attributed to the hysteretic behavior of the contact angle [34] and to the existence of multiple morphologies for a liquid drop in contact with more than two grains, as it was underlined in the case of a triplet of spheres in Semprebon *et al.* [35]. Coalescence and

50 rupture of water bridges in assemblies of more than two grains also lead to a hys-
51 teresis in the evolution of the capillary forces. Coalescence of axisymmetric bridges
52 between pairs of grains into more complex bridges in contact with more than two
53 grains has been studied experimentally [36,37]. Experimental desiccation of water
54 in assemblies of 3 grains and more was performed in [38]. Numerically, the coales-
55 cence of three bridges between equidistant spheres has been considered by solving
56 the Laplace-Young equation both in 2D [39,40] and in 3D [41], and the resulting
57 coalesced bridge was studied in [42]. The rupture of a coalesced bridge into two
58 separate pendular bridges was studied using an energy minimization method [43].
59 However, more complex assemblies are difficult to handle directly through the
60 Laplace-Young equation because of the lack of symmetry [and advanced numerical](#)
61 [methods are needed](#) [10–12].

62 In this paper, we propose an [alternative](#) advanced method ([computationally](#)
63 [less expensive](#)) to compute capillary forces in an assembly of three grains, based on
64 an energy minimization approach. To this respect, the energy minimization soft-
65 ware Surface Evolver is used [44]. This method has been implemented to solve
66 different problems, such as capillary bridges between two planes [45] or non-
67 symmetric capillary bridges [46]. The main benefit of this method is that the
68 energy minimization approach provides the geometrical shape of capillary bridges,
69 for any grain configurations and for any given water volume, knowing the contact
70 angle. This method is also truly efficient to include gravity effect on the morphol-
71 ogy of a bridge. However, it does not account automatically for coalescence and
72 rupture of bridges. This method has already been used to model water bridges
73 between more than two grains [43], but to the best of our knowledge, no study
74 about the influence of contact angle and gravity on the coalescence of two capillary
75 bridges in a triplet of grains has been carried out so far. In this paper, a compar-
76 ison between an experimental study of the coalescence of two capillary bridges in
77 a triplet of grains by El Korchi *et al.* [37] and numerical results obtained from
78 energy minimization provides the opportunity to capture the effect of surface ten-
79 sion, contact angle and gravity on the capillary force, the volume of coalescence
80 and the morphology of the coalesced bridge. The present results pave the way for
81 the development of enriched micromechanical models in which the constitutive
82 behavior is deduced from the behavior of a collection of mesostructures composed

83 of a few grains. In particular, the method seems to be perfectly adapted for the
 84 calculation of the capillary forces in the ten-grain mesostructure of the so-called
 85 H-model [47].

86 This paper is organized as follows. We first present the energy method used
 87 to compute the capillary forces in an assembly of grains. This approach is next
 88 validated for an axisymmetric capillary bridge between two grains, by comparing
 89 the results with an exact numerical solution [9] and related empirical approxima-
 90 tion [16, 26], an analytical expression based on a cylindrical approximation of the
 91 bridge [18] and several experimental results [48]. Capillary forces calculations are
 92 then performed on an assembly of three grains with two merging capillary bridges.
 93 The results are compared with the experimental results obtained by El Korchi *et*
 94 *al.* [37] and eventually discussed, including detailed analyses on the influences of
 95 the main numerical parameters such as contact angle, surface tension and gravity.

96 2 Energy method for capillary forces calculation

97 2.1 Capillary forces calculation

98 The capillary bridges and related forces for a given geometric arrangement of
 99 spherical grains and a given volume of water are calculated by means of a surface
 100 energy minimization method, using the open source software Surface Evolver [44].

101 For an unsaturated granular assembly composed of N grains, the surface energy
 102 E_s is given by:

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

103 where γ^{lg} is the surface tension and A^{lg} the area of the liquid/gas (i.e. water/air)
 104 interface, γ_i^{sl} and A_i^{sl} as well as γ_i^{sg} and A_i^{sg} are respectively the surface tension
 105 and the area of the interface between grain i and liquid (i.e. water), and between
 106 grain i and gas (i.e. air).

107 In addition, the surface tensions of the different interfaces are related by the
 108 Young-Dupré equation [49]:

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

109 where θ_i stands for the contact angle of water on grain i .

110 Thus, the surface energy of the system can be expressed as follows:

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

111 where $C = \sum_{i=1}^N \gamma_i^{sg} A_i^s$ is a constant for a given grain assembly, with $A_i^s = A_i^{sg} +$
 112 A_i^{sl} the total area of grain i . Eventually, it appears from Eq. (3) that the variation
 113 in surface energy depends solely on the overall geometry of the liquid interfaces.

114 The geometry of the liquid interfaces minimizing surface energy is computed
 115 using the gradient descent method implemented in Surface Evolver. As energies
 116 are usually defined up to a constant, only energy differences are tracked for the
 117 capillary force calculation. The constant C is thus not calculated and left aside,
 118 which means that the solid/gas interfaces do not need to be modeled. Conse-
 119 quently, the problem to be solved is an energy minimization calculation on the
 120 liquid phase under constraints on the positions of solid/liquid interfaces and on
 121 the liquid volume. The specificity of this gradient descent method concerns its
 122 application on a mesh of the liquid phase interfaces that is refined several times
 123 during the calculation [44]. As a result, the number of degrees of freedom handled
 124 in the gradient descent steps regularly increases during the process.

125 Figure 1 illustrates the different steps of the surface energy minimization
 126 scheme. First, a basic geometry with few vertices and an arbitrary volume is de-
 127 fined. Then, many iterations of gradient descents are carried out while remeshing
 128 is performed periodically, in order to increase progressively the number of ver-
 129 tices and improve the precision of the calculation. During remeshing phases, the
 130 size distribution of edges lengths is kept small enough by removing and refining
 131 short and long edges, respectively [35]. The iterative numerical process is thus a
 132 succession of energy minimization and remeshing steps.

133 Once the optimized geometry is reached, capillary forces acting on a given
 134 grain assembly are determined relying on the Virtual Work Principle. Note that,
 135 even though the capillary force acting on a grain could also be calculated with

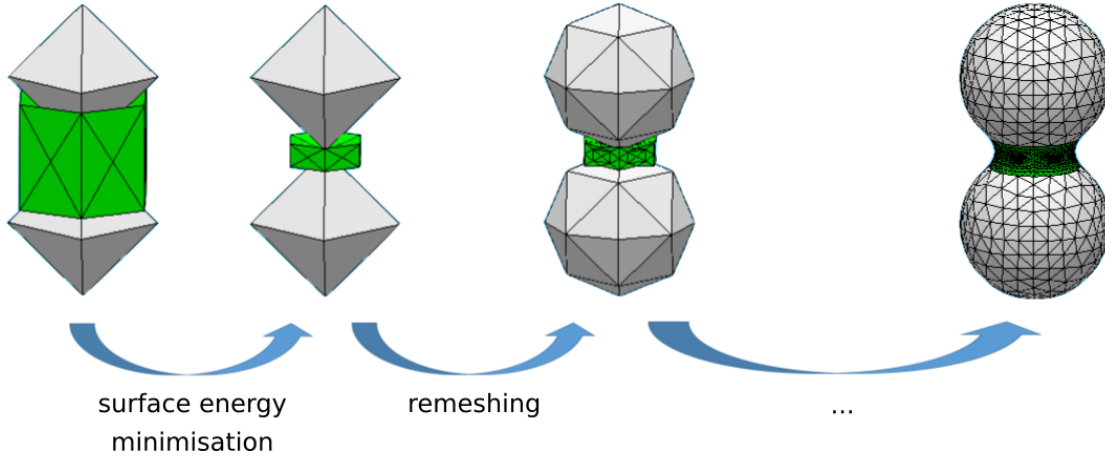


Fig. 1 Illustration of the energy minimization procedure scheme for a capillary bridge between two grains from the initial to the optimized geometry. Note that the grains are plotted only for the sake of illustration. The grain surface is accounted for by a geometric constraint in the Lagrangian formulation of the problem.

136 the boundary method [35], the Virtual Work Principle provides directly the ex-
 137 ternal forces of a system of several grains with capillary bridges. The formalism
 138 obtained with this method is thus well adapted to account for capillary effects in
 139 micromechanical models as for instance the H-model relying on mesostructures of
 140 10 grains [47]. Such a work is currently under development [50]. The system is
 141 consequently stretched in a given direction corresponding to a virtual incremental
 142 displacement $\delta\vec{d}$ (Figure 2), and the surface energy is estimated independently
 143 in both initial and stretched configurations. Assuming that the system is closed
 144 (no change in water volume), static (no kinetic energy) and non-dissipative, the
 145 incremental work δW of the external force \vec{F}_c can be expressed as:

$$\delta W = \vec{F}_c \cdot \delta\vec{d} = \delta E_s + \delta E_p \quad (4)$$

146 with δE_s the incremental variation in surface energy between the two configura-
 147 tions and δE_p the incremental variation in potential energy. Here, only potential
 148 energy due to gravity can be optionally considered (see Section 3.4).

