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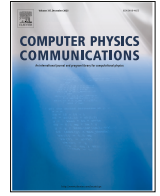
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Computational Physics

A soft particle dynamics method based on shape degrees of freedom for core-shell particles



Yohann Trivino ^{a,b}, Vincent Richefeu ^c, Farhang Radjai ^a, Komlanvi Lampoh ^b,
Jean-Yves Delenne ^{b,*}

^a LMGC, CNRS, University of Montpellier, 34090, Montpellier, France

^b IATE, INRAE, Institut Agro, University of Montpellier, 34000, Montpellier, France

^c Laboratoire 3SR, CNRS, University Grenoble Alpes, 38400, Grenoble, France

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ABSTRACT

In this paper, we present a 2D numerical model developed to simulate the dynamics of soft core-shell particles. To accommodate large particle deformations, the particle surface is represented as a thin shell composed of mass points that interact through elasto-plastic force laws governing their linear and angular relative displacements. Particle shape changes are controlled by these interactions, in conjunction with a uniform particle core stiffness. This model can be applied to simulate flexible beams and core-shell particles of arbitrary shape. We calibrate and verify this model by comparing the deformation of constrained beams under load with theoretical predictions. Subsequently, we explore the diametral compression of a single particle between two walls, focusing on the influence of the particle core stiffness and shell plasticity. Our findings indicate that increased core stiffness reduces particle volume change and promotes the development of flat contact areas with the walls. To further illustrate the model capabilities, we apply it to the uniaxial compaction of a granular material composed of core-shell particles. We show that, depending on the core stiffness and shell plastic threshold, the compaction leads to either a significant reduction of particle volumes or an improved pore filling due to particle shape changes. At high compaction, particle shapes vary such that elastic particles without core stiffness become mostly elongated, elastic particles with core stiffness form polygonal shapes, while plastic particles develop elliptical or highly irregular forms. Finally, we simulate the tensile fracture of a tissue composed of elastic or plastic cells, illustrating the model's potential applicability to soft tissues that undergo both large cell deformations and fracture.

1. Introduction

The study of soft particles is a diverse and rapidly evolving field within materials science and the physics of complex systems. These soft particles encompass a wide range of materials, including hydrogels [1], polymers [2,3], colloids [4–6], emulsions [7], plant cells [8,9], and red blood cells [10]. Understanding the mechanical behavior of these materials has broad implications across multiple disciplines. For instance, deformable polymer particles can be engineered to create innovative materials with customized properties [11–13].

Plant cells and red blood cells belong to the broader class of core-shell particles, which consist of solid, liquid, or gas cores surrounded by solid shells [14–17]. The combined effects of their core and shell materials make them suitable for many applications such as drug delivery, chromatography, catalysis, and design of artificial cells. The core-shell particles are assembled from inorganic, organic, polymeric, or crys-

talline materials with sizes ranging from nanometer to micrometer. Hollow nanoparticles are of particular interest because of their lower density compared to their solid counterparts, and they have been explored for their use in catalysis. The mechanical properties of core-shell particles are essential for their performance in applications. In exception to a few studies [17–19], most past studies have been concerned with the fabrication and initial biological characterization of core-shell particles rather than their mechanical behavior.

What connects these materials, despite their diverse physical natures, is their common ability to undergo significant deformation due to both collective particle rearrangements and changes in particle volume or shape under external and internal stresses. These characteristics alter the space-filling properties of soft-particle systems compared to hard particle packings, where the packing fraction cannot exceed the random close packing (RCP) limit [20,21]. The rheological behavior of highly deformable particle systems confined

* Corresponding author.

E-mail address: jean-yves.delenne@inrae.fr (J.-Y. Delenne).

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beyond this jamming limit has only recently been studied systematically [22–24].

