

A Phase-Field Discrete Element Method to study chemo-mechanical coupling in granular materials

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ABSTRACT

This paper presents an extension of the discrete element method using a phase-field formulation to incorporate grain shape and its evolution. The introduction of a phase variable enables an effective representation of grain geometry and facilitates the application of physical laws, such as chemo-mechanical couplings, for modeling shape changes. These physical laws are solved numerically using the finite element method coupled in a staggered scheme to the discrete element model. The efficacy of the proposed Phase-Field Discrete Element Model (PFDEM) is demonstrated through its ability to accurately capture the real grain shape in a material subjected to dissolution only and compute the stress evolution. It is then applied to model the phenomenon of pressure solution involving dissolution and precipitation in granular materials at the microscale and enables to reproduce the creep response observed experimentally. This framework contributes to the enhanced understanding and simulation of complex behaviors in granular materials and sedimentary rocks for many geological processes like diagenesis or earthquake nucleation.

1. Introduction

The intricate interplay between chemical and mechanical processes in soil and rocks has emerged as a key factor to consider for many engineering applications like underground storage or geothermal energy [1] or to understand geological processes like diagenesis or earthquake nucleation [2]. In particular, underground storage strategies envisioned to store large amounts of CO₂, captured from large point sources like power generation facilities, or H₂, produced during overproduction periods of renewable energies like solar or wind, involve the injection of a fluid into a reservoir rock. This fluid reacts with the surrounding rock inducing dissolution and/or precipitation that affects rocks' permeability [3], but also their mechanical behavior [4]. To ensure the long-term success and safety of such storage solutions, the role of chemo-mechanical couplings needs to be understood and modeled as they can influence settlement at the surface [5], the stability of the caprock [6,7] or induced seismicity [8].

Chemo-mechanical couplings are also fundamental to many geological processes. For example, understanding of diagenetic transformations and in particular the phenomenon of pressure solution [9] relies on a comprehensive grasp of these couplings. During the diagenetic processes sediments are transformed into sedimentary rocks. These processes influence reservoir quality in hydrocarbon exploration and the formation of economically valuable mineral deposits. Moreover, Pressure solution [10], has also a pivotal role in earthquake nucleation and recurrence. It involves three chemo-mechanical processes at the micro-scale [11]: dissolution due to stress concentration at grain contacts, diffusive transport of dissolved mass from the contact to the pore space,

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and precipitation of the solute on the less stressed surface of the grains. These processes lead to a time-dependent compaction of the rock by changing its microstructure, pore structure and composition [11]. It also induces a modification of the strength of a wide range of geological materials. As such, it has been suggested as a mechanism for long-term evolution of fault strength during interseismic periods [12], but also to control faults' frictional behavior at low speed and thus influences earthquake nucleation [10].

Chemo-mechanical couplings have already been investigated with finite-element models at the meso/macro scale [13] but this kind of formulation strongly depends the chosen constitutive equations, which are not well constrained as they depend on the specific microstructure and chemical reactions considered. To better understand the driving processes simulations on the microstructure should be considered. To do so, the discrete model (DEM) [14] is used in the present study as it enables the micromechanical analysis of granular materials and sedimentary rocks by reproducing the interactions among individual grains and grains' rearrangement [15]. Traditional DEM formulations assume grains as disks in two dimensions (2D) or spheres in three dimensions (3D). The dissolution/precipitation is then taken into account as a homogeneous decrease/increase of the grain diameter [16,17] or with an addition/subtraction of a dissolved/precipitated layer thickness at the contacts [18]. The extrapolation of the results obtained from those approaches to geological applications is limited as they only consider disks or spheres as grains, but real particles often exhibit highly irregular shapes. These complex geometries of the grains significantly influence the macroscopic mechanical behavior of granular materials [19,20]. Therefore, accurate models should aim to capture this complexity. Various approaches have been developed within the framework of DEM to account for irregular grain shapes. These include incorporating rolling resistance calibrated with grain geometry [21,22], utilizing grain clusters [23], using ellipsoids [24], employing superquadric particles [25], and even considering polyhedral shapes [26–28]. More recently, a level-set discrete element model was developed to capture the complex shapes of grains and reproduce experimental results [29,30]. However, none of those approaches consider a grain shape evolution due to chemo-mechanical couplings.

Considering the granular material as a phase, the phase-field theory (PF) [31–34] provides a suitable framework for modeling the local addition or reduction of material quantity using physics-based laws. Dissolution/precipitation at the contact interfaces is controlled by introducing mechanical and chemical energy into the Allen–Cahn formulation of the phase variables, while the mass conservation and the solute diffusion are addressed through a coupled diffusion formulation of the solute concentration [35]. Notice that phase-field description is not sufficient alone to describe the microstructure evolution. In granular matter, grain reorganization is described as discrete displacements of the grains. Phase-field formulation is solved with a Finite Element Method, so it is a continuous description, which is less suited than DEM approaches to model at the grain scale large deformation and contact topology changes as involved in grain reorganization.

Previous studies have already explored the coupling between finite element modeling and discrete element methods to study deformable grains [36] or grain growth and sintering [37]. In this study, we present an extension of the discrete element method to simulate irregular particle shapes in granular materials and their heterogeneous evolution using the phase-field variable as a geometric descriptor. We apply this method to two cases: (i) an oedometric test with partial dissolution and (ii) the pressure solution phenomenon involving two or multiple grains. The first case highlights the influence of grain shape and dissolution on the mechanical behavior, while the second case investigates the effects of heterogeneous dissolution and precipitation on the rate of material compaction.

2. Methodology

The objective of this paper is to present a novel coupling between a Phase-Field (PF) model and a Discrete Element Model (DEM). In this section, the algorithms and constitutive equations for discrete element models and the phase field are presented separately. The framework of the model is then presented to give an overview of the algorithm and how each model involved in the coupling scheme is used.

2.1. DEM

Time integration

The linear kinematics of grains are described by their center C . Various integration methods can be used [38], but for computational efficiency, an explicit method is chosen, the Symplectic Euler method. It is selected for its suitability and accuracy in the simulation [38], with time discretization playing a significant role in the simulation outcome. The rotation of the grains is also considered, especially in shearing problems. The rotation integration follows the same scheme. A rigid body rotation is used to compute the coordinates of the grain vertices.

Mass m and inertia I of the grains, used to solve the momentum balances [15], must be updated during a simulation as chemical reactions will modify the shape of the grain (dissolution/precipitation occurring). A Monte Carlo method [39] is used after each phase-field simulation to solve this problem, see Section 2.3.

Contact detection

As the particles are polygonal, an algorithm is needed to detect contact between grains i and j . First, the nearest vertex of grain j to grain i needs to be determined. This is achieved by applying a virtual displacement, as described in Eq. (1), to the vertices of grain j .

$$\mathbf{p}^v = \mathbf{p} + \max(R_i, R_j) \times \frac{\mathbf{C}_j - \mathbf{C}_i}{\|\mathbf{C}_j - \mathbf{C}_i\|} \quad (1)$$

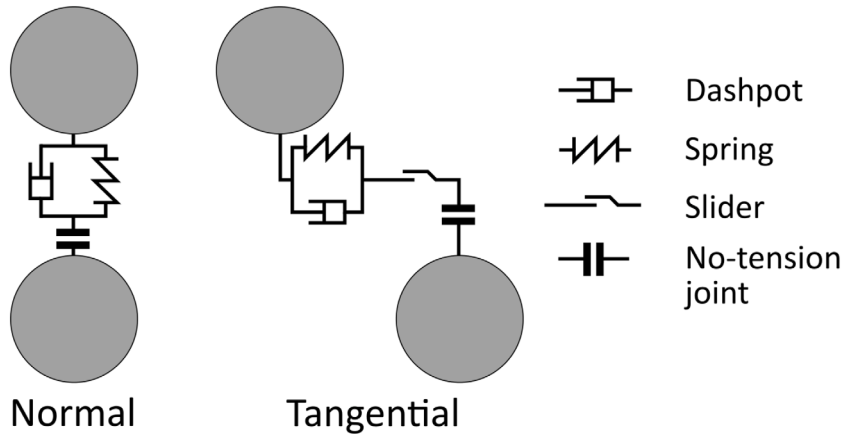


Fig. 1. Model for the interaction between two particles.

Here, $\mathbf{p}^v$ represents the virtual coordinates of the vertex, $\mathbf{p}$ denotes the coordinates of the vertex, $R_{i,j}$ is the maximum radius of the grain i, j (grains have different radii depending on the direction), and $\mathbf{C}_{i,j}$ denotes the coordinates of the center. This virtual translation assumes that the grains are not in contact (even if they were before this operation). After the virtual displacement, the distances between vertices of grains i and j are computed. The vertices used for contact detection are determined by considering the nearest ones after the virtual displacement.

Next, the algorithm of the common plane is applied to compute the contact normal vector $\bar{\mathbf{n}}$ [25–27] and the normal distance between grains is defined as $\delta_n = d^j - d^i$ where $d^{i,j}$ is the distance between grain and the common plane. It is important to note that particles are in contact only if the overlap δ_n is negative.

This contact algorithm, especially the virtual displacement approach, is conventional for spherical particles but its robustness is questionable for very complex shapes. Other proximity detection algorithms are available in the literature [40–42] and work better in the latter case. However, the performances of this algorithm are acceptable for grains with shapes close to spheres (as is the case here). A more suitable algorithm for contact detection will be the focus of future works.

Interaction between grains

The interaction between two grains is illustrated in Fig. 1 and described by the following constitutive laws. The normal response consists of a nonlinear spring and a dashpot in parallel, along with a no-tension joint. Similarly, the tangential response includes a nonlinear spring and a dashpot in parallel, a slider, and a no-tension joint. This description used here is the classical idealized interaction between two bodies. A more realistic one will be the subject of further work. Indeed, it appears in Section 4 that the contacts can become flat. Considering this observation, a distributed contact stiffness or a surface (2D)/volume (3D) stiffness would be more suitable.

The normal spring in the contact model is defined by Eq. (2). It is worth noting that some equivalent parameters, such as the Young's modulus Y_{eq} and the radius R_{eq} , are used and depend on the grain properties.

$$k = \frac{4}{3} Y_{eq} \sqrt{R_{eq}}$$

$$\text{where } \frac{1}{Y_{eq}} = \frac{1 - \nu_i^2}{Y_i} + \frac{1 - \nu_j^2}{Y_j} \text{ and } \frac{1}{R_{eq}} = \frac{1}{R_i} + \frac{1}{R_j} \quad (2)$$

Here, k represents the stiffness of the normal spring, $Y_{i,j}$ is the Young's modulus of the grain i or j , $\nu_{i,j}$ is the Poisson's ratio of the grain i or j , and $R_{i,j}$ is the mean grain radius of the grain i or j .

To introduce energy dissipation and reach an equilibrium, a linear damping term is added. The damping coefficient η is defined in Eq. (3) based on a restitution coefficient ($e = 1$ for perfect elastic contact, $e = 0$ for complete energy dissipation).

$$\eta = 2 \times \gamma \sqrt{m_{eq} \times k}$$

$$\text{where } \gamma = -\frac{\ln(e)}{\sqrt{\pi^2 + \ln(e)^2}} \text{ and } m_{eq} = \frac{m_i \times m_j}{m_i + m_j} \quad (3)$$

Here, η denotes the damping coefficient, $m_{i,j}$ is the mass of the grain i or j , k is the stiffness of the normal spring, and e is the restitution coefficient.

Next, the Hertz theory is applied in Eq. (4) to obtain the normal force [43–45]. A 3D formulation has been applied as the PFDEM aims to be applied for 3D geometries. It is important to note that this mechanical response is nonlinear with respect to the overlap. The stiffness increases as the overlap becomes larger. The damping term is also included.

$$F_n = F_{s_n} + F_{d_n} = -k \times \delta_n^{3/2} - \eta \times (\bar{\mathbf{v}}_i - \bar{\mathbf{v}}_j) \cdot \bar{\mathbf{n}} \quad (4)$$

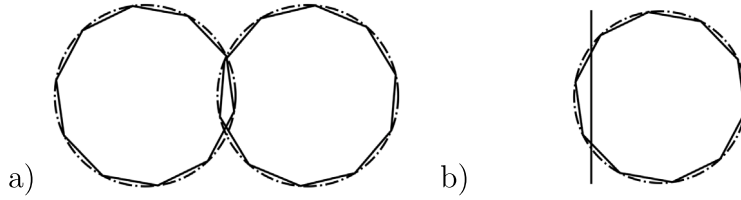


Fig. 2. Two cases are considered: (a) a contact grain–grain and (b) a contact grain–wall. The dashed lines represent perfectly circular grains.