149 The capillary force component acting in an arbitrary direction \vec{u} is then directly
 150 related to the variation of the surface energy and the incremental displacement,
 151 and reads:

$$\vec{F}_c \cdot \vec{u} = \frac{\delta E_s + \delta E_p}{\delta \vec{d} \cdot \vec{u}} \quad (5)$$

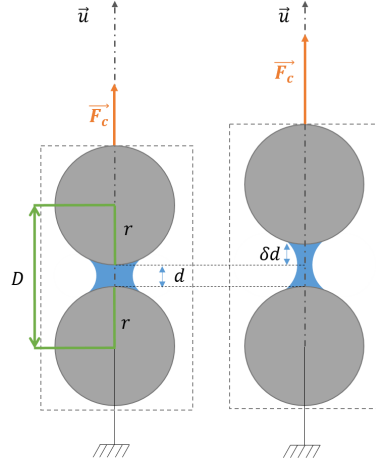


Fig. 2 Determination of a capillary force along direction \vec{u} with the Virtual Work Principle.

152 Compared with standard energy minimization techniques performed over a
 153 fixed number of degrees of freedom, the main difficulty of the present procedure
 154 lies in the selection of an optimal number of gradient descent steps between two
 155 successive remeshing steps in order to prevent a stalling of gradient descent method
 156 due to a too small scale factor. The choice in $\delta \vec{d}$ should allow energy variations
 157 larger than numerical noise but small enough for non-linear effects to be neglected.
 158 A parametric study is thus necessary to determine the most efficient parameters
 159 for any given grain assembly. An example of such a parametric study is given in
 160 Appendix A for the triplet of grains considered in the forthcoming Section 3, with
 161 restriction to $\theta = 0^\circ$.

162 2.2 Capillary force in a single bridge between two grains

163 The purpose of this subsection is to [check the validity of the numerical protocol](#)
 164 [based on the energy method presented in the previous section.](#) The most standard
 165 [example of an axisymmetric liquid bridge connecting two spheres is modeled.](#) This

166 very simple [benchmark](#) case was widely discussed in the literature [15–25]. More
167 complex configurations will be addressed thereafter.

168 Thus, we consider here two spherical grains with the same radius r and the
169 same contact angle with liquid, namely $\theta = 0^\circ$. The distance between the centers
170 of the spheres is $D = 2r + d$, with d the intergranular distance. A given volume
171 V of liquid is entirely used to form a capillary bridge connecting the two grains.
172 Because the geometry of the capillary doublet is left invariant by rotation around
173 the axis joining the two grain centers, the axisymmetric liquid bridge generates a
174 capillary force F_c along this direction denoted by \vec{u} (Figure 2). All the quantities
175 of interest are normalized with the radius and the surface tension of the liquid/gas
176 interface γ^{lg} and the star superscript refers to dimensionless quantities in the
177 following. Accordingly, the dimensionless capillary force $F_c^* = F_c/(2\pi\gamma^{lg}r)$ in the
178 axial direction \vec{u} is calculated as a function of the dimensionless intergranular
179 distance $d^* = d/r$, for different dimensionless volumes of water $V^* = V/r^3$.

180 The results from this energy minimization method are compared to some previ-
181 ous studies published in the literature. Since the capillary bridge has axial symme-
182 try, the Laplace-Young equation can be solved numerically [9], or analytically with
183 a cylindrical approximation. Cylindrical approximation leads to a straightforward
184 relationship between the capillary force and the intergranular distance [18]:

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

185 This relationship is only valid for small volumes of water, typically for $V^* <$
186 0.01 . An expression has also been proposed by Richefeu *et al.* [26] in order to fit
187 the numerical solution of Laplace-Young equation in monodisperse condition (i.e.
188 grains of the same diameter):

$$F_c^* = \cos \theta \exp \left(\frac{-d^*}{0.9\sqrt{V^*}} \right) \quad (7)$$

189 Another more complex and precise expression obtained with an approximation
190 of the numerical solution of Laplace-Young equation is provided by Willett *et*
191 *al.* [16]. Moreover, this relationship is valid for a larger range of volumes than
192 equations (6) and (7) are, namely for $V^* < 0.1$.

193 The expressions of the dimensionless capillary force obtained with the different
 194 models are plotted in Figure 3, as a function of the dimensionless intergranular
 195 distance for two values of dimensionless water volume: $V^* = 0.008$ and $V^* = 0.156$,
 196 which had been used in the experiments realized by Mielniczuk *et al.* [48]. In all
 197 cases, the capillary force decreases with the intergranular distance, except in the
 198 experiments with the highest water volume where a slight increase is observed at
 199 very small intergranular distances, namely $d^* < 0.05$.

200 The capillary force deduced from surface energy minimization matches fairly
 201 well with the numerical solution of Laplace-Young equation [9] and the expres-
 202 sion proposed by Willett *et al.* [16]. This agreement can be partly justified from
 203 the equivalence between resolution of Laplace-Young equation and surface energy
 204 minimization (as implemented in Surface Evolver) which has been discussed in
 205 this particular case in Lambert *et al.* [51]. The obtained results are also in good
 206 agreement with the experimental results [48], even if the capillary force obtained
 207 from the energy method is systematically higher for the small intergranular dis-
 208 tances, especially for the large dimensionless volume. It is worth noting that the
 209 differences between numerical and experimental results at low intergranular dis-
 210 tances can have two possible explanations. First, for low intergranular distances,
 211 the optimized incremental displacement δd must be sufficiently large to induce a
 212 significant variation of energy, but smaller than the intergranular distance, in order
 213 to avoid having an interpenetration of the grains. Secondly, in the experiments,
 214 for low intergranular distance, a contact between grains is possible, which could
 215 substantially affect the measurement of the capillary force with the laboratory
 216 balance. Finally, the results obtained from the energy minimization method agree
 217 also fairly well with the analytical equations (6) and (7), demonstrating the good
 218 ability to predict experimental and numerical results over a wide range of water
 219 volumes.

220 **3 Capillary forces in an assembly of three spheres**

221 This section is devoted to (i) an extension of the model to calculate capillary
 222 forces for higher volumes of water involving larger grain assemblies, and (ii) a
 223 practical way to account for the possible coalescence of capillary bridges. Indeed,

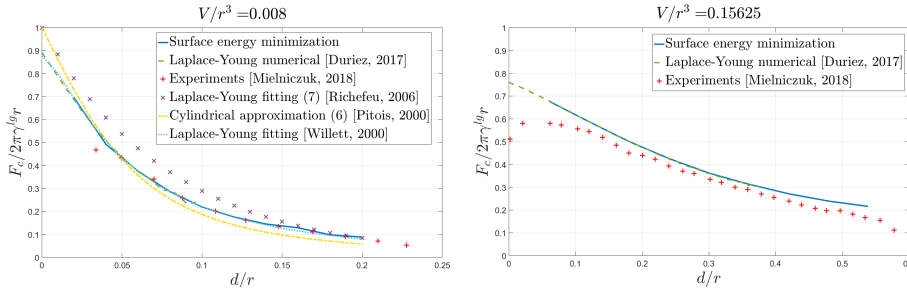


Fig. 3 Dimensionless capillary forces in a liquid bridge, as a function of the dimensionless intergranular distance, obtained with Surface Evolver (blue solid line), by solving Laplace-Young equation numerically (green dashed line) or analytically with a cylindrical approximation (yellow dash-dot line), with fittings of Laplace-Young relationship provided by Richefeu *et al.* [26] (crosses) and by Willett *et al.* [16] (light blue dotted line), and experimentally (red plus symbols). Note that the cylindrical approximation cannot be plotted for $V^* > 0.01$ and fittings of Laplace-Young equation for $V^* > 0.1$.

224 when a capillary bridge connects more than two grains, the axisymmetry of the
 225 geometry is usually broken. Such a lack of symmetry makes the resolution of
 226 Laplace-Young equation far more complex, underlying the relevance of the surface
 227 energy minimization method. The methodology presented in the previous section
 228 is thus extended here to analyze the coalescence of two liquid bridges in a triplet
 229 of grains, taking the opportunity of a direct comparison with the experimental
 230 results from [37]. The objectives are to show the ability of the numerical procedure
 231 to handle complex grain configurations for a wide range of water volume and to
 232 analyze the influences of several physical parameters.

233 3.1 Description of the experiments

234 The experimental set-up developed in [37] consists of a triplet configuration with
 235 three identical spherical glass beads of the same radius $r = 4$ mm. The base of
 236 the assembly is constituted of two beads, the centers of which are separated by a
 237 distance $D_2 = 8.3$ mm. The third bead is placed above, in the median plane, at a
 238 distance $D_1 = 8.7$ mm from the centers of the other beads as presented in Figure
 239 4. Two capillary bridges between the upper bead and each of the two lower beads
 240 are initially created, using a micro-syringe. Then water is progressively added by
 241 steps of $2 \mu\text{l}$ in each bridge until they merge. Afterward, water is added by steps
 242 of $4 \mu\text{l}$ in the coalesced bridge.

243 The vertical capillary force is measured by differential weighing of the system
 244 composed of the volume of water and the two lower beads. Indeed, while the upper
 245 bead remains fixed, the two lower ones lie on a precision scale. If water bridges
 246 were not attached to the upper bead, the scale would measure the mass of water
 247 plus the mass of the beads. In practice, this maximal available force is reduced by
 248 the capillary force exerted on the upper bead and the vertical capillary force is
 249 thus deduced from the difference between the theoretical maximal weight and the
 250 actual measurement.

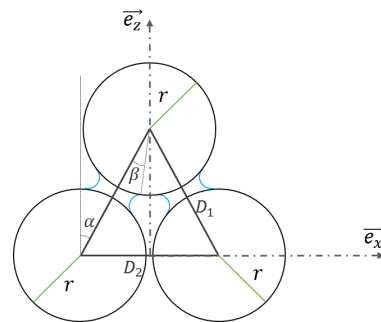


Fig. 4 Geometry of the triplet of grains with definition of both the half-filling angle β of a bridge and the opening angle α .