The standard method for simulating granular materials is the Discrete Element Method (DEM) [25,25–27]. This technique consists in integrating the equations of motion for the translational and rotational degrees of freedom of each particle, accounting for their contact interactions, and employing a time-stepping scheme [28]. The primary assumption of DEM is that particles are undeformable and lack therefore shape degrees of freedom, though small overlaps are permitted to represent contact elastic or plastic deflections between particles. Consequently, DEM in its basic formulation is unsuitable for simulating soft particles, which require shape degrees of freedom. However, numerical methods incorporating shape degrees of freedom within the DEM have been proposed. For instance, Mollon developed a Soft DEM, where rotations and center-of-mass displacements are managed similarly to DEM, but elliptical particles can adjust their aspect ratio through stepwise variations in strain (assumed to be uniform) in response to changes in average stress due to contact forces [29]. This model is limited to elliptical particles and cannot be used to simulate arbitrary particle shapes. Boromand et al. introduced a versatile Deformable Particle (DP) method, where the degrees of freedom are represented by mass points (or vertices) on the particle boundary [23]. The evolution of these boundary points is governed by a shape-energy function, which is minimized with each increment of imposed displacements to determine the new positions of the points. This approach allows for arbitrary deformations from a reference shape defined by the initial positions of the vertices. The DP model has been applied to study the jamming of soft grains [23] as well as the isotropic compaction and hopper flow of deformable particles [24,30]. From the viewpoint of mechanical behavior, the DP model can be considered as a method for the simulation of hollow-core thin-shell particles.

It is noteworthy that continuum methods such as Finite Element Method (FEM) and Material Point Method (MPM) can also be used to simulate soft particles [22,31–37]. In particular, these methods can be adapted to core-shell particles, which are at the focus of this paper. But, such models may be delicate to handle for the simulation of core-shell particles with vanishing shell thickness or for the treatment of frictional contacts [22].

In this paper, we present a 2D numerical method that builds on the principles of the DEM with frictional contact interactions between individual particles, but with the added capability of handling large deformations. In close analogy with the DP model, as previously discussed, our model introduces shape degrees of freedom by representing the particle surface as a shell composed of mass points interacting through elasto-plastic force laws.

As in DP model, our Soft Particle Dynamics (SPD) model relies on a limited number of degrees of freedom per particle, enabling efficient simulations of core-shell particles. A key distinction lies in the treatment of dynamics by SPD and DP: the DP model is inherently quasi-static, whereas SPD is based on a fully dynamic algorithm, making it better suited for applications involving time-dependent behavior such as viscous damping and collisions with finite energy restitution. In addition, an explicit elastic limit on shell flexion is introduced in SPD to allow for plastic deformations. In contrast to DP, we also account for friction between particles via a Coulomb friction law. For modeling cellular tissues or core-shell aggregates, we have also implemented a multi-directional adhesion law between soft particles. Finally, to account for liquid core in the simulations of a broad class of systems such as living cells, the model incorporates a core stiffness of pressure in addition to the stretch and bending stiffness parameters associated with the shell elements.

We shall see that the mechanical behavior of a single particle can vary significantly based on the values of stiffness parameters and shell plasticity. We highlight the versatility of this method by applying it to the compaction of deformable core-shell particles and the fracture of cellular tissues.

Section 2 presents a detailed description of the approach. Section 3 presents the software implementation of this approach, describes the

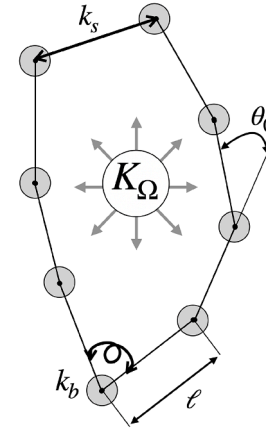


Fig. 1. Representation of a particle composed of 8 mass points and 8 segments in the xy plane.

neighbor search and optimization strategies, and analyzes performance and scalability. Section 4 considers the calibration of the method, focusing on its application to beams subjected to point forces. In Section 5, we examine how model parameters affect the mechanical response of a single particle under diametral compression between two flat walls. For the sake of demonstration, in Section 6 we present simulations of the compaction of an assembly of deformable particles. To showcase the applicability of the method to cellular materials, in Section 7 two examples of cellular tissue fracture under tensile deformation are presented and briefly discussed. Finally, Section 8 concludes with a summary of the key findings and potential future directions for this work.