Here, $\vec{v}_{i,j}$ is the speed of the grain i or j , and $\vec{n}$ is the normal vector of the contact.

Concerning tangential behavior, a tangential overlap vector $\vec{\delta}_t$ is computed incrementally by $\Delta\vec{\delta}_t$, defined Eq. (5).

$$\Delta\vec{\delta}_t = [\vec{v}_{ij} - \vec{n}(\vec{n} \cdot \vec{v}_{ij})] \times dt$$

where $\vec{v}_{ij} = (\vec{v}_i - \vec{v}_j) + R_i \vec{n} \times \vec{\omega}_i + R_j \vec{n} \times \vec{\omega}_j$ (5)

Here, $\vec{v}_{i,j}$ is the grain linear velocity vector, $\vec{\omega}_{i,j}$ is the grain angular velocity vector, dt is the time step.

It is important to notice that the orientation of the tangential vector can evolve with time. An update of this vector is done at each step, see Eq. (6).

$$\vec{\delta}_t = \vec{\delta}_t' - \vec{n}(\vec{n} \cdot \vec{\delta}_t') \quad (6)$$

Here, $\vec{\delta}_t$ is the tangential displacement updated and $\vec{\delta}_t'$ is the tangential displacement not updated.

The tangential spring in the contact model is defined by Eq. (7). Similar to the normal spring, it uses equivalent parameters (shear modulus G_{eq} and radius R_{eq}) that depend on the grain properties. Additionally, this parameter is obtained using the Mindlin and Deresiewicz theory [44–46]. The tangential stiffness depends on the normal overlap δ_n , with a stiffer spring for larger overlaps. Moreover, it is nonlinear, depending on the value of the norm of the tangential overlap $\vec{\delta}_t$, with a softer spring for larger tangential overlaps.

$$k_t = k_{t0} \sqrt{1 - \frac{2 \times k_{t0} \times \vec{\delta}_t}{3 \times \mu \times F s_n}}$$

where $k_{t0} = 8 \times G_{eq} \sqrt{R_{eq} \times \delta_n}$

and $\frac{1}{G_{eq}} = \frac{1 - \nu_i}{G_i} + \frac{1 - \nu_j}{G_j}$ and $G_i = \frac{Y_i}{2(1 + \nu_i)}$ (7)

Here, k_t represents the stiffness of the tangential spring, μ is the friction coefficient, and $G_{i,j}$ is the shear modulus of the grain i or j .

Similar to the normal contact, a linear damping term is added for energy dissipation, and the damping coefficient is defined in Eq. (8).

$$\eta_t = 2 \times \gamma \sqrt{m_{eq} \times k_t} \quad (8)$$

To obtain the tangential force vector $\vec{F s}_t$, the Coulomb criterion is applied, allowing sliding between grains.

$$\vec{F s}_t = -k_t \times \vec{\delta}_t$$

$$\vec{F s}_t \leq \mu F s_n \quad (9)$$

The total tangential force is the sum of the spring term and the damping term, as explained in Eq. (10).

$$\vec{F}_t = \vec{F s}_t + \vec{F d}_t = -k_t \times \vec{\delta}_t - \eta_t \times (\vec{v}_i - \vec{v}_j) \cdot \vec{t} \quad (10)$$

Note that the equations for the Discrete Element Method outlined in this Section and used in the present paper are frequently applied in the literature for geomaterials [15]. Multiple adaptations and expansions of this model exist, tailored to the specific applications targeted or couplings considered [47] and could be easily added to the present framework.

Influence of grain discretization

The discretization of the grain (= the number of vertices) is the main issue for the quality of the result for polyhedral particles. Hence, if the discretization is coarse, the shape is not well described and some errors can occur for contact computation. The goal of this paragraph is to study the influence of this parameter on the quality of the results. First, two simple cases illustrated in Fig. 2 are considered: two grains in contact and one grain in contact with a wall. Those cases represent the elementary phenomena in a granular sample.

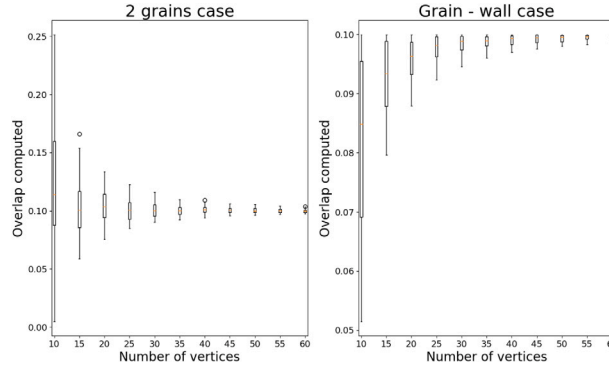


Fig. 3. Influence of the grain discretization on the overlap estimation (the targetted value is 0.10).

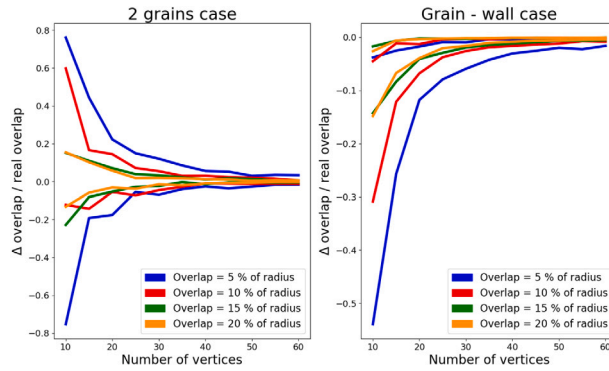


Fig. 4. Influence of the grain discretization on the overlap estimation for different solicitations. Only the first and the third quartiles of each data set are plotted.

Different grains with 10 to 60 (with a step of 5) vertices are generated to see the influence of grain discretization. Then, the grains are randomly rotated and the overlap is estimated with the common-plane algorithm [27]. The statistical result obtained with 100 repetitions is shown in Fig. 3. It appears the variation of estimated overlap (see the size of the boxes) decreases with grain discretization.

This study is repeated for different real overlaps. Indeed, for coarse discretization and low contact force, a theoretical contact cannot be detected because of the discretization. Fig. 4 shows that grain discretization greatly influences the results' quality for small overlap, as is the case in the granular sample.

Secondly, a more complex case is considered: a granular assembly composed of 300 grains is loaded under oedometric conditions. To see the influence of grain discretization, a sample composed of perfect disks is loaded. Then the grains are divided into 20, 30, 40 or 60 vertices. For each case, 10 simulations are run. Fig. 5 shows the evolution with time of the total kinetic energy, the coefficient $K_0 = \sigma_{II}/\sigma_I$, the upper wall position and the force applied on the upper wall for one run and different numbers of vertices. The number of vertices for one grain has a large influence on the global behavior of the sample. Indeed, with few vertices, a lot of fluctuation is introduced in the computing of the contacts. This fluctuation is reflected in the estimation of the coefficient K_0 . Moreover, the total kinetic energy stays at a large value with few vertices by grains. The equilibrium cannot be reached.

A statistical analysis of the total kinetic energy and the estimation of the coefficient K_0 of all the runs is presented in Fig. 6. For all runs, the difference between the third quartile and the first one is estimated. Then, a mean value is computed for the different numbers of vertices. It appears the fluctuation is decreasing with the quality of the discretization.

It appears the discretization of the grains is a main parameter to capture accurately the interactions at the particle level and to minimize the noise in more complex granular media. At least 60 nodes are considered in this work to discretize the grains (80 nodes are considered for more complex shapes).

2.2. Phase-field

A granular medium is composed of grains and pores. As illustrated in Fig. 7, this porous matter is represented here in the phase-field space by a combination of phase variables (one phase per grain). This phase variable equals 1 if it is inside the grain associated and equals 0 elsewhere.

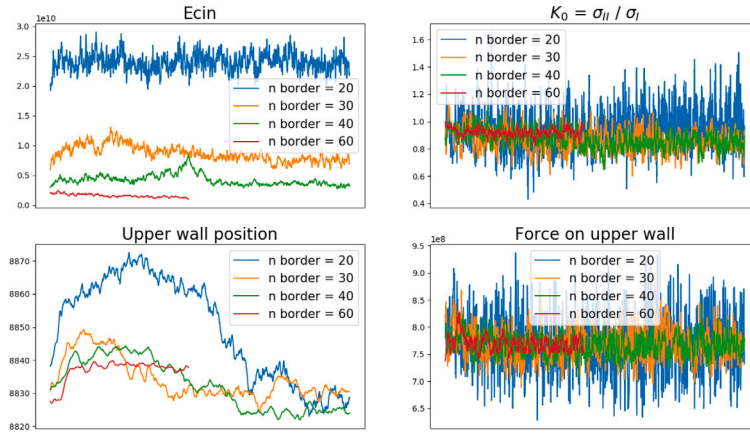


Fig. 5. Evolution with time of the total kinetic energy, the coefficient $K_0 = \sigma_{II}/\sigma_I$, the upper wall position and the force applied on the upper wall for different numbers of vertices.

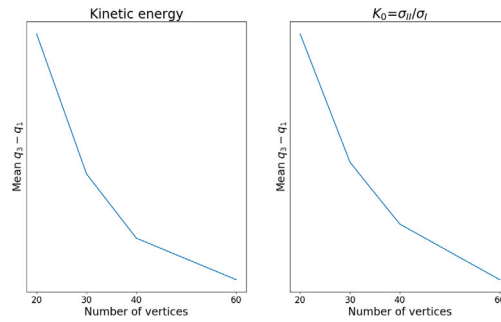


Fig. 6. Statistical analysis about the fluctuation of the coefficient $K_0 = \sigma_{II}/\sigma_I$ for different numbers of vertices.

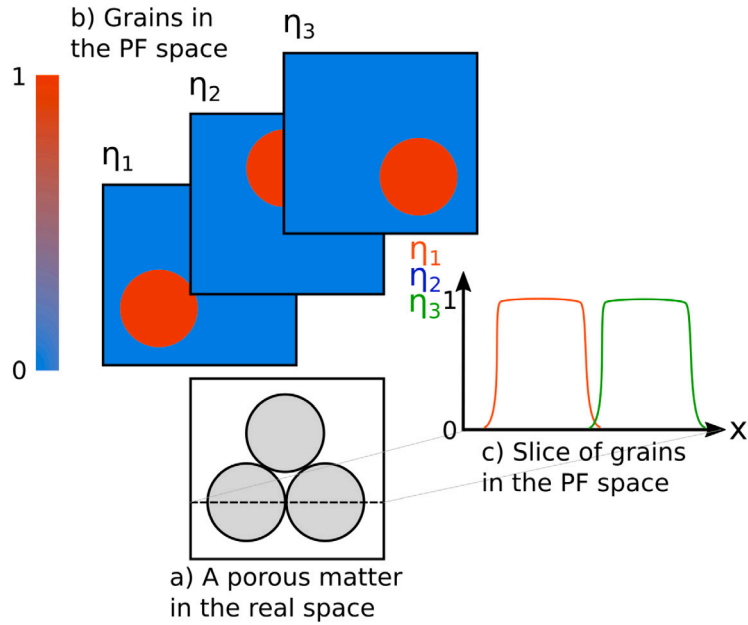


Fig. 7. The phase-field method is applied to granular matter: (a) a granular matter is composed of grains and by pore, (b) one phase variable η_i is generated by grain, (c) the phase variable is equal to 1 if it is inside the grain associated and equal to 0 elsewhere.

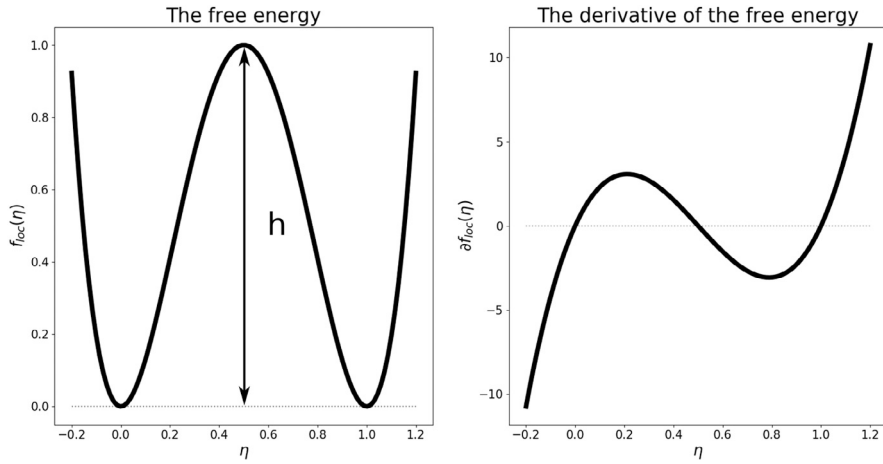


Fig. 8. A double-well function as a local free energy density f_{loc} and its derivative $\frac{df_{loc}}{d\eta}(\eta)$ (the energy barrier $h = 1$ in this example).