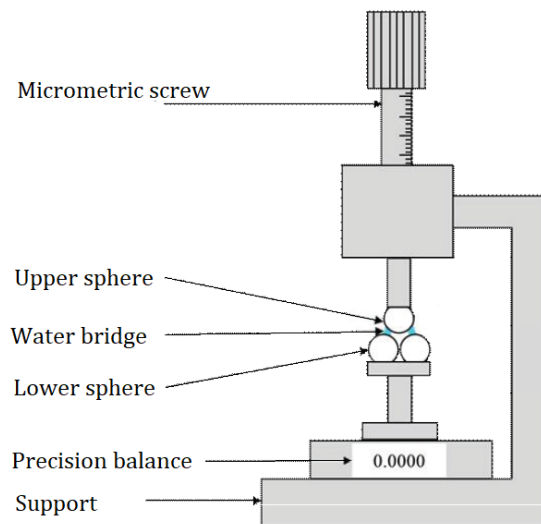


Fig. 5 Scheme of the experimental set-up from [37].

251 3.2 Modeling of imbibition of a triplet of grains

252 In order to model the experiment presented above, the standard value of the
253 surface tension between pure water and air at 20°C is first selected, namely $\gamma^{lg} =$
254 0.073 N/m [52]. The contact angle θ is taken as zero and gravity is not considered
255 as a preliminary approximation. The relative influence of these different control
256 parameters will be discussed later, in sections 3.3 and 3.4.

257 For low volumes of water, two inclined capillary bridges exist between the
258 upper sphere and each of the two other spheres. Consequently, the vertical capillary
259 force is directly deduced from the previous results obtained for a capillary bridge
260 between two grains (Section 2.2) by simple addition of the vertical components of
261 the axial capillary force of the two inclined bridges. This approach remains valid
262 as long as the two inclined bridges in Figure 4 do not merge. As the energetic
263 approach is not capable of predicting merging of water volumes, a geometrical
264 criterion is alternatively proposed in order to evaluate the volume corresponding
265 to the merging of the two capillary bridges into a unique coalesced bridge. The
266 half-filling angle β^1 of the bridge, as defined in Figure 4, is measured in order
267 to detect the volume V_{coal} for which $\beta = \alpha$ [39]. At this point, the water in the
268 two bridges forms a common volume, which will evolve to a substantially different
269 geometric configuration when minimizing the surface energy. For $V \geq V_{coal}$, the
270 coalesced bridge is modeled using the numerical parameters determined in the
271 parametric study presented in Appendix A.

272 In Figure 6, the results, obtained first for two uncoalesced bridges and second
273 for a unique coalesced bridge, are compared with the experimental results. The
274 latter shows an increase in the capillary force as a function of the water volume
275 added in the two capillary bridges. The force increase gets progressively smaller
276 until a plateau is almost reached. Coalescence of the two bridges occurs between
277 16 μl and 20 μl , together with a substantial increase in the capillary force. For
278 water volumes greater than 24 μl , when water is added in the coalesced bridge,
279 the capillary force is found to decrease slightly.

¹ In the literature, the half-filling angle is generally denoted δ , but, in order to avoid any confusion with the symbol used before for infinitesimal variation, it is here denoted β .

280 In the numerical simulations with the standard values chosen for the control
 281 parameters, the capillary force also increases until the geometrical coalescence
 282 criterion is met, for a total volume between $14 \mu\text{l}$ and $14.5 \mu\text{l}$. However, several
 283 major differences must be pointed out. First, the values of the capillary force are
 284 systematically about 1.5 to 2 times larger than the experimental values. Secondly,
 285 the capillary force is found to drop at coalescence and not to increase as measured.
 286 Finally, the capillary force further increases at larger volumes, presumably tending
 287 to a plateau.

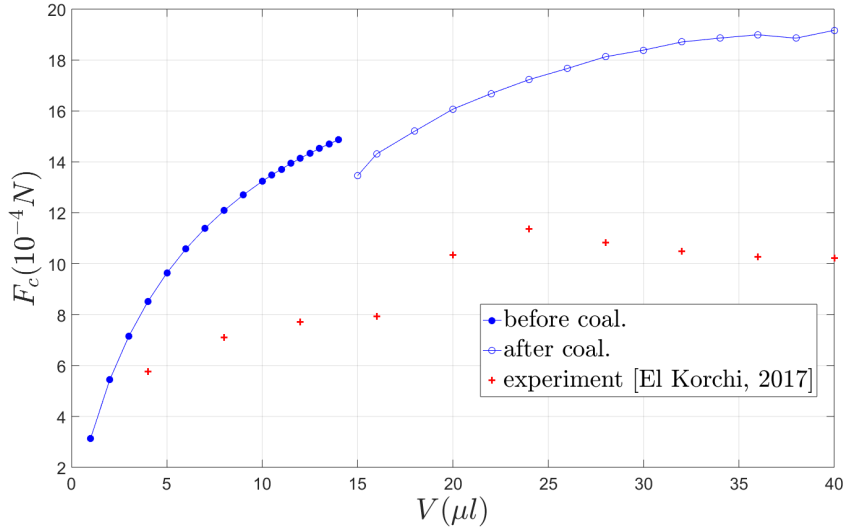


Fig. 6 Capillary force in a triplet of spheres, as a function of the injected volume of water. Numerical results are obtained with Surface Evolver for a contact angle $\theta = 0^\circ$, with the standard surface tension value $\gamma^{lg} = 0.073 \text{ N.m}^{-1}$. The solid and open symbols stand for the uncoalesced (two bridges) and coalesced (single cluster) regimes, respectively. The experimental data (red plus symbols) are taken from [37] (plus symbols). Coalescence occurs for V between $14 \mu\text{l}$ and $15 \mu\text{l}$ with the numerical method, and for V between $16 \mu\text{l}$ and $20 \mu\text{l}$ in the experiment.

288 Although the proposed energetic approach has been validated in previous sec-
 289 tion for the modeling of a simple liquid bridge between a pair of spherical grains,
 290 it clearly fails to predict quantitatively the experimental data with standard pa-
 291 rameter values, even in the uncoalesced regime. This suggests that the effective
 292 values of the main physical parameters (such as surface tension and contact angle)
 293 may differ from the classically admitted values, namely $\gamma^{lg} = 0.073 \text{ N.m}^{-1}$ at 20°C

294 (see for instance Molenkamp and Nazemi [52]) and $\theta \leq 10^\circ$ for glass beads (see
295 for instance Scheel *et al.* [53], or Duriez and Wan [9]) and that gravity needs to
296 be taken into account. Further investigations on the influence of these parameters,
297 including gravity, are thus carried out in the following sections.

298 3.3 Influence of the contact angle

299 Although contact angle is a key parameter in all capillary phenomena, an exper-
300 imental measure of its value is complex. Pictures of the experiments presented
301 in [37] show that the contact angle changes with the volume of water and the po-
302 sition of the triple line (i.e. the intersection of liquid, gaseous and solid interfaces).
303 The roughness and the cleanliness of the beads surface are known to affect locally
304 its value, as well as the presence of adsorbed water at the solid surface. By way of
305 illustration, in a bridge between two grains separated by 0.7 mm, with a radius of
306 8 mm and a volume of 1 μl , 4 μl and 10 μl , the contact angle may vary between
307 7.2° and 13.7° , according to [48]. In a triplet of grains, the contact angle of a water
308 coalesced bridge was measured in Wang *et al.* [43] with values ranging between 10°
309 and 70° . In the coalesced domain, the pictures of the experiment show that the
310 water cluster can even become convex along particular triple lines. This is visible
311 for instance in Figure 7, where a contact angle greater than 90° can be observed.
312 Figure 7 depicts the profile of water interfaces before and after coalescence in both
313 numerical simulations and experiments. After coalescence, part of the triple lines
314 lies on surfaces that were previously covered by water before coalescence (the two
315 interfaces between the top and bottom grains in the 2D cut in Figure 7), while
316 some other portions of the triple line lie on surfaces that were dry before coales-
317 cence (the interfaces between the bottom grains in the 2D cut in Figure 7). The
318 past state and history of the surface (wet or dry) are thus likely to generate large
319 heterogeneities in contact angle at the surface of a same grain.

320 It is also worth pointing out a striking difference in the geometry of the co-
321 alesced bridge, the lower meniscus of which is located above the horizontal line
322 joining the centers of the two bottom grains in the experiments, forming a so-called
323 dimmer [35] whereas it is located below this line in the simulations presented in
324 this manuscript, forming a so-called trimmer. As depicted in Figure 8, a lower po-

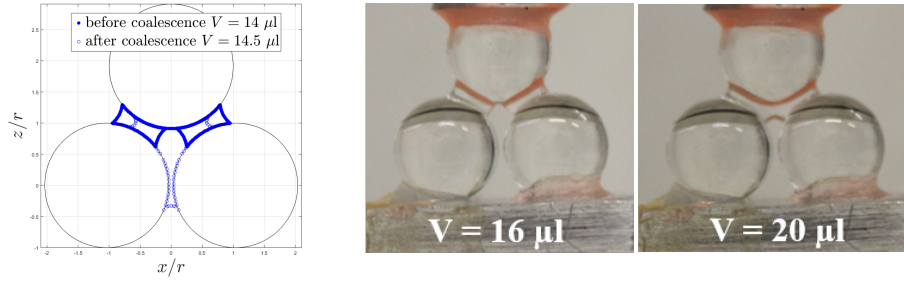


Fig. 7 Profile of water interfaces before and after coalescence. Left: position of the interfaces obtained numerically, in the plane formed by the centers of the grains just before coalescence for $V = 14 \mu\text{l}$ (full circles) and just after coalescence for $V = 14.5 \mu\text{l}$ (empty circles). Middle and right: photographs of the water between the three grains in the experiment [37], before coalescence for $V = 16 \mu\text{l}$ and after coalescence for $V = 20 \mu\text{l}$.