2. Model description

In this section, we outline the main ingredients of the model and introduce the notations that will be used throughout the paper. It is important to note that both the model and the examples discussed are in two dimensions under plane-stress conditions.

2.1. Geometric representation of particles

In the model, we refer to various basic units—such as plant cells, grains, microcapsules, nanotubes, and vesicles—as “particles.” Each particle can undergo significant elastic or plastic deformations without breaking and interacts with other particles through elastic and cohesive contact forces. These deformations involve changes in both the volume and shape of the particles, which are modeled by representing each particle’s periphery as an array of mass points connected by elastic-plastic force laws. These force laws can be viewed as extensible elements (beams) linking the mass points; however, the mass and dynamics of the system are carried by the mass points themselves, which we will also refer to as nodes or vertices. It is important not to confuse this approach with alternative methods that represent the particle surface as an array of beam elements articulated at their endpoints, where the mass and dynamics are carried by the elements rather than the nodes.

In our model, the mechanical integrity of a particle is maintained through the interactions between adjacent pairs of mass points and by a flexural or bending stiffness at each vertex formed by two adjacent segments (elements), which involves three mass points. These mass points at the vertices are the discrete elements of the model and represent the shape degrees of freedom of a particle. Changes in particle shape are governed by variations in the angles between adjacent segments (the bending mode), while variation of the particle’s perimeter depends on the elongation of these segments (the stretch mode). Although the dynamics is carried by the vertices, we assume that for interactions between particles, the segments behave as sphero-segments—thick lines

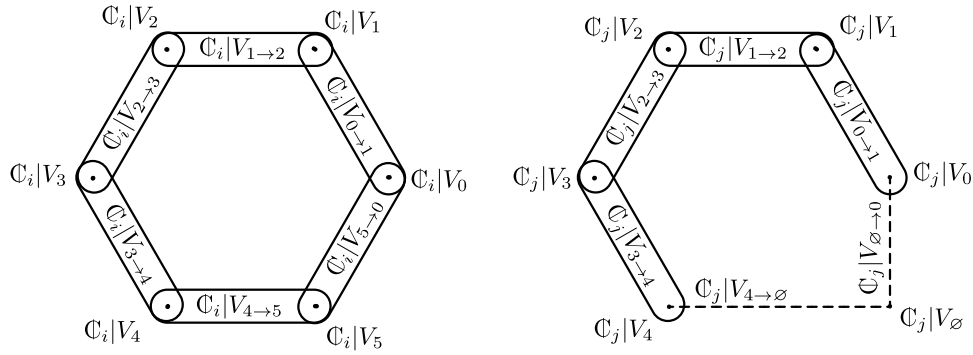


Fig. 2. Identification of vertices and segments in each particle. Each vertex has a local number within the particle; to refer to it globally, both the particle number and the local vertex number are needed. For instance, the bottom-right vertex is identified as $C_j|V_4$, where j is the particle number and 4 is the local vertex number. Similarly, any vertex in particle i is denoted as $C_i|V_k$, where k specifies the vertex within that particle.

with rounded caps—that can come into contact with the vertices of other particles.

Fig. 1 illustrates a 2D particle consisting of vertices and elements of varying lengths ℓ in the xy plane. The initial shape of the particle is defined by the equilibrium lengths ℓ_0 of its sides and the angles θ_0 between adjacent elements. The corresponding stretch and bending stiffnesses are denoted by k_s and k_b , respectively. The particles are assumed to have a length s along the z axis. The set of vertices defines a thin shell, but we numerically replace each vertex by a disk of radius r and each segment joining two vertices by a sphero-segment or rounded-cap rectangle of thickness $2r$. The centers of the disks at the vertices of two adjacent elements coincide.