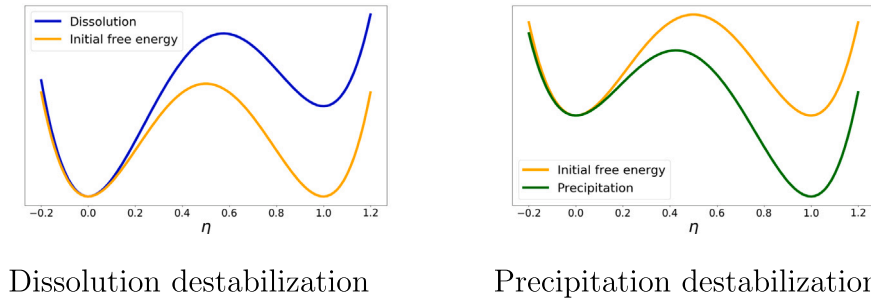


Fig. 9. The double-well function is destabilized to favor dissolution/precipitation.

The phase-field method, specifically the Allen–Cahn equation described in Eq. (11), is employed to describe the dissolution/precipitation of the material [33]. In this approach, nonconserved order parameters η_j are utilized to represent the phase transformation.

$$\frac{\partial \eta_j}{\partial t} = -L_j \left(\frac{\partial (f_{loc} + E_d)}{\partial \eta_j} - \kappa_j \nabla^2 \eta_j \right) \quad (11)$$

In this equation, the terms L_j and κ_j correspond to the order parameter mobility and the gradient energy coefficient, respectively. The order parameter mobility affects the overall dissolution/precipitation kinetic, while the gradient energy coefficient influences the interface width and reaction. The term E_d encompasses additional sources of energy introduced into the system, such as mechanical, chemical, or thermal loading. The local free energy density f_{loc} is specified in Eq. (12) and is visualized in Fig. 8.

$$f_{loc} = 16 \times h \times \left(\sum_j \eta_j^2 (1 - \eta_j)^2 \right) \quad (12)$$

The local free energy density f_{loc} employs a double-well function with a barrier height h [48]. Notice that the minima of this potential energy are located at $\eta_j = 0$ and $\eta_j = 1$. At the equilibrium and without external destabilization, the phase variables stay at $\eta_j = 0$ or $\eta_j = 1$ (no dissolution/precipitation). Fig. 8 illustrates the double-well function as a representation of the local free energy density f_{loc} and its derivative regarding the phase variable η .

To obtain localized dissolution/precipitation, the idea is to add external source term E_d to tilt the initial free energy to favor dissolution/precipitation, as depicted in Fig. 9. When the dissolution phenomenon dominates, the double-well function is tilted towards $\eta_j = 0$, causing the material to aim for dissolution. Conversely, when the precipitation phenomenon dominates, the double-well function is tilted towards $\eta_j = 1$, indicating the material's tendency to precipitate.

To model solute concentration in the pore fluid, a new variable, denoted as c , is introduced in the phase-field formulation. The Eq. (11) is solved along with a new equation for the variable c , as given in Eq. (13).

$$\frac{\partial c}{\partial t} = - \sum_j \left(\frac{\partial \eta_j}{\partial t} \right) + \kappa_c \nabla^2 c \quad (13)$$

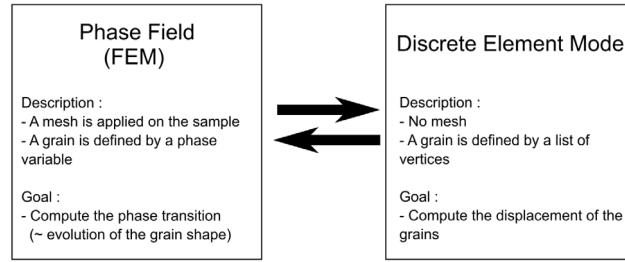


Fig. 10. Data exchange between the phase-field simulation and discrete element modelization.

The Eq. (13) represents the conservation of solute mass and is solved using the variations of phase-field variables η_j as a source term. Here, κ_c represents the gradient energy coefficient that controls the diffusion rate. Notably, the gradient energy coefficient κ_c is assumed to be 0 within the grains, so that the solute concentration c is nonzero outside the grains and diffuses from the contact area to the pore surface. The algorithm's implementation for building the heterogeneous gradient energy coefficient κ_c is described in Appendix B. The terms $\frac{\partial c}{\partial t} = - \sum_j \frac{\partial \eta_j}{\partial t}$ in Eq. (13) ensure the conservation of mass. When a grain (η_j) dissolves, solute concentration (c) is generated, and vice versa, when η_j is generated through precipitation, some solute disappears.

Eqs. (11) and (13) are solved with the open-source finite element software MOOSE [49]. This software uses automatic differentiation to solve the system of equations with an implicit formulation.

A special focus is placed on the mesh dependency of the problem. Indeed the mesh resolution influences the resolution of the Phase-Field equations and the discretization of the grain, see Section 2.1.

The mesh should be fine enough to obtain accurate results for solving the Phase-Field equations. The critical element is the interface thickness. In the literature, the criteria $w \sim 4\Delta x - 8\Delta x$ and $\Delta x \leq R/5$ are advised [48,50] where w is the interface width, Δx is the mesh size and R is the grain radius. Combining the two criteria, a third one is obtained: $w \leq 4R/5$. In this study, a finer interface has been selected ($w \sim R/10 \iff \Delta x \sim R/40$) to be sure the mesh has no influence on the numerical results and to have a fine interface compared to the grain size [50].

Concerning the discretization of the grain, the mesh limits the maximal number of vertices defining a grain, see the algorithm presented in Section 2.3. Considering the mesh size described earlier in this section ($\Delta x \sim R/40$) it appears that the maximum discretization is ≈ 160 nodes (2 vertices per slice). This value is much larger than the discretization considered in Section 2.1.

To summarize, assuming a fine interface compared to the size of the grain induces mesh independence of the numerical results.

2.3. PF-DEM couplings

The data exchange and global scheme of the PF-DEM couplings are illustrated in Fig. 10 and in Algorithm 1, respectively.

In the phase-field simulation, the sample geometry is discretized into a mesh, and the grains are represented by phase variable maps. A grain detection algorithm is applied to determine the new grain shape and solute configuration based on the phase-field outputs. On the other hand, in the discrete element modelization, grains are represented as a collection of vertices. This model aims to compute the new positions of the grains and the mechanical energy at each contact.

It is important to note that although PF and DEM operate on different time scales, they are still connected. The mechanical equilibrium (DEM) is assumed to be instantaneous, while grain dissolution or precipitation occurs over longer time periods, typically several hours to days.

Algorithm 1 Global scheme of the simulation. Two time scales are used: one for DEM and one for PF.

```

while work not finished do
  Build grains from PF data
  Update geometric parameters
  while not DEM equilibrium do
    Compute solicitations
    Solve the momentum balances
    Check the equilibrium criteria for DEM
  end while
  Recreate the maps of phase variable
  Solve PF equations
end while

```

▷ Start the DEM simulation

▷ Start the PF simulation

After a phase-field step, the system does not immediately reach a mechanical equilibrium due to ongoing dissolution or precipitation. Therefore, the new grain boundaries need to be detected. Fig. 11 illustrates the division of the phase-field into multiple layers (along the different axes), assuming the grain boundary occurs at $\eta_j = 0.5$ and using a linear approximation.

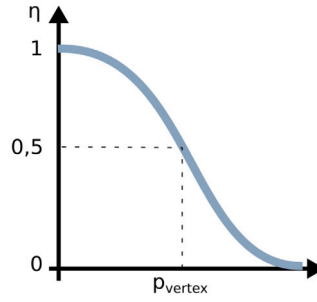


Fig. 11. The phase field is divided into layers, and the grain boundary is assumed to occur at $\eta_j = 0.5$.

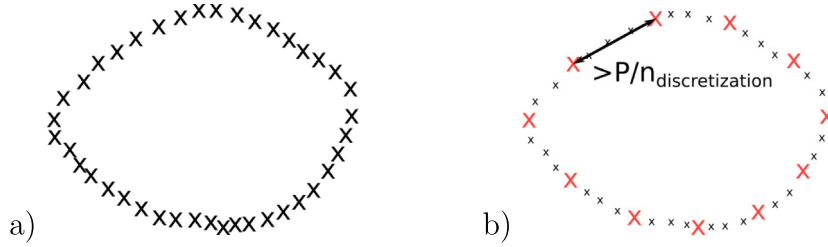


Fig. 12. Even if (a) the grain is described as a list of vertices, (b) only a part of this list is considered to save computational cost.

Table 1

Comparison of the Deconstruction-Rebuild (DR) and the Interpolation (Int) algorithms to build phase map after a DEM step.

	DR	Int
Assume the interface width w constant	x	
Generate a new mesh at each PF simulation	x	
Conservation of the information between PF simulations		x
Can track the solute concentration c		x

A polygonal particle is obtained based on the vertex positions. To reduce computational cost, only a certain number of vertices are used. As explained in Fig. 12a, all nodes are considered initially. Then, the perimeter of the polygon is computed by summing the distance of the nearest nodes all over the grain. An average node distance is computed considering the perimeter and the grain discretization $d_{min}^{dis} = \text{Perimeter} / n_{discretization}$. Finally, an iterative step is used, considering a random starting vertex. As illustrated in Fig. 12b, the vertices list is read until the distance between the two vertices (starting and the list's ones) is at least the average node distance d_{min}^{dis} . The iteration keeps going, considering the list's vertex as the new starting one. This method helps to minimize the number of nodes and to have a homogeneous discretization of the grain.

The discretization of the grain boundary is crucial, and the quality of overlap estimation depends strongly on this parameter, as explained in Section 2.1. The geometric properties of the grain, such as its center, surface area, and inertia, can be computed from the list of vertices using a Monte Carlo method [39] described in Appendix A.

Once the grain boundaries are known, a series of DEM iterations takes place until the system reaches an equilibrium. To dissipate mechanical energy, some damping is introduced, as explained earlier in this section. The convergence criteria for detecting the equilibrium may vary depending on the problem. In this work, the equilibrium is detected when the three following criteria are verified :

- the sum of the kinetic energy over the grains is smaller than a threshold value.
- the confining pressure applied is in the window defined by 0.95 and 1.05 the confining pressure targetted.
- the position of the top wall (controlled to apply the load) is stable. The variance of the latest positions is below a threshold value.

Moreover, a maximum number of iterations is set to avoid an infinite loop. Once the equilibrium is reached before the maximum number of iterations, new phase maps are constructed to update the geometry of the phase field problem based on the results of the DEM step.

Two methods have been designed to construct the new phase maps: the Deconstruction-Rebuild and the Interpolation algorithms. A comparison of their features is shown in Table 1.

In the simulations presented in Section 3, a Deconstruction-Rebuild algorithm is employed, assuming that the interface width (w) remains constant throughout the study. Indeed, the solute concentration does not need to be tracked as it is assumed immediately

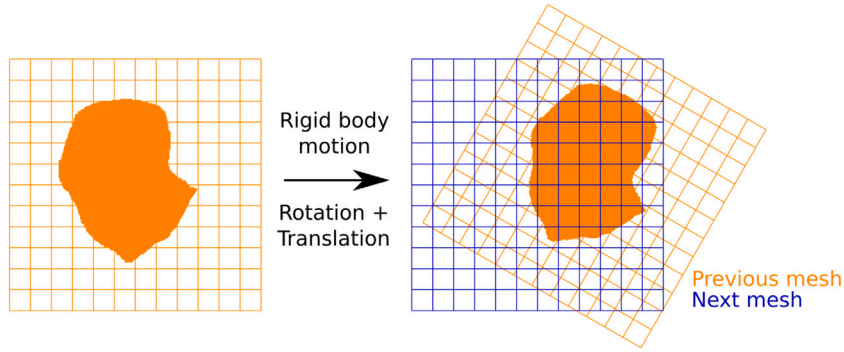


Fig. 13. Scheme of the interpolation algorithm. The next mesh is computed from the previous mesh by applying an inverse rigid body motion.

evacuated [17,51]. Moreover, this algorithm is faster than the Interpolation one. Given the knowledge of the center and vertices of a grain (the Deconstruction part), a distribution of the radius R following the angle can be computed (the choice of the angle origin is arbitrary; for this study, the +x-axis is considered). Subsequently, the new phase variable η_j is calculated using a cosine profile described by Eq. (14) for all nodes of the mesh (the Rebuild part).

$$\eta_j = \begin{cases} 1 & \text{for } r \leq R - \frac{w}{2} \\ 0.5 \times \left(1 + \cos \left(\pi \frac{r - R + \frac{w}{2}}{w} \right) \right) & \text{for } R - \frac{w}{2} \leq r \leq R + \frac{w}{2} \\ 0 & \text{for } r \geq R + \frac{w}{2} \end{cases} \quad (14)$$

Here, r represents the distance between the node and the center, R is the radius in the considered direction, and w denotes the interface width.