325 sition of the meniscus will increase the horizontal component of the capillary force
 326 and decrease the vertical one. Moreover, a dimmer instead of a trimmer configu-
 327 ration tends to concentrate the volume of water in the upper part of the coalesced
 328 bridge, which increases in return the radius of curvature of the upper meniscus
 329 and then the vertical capillary force, according to [54]. Consequently, the vertical
 330 capillary force **increases after coalescence in the experiments while it decreases in**
 331 **the simulations**. For the present geometric configuration, no static equilibrium in
 332 a dimmer configuration was found. This suggests that the dimmer configuration
 333 observed experimentally is a metastable configuration.

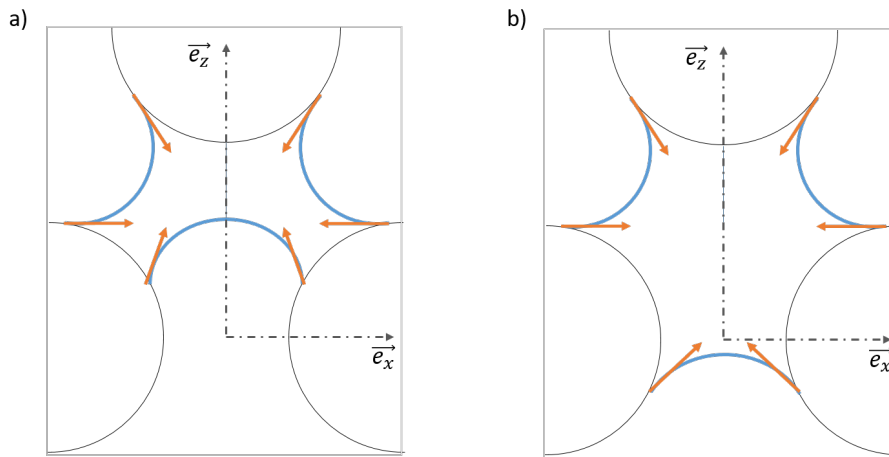


Fig. 8 Schemes of the influence of the meniscus position on the capillary force components: a) for a lower meniscus above the centers of the lower grains. b) For a lower meniscus below the centers of the lower grains.

Figure 9 shows the capillary force acting on the top grain of the triplet as a function of the volume for a large range of contact angles. From $\theta \geq 30^\circ$, the capillary force no longer decreases but starts to increase at the coalescence transition, from two liquid bridges to a single capillary cluster. Keeping the standard value $\gamma^{lg} = 0.073 \text{ N.m}^{-1}$, the numerical curve approximately fits the experimental curve before coalescence for $\theta \simeq 60^\circ$. After coalescence, the experimental curve lays between the numerical curves obtained for $\theta = 50^\circ$ and $\theta = 60^\circ$, which seems plausible according to [43] and to the pictures of the experiments presented in Figure 7. As mentioned previously, it is known that the contact angle depends on whether the surface was previously wet or dry. Based on the observations in Figure 7, a change in the contact angle is thus physically relevant.

In addition to the change in capillary force at coalescence, Figure 10 also highlights that the total volume of water at coalescence V_{coal} increases with the contact angle, perfectly linearly:

$$V_{coal} = V_{coal}^0 + \frac{\theta}{\Delta\theta} \Delta V_{coal} \quad (8)$$

with $V_{coal}^0 = 14.5 \mu\text{l}$, $\Delta V_{coal} = 18 \mu\text{l}$ and $\Delta\theta = 90^\circ$.

Such a linear relationship is reminiscent of the one observed between the rupture distance and the contact angle in a capillary bridge between two grains, proposed by Lian *et al.* [20]. However, these similar behaviors are most probably coincidental or fortuitous since the two criteria of regime change do not have the same origin. The rupture distance in a capillary bridge is considered during drying or when intergranular distances increase, and depends on the surface energy of the liquid bridge. On the other hand, the volume of coalescence of capillary bridges has to be evaluated during imbibition or when intergranular distances decreases, and depends on the geometry of the grains assembly.

3.4 Influence of gravity

The effect of gravity can also partly explain the difference between experimental and numerical capillary forces. Indeed, gravity tends to deform the two inclined bridges and consequently modifies the capillary force applied on the top grain. The

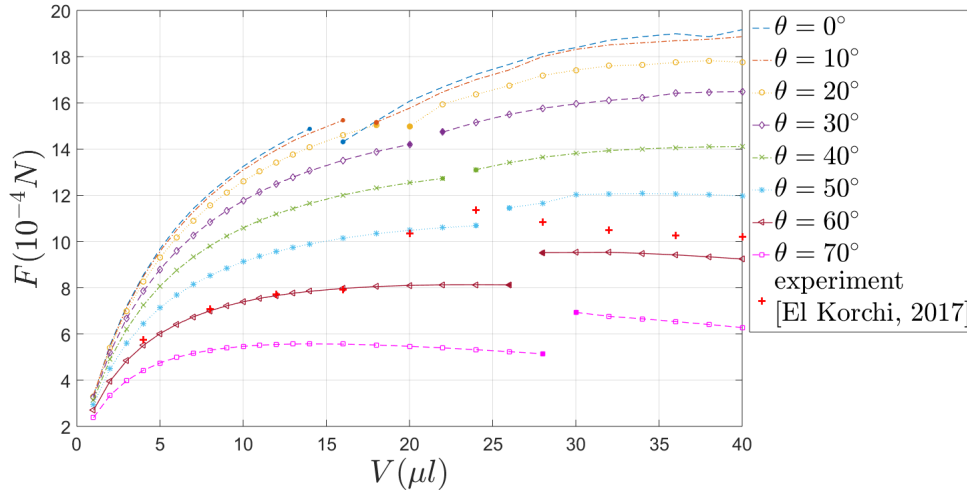


Fig. 9 Capillary force in a triplet of grains, as a function of the volume of water, calculated with Surface Evolver for $\gamma^{lg} = 0.073 \text{ N.m}^{-1}$ and for different contact angles (dashed lines), and obtained experimentally in [37] (red plus symbols).

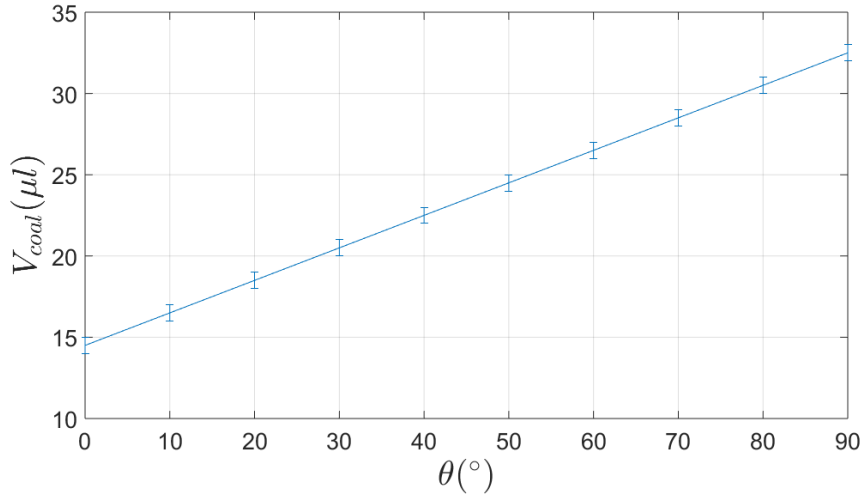


Fig. 10 Total volume of water at coalescence as a function of the contact angle. The solid line stands for the linear relationship: $V_{coal} = V_{coal}^0 + \frac{\theta}{\Delta\theta} \Delta V_{coal}$ with $V_{coal}^0 = 14.5 \mu\text{l}$, $\Delta V_{coal} = 18 \mu\text{l}$ and $\Delta\theta = 90^\circ$.

362 dimensionless Bond number can be introduced to compare gravitational effect to
 363 capillary forces in a system, apart from any water content consideration. A Bond
 364 number negligible with respect to 1 allows neglecting the gravity. Here, the Bond
 365 number given by the classical definition reads:

$$Bo = \frac{r^2 \Delta \rho g}{\gamma^{lg}} = 2.14 \geq 1 \quad (9)$$

with $g = 9.81 \text{ m.s}^{-2}$ the acceleration of gravity and $\Delta \rho = 997 \text{ kg.m}^{-3}$ the difference between liquid and gas density at 20°C . Consequently, gravity cannot be neglected in the present case.

Fortunately, accounting for gravity is quite straightforward in our energy based approach as it simply consists in adding the potential energy term in the expression of the energy (in Eq. (4)) while keeping the minimization procedure unchanged.

The capillary forces in the assembly of three grains, with or without gravity, are plotted in Figure 11. As can be seen, gravity tends to decrease the capillary forces, as it is observed in [55], moving closer to the experimental data. On the contrary, the volume of coalescence remains almost the same, between $14 \mu\text{l}$ and $14.5 \mu\text{l}$, which means that the influence of gravity on the position of the triple line at the upper grain surface before coalescence is small.