We employ a local numbering scheme for vertices within each particle to ensure precise identification. As illustrated in Fig. 2, this method assigns each vertex a pair of indices, denoted as $C_i|V_k$, where i represents the particle number and k indicates the local vertex number. An element connecting two successive vertices k and $k + 1$ within the same particle i is labeled as $C_i|V_{k \rightarrow k+1}$. Additionally, our data structure accounts for cases where an element may have a missing endpoint, which is useful for modeling open or breakable cells, though such cases are beyond the scope of this paper. To accommodate these scenarios, we introduce the concept of an “absent” vertex, denoted by \emptyset , as seen in $C_i|V_{4 \rightarrow \emptyset}$. This linked list structure, whether closed or open, is both concise and easy to implement.

2.2. Internal forces and moments

Two mass points k and $k + 1$ are assumed to interact through a harmonic potential energy with a plastic threshold. In other words, the extensional incremental deformation $\delta \ell_{(k,k+1)}$ of the segment $C_i|V_{k \rightarrow k+1}$ joining the two points is governed by a linear elastic-perfectly plastic law:

$$\delta F_{(k,k+1)} = [k_s \delta \ell_{(k,k+1)}]_{\pm} F_s^Y, \quad (1)$$

where k_s is the stretch (extensional) stiffness, $\delta F_{(k,k+1)}$ is the extensional force increment, and F_s^Y is the elastic limit or plastic threshold force. The notation $[\Delta \mathcal{X}]_{\pm \mathcal{P}}$ is defined as:

$$[\Delta \mathcal{X}]_{\pm \mathcal{P}} = \begin{cases} \Delta \mathcal{X} & \text{if } |\mathcal{X} + \Delta \mathcal{X}| < \mathcal{P}, \\ 0 & \text{otherwise.} \end{cases} \quad (2)$$

In this notation, compressive forces and contractions of a segment are counted as positive, whereas tensile forces and extensions are considered negative.

Shear deformation across the shell wall is neglected. However, to endow a particle with an equilibrium shape, we must also incorporate resistance to bending at all vertices of the particle. We assign a reference angle θ_{0k} to each node $C_i|V_k$, and the variations $\delta \theta_k$ of the angles follow

a linear elasto-plastic law:

$$\delta M_k = [k_b \delta \theta_k]_{\pm} M_b^Y, \quad (3)$$

where k_b is the bending stiffness, δM_k is the torque increment at node k due to internal or external forces, and M_b^Y is the elastic limit or plastic threshold for the torque. The initial values $\ell_{0(k,k+1)}$ of segment lengths and θ_{0k} of vertex angles define the particle’s initial shape. Any changes in shape require external forces. In the elastic regime, the initial shape represents the reference state such that if external forces are removed, the particle will return to this initial shape.

When plastic deformations occur at some nodes under the action of external forces, the torque M_k at those nodes remains equal to M_b^Y while the angles and consequently the shape of the particle change. In the same way, an element may reach its extensional elastic limit, in which case the force will remain at its plastic limit F_s^Y unless the direction of loading changes. Once external forces are removed, the new reference state is defined by the cumulative plastic deformations at all nodes and elements. As we shall see in Section 2.4, since our model assigns degrees of freedom only to mass points, an interaction law like (3), which involves the angle $\delta \theta_k$ as a variable, represents a three-body interaction between the three nodes $k - 1$, k , and $k + 1$. This interaction is handled by substituting the torques with moments of forces acting on the segments.

To accurately model the physical behavior of systems such as cellular tissues, it is crucial to account for the effect of fluid inside the particle. Let V denote the volume of the particle, V_0 its initial volume, and p the fluid pressure. We assume that the fluid is inviscid, and the variations δp of pressure follow a linear isotropic elastic behavior:

$$\delta p = -K_{\Omega} \frac{\delta V}{V_0}, \quad (4)$$

where K_{Ω} is the core modulus due to the presence of the fluid. While the fluid can possess viscosity or exhibit more complex behaviors, this model assumes an inviscid fluid for simplicity. Under undrained conditions, where the fluid is confined within the particle, the fluid pressure p adjusts in response to changes in the particle’s volume. Conversely, under drained conditions, where the fluid is in equilibrium with the surrounding environment, p remains constant and equal to the external pressure. As discussed further below, the overall bulk modulus K of a particle is a combination of K_{Ω} and k_s .