In the simulations presented in Section 4, an Interpolation algorithm is used. This algorithm considers that the interface width (w) is not constant during the study, particularly increasing in the contact zone during pressure solution modeling. Moreover, it becomes important to track the solute concentration c . The new phase map is obtained through interpolation from the previous one. As illustrated in Fig. 13, at each iteration, the next mesh is computed based on the previous mesh by applying an inverse rigid body motion. Since the two meshes often do not perfectly match, bilinear (2D) or trilinear (3D) interpolation is performed to estimate the values of the next mesh.

The deformation induced by the phase-field simulation and the grain displacements computed in the discrete element modelization are closely interconnected. It is important to ensure that the deformation remains in the small-strain range. For fluid–structure interaction problems, an Aitken method [52] is commonly used to adapt the deformation of the structure. Here, the deformation of the grain during a phase-field simulation can be controlled with an adaptive time step (relative to shape evolutions). A classical threshold values system is used in this problem. The duration of the simulation, and consequently the grain deformation during the phase-field simulation, depends on the mean absolute value per contact node of the total energy E_d . This parameter is related to the deformation known in the phase-field simulation. The importance of this method is illustrated in Fig. 14 where a lateral displacement for 2 grains pressure solution configuration, see Section 4, is plotted without the inspired Aitken method. Oscillations appear, revealing large deformation in the Phase-Field simulations. At step i , a large amount of grain dissolves, a lot of solute is available, and the grains get closer. At step $i + 1$, the solute available generates a large amount of grain precipitation, and the grains get further. The inspired Aitken method allows the use of an efficient Phase-Field simulation duration, verifying a small deformation criterion.

By initializing the sum of the absolute total energy as $E_{d,abs}$ and the number of contact nodes as $node_contact$, the mesh is scanned. If a contact zone is detected (where η_i and η_j are both larger than 0.5), the absolute value of the total energy E_d is added to the indicator $E_{d,abs}$, and the number of contact nodes is incremented. The mean absolute value per contact node of the total energy $\overline{E_{d,abs}}$ is then computed $= E_{d,abs} / node_contact$. This mean parameter plays the role of the discriminant value and depending on the threshold values, a time step dt is determined for the phase-field simulation.

3. Application to irregular shapes and homogeneous dissolution

This Section aims to demonstrate the capability of the PFDEM to handle irregular grain shapes. The simulations conducted here are intended to be compared with previous experiments and numerical simulations conducted by Shin et Santamarina and Cha et Santamarina [51,53]. Fig. 15 illustrates the setup where a sample is subjected to a constant stress in oedometric conditions while acid is injected. The granular material consists of two types of grains: dissolvable and undissolvable.

The distribution between dissolvable and undissolvable grains is determined by the ratio of the total surface area of dissolvable grains to the total surface area of all grains. As the acid is injected, it tends to reduce the size of the dissolvable grains. It has been

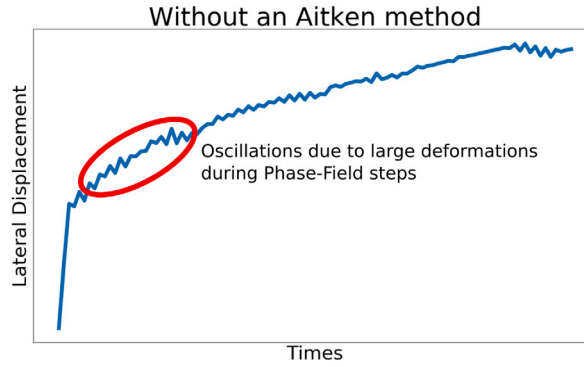


Fig. 14. Lateral displacement for a 2 grains pressure solution configuration, see Section 4, without an inspired Aitken method. Oscillations appear because of the large deformation in the Phase-Field simulations.

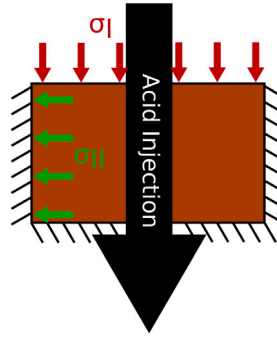


Fig. 15. Scheme of the sample under oedometric condition and acid injection.

Table 2

Parameters used for the simulation campaign, concerning the acid injection inside a sample under oedometric condition.

Parameters	Unit	Value
Number of grains	–	300
Particle size distribution for undissolvable grains (radius and percentage of the number of undissolvable grains)	$\mu\text{m}(\%)$	420 (17), 385 (33), 315 (33), 280 (17)
Percentage of grain dissolvable ($= S_{\text{dissolvable}} / (S_{\text{dissolvable}} + S_{\text{undissolvable}})$)	%	5 or 15
Particle size distribution for disks as dissolvable grains (radius and percentage of the number of dissolvable grains)	$\mu\text{m}(\%)$	360 (17), 330 (33), 270 (33), 240 (17)
Particle size distribution for squares as dissolvable grains (dimension and percentage of the number of dissolvable grains)	$\mu\text{m}(\%)$	500 (17), 460 (33), 380 (33), 440 (17)
Young modulus	GPa	70
Poisson's ratio	–	0.3
Density	kg/m^3	2500
Friction grain–grain	–	0.5
Friction grain–wall	–	0
Restitution coefficient	–	0.2
Mobility for phase-field	–	1
Gradient coefficient for phase-field	–	3
Time step for discrete element model	s	$\Delta t_{\text{crit}}/8$
Linear force applied on the upper wall	N/m	$4 \times Y R_{\text{mean}}/2000$
Percentage of the mean dimension dissolved between each iteration	%	0.5

observed that the coefficient $K_0 = \sigma_{II}/\sigma_I$ evolves with the dissolution process due to internal reorganization around the dissolvable grains.

The simulation campaign parameters are provided in Table 2. The mean behavior is obtained by extrapolating results from three simulations for each configuration.

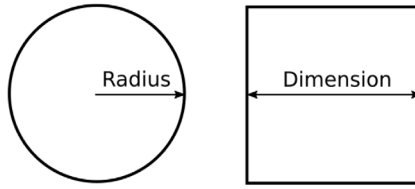


Fig. 16. Definition of the characteristic length for a disk and a square.

Table 3

Different samples are tried with different numbers of grains. Each configuration is run several times to make a statistical study of the results.

Number of grains	50	100	200	300	400	500	700
Number of runs	10	10	10	9	10	5	5

In the simulations presented in this study, the undissolvable grains are always assumed to be disks, while the dissolvable grains can be either disks or squares (although other shapes are possible, the simulation is restricted to these two). The main objective of this Section is to discuss the influence of grain shape on overall behavior. The latter choice is only possible in the present framework and represents more accurately the experimental setup as the undissolvable grains are glass beads and the dissolvable ones are salt grains with a cubic shape. The size of the grains is defined as shown in Fig. 16, where a disk is characterized by its radius and a square is determined by the length of one side.

The choice of grain shape affects certain material properties, such as surface density. For disk particles, the surface density is given by $\sigma_m = \frac{4}{3}\rho R_{\text{mean}}$, while for square particles, it is $\sigma_m = \rho L_{\text{mean}}$, where R_{mean} is the mean radius, L_{mean} is the mean dimension, and ρ is the density.

The time step for the DEM is computed based on the critical time step defined for a sphere using the Hertzian contact model, as shown in Eq. (15) [54]:

$$\Delta t_{\text{crit}} = \frac{\pi L_{\text{min}}}{0.1631\nu + 0.88} \sqrt{\frac{\rho}{G}} \quad (15)$$

Here, L_{min} represents the minimal characteristic length for the grains (half of the dimension for squares), ν is the Poisson's ratio, ρ is the density, $G = \frac{Y}{2(1+\nu)}$ is the shear modulus, and Y is the Young's modulus.

A linear vertical force is applied to the upper wall to confine the sample. The intensity of this force is proportional to the normal stiffness, considering an isotropic 3D material model with $k_n = 4 \times Y \times R_{\text{mean}}$ [55], where Y is the Young's modulus and R_{mean} is the mean radius of the undissolvable grains.

To establish the initial configuration, perfect disks are assumed (using the circumscribed circle for non-disk grains). These disks are randomly generated without overlap within the sample and then loaded. Once an initial equilibrium is reached, the disks are discretized, and their shapes are maintained. Another loading step is performed to reach a second equilibrium. A sample geometry with a height-to-diameter ratio of 0.6 is chosen to minimize boundary effects at the top and bottom [51], and the sample generation process ensures this geometry is achieved.

3.1. Influence of the number of grains

The definition of the particle size distribution depends on the specific case and is presented in Table 2. The total number of grains has been chosen to minimize computational cost while respecting the assumption of a representative element volume, as determined by a preliminary study presented in the following.

Circular particles are used for this analysis on the representative number of particles to optimize the computational cost. Parameters from Table 2 are used to define the material constitutive laws, the DEM time step, and the particle's geometry. As described by Table 3, the number of grains varies between 50 and 700. The table also describes the number of simulations run for each number of grains (between 5 and 10 times). 15% of the grains selected randomly are assumed as dissolvable. After equilibrium is found, the radius of the dissolvable particles decreases by 1% of the initial mean radius (350 μm).

The results are presented in Figs. 17–19. A statistical study is done on the evolution of the $K_0 = \sigma_{II}/\sigma_I$ with dissolved material quantity to determine the representative equivalent volume.

We can observe that the results obtained with only 50 grains are scattered and therefore not representative. Even if Fig. 18 shows that mean curves are the same for samples with 100, 200 or more than 300 grains, Fig. 19 highlights the large variance for the case of 100 grains. The representative equivalent volume can be assumed with 200 grains as the variance is much lower. As the sample is a granular material, the results are always noisy. Even if the sample is with a representative element volume, several simulations at the same configuration should be done to work with a mean evolution.

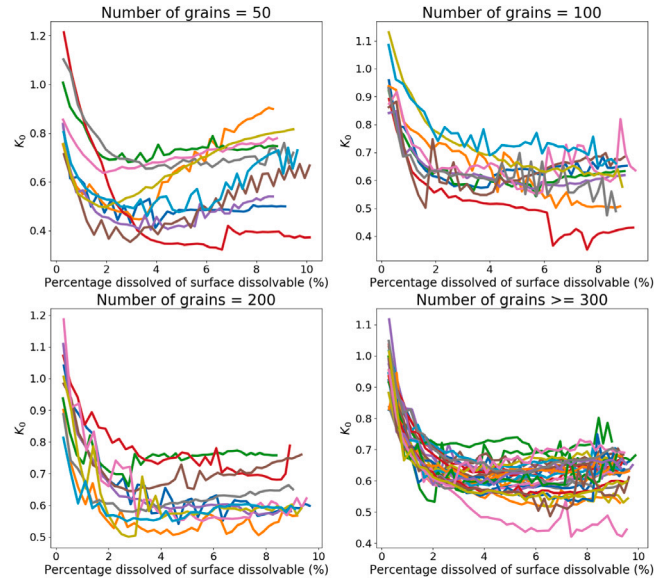


Fig. 17. All curves of the preliminary campaign sorted following the number of grains in the sample.

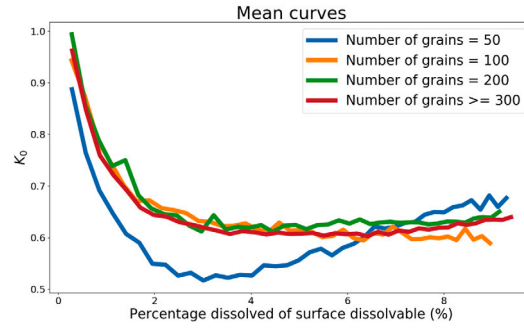


Fig. 18. Mean curves for different numbers of grains in the sample.