It is worth noting that gravity increases the drop in capillary force at coalescence and affects more strongly the small volume cases in the subsequent coalesced regime. This can be explained by the shape of the liquid interfaces as illustrated in Figure 12 where is plotted the profile of the interfaces of a coalesced bridge in the plane formed by the centers of the grains, for $V = 16 \mu\text{l}$ and $V = 30 \mu\text{l}$:

- At the top of the bridge, the displacement of a part of the water due to gravity decreases the radius of curvature of the meniscus contributing to the capillary force between the lower grains and the upper grain. As the capillary force tends to decrease with the radius of curvature [54], the contribution of the upper parts of the coalesced bridge to the vertical capillary force decreases. For the highest volumes, the displacement of the water in the upper part of the capillary bridge is relatively less important than for small volumes (a larger proportion of the water weight is supported by the bottom grains for large volumes, which limits water transfers), and the radius of curvature is less affected.
- At the bottom of the bridge, the displacement of the liquid/gas interface induces an increase in the vertical capillary force but with a smaller effect as the curvature is orthogonal to the force. Indeed, this portion of the capillary bridge contributes mainly to horizontal attraction between the bottom grains,

396 which could not be measured with the experimental set up. The displacement
 397 of the liquid/gas interface at the bottom is larger for the highest volumes since
 398 the weight of the water bridge increases with its volume.

399 – In the end, as the displacement at the top of the bridge is less significant for
 400 higher volumes than for smaller ones, and more significant at the bottom, the
 401 impact of gravity on the vertical capillary force is consequently less important
 402 for the highest volumes.

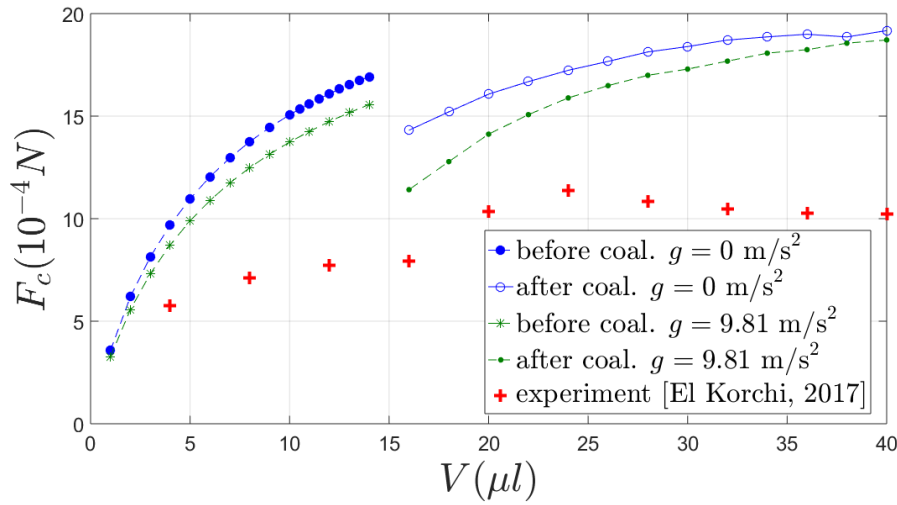


Fig. 11 Capillary force in a triplet of grains calculated numerically without gravity (blue circles) and with gravity (green stars and points), as a function of the volume of water, with $\gamma^{lg} = 0.073 \text{ N}\cdot\text{m}^{-1}$ and $\theta = 0^\circ$, and obtained experimentally in El Korchi *et al.* [37] (red plus symbols).

403 3.5 Influence of the surface tension of the liquid/gas interface

404 The value to be used for the liquid/gas surface tension is questionable since it
 405 was inferred but not directly measured in the experiments [37]. If the standard
 406 value $\gamma^{lg} = 0.073 \text{ N}\cdot\text{m}^{-1}$ corresponds to pure water in air at 20°C [52], water
 407 is known to be a polar liquid that easily captures impurities from the external
 408 environment, inducing substantial reduction in surface tension. In this context, a
 409 calibration of the surface tension value in a capillary bridge between two grains

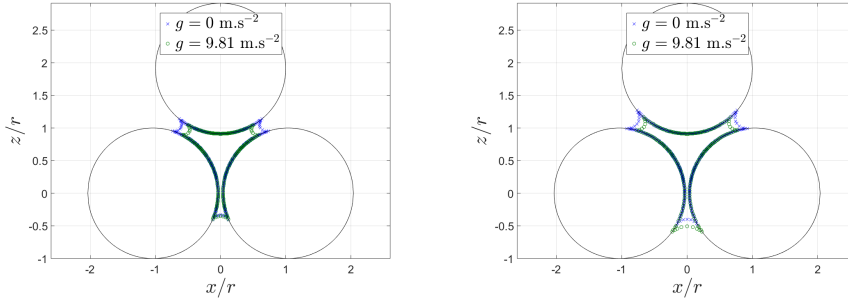


Fig. 12 Positions of the water interfaces obtained numerically in the plane formed by the centers of the grains for $V = 16 \mu\text{l}$ (left) and $V = 30 \mu\text{l}$ (right), without gravity (empty blue circles) and with gravity (green points).

410 was realized in [56] and shows that a value around 0.0693 N.m^{-1} can reasonably
 411 be adopted. When gravity is not accounted for, surface energy and capillary force
 412 are basically proportional to surface tension. A decrease in surface tension induces
 413 a decrease in the same proportion for the capillary force, which may explain part
 414 of the discrepancy observed between the experimental and numerical curves in
 415 Figure 6.

416 When gravity is taken into account, a decrease in the surface tension will de-
 417 crease proportionally the surface energy and will increase the relative contribution
 418 of gravity to the total energy of water. Thus, the decrease in the surface tension
 419 has a twofold effect on the capillary force decrease. Figure 13 shows the capil-
 420 lary forces before and after coalescence for the classical value $\gamma^{lg} = 0.073 \text{ N.m}^{-1}$
 421 ($Bo = 2.14$) and for the value from [56] $\gamma^{lg} = 0.0693 \text{ N.m}^{-1}$ ($Bo = 2.26$), with
 422 and without gravity, for $\theta = 0^\circ$. The upper chart confirms that the dimensional
 423 capillary force decreases with gravity and decreasing surface tension. This obser-
 424 vation is in agreement with the results from Murase *et al.* [55], which show that
 425 the vertical capillary force in a triplet decreases when Bond number increases.
 426 On the lower chart, the dimensionless capillary forces $F_c^* = \frac{F_c}{2\pi r \gamma^{lg}}$ are plotted.
 427 It can be deduced from this chart that before coalescence, gravity and surface
 428 tension influence significantly and independently the capillary force. However, the
 429 relative importance of gravity over surface tension is not affected by the value of
 430 the surface tension. After coalescence, the differences between the dimensionless
 431 curves with gravity show that decreasing the value of γ^{lg} increases the relative

432 importance of gravity. Thus, the slight difference in the Bond number between the
 433 two cases is almost negligible before coalescence but becomes significant beyond
 434 coalescence.

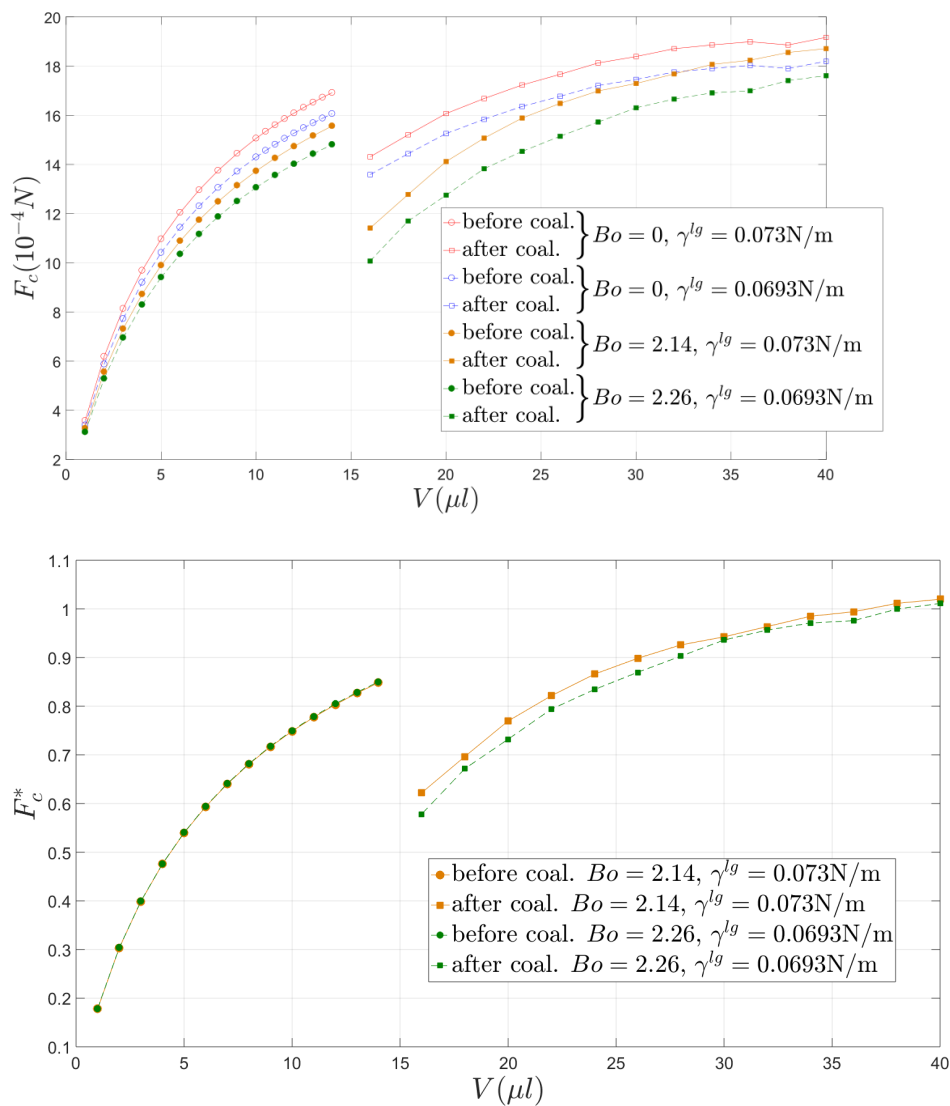


Fig. 13 Capillary force in a triplet of grains calculated numerically without gravity (empty symbols) and with gravity (full symbols), for $\gamma^{lg} = 0.073 N/m$ (solid line) and $\gamma^{lg} = 0.073 N/m$ (dashed line), with $\theta = 0^\circ$, as a function of the volume of water. Upper: dimensional capillary forces, lower: dimensionless capillary forces.