2.3. Particle interactions

In 2D, the interactions between two particles C_i and C_j reduce to interactions between their vertices and elements. A vertex-vertex contact occurs between two disks, while a vertex-element contact is a contact between a disk and a thick line. An element-element contact can involve either one vertex-vertex contact along with one vertex-element contact,



Fig. 3. An element-element contact can involve either one vertex-vertex contact, indicated by two arrows, along with one vertex-element contact, or it can involve two vertex-element contacts, each marked by a single arrow.

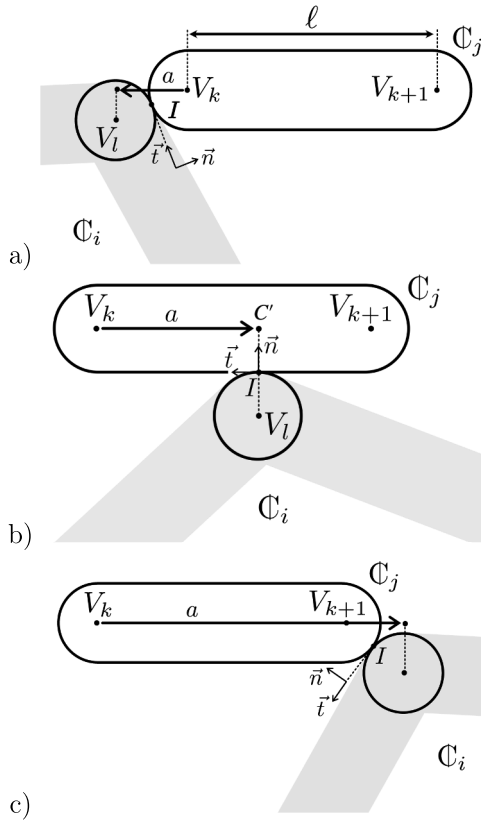


Fig. 4. Possible contact configurations between two elements.

or two vertex-element contacts, as illustrated in Fig. 3. Therefore, for detecting the contacts between two particles, it is sufficient to consider only vertex-vertex and vertex-element interactions.

Fig. 4 illustrates the three possible interactions between a vertex of \mathbb{C}_i and an element $\mathbb{C}_j|V_{k \rightarrow k+1}$ of the cell \mathbb{C}_j : $\mathbb{C}_i|V_l - \mathbb{C}_j|V_k$ (Fig. 4a), $\mathbb{C}_i|V_l - \mathbb{C}_j|V_{k \rightarrow k+1}$ (Fig. 4b), and $\mathbb{C}_i|V_l - \mathbb{C}_j|V_{k+1}$ (Fig. 4c). For the sake of simplicity we denote by A and B the vertices V_k and V_{k+1} endpoints of the element $\mathbb{C}_j|V_{k \rightarrow k+1}$, and by C the vertex V_l of \mathbb{C}_i in contact with the element. I is the contact point of C with the element, and C' is the projection of C over the line (AB) .

These cases can be algebraically distinguished by analyzing the length $a = \overline{AC} \cdot \overline{AB} / \|\overline{AB}\|$ and considering the different in-plane thicknesses $2r_i$ and $2r_j$ of cells \mathbb{C}_i and \mathbb{C}_j :

1. for $a < 0$, the normal vector at contact is $\vec{n} = \overline{CA} / \|\overline{CA}\|$ and the overlap is $\delta_n = \|\overline{CA}\| - (r_i + r_j)$,
2. for $0 \leq a \leq \ell$, $\vec{n} = \overline{CC'} / \|\overline{CC'}\|$ and $\delta_n = \|\overline{CC'}\| - (r_i + r_j)$,
3. for $a > \ell$, $\vec{n} = \overline{CB} / \|\overline{CB}\|$ and $\delta_n = \|\overline{CB}\| - (r_i + r_j)$.

We also denote by (I, \vec{n}, \vec{t}) the local frame attached to the contact point with $\vec{t} = \vec{n} \times \vec{z}$.