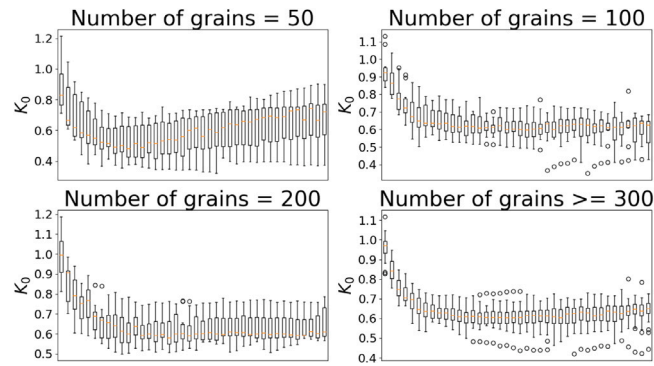


Fig. 19. Statistical study to justify that a sample with 200 grains is a representative equivalent volume.

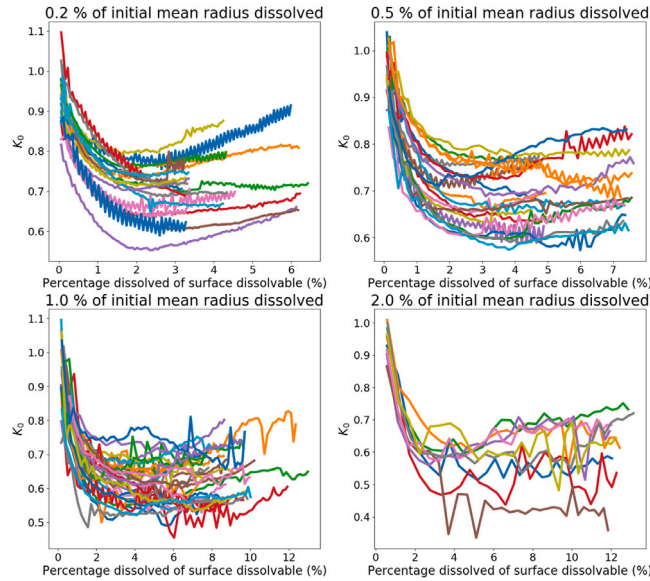
3.2. Influence of the step in the grain dissolution

In this case, the external source term E_d in the phase-field formulation (as described in Eq. (11)) models the acid. It is assumed that the solute quantity generated by dissolution is instantaneously evacuated (the diffusive-conservative Eq. (13) is not solved and the solute concentration c is not tracked). The formulation of this source term is explained in Eq. (16). It should be noted that this

Table 4

Different radius reductions between iterations are tried. Each configuration is run several times to make a statistical study of the results.

Radius reduction (% of the initial mean radius)	0.2	0.3	0.5	0.6	0.7	1.0	2.0	5.0
Number of runs	21	9	13	9	9	13	9	5

**Fig. 20.** All curves of the preliminary campaign sorted following radius reduction.

term is applied only to dissolvable grains, as there is no interaction between grains during the phase-field simulation. Therefore, it is possible to extract dissolvable grains individually for separate simulations, and undissolvable grains are not included in the phase-field simulation as they remain unchanged.

$$E_d = e_{\text{diss}} \times \left(\sum_j \eta_j^2 (3 - 2\eta_j) \right) \quad (16)$$

Here, e_{diss} represents the energy of dissolution, and η_j is a phase variable that models a dissolvable grain.

The amount of material dissolved during each phase-field simulation step depends on the grain size, the energy of dissolution e_{diss} , and the duration of the simulation. It is important to ensure proper discretization between DEM steps. In this regard, the DEM step models mechanical equilibrium, while the PF step models dissolution as the source of perturbation. Mechanical equilibrium is assumed to be instantaneous, and the amount of material dissolved between DEM simulations must be sufficiently small. A simulation campaign presented in the following was conducted to verify this criterion.

To have faster results, perfect circle particles are used. Parameters from Table 2 are used to define the material, the discrete element model time step, and the particle's geometry. According to the preliminary work about the representative equivalent volume presented in this Section, the number of grains is 300. 15% of the grains selected randomly are assumed as dissolvable. As described by Table 4, the radius of the dissolvable particles is decreasing by 0.2%, 0.5%, 1.0% or 2.0% of the initial mean radius (350 μm). The table also describes the number of simulations run for each radius reduction (between 8 and 15 times). The radius reduction between iterations defines the representative dissolution.

The results are presented in Figs. 20–22. A statistical study is done on the evolution of the $K_0 = \sigma_{II}/\sigma_I$ with dissolved material quantity to determine the representative dissolution.

The results obtained with a radius reduction equivalent to 2.0% of the initial mean radius are dispersed and thus not representative. Moreover, the steps are too large to describe the initial fast decrease of K_0 . Figs. 21 and 22 show the curves obtained with a radius reduction lower than 0.5% of the initial mean radius are reproducible and the initial fast decrease is well captured by those configurations. The representative dissolution can be assumed with a radius reduction equivalent to 0.5% of the initial mean radius. Notice that in this study no inspired Aitken method is needed. Indeed, the deformation of the grains aims to stay constant during the phase-field simulation. As the sample is a granular material, the results are noisy. Even if the sample is with a representative dissolution, several simulations at the same configuration should be done to work with a mean evolution.

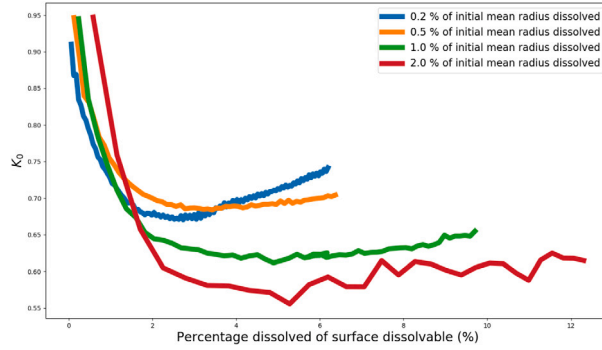


Fig. 21. Mean curves for different radius reduction.

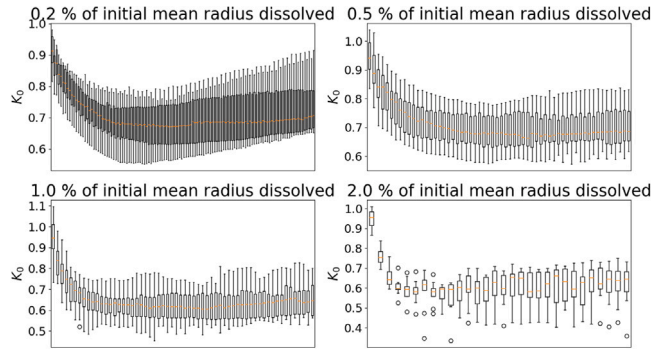


Fig. 22. Statistical study to justify that 0.5% of the initial mean radius dissolved at each iteration is a representative dissolution.

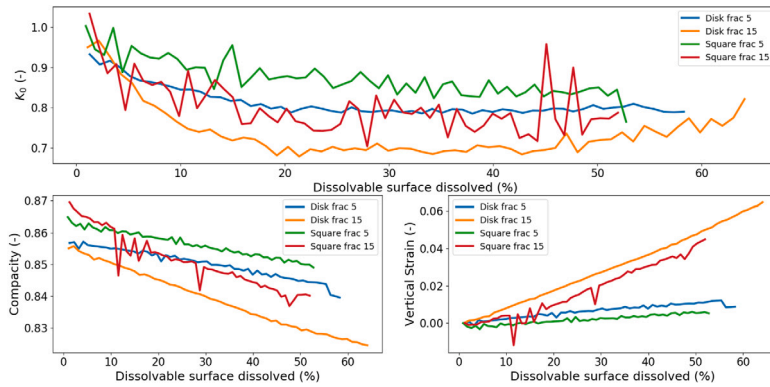


Fig. 23. Mean evolution of K_0 (top), of the compacity (left) and the vertical strain (right) with the dissolution of the dissolvable material, considering dissolvable grains as disks or as squares. Two ratios of the dissolvable surface over the total surface are studied.

3.3. Influence of the particle shape

The results of the simulation campaign are shown in Figs. 23 and 24. Additionally, four example movies are linked to this article, demonstrating the evolution of grain configuration and chain forces for both disk-shaped and square-shaped dissolvable grains with a dissolvable surface ratio of 0.15 relative to the total surface.

Fig. 23 illustrates the mean evolution of K_0 (top), compacity (left), and vertical strain (right) with the dissolution of dissolvable material, considering dissolvable grains as disks or squares. Two different ratios of dissolvable surface to total surface are studied. As highlighted by Shin et Santamarina and Cha et Santamarina [51,53] and observed in Fig. 23, the dissolution of grains leads to an evolution (increase or decrease) of the coefficient $K_0 = \frac{\sigma_{II}}{\sigma_I}$. In this paper, a stronger reduction in K_0 is observed when the percentage of dissolvable grains is larger. This reduction occurs due to the reorganization of grains around the dissolved grains,

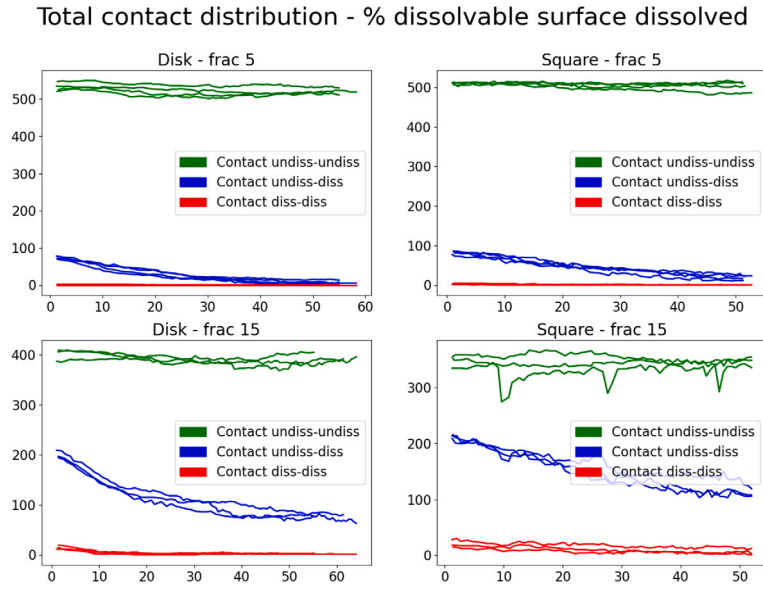


Fig. 24. Evolutions of contact distribution with the dissolution of the dissolvable material, considering dissolvable grains as disks or as squares. Two ratios of the dissolvable surface over the total surface are studied.

as shown in Fig. 24. The number of undissolvable–dissolvable contacts decreases with material dissolution, while the number of undissolvable–undissolvable contacts remains relatively constant.

It should be noted that the simulations by Shin et Santamarina and Cha et Santamarina constrained particle rotation to account for grain angularity and interlocking, while in our simulations, particle rotation remains free. Figure 3 from Cha et Santamarina [53] highlights that hindering the grains rotation tends to decrease the coefficient K_0 . Hindering particle rotation is often used as a proxy for grains angularity [56], so their simulations results tend to show that more angular grains would have a larger decrease of K_0 , which is the opposite that what we observe on 23. This highlights the importance of considering explicitly the grain shape to obtain an accurate response of the system. A parametric study would be relevant to better understand the influence of confinement, particle size distribution, rolling model, and initial compressibility to better understand in which conditions a rolling model can be used as a proxy for grains angularity when chemo-mechanical couplings are involved.

Furthermore, simulations with square dissolvable grains exhibit more fluctuation, even though the grain discretization was increased to 80 vertices for these simulations. This phenomenon is common in simulation with polygons [20,57,58] and it is explained due to the applied moments on square particles, arising from the arm moment and the force at the contacts [59]. With disk particles, the forces at the contacts are more often directed towards the center of the grains, resulting in smaller applied moments. Fig. 24 also reveals that the number of undissolvable–undissolvable contacts is smaller for square grains compared to disk grains. While this type of contact does not introduce fluctuation (as it involves two disk grains), the contact undissolvable–dissolvable becomes more significant as it includes a square-shaped grain. The difference in contact numbers arises from the fact that there are more dissolvable grains in the case of squares than disks. Consequently, the percentage of dissolvable grains is defined as the ratio of dissolvable surface area ($S_{\text{dissolvable}}$) to the sum of dissolvable and undissolvable surface areas ($S_{\text{dissolvable}} + S_{\text{undissolvable}}$), and the square-shaped grain has a smaller surface area than the disk-shaped grain. For a percentage of 15%, a simulation with 300 grains contains 58 grains (in the case of disks) or 83 grains (in the case of squares).