435 3.6 Calibration of the physical parameters

436 Investigating the influence of the physical parameters has pointed out that the
 437 vertical capillary force decreases with decreasing surface tension, increasing contact
 438 angle and addition of gravity. Consequently, accounting for gravity and using the
 439 more realistic value of the surface tension $\gamma^{lg} = 0.0693 \text{ N.m}^{-1}$ [56], we investigate
 440 on a plausible range of contact angle values compatible with the experimental
 441 data by El Korchi *et al.* In Figure 14, the capillary forces have been plotted for
 442 two different values of the contact angle, when adding gravity, and with $\gamma^{lg} =$
 443 0.0693 N.m^{-1} . Before coalescence the numerical curve with $\theta = 60^\circ$ matches quite
 444 well the experimental curve. The differences between the two curves tend to show
 445 that the contact angle is slightly lower for small volumes and a little higher just
 446 before coalescence. As regards the highest volumes, the capillary forces obtained
 447 numerically with $\theta = 55^\circ$ are in good agreement with the experimental results.
 448 However, the fitted parameters should be considered with care as the comparison
 449 is made with a single experimental set.

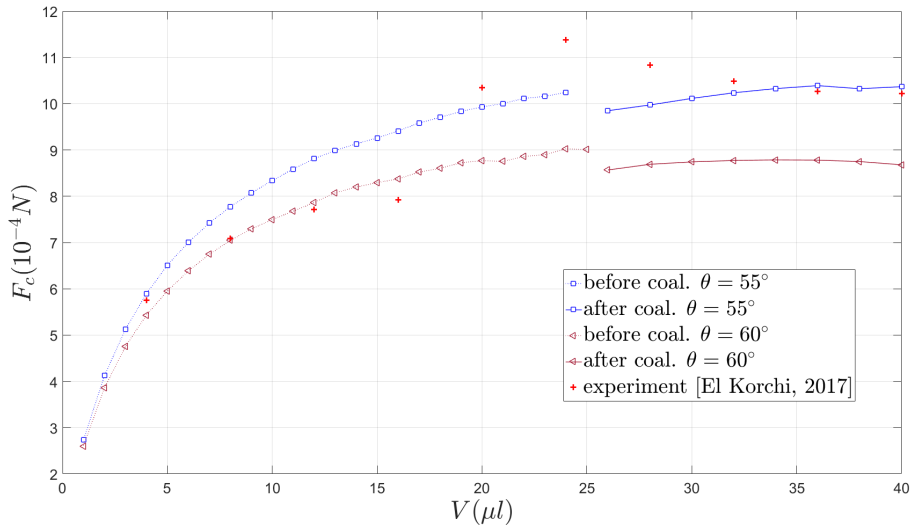


Fig. 14 Capillary force in a triplet of grains, as a function of the volume of water, calculated with Surface Evolver with $\gamma^{lg} = 0.0693 \text{ N.m}^{-1}$ with $g = 9.81 \text{ m.s}^{-2}$, $\theta = 60^\circ$ (triangles) and $\theta = 55^\circ$ (squares), before (dotted line) and after (solid line) coalescence, against experimental results from [37] (crosses).

450 This range of contact angle values is in reasonable agreement with the experi-
451 ment pictures (Figure 7 and El Korchi *et al.* [37]), where the contact angle varies
452 roughly from 30° to 60° . The picture tends to show that the contact angle is not
453 the same on the upper and the lower beads, depending on the position of the
454 triple line on each bead and then on the volume of water. At coalescence, the up-
455 per parts of the triple lines lie on areas previously wet, where a thin layer of water
456 may remain. This leads to a contact angle different from the uncoalesced bridges
457 and from the lower part of the coalesced bridge that took place on a previously
458 dry surface, due to the hysteresis of the contact angle [33,34]. However, it should
459 be underlined that the present formulation of the minimization problem in Surface
460 Evolver does not allow for defining different contact angle values on the surface of
461 a same given grain.

462 Depending on the contact angle value, coalescence now occurs for V between
463 $24 \mu\text{l}$ and $26 \mu\text{l}$, which is more than the experimental coalescence volume, in
464 between 16 and $20 \mu\text{l}$. Figure 15 shows that for $V = 20 \mu\text{l}$, the half-filling angle
465 β is less than 3° under the value of the opening angle α , which means that the
466 two bridges are very close. It is therefore plausible that the contact could occur
467 in practice for a smaller volume, due to some slight loss of symmetry, or to the
468 presence of impurities in the water or at the surface of the beads.

469 As observed, this range of contact angle values provides satisfactory agreement
470 between the numerical curve and the experimental data both before coalescence
471 and after coalescence, but only for the highest volumes ($V \geq 32 \mu\text{l}$). However, just
472 after coalescence, for V between $25 \mu\text{l}$ and $32 \mu\text{l}$, the calculated capillary forces
473 are smaller than the measured ones.

474 Finally, Figure 16 depicts the geometry of the water interfaces with $\theta = 55^\circ$
475 just after coalescence, for $V = 26 \mu\text{l}$, and later, for $V = 36 \mu\text{l}$. Obviously, the
476 meniscus between the lowest spheres is still below the centers of the grains just
477 after the coalescence, unlike the experiment. These results suggest that the energy
478 minimization approach is able to reproduce the experimental observations before
479 and far enough after coalescence. However, because of the differences observed at
480 its vicinity, one could speculate on a transient state where the energy required to
481 move the water to the configuration with the smallest energy is higher than the
482 difference between the energy of the current geometry, and the smallest energy.

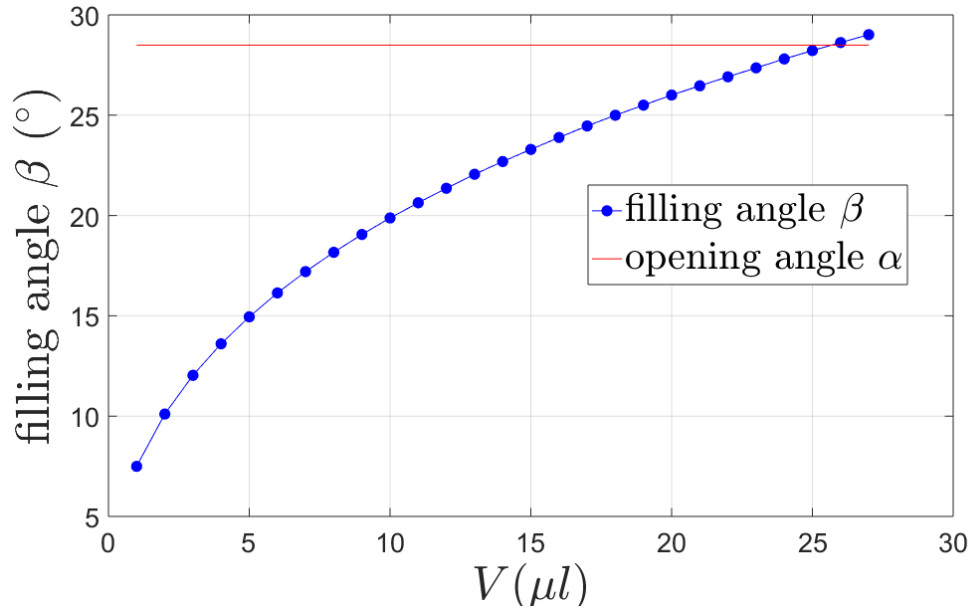


Fig. 15 Filling angle β as a function of the volume of water in two uncoalesced bridges, obtained with $g = 9.81 \text{ m.s}^{-2}$, $\gamma^{lg} = 0.0693 \text{ N.m}^{-1}$ and $\theta = 60^\circ$. The opening angle α characterizing the triplet geometry as shown in Figure 4 is marked as a horizontal solid line.

483 Moreover, dynamics effects on the surface tension value have been observed in
 484 Hauner *et al.* [57]. It can lead to an important increase in the surface tension value
 485 around 0.09 N.m^{-1} , which implies an increase in the capillary force. As these
 486 effects occur at the atomic and molecular scales, the surface energy minimization
 487 method cannot reproduce this transient state.