The total contact force \vec{f} at the contact I is defined by its normal and tangential components f_n and f_t in the local frame:

$$\vec{f} = f_n \vec{n} + f_t \vec{t}. \quad (5)$$

In all cases, the normal elastic repulsion force is given by:

$$f_n = k_n \delta_n, \quad (6)$$

where k_n is the normal contact stiffness. The tangential elastic force follows the Coulomb friction law, which can be expressed using force increments δf_t as follows:

$$\delta f_t = [-k_t \delta u_t]_{\pm \mu f_n}, \quad (7)$$

where μ is the friction coefficient, k_t is the tangential elastic stiffness, and δu_t is the incremental tangential displacement of \mathbb{C}_j with respect to \mathbb{C}_i at the contact point. This is equivalent to the following expression:

$$f_t = \begin{cases} -k_t u_t & \text{for } |f_t| \leq \mu f_n, \\ -\mu f_n \frac{\dot{u}_t}{|\dot{u}_t|} & \text{otherwise,} \end{cases} \quad (8)$$

where u_t is the cumulative tangential displacement and \dot{u}_t is the tangential relative velocity.

2.4. Time stepping scheme

Given that the discrete degrees of freedom for the particles are carried by their vertices, we assign a mass m to each vertex, resulting in a total particle mass of Nm for a particle composed of N vertices. The classical velocity Verlet time-stepping scheme is applied to each mass point. This scheme, widely used in DEM, is recognized for its balance between accuracy and computational cost. As a symplectic integrator, it conserves the phase-space volume over time, making it well suited for Hamiltonian systems. Unlike DEM, rotational degrees of freedom for the mass points are not required, as particle rotations naturally arise from the displacement of vertices. The time step δt must be kept below the critical threshold $\delta t_c = \sqrt{m/k_{\max}}$, where k_{\max} represents the largest stiffness parameter of the system.

Although the elements are massless, they can still receive forces at their contact points with other particles. Since the dynamics is entirely governed by the mass points located at the vertices, any force acting on an element must be transferred to the vertices at its endpoints, as illustrated in Fig. 5. Let \vec{f} represent a force vector acting on an element of length ℓ , applied at a point located a distance a from one end, denoted as k , and a distance $\ell - a$ from the other end, denoted as $k + 1$. Assuming the element is in equilibrium under the action of \vec{f} and the reaction forces at the two vertices, the force \vec{f} is fully transferred to these endpoints. The forces acting at the vertices k and $k + 1$ are given by $\vec{f}_k = w_k \vec{f}$ and $\vec{f}_{k+1} = w_{k+1} \vec{f}$, respectively, where $w_k = (\ell - a)/\ell$ and $w_{k+1} = a/\ell$.

The core pressure within a particle manifests through the force it exerts on each vertex. This process occurs in two distinct steps. First, a force increment $\delta \vec{F}_{(k,k+1)}^{\text{in}}$ due to the core pressure increment δp acts on each element $(k, k + 1)$. Given the isotropic nature of the pressure, this force increment is perpendicular to the element at its midpoint and is calculated as $s \ell_{(k,k+1)} \delta p$, where $\ell_{(k,k+1)}$ is the length of the element. Second, this force is equally distributed between the two vertices k and $k + 1$, in accordance with the rule outlined in Section 2.3. The variation

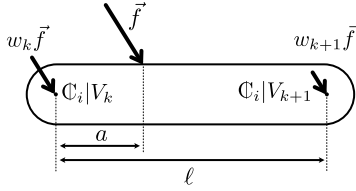


Fig. 5. Representation of force transfer from the contact point to the nodes belonging to $C_i | V_{k \rightarrow k+1}$.

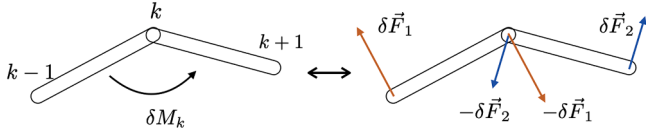


Fig. 6. Equivalence between a torque acting at the node k and a pair of couples acting on the elements $(k - 1, k)$ and $(k, k + 1)$.