Fig. 24 demonstrates that the number of undissolvable–dissolvable contacts evolves differently depending on the shape of the dissolvable grains, especially when the dissolvable surface ratio is 0.15. The number of contacts for disks decreases in two steps: a sharp slope (around 5 contacts lost per percentage) from 0% to 15% dissolvable surface dissolved, followed by a slight slope (around 1 contact lost per percentage) from 15% to 60% dissolvable surface dissolved. On the other hand, the number of contacts for squares decreases in a single step, with a slight slope (around 1–2 contacts lost per percentage). It is worth mentioning that the initial configuration algorithm assumes perfect disks. Once the first equilibrium is reached, the shapes of the particles are generated, and the circumscribed disks are replaced by disks or squares. In the case of squares, this operation suddenly reduces the number of undissolvable–dissolvable contacts. When dissolution begins in the case of disks, many contacts with small overlaps are deleted in the initial iterations. In contrast, these contacts with small overlaps are already deleted during the initial configuration generation for squares.

Fig. 23 illustrates that the evolution of compacity ($= \frac{S_{\text{grains}}}{S_{\text{box}}}$) and vertical strain seems to depend solely on the percentage of dissolvable grains. The slope is sharper when the percentage of dissolvable grains is larger. For a given percentage, regardless of the shape (disk or square), the same amount of material is dissolved at each iteration.

In conclusion, this Section emphasizes the ability of PFDEM to handle irregular grains. The shape of the grains has a significant influence on granular behavior, and considering the true shape instead of perfect disks/spheres is important.

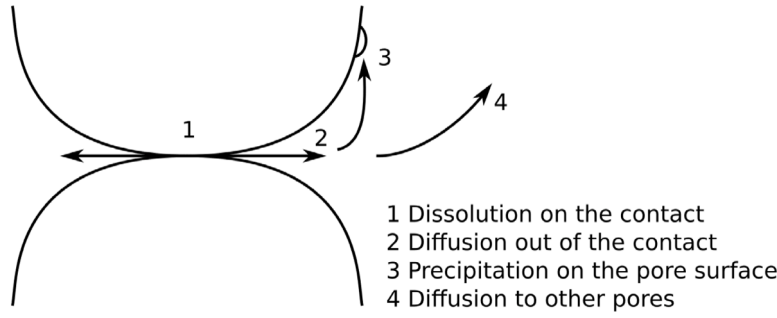


Fig. 25. Scheme of pressure solution phenomena.

4. Application to irregular shapes, heterogeneous dissolution and precipitation

In the context of PFDEM simulations, the heterogeneous dissolution/precipitation process can be modeled. This Section aims to demonstrate the capability of PFDEM to simulate such processes. In particular, we consider the example of the pressure solution phenomenon that involves both processes at the microscale and compare the simulation results with experimental findings reported by De Meer et al. [60].

The pressure solution phenomenon arises from the premise that in densely packed granular materials intergranular forces are substantial and this mechanism is dependent on temperature and mineral composition. This process involves the dissolution of material in high-stress areas and precipitation in low-stress areas, facilitated by diffusive mass transfer through the pore fluid [61–63].

Fig. 25 provides a schematic representation of the pressure solution process at the boundaries between two grains. In this scheme, the compacted granular medium is subjected to stress, leading to the formation of high-stress and low-stress regions. Within the high-stress regions at the contact, dissolution takes place due to a modification of the chemical potential, resulting in the removal of material. This dissolved material is then transported through the pore fluid to the low-stress regions far from the contact, where precipitation occurs, leading to the formation of new material.

Here, Eq. (13) is solved to track the solute generation, and its diffusion, and to ensure the total mass is conserved.

In the phase-field formulation, Eq. (11), the external source term E_d (presented in Eq. (11)) models both the mechanical energy at the contact level (E_{mec}) and the chemical energy due to the solute (E_{che}). As explained in Fig. 9, the mechanical energy induces dissolution, whereas the chemical energy induces precipitation. The formulation of this source term is given by Eq. (17).

$$E_d = E_{mec} - E_{che} = \sum_j \alpha \min(\eta_i) e_{mec} \times \eta_j^2 (3 - 2\eta_j) - \chi c \times \eta_j^2 (3 - 2\eta_j) \quad (17)$$

In Eq. (17), E_d is defined as the difference between the mechanical energy (E_{mec}) and the chemical energy (E_{che}). The mechanical energy term is computed based on the contact level from the DEM simulation and is applied to the contact area. The solute concentration c is multiplied by a coefficient χ representing the chemical energy term. A function of interpolation $\eta_j^2 (3 - 2\eta_j)$ is used to apply the source term E_d only at the interface of the phase variables ($\eta_j \neq 1$ or 0).

The source term E_{mec} is non-zero only if both phase variables η_i involved in the contact are non-zero, approximately representing the contact area. This assumption generates a heterogeneous dissolution focused on the contact area. To ensure stability, it is recommended to work with a source term E_{mec} lower than 0.2. The coefficient α is used to normalize the mechanical energy term. The term e_{mec} , defined in Eq. (18), represents the potential mechanical energy at the contact level and is computed as a potential normalized according to the relation (2).

$$e_{mec} = \frac{\int F s_n d\delta_n}{\sum_{\Omega} \min(\eta_i)} = \frac{\int k \delta_n^{3/2} d\delta_n}{\sum_{\Omega} \min(\eta_i)} = \frac{\frac{2}{5} k \delta_n^{5/2}}{\sum_{\Omega} \min(\eta_i)} \quad (18)$$

The quantity $\sum_{\Omega} \min(\eta_i)$ represents the sum over the contact area of the minimal value between phase variables involved η_i at each node. This variable is equivalent to the contact surface and ensures that the amount of energy introduced in the system from the interaction between grains remains constant. For example, if only two grains are in contact, the introduced energy term $\sum_{\Omega} E_{mec}$ is proportional to $\frac{2}{5} k \delta_n^{5/2}$. Thus, the term remains constant with time as $\sum_{\Omega} E_{mec} = \sum_{\Omega} \alpha \min(\eta_i) e_{mec} = \sum_{\Omega} \alpha \min(\eta_i) \frac{\frac{2}{5} k \delta_n^{5/2}}{\sum_{\Omega} \min(\eta_i)} = \alpha \frac{2}{5} k \delta_n^{5/2} \frac{\sum_{\Omega} \min(\eta_i)}{\sum_{\Omega} \min(\eta_i)} = \alpha \frac{2}{5} k \delta_n^{5/2}$.

As explained in Section 2.3, the deformation induced by the phase-field simulation and the grain displacements computed in the discrete element modelization are closely interconnected. Following an inspired Aitken method [52], a variable time step is used during phase-field simulations to minimize grain deformation. The values of the thresholds are obtained by trial and error.

Table 5
Parameters used for the two grains pressure solution simulation.

Parameters	Unit	Value
Mobility for phase-field η_j	–	1
Gradient coefficient for phase-field κ_j	–	0.01
Gradient coefficient for solute κ_c	–	50
Initial time step for phase-field simulation	s	0.2
Duration of the phase-field simulation	s	$6 \times$ the time step
Overlap applied	μm	10% of the initial radius
Chemical energy coefficient χ	–	0.5
Mechanical energy coefficient α	–	Initial $\sum_{\Omega} \min(\eta_i)$

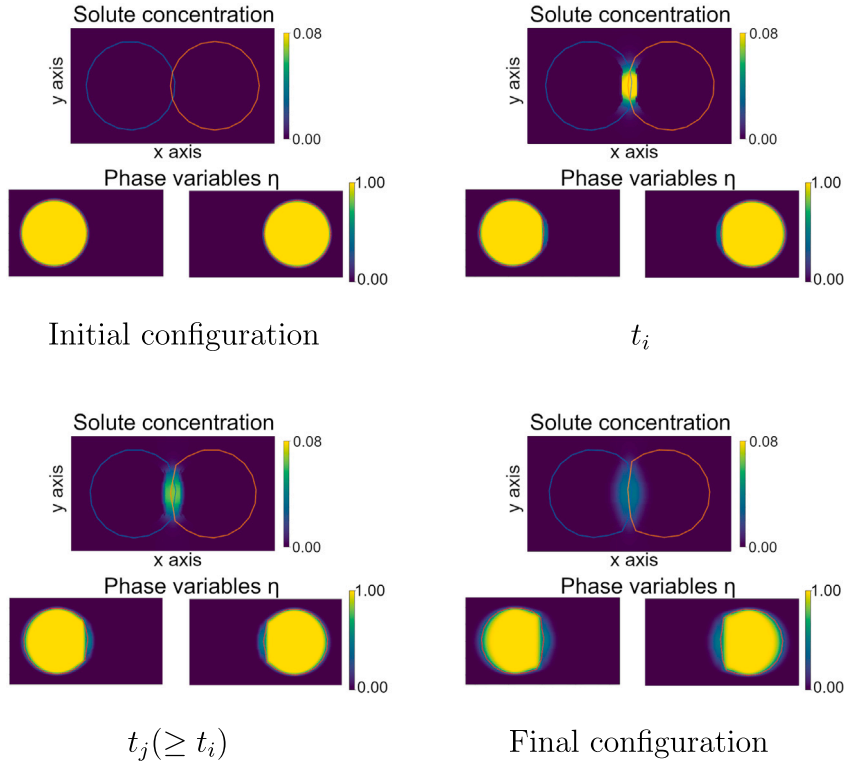


Fig. 26. Pressure solution phenomena between two grains. For each time, the upper plot represents the position of the grains and the solute concentration whereas the lower plots represent the phase-field variable of each grain. Between the initial and the final steps, solute has been generated and the shape of the grains have become less and less spherical.

4.1. 2 grains configuration

A first simulation campaign was conducted using only two grains with the same radius, and the parameters used for this pressure solution simulation are listed in Table 5. Since the configuration is relatively simple, the discrete element method (DEM) step can be simplified by using an analytical solution. In this case, the steady overlap between the two grains can be computed from the applied external load, and only an overlap is applied to move the grains.

The configuration of the two-grain system at different times is depicted in Fig. 26, and a movie is linked to the article for a more comprehensive visualization. The initial configuration consists of two grains in contact with no solute in the sample. As the simulation progresses, dissolution occurs at the contact, resulting in a decrease in the phase-field variables and the generation of solute. The dissolution process continues, and the solute diffuses throughout the sample. The amount of solute generated decreases as the chemical energy at the contact balances the mechanical energy. Eventually, a steady-state is reached, where grains continue to dissolve at the contact, while an equal amount of solute precipitates far from the contact.

Various curves presented in Figs. 27, 28, 29, and 30 provide further insights into the simulation. Fig. 27 shows the evolution of lateral strain with time, highlighting a creep phenomenon. This behavior is consistent with previous research findings on the topic [35,60]. The slowdown in the strain evolution can be attributed to two scenarios: (i) the expanding contact area reduces the

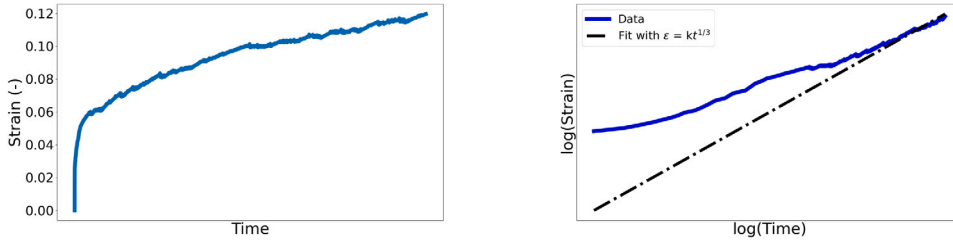


Fig. 27. Evolution of the lateral strain with times (left) and fit with the Andrade creep law (right).

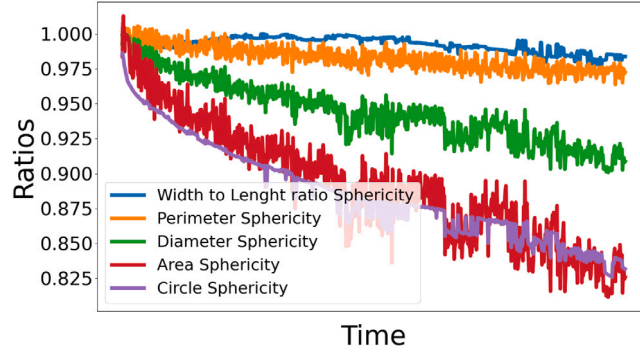


Fig. 28. Evolution of different indices to appreciate the sphericity of the grain 1.

introduced mechanical energy, and (ii) the pore water becomes saturated with the solute concentration. This creep phenomenon is known as the Andrade creep response, and it has been observed in various geomaterials [64]. The lateral strain evolves proportionally with the cubic root of time ($\epsilon = k t^{1/3}$), and the slope of $1/3$ is verified for long-term times. Concerning the short-term times, the result and the Andrade creep law must not be compared as the validity of the latter is limited to the long term. This short term is dominated by dissolution only (not enough solute for precipitation). The lateral strain is computed incrementally, $\epsilon = \sum_i \Delta_i / (2 R)$, where Δ_i is the rigid body motion applied to verify the targetted overlap and R is the initial radius of the particles.