488 4 Concluding remarks

489 To sum up this contribution, a numerical method based on surface energy mini-
 490 mization has been presented in order to estimate capillary forces in small assem-
 491 blies composed of a few spherical grains. Firstly, the method has been challenged
 492 to model a single capillary bridge between two grains, in order to determine the
 493 evolution of the related capillary force as a function of both the intergranular dis-
 494 tance and the volume of liquid. The results have been successfully compared with
 495 published experimental and numerical results. Secondly, the method was used to

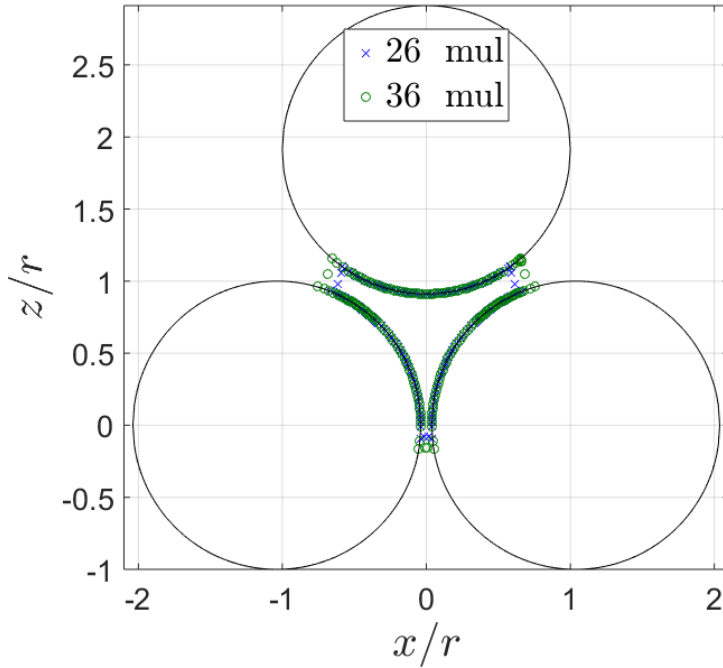


Fig. 16 Profile of water interfaces after coalescence, for $V = 26 \mu\text{l}$ (blue crosses) and $V = 36 \mu\text{l}$ (green open circles), with gravity and for $\gamma^{lg} = 0.0693 \text{ N.m}^{-1}$ and $\theta = 55^\circ$.

496 investigate the evolution of capillary forces during coalescence of two capillary
 497 bridges in a triplet of spherical grains.

498 A comparison with published experimental results by El Korchi *et al.* [37] pro-
 499 vides the opportunity to discuss the influence of physical parameters. The contact
 500 angle value was first investigated. It is shown to have a large influence on the cap-
 501 illary force, which decreases substantially when the contact angle increases. The
 502 contact angle has also an effect on the overall shape of the capillary force curve
 503 that can affect the evolution of capillary force after coalescence. It also has an
 504 important effect on the shape of the bridges, and a linear relationship between co-
 505 alescence volume and contact angle has been found. Comparison with experiments
 506 shows that the contact angle depends on the volume of water and on the position
 507 of the triple line on the grain. Imperfections on the spheres surface are thought to
 508 influence the position of the triple line, leading to the hysteresis of contact angle.
 509 A plausible range of value has been found between 55° and 60° .

510 Considering the size of glass beads radius, gravity cannot be neglected. Gravity
511 tends to decrease capillary force value. Its influence before coalescence is quite
512 low, and the changes in coalescence volume is not significant. In the coalesced
513 bridge, the influence of the gravity is more important. Paradoxically, the influence
514 of gravity on capillary force is more important for the smallest volumes of the
515 coalesced bridge, which can stem from the evolution of the morphology of the
516 bridge with gravity.

517 Then, the influence of the surface tension has been investigated with and with-
518 out gravity. In the absence of gravity, surface tension has a proportional effect on
519 the capillary forces value, with no impact on the morphology of the bridge. How-
520 ever, when adding gravity, a decrease in the surface tension increases the Bond
521 number value and then the relative contribution of the gravity in the total en-
522 ergy. The effects of the variation of the Bond number is quite negligible before
523 coalescence but is more important after.

524 Finally, this sensitivity analysis gives a plausible range of values for the physical
525 parameters. The present work underlines the relative influence of different phys-
526 ical parameters on the contact force value. It was found that the contact angle
527 is the most important parameter to be calibrated to reproduce the experimental
528 results. A convenient choice of contact angle should allow reproducing accurately
529 experimental results before coalescence and sufficiently long after the coalescence.
530 However, the coalescence of bridges is difficult to reproduce with a static method
531 because of transient phenomena that are not governed by a simple energy crite-
532 rion. The impossibility for the energy minimization software to account for spatial
533 variations in the contact angle on the grain surfaces can also explain the remaining
534 discrepancies between experimental and numerical data.

535 A reciprocal investigation of the rupture of liquid bridges in grains assemblies
536 during drying will be considered in future work. By assuming that the rupture of
537 a coalesced volume occurs when the energy of the non-coalesced configuration is
538 lower than the energy of the coalesced configuration, it could be possible to predict
539 the volume at rupture and the resulting evolution of capillary forces in drying with
540 the presented numerical method. In addition, benefiting from the present approach
541 to compute capillary forces in the case of well-defined geometry assemblies with
542 small numbers of grains under a quasi-static loading, an extension to larger grain

543 assemblies is currently in progress for potential enrichment of existing microme-
544 chanical and multiscale models, such as the H-model [47]. First results pertaining
545 to the pendular regime are about to be published [50].

546 **Acknowledgements** The authors acknowledge F. Rouyer for the helpful discussions on the
547 Surface Evolver software. The authors also express their sincere thanks to the French Research
548 Network GeoMech (GDRI CNRS) for promoting and favoring interactions between researchers.
549 It helped improving the work by quality discussions.

550 Compliance with ethical standards

551 The authors declare that there is no conflict of interests regarding the publication
552 of this article. Publication has been approved by all authors. None of the material
553 presented in the paper is submitted or published elsewhere.

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684 **A Parametric study of numerical parameters in surface energy** 685 **calculation with Surface Evolver**

686 Compared to the calculation for a bridge between two grains, the convergence of the surface
687 energy minimization process is found to be more sensitive to the incremental distance δd
688 and to the numbers of gradient descent iterations and remeshings. The optimum calculation
689 parameters are determined by a parametric study.

690 The first parameter to determine is the incremental distance δd^* to apply to the system.
691 The first criterion is to find a δd^* not too large compared to the intergranular distances,
692 but large enough to obtain a significant difference between the surface energies of the two

693 configurations. The second criterion is to obtain a smooth variation of capillary forces with
 694 respect to the total volume of water contained in the cluster. In Figure 17, the capillary forces
 695 have been plotted as a function of the volume of water in funicular regime, for different value
 696 of δd^* between 1.10^{-4} and 9.10^{-2} . For $\delta d^* \leq 1.10^{-2}$, the values of capillary forces seem really
 697 imprecise, as the value of δE_s is too small compared to the precision on E_s , which means that
 698 δd^* requires being higher. For $\delta d^* > 1.10^{-2}$, the impact of δd^* on the capillary forces is less
 699 visible. In the following, we fix $\delta d^* = 0.06$ as the curve obtained with this value presents the
 700 smoothest shape.

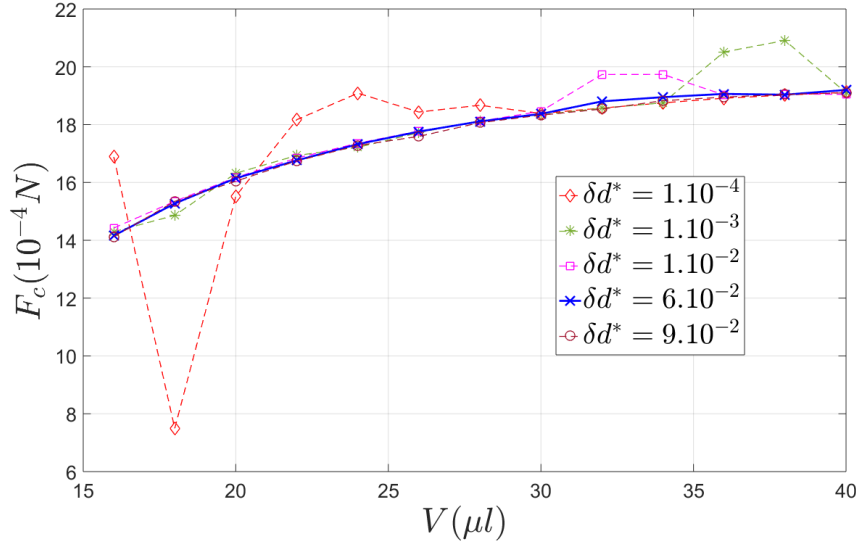


Fig. 17 Capillary force in a coalesced bridge between three grains, as a function of the volume of water, for different incremental intergranular distances δd^* , with 5 remeshings and 36 iterations between remeshings and after the last remeshing.

701 Sometimes, too much iterations of gradient descent method before a remeshing can lead
 702 to a divergence of the surface energy, when additional solid/gas interfaces are created outside
 703 the volume. Therefore, an optimized number of iterations between two remeshings has to be
 704 found. As shown in Figure 18, the number of iterations performed between remeshings affects
 705 the value of the capillary forces. We choose to perform 36 iterations between two remeshings
 706 since this curve is the smoothest.