δp in core pressure during each time step is given by the corresponding volume change, which is based on the displacements of the vertices at the midpoint of each time step, similar to how contact forces with other particles are handled.

As previously mentioned, the torque Eq. (3) represents a three-body interaction, given that the primary variables of the system are the displacements of the mass points. The variation $\delta\theta_k$ of the angle at a vertex k is computed at the midpoint of each time step. Using Eq. (3), the increment δM_k is calculated. As shown in Fig. 6, this torque increment can be replaced by two couples $(\delta\vec{F}_1, -\delta\vec{F}_1)$ and $(\delta\vec{F}_2, -\delta\vec{F}_2)$, with the force magnitudes given by:

$$\delta F_1 = \frac{\delta M_k}{2\ell_{(k-1,k)}} \quad (9)$$

$$\delta F_2 = \frac{\delta M_k}{2\ell_{(k,k+1)}}. \quad (10)$$

The forces $\delta\vec{F}_1$ and $-\delta\vec{F}_1$ are perpendicular to the element $(k - 1, k)$ and act on the vertices $k - 1$ and k , respectively. Similarly, the forces $\delta\vec{F}_2$ and $-\delta\vec{F}_2$ are perpendicular to the element $(k, k + 1)$ and act on the vertices k and $k + 1$, respectively. The sum of the two couples equals δM_k .

Finally, a combination of forces and velocities can be imposed on the particles through their vertices. Specifically, a particle can be made perfectly rigid by freezing its surface degrees of freedom. In the same way, wall boundary conditions can be enforced by imposing force or velocity components on selected vertices of a particle.

3. Implementation and performance analysis

With the model now fully defined, this section provides insights into its software implementation and evaluates its expected performance characteristics. The implementation was developed within a computational code named l-hyphen, written in C++ and distributed under the CeCILL-B license (available at <https://github.com/richefeu/l-hyphen>). A distinctive feature of l-hyphen is that it relies exclusively on the toofus framework [38], without introducing any additional external dependencies. Visualizations and graphical processing are handled through a dedicated application built on OpenGL [39], ensuring the software remains self-contained, multi-platform and user-friendly.

Given that core-shells can exhibit extremely large deformations, their construction involves sub-elements, that are thin lines and disks. Consequently, the classical Verlet radial-distance method is insufficient when applied to significant deformations, leading to inaccurate determination of neighboring elements. Therefore, an approach based on a hierarchical neighborhood definition has been developed to address this issue.

By defining the axis-aligned bounding box (AABB) that encompasses each core-shell, their proximity can be stated when the expanded boxes

by a margin using an alert distance d_{alert} overlap. For this very initial broad phase step, an algorithm with complexity $\mathcal{O}(N_{\text{shell}}^2)$ was used in the performance analysis. Additionally, we implemented a linked-cell algorithm which has a complexity of $\mathcal{O}(N_{\text{shell}})$. Following the broad phase, the proximity of all pairs of node-bar and node-node elements is tested using the smallest segment-point or point-point distances, with half the thicknesses of the shells subtracted. This fine phase has a complexity of $\mathcal{O}(n_{\text{sub}}^2)$, where n_{sub} represents the number of sub-elements on adjacent core-shells. It could be optimized by considering a hierarchical structure of sub-elements using binary trees of bounding boxes, but this strategy has not yet been fully implemented as it was not currently absolutely necessary.

The performance analysis is accomplished using a simulation setup that models a column collapse on a horizontal plane consisting of soft core-shell particles. The core-shell particles are initially arranged into a column using an algorithm that is beyond the scope of this analysis.

To assess the simulation time as a function of the number of nodes in the system, two parameters were systematically varied for a column of fixed size: ① the number of particles was incrementally increased while maintaining approximate homothety, ② the number of nodes was augmented in the configuration with the smallest number of particles by subdividing the particle faces; Fig. 7(a).

For all simulations, the total duration t_{total} was recorded. Additionally, the time spent was measured in three key phases: (1) the reconstruction of the neighbor list, denoted as $t_{\text{neighbors}}$, (2) the computation of internal forces and moments within the particles (Section 2.2), denoted as t_{shell} , and (3) the calculation of interaction forces between particles (Section 2.3), denoted as $t_{\text{interaction}}$.