Fig. 28 illustrates the shape evolution of the grains using different sphericity indices. The shape of a 2D grain is characterized by five sphericities, as defined in Eq. (19) [65]. The sphericities decrease over time, indicating that the shape of grain 1 deviates from a perfect circle as pressure solution occurs. It is worth noting the evolution of the width-to-length ratio sphericity, which initially decreases, then increases, and finally decreases again. This suggests that the particle shape tends to transition from a circle to a square and then to a rectangle.

$$\begin{aligned}
 \text{Area sphericity} & \frac{A_s}{A_{cir}} \\
 \text{Diameter sphericity} & \frac{D_c}{D_{cir}} \\
 \text{Circle ratio sphericity} & \frac{D_{ins}}{D_{cir}} \\
 \text{Perimeter sphericity} & \frac{P_c}{P_s} \\
 \text{Width to length ratio sphericity} & \frac{d_2}{d_1}
 \end{aligned} \tag{19}$$

Here, A_s is the surface of the grain, A_{cir} is the surface of the minimum circumscribing circle, D_c is the diameter of the perfect circle having the same area as the grain ($= 2\sqrt{A_s/\pi}$), D_{cir} is the diameter of the minimum circumscribing circle, D_{ins} is the diameter of the largest inscribing circle, P_c is the perimeter of the perfect circle having the same area as the grain ($= 2\sqrt{A_s\pi}$), P_s is the perimeter of the grain, and d_1 and d_2 are the length and the width of the grain.

The evolution of the chemical ed_{che} , mechanical ed_{mec} , and total energy ed at the center point of the sample (0, 0) is depicted in Fig. 29. This point is selected because it always remains in the contact area during the simulation. As explained in Eq. (17), the chemical and mechanical energy terms are proportional to the solute concentration at the selected point and the contact surface, respectively. The simulation starts with significant dissolution of the grains, followed by solute diffusion and precipitation. These phenomena increase the size of the contact area, leading to a decrease in the mechanical energy term. By choosing appropriate parameters, the two limiting scenarios described by Lu et al. [66] can be reproduced.

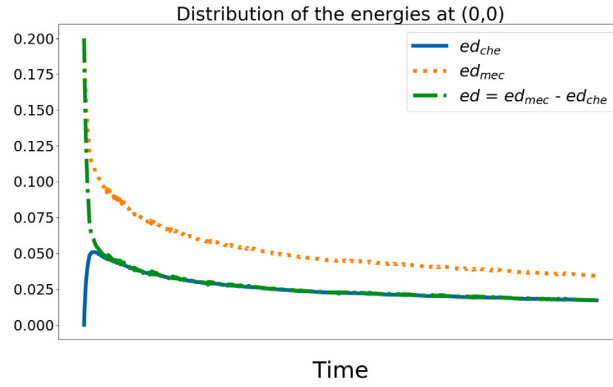


Fig. 29. Evolution of the chemical, mechanical and total energy at the center point of the sample (always in the contact area).

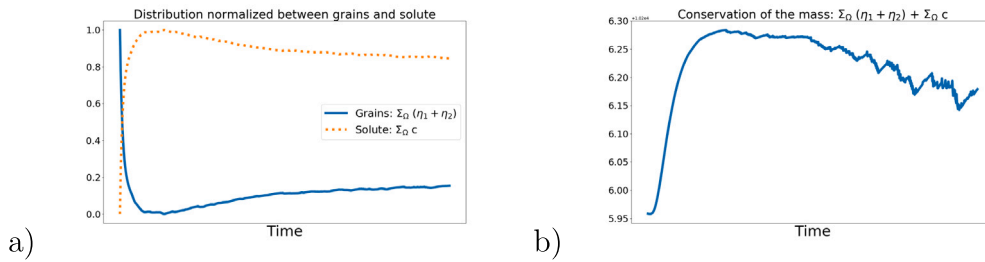


Fig. 30. Evolution of the grains and solute quantities (first steps have been removed to facilitate the curve reading): (a) A decrease in the grain quantity leads to an increase in the solute one. (b) The conservation of the mass is verified.

Fig. 30 presents the material distribution between the grains and the solute. A normalized distribution is shown for a clearer plot. The normalization is presented in Eq. (20).

$$v^n(t) = \frac{v(t) - v_{min}}{v_{max} - v_{min}} \quad (20)$$

where $v^n(t)$ is the normalized value (grain or solute quantity in the entire domain) at the time t , $v(t)$ is the value at the time t , v_{min} is the minimum reached of the value and v_{max} is the maximum reached of the value.

The evolution of the grain quantity is computed by summing the phase-field variables over the sample, while the evolution of the solute quantity is computed by summing the solute concentration over the sample. Fig. 30b demonstrates the mass conservation, as the sum of the two variables remains constant (with a negligible difference due to mass loss during phase-field generations). In conjunction with Fig. 29, it appears that a steady-state is reached. At the center point (in the contact area), material dissolution occurs (indicated by the positive sum of energy), but at the same time, the sum of the solute concentration over the sample remains constant. This indicates that the same quantity of solute generated at the contact is precipitated far from the contact, ensuring mass conservation.

Fig. 31 illustrates the computing time distribution between the four main steps: DEM, DEM to PF, PF and PF to DEM. It appears the DEM part is negligible. Indeed, in this two grains configuration, an analytical solution can be used, decreasing hugely the time cost. The PF part is the most important cost. Of course, this distribution is here only for example purposes. It depends on multiple parameters such as the mesh size, the number of processors used or the duration of the phase-field simulation (similar to the deformation induced by this step), among others.

4.2. Multiple grains configuration

Once a standard configuration with only two grains has been studied, a multiple grains configuration is considered using the parameters presented in Table 6. In the multiple grains configuration, a new algorithm described in Appendix C is applied to move the solute with the grains.

To define the initial configuration, perfect disks are assumed. They are randomly generated without overlap between them in the sample and then loaded. Once an equilibrium is reached, the disks are discretized. The sample generation aims to achieve a ratio between the sample diameter (D) and the sample height (H) equal to 0.6.

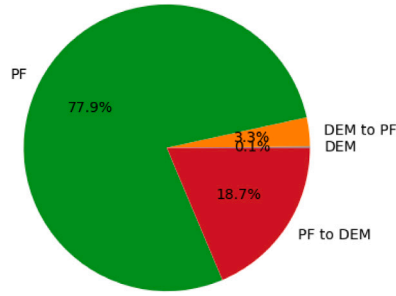


Fig. 31. Computing time distribution between the four main steps: DEM, DEM to PF, PF and PF to DEM. The part of the DEM is negligible in this case because an analytical result is possible for the two grains configuration.

Table 6

Parameters used for multiple grains pressure solution simulation.

Parameters	Unit	Value
Number of grains	–	30
Particle size distribution for grains (radius and percentage of the number of grains)	$\mu\text{m}(\%)$	420 (17), 385 (33), 315 (33), 280 (17)
Young modulus	GPa	70
Poisson's ratio	–	0.3
Density	kg/m^3	2500
Friction grain–grain	–	0.5
Friction grain–wall	–	0
Restitution coefficient	–	0.2
Time step for discrete element model	s	$\Delta t_{\text{crit}}/8$
Mobility for phase-field	–	1
Gradient coefficient for phase-field κ_j	–	0.01
Gradient coefficient for solute κ_c	–	50
Initial time step for phase-field simulation	s	0.01
Duration of the phase-field simulation	s	$8 \times \text{the time step}$
Linear force applied on the upper wall	N/m	$4 \times Y R_{\text{mean}}/1000$
Chemical energy coefficient χ	–	0.5
Mechanical energy coefficient α	–	Calibrated $\sum_{\Omega} \min(\eta_i)$

The coefficient α is computed from a calibration simulation. Two grains with a radius equal to the mean radius of the particle size distribution are generated. Then, a vertical confinement force is applied to the two grains to obtain an overlap. Finally, the coefficient α is equal to $0.06 \times \sum_{\Omega} \min(\eta_i)$, where $\sum_{\Omega} \min(\eta_i)$ is the sum over all the calibration sample of the minimal value of η_i at each node.

Fig. 32 shows some pictures of the configuration, and a movie is linked to the article for a more comprehensive visualization. Initially, there is no solute in the sample. After several iterations, some solute is generated and localized at the contact level. Grain reorganization occurs as shape deformation takes place. Strong concentrations of solute appear, and solute leakage can be observed at the top of the sample. In this configuration, the interaction with the top wall is not considered, and nothing forces the generated solute to follow the movement of the grains.

The evolution of the shape of the grains is illustrated in Fig. 33 by the evolution of the mean sphericity indices. In the case of multiple grains, the mean value over the grains is considered. It can be observed that the grains become less and less similar to a sphere over time.

Fig. 34 shows the sample's vertical strain and compacity. The evolution of compacity is important to comment on, as it is noisy and does not evolve linearly with the vertical strain. It is computed with the ratio of the surface grains over the sample surface. In this configuration, the confinement force is large, and overlaps are quite large as well. To obtain a corrected compacity index, it becomes important to reduce the contact surface and not count the material surfaces twice.

A fit with an Andrade creep response has been attempted in Fig. 35. The results of the simulation seems to be aiming to reach the tendency of the Andrade fit.

The normalized distribution (presented Eq. (20)) between grains and solute is illustrated in Fig. 36a. The mass conservation is studied in Fig. 36b. It is observed that a small loss of mass occurs, approximately 1% of the initial mass. This loss is due to the grain displacement and detection algorithms, as these algorithms use a window around the grain to limit the computational cost and cut everything outside this window.

Fig. 37 illustrates the computing time distribution between the four main steps: DEM, DEM to PF, PF and PF to DEM. The PF part is the most important cost and the DEM part is quite important also (as no analytical solution is used here compared to Fig. 31). This distribution is here only for example purposes as explained in Section 4.1. It depends on multiple parameters listed above but also

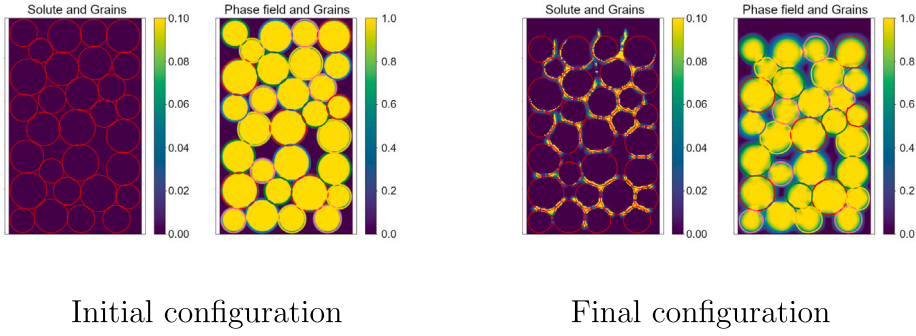


Fig. 32. Pressure solution phenomena between multiple grains. For initial and final configurations, the left plot shows the position of the grains and the solute concentration, and the right plot shows the phase variables. Between the initial and the final steps, solute has been generated and the shape of the grains has become less and less spherical. The granular material becomes denser while the pressure solution phenomenon occurs.

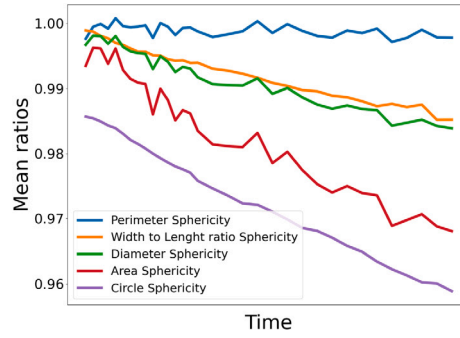


Fig. 33. Evolution of different mean indices to appreciate the sphericity of the grains.

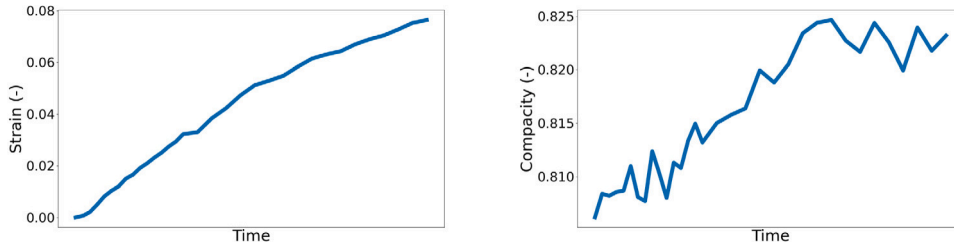


Fig. 34. Evolution of the vertical strain and the sample compacity.