707 Then, an optimized number of remeshings is determined from Figure 1. The capillary forces
 708 are calculated for a number of remeshings between 0 and 7, in order to observe a convergence in
 709 Figure 19. Between 5 and 7 remeshings, we observe a maximal relative difference of 0.35 %, and
 710 a mean relative difference of 0.21 %. Between six and seven remeshings, we observe a maximal
 711 relative difference of 0.07 % and a mean relative difference of 0.04 %. In the following, we
 712 perform six remeshings of the water interfaces.

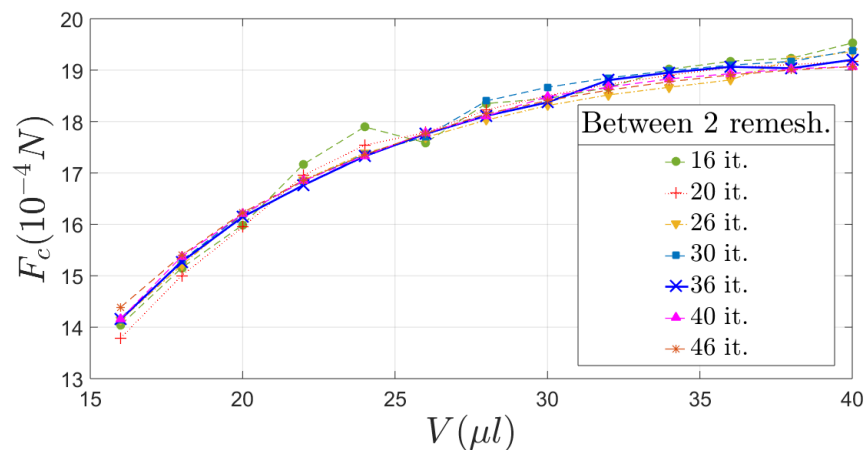


Fig. 18 Capillary force in a coalesced bridge between three grains, as a function of the volume of water, for different numbers of iterations between two remeshings, with $\delta d^* = 0.06$.

δd^*	0.06
nb. of iterations between remeshings	36
nb. of remeshings	6
nb. of iterations after the last remeshing	1400

Table 1 Values of the calculation parameters used in a coalesced bridge in a triplet of grains with $\theta = 0^\circ$

713 After the last remeshing, we have to control the convergence of the force calculation. Figure
 714 20 shows the capillary force in the coalesced bridge as a function of the volume of water, for
 715 different numbers of iterations after the last remeshing. This curves show a convergence of the
 716 capillary force, as we observe a mean relative error of 0.05 % between 1186 iterations and 1386
 717 iterations, and of 0.02 % between 1286 and 1386 iterations. In the following, we perform 1386
 718 iterations after the last remeshing.

719 Finally, for a coalesced bridge between three grains, with a contact angle $\theta = 0^\circ$, the
 720 following calculation parameters are chosen.

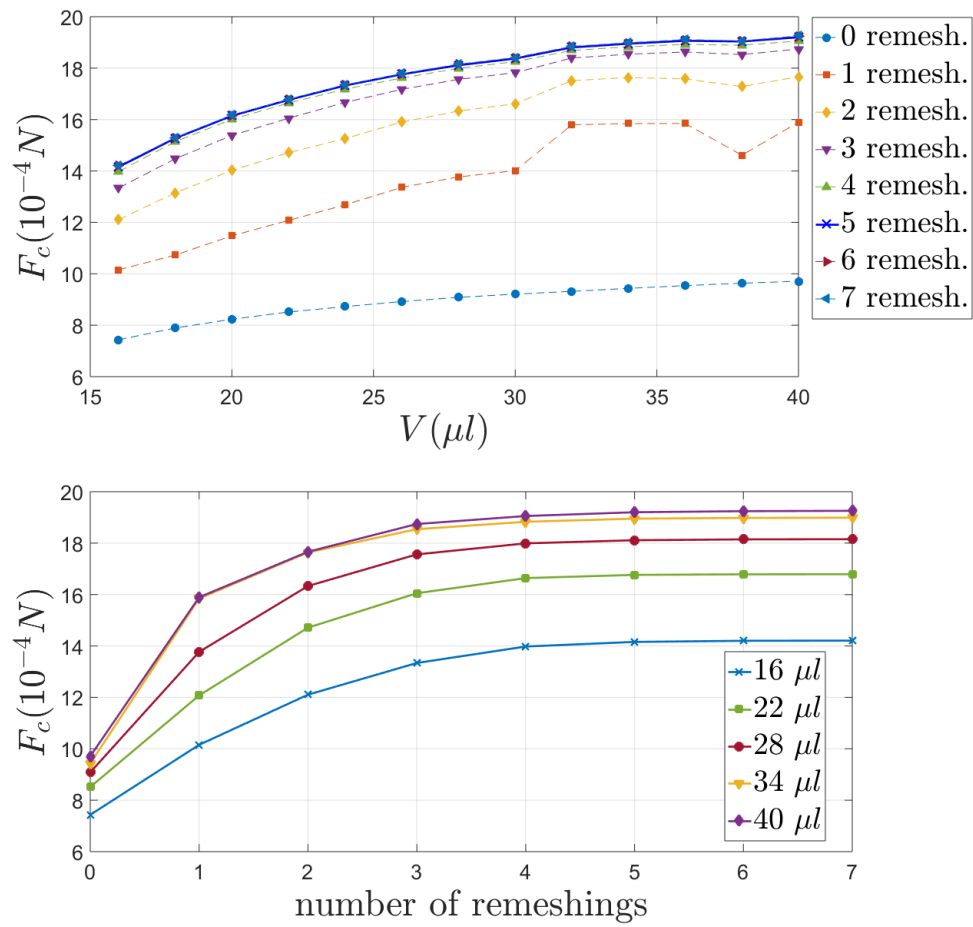


Fig. 19 Capillary force in a coalesced bridge between three grains, as a function of the volume of water, for different numbers of remeshings, (up), and as a function of the number of remeshings for different volumes of water (down), calculated with $\delta d^* = 0.06$ and 36 iterations between two remeshings.

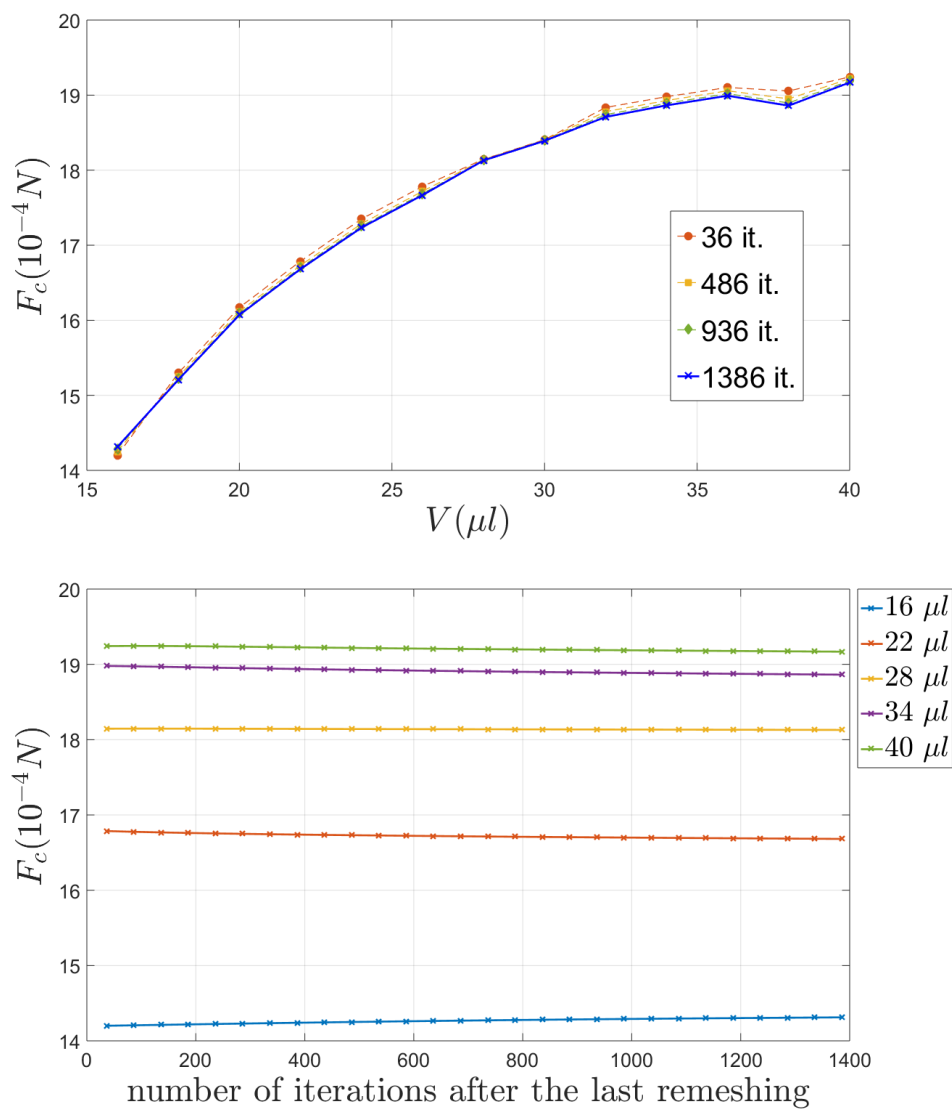


Fig. 20 Capillary force in a coalesced bridge between three grains, as a function of the volume of water, for different numbers of iterations after the last remeshing (up), and as a function of the number of iterations after the last remeshing for some volumes of water (down).