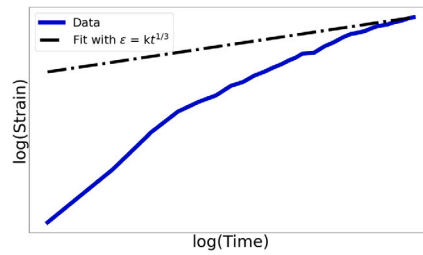


Fig. 35. Comparison between the numerical results and the Andrade creep law for the evolution of strain with time.

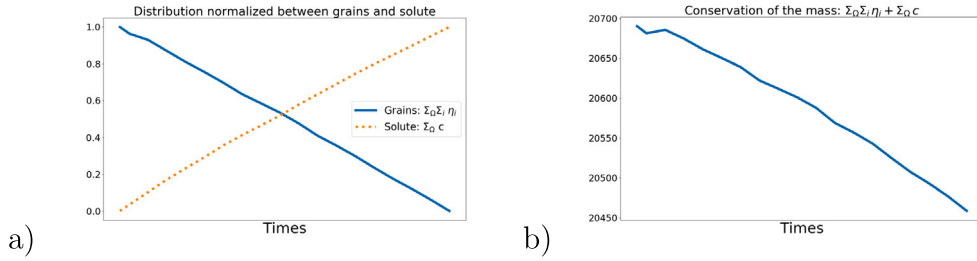


Fig. 36. Evolution of the grains and solute quantities. A small loss of mass (because of the grain displacement and detection algorithms) is detected.

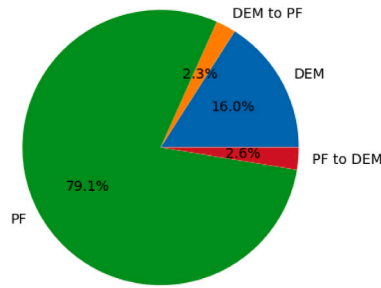


Fig. 37. Computing time distribution between the four main steps: DEM, DEM to PF, PF and PF to DEM.

in this case, the discretization of the grains, the criteria to define the DEM steady-state or the duration of the phase-field simulation (similar to the deformation induced by this step), among others.

The goal of this Section was to highlight the PFDEM's capability to handle heterogeneous dissolution/precipitation processes. The observed grain shape evolution during the pressure solution phenomena is not uniform, as it varies from the contact point (high-stress area) to the pore surface (low-stress area). To capture this behavior, a solution concentration and a chemo-mechanical formulation have been developed and incorporated into the phase-field equations. The results demonstrate that the sphericities of the grains decrease over time, indicating that the grains become less disk-like. Additionally, the sample tends to an Andrade creep response, which is commonly observed in geomaterials during pressure solution. These findings illustrate the PFDEM's ability to accurately simulate and analyze the complex behavior of pressure solution phenomena, taking into account heterogeneous dissolution/precipitation effects.

5. Conclusions

This work presents an extension of the classical discrete element model by coupling it to the phase-field theory, enabling the capture of real grain shape and its evolution based on physical laws. The study was conducted in two steps. Firstly, the effect of grain shape was investigated through a sample subjected to constant stress in oedometric conditions with partial dissolution. The results highlighted the importance of considering the actual grain shape instead of relying solely on modeling with rolling resistance as the increase of grain angularity showed opposite evolution for the lateral pressure coefficient evolution K_0 . Secondly, the pressure solution phenomena was examined, considering a heterogeneous dissolution/precipitation simulation. A comparison with experimental data was performed, demonstrating that the simulated data tends to the Andrade creep response, a characteristic behavior observed in granular materials undergoing pressure solution.

The proposed formulation opens up avenues for further exploration into the influence of various parameters on the creep behavior and the effect of grains characteristics. Parameters such as solute diffusivity, chemical energy factor, and mechanical energy factor can now be systematically studied to gain insights into their impact on the overall behavior. This coupling of discrete element modeling with phase-field theory provides a useful framework for investigating the complex interplay between grain characteristics and the mechanical response of geomaterials undergoing dissolution/precipitation processes.

6. Software

The PF model is solved using the MOOSE software [49], while the DEM is solved using a custom-developed Python software. The scripts and algorithms used in this study are available on GitHub at the following links:

- https://github.com/AlexSacMorane/PFDEM_AC
- https://github.com/AlexSacMorane/PFDEM_ACS
- https://github.com/AlexSacMorane/PFDEM_ACS_MultiGrains

CRediT authorship contribution statement

Alexandre Sac-Morane: Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Methodology, Investigation, Formal analysis. **Manolis Veveakis:** Writing – review & editing, Writing – original draft, Supervision, Funding acquisition, Conceptualization. **Hadrien Rattiez:** Writing – review & editing, Writing – original draft, Supervision, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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Appendix A. A Monte Carlo method algorithm to characterize a polygonal particle

A polygonal particle is defined by the coordinates of the vertices and some essential information as center, surface and inertia must be known for the DEM algorithm. A Monte Carlo [39] is used to compute them [28] this method is based on the creation of a box around the grain. Then, a point is generated randomly inside the box. A point-inside-polygon test is used to determine if the point is inside or not the polygonal particle (this test is explained in the following). This step is repeated a large number of time. The mass, the center and the inertia of the particle can be determined with the Eqs. (A.1)–(A.3).

$$mass = \frac{A_{box}}{N_p} \sum_{i=1}^{N_p} \chi(\bar{X}_i) \sigma \quad (A.1)$$

$$mass \times \bar{r} = \frac{A_{box}}{N_p} \sum_{i=1}^{N_p} \chi(\bar{X}_i) \sigma \bar{X}_i \quad (A.2)$$

$$I + mass \|\bar{r}\|^2 = \frac{A_{box}}{N_p} \sum_{i=1}^{N_p} \chi(\bar{X}_i) \sigma \|\bar{X}_i\|^2 \quad (A.3)$$

with A_{box} is the area of the box, $\bar{X}_i$ the coordinate of the random point, N_p the total number of random point, σ the surface mass, $\bar{r}$ the center of mass and I the moment of inertia. The function $\chi(\bar{X}_i)$ is the characteristic function, which returns 1 if the point is inside the grain and 0 otherwise.

This characteristic function follows the point-inside-polygon test developed by Franklin [67]. A semi-infinite ray is generated from the point in the direction of the increasing x. Every time this ray crosses an edge the point switches between inside and outside.

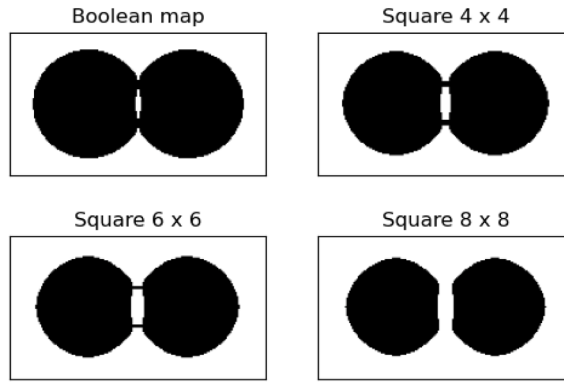


Fig. B.38. Diffusion coefficient maps for different morphological operators.

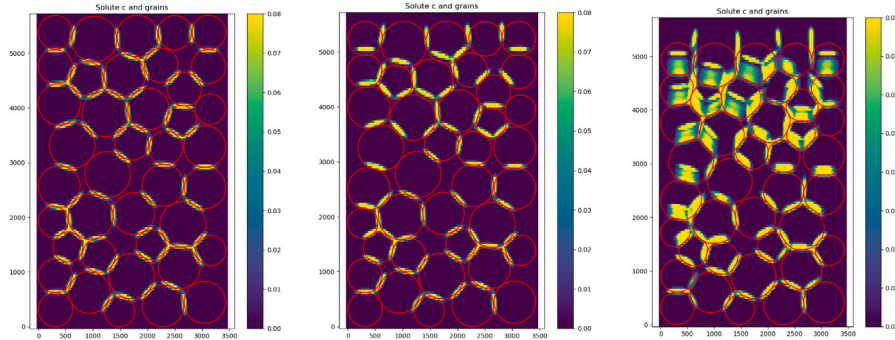


Fig. C.39. Solute is generated initially (left). Then, the grains move after the DEM step to find a new equilibrium whereas the solute stays at the same place (center). Finally, it appears after multiple iterations that the solute needs to follow the grains (left).

Appendix B. Method to build the field of the solute diffusion coefficient

In the case of pressure solution, the problem asks for a heterogeneous solute diffusion coefficient field. The goal is to have diffusion at the contact area (to evacuate the solute generated) and in the pore area (as some fluid is assumed). However, it should not have diffusion in the grain material. The map of this coefficient is following the different steps :

1. for each node of the mesh, a Boolean value is attributed, depending on the different phase variable (if $\eta_i > 0.5$ and $\eta_j > 0.5$ returns True; if $\eta_i < 0.5$ and $\eta_j < 0.5$ returns True; else return False). A Boolean map is generated.
2. a dilation method `scipy.ndimage.binary_dilation` is applied to the Boolean map to generate a dilated map.
3. The diffusion coefficient map is generated. For each node, if the value of the dilated map is True, κ_c is attributed to the diffusion map; else, 0 is attributed to the diffusion map.

As Fig. B.38 highlights, the dilation step is needed to be sure the contact zone is connected to the pore space. Depending on the configuration, the selection of the morphological operator is the main choice. The larger the size of the operator is, the more diffusion inside the grains occurs.

Appendix C. Method to move solute out of a grain

Compare to the two grains pressure solution simulation, the multi-grain one faces trouble concerning the solute and the grain moves. As illustrated by Fig. C.39, the solute generated does not follow the grain moves and it produces nonphysical results. It can be noticed the troubles are located more at the top of the sample. Hence, the simulation is made as the upper wall moves to verify the confinement pressure. Grains at the top move more than grains at the bottom. A new algorithm must be designed to move the solute with the grains.

The fundamental assumption is a small displacement of the grains. As illustrated by Fig. C.40, all nodes are said available (in the pore space or in the contact area) or not (in only one grain) to host solute. Then, for nodes not available the solute is distributed to the nearest node available as illustrated in Fig. C.40. If there are multiple nodes available at the same distance, the concentration to move is divided into equivalent parts.

The algorithm can be resumed by the following steps :

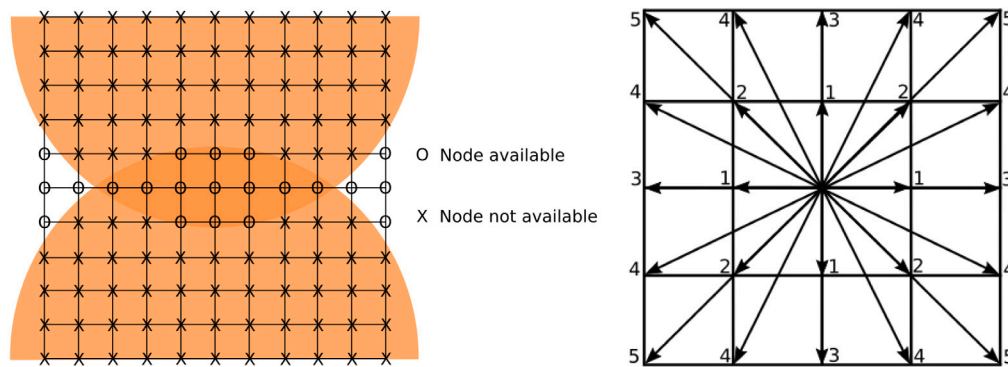


Fig. C.40. A node is considered available to host solute if it is a pore space or a contact area (left) and an illustration of the priorities to move the solute to the nearest node (right).

1. a Boolean map is generated depending if the node can host or not solute.
2. a dilation method `scipy.ndimage.binary_dilation` is applied to the Boolean map to generate a dilated map.
3. For all nodes of the dilated map not available to host the solute, the nearest nodes are searched:
 - (a) It is checked if at least one node of the priority i can host solute.
 - (b) If no node is available: the previous step is repeated with priority $i + 1$.
 - (c) If at least one node is available: the solute is moved with the relation at every available node $c_{available} = c_{available} + c_{not\ available}/n_{available}$, where $c_{available}$ is the solute concentration at the available node, $c_{not\ available}$ is the solute concentration at the not available node and $n_{available}$ the number of available nodes at the priority i . The solute concentration at the not available node is set to 0.

Appendix D. Supplementary data

Supplementary material related to this article can be found online at <https://doi.org/10.1016/j.cma.2024.116900>.

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