Fig. 7(b) shows the relative contributions of the different calculation steps as a function of the total number of nodes N . The times have been normalized by the total time of each simulation $t_i(N)/t_{\text{total}}(N)$ (hence the red/disk curve equals 1). The three main contributions observed are: calculations of interactions between elements (yellow/diamond), construction of neighbor lists (green/triangle), and calculation of internal forces (blue/square). For configuration ①, where the number of particles is increased while maintaining node density, the relative share of time spent on interactions $t_{\text{interaction}}$ increases with N according to a power law, while the relative times spent on searching for neighbors $t_{\text{neighbors}}$ and calculating internal forces t_{shell} tend to decrease. When only the number of nodes per particle is increased (configuration ②, 381 fixed particles), the trends remain the same but with a different distribution of costs: the relative share of interaction calculations is lower than in configuration ①, at the cost of a relative increase in the time spent searching for neighbors and calculating internal forces. In other words, densifying local meshes increases the local processing cost per cell without causing as many inter-particle interactions as when increasing the number of particles. The inset confirms that the total computation time generally follows a quadratic growth $t_{\text{total}} \propto N^2$ for both configurations. However, the growth is less pronounced in configuration ②, which is consistent with a lower number of inter-particle interactions (the overall interaction pairs increase less rapidly).

4. Calibration and verification

The parameters of the force laws used in the model must be expressed as functions of the material properties and the number N of segments or their lengths ℓ . We assume that each particle represents a core-shell tube of shell thickness h and length s . If the shell is made of a material of Young modulus E and Poisson ratio ν , according to shell theory, the extensional stiffness is given by [18]

$$k_s = \frac{Eh}{1 - \nu^2}, \quad (11)$$

whereas the bending rigidity is

$$k_b = \frac{Eh^3}{12(1 - \nu^2)}. \quad (12)$$

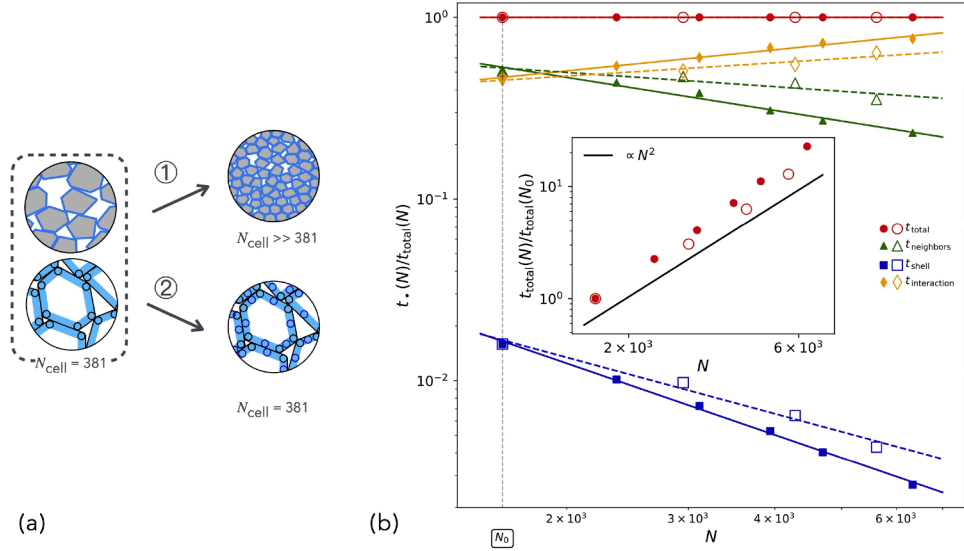


Fig. 7. (a) Sketch of the two tested configurations to increase the number of nodes. (b) Evolution of the different relative computation times as a function of the number of nodes. The solid symbols correspond to an increase in the number of particles (1) and the empty symbols to configuration (2), where the number of nodes per particle is increased in the 381-particle reference sample. The inset shows that the total durations evolve overall as the number of nodes squared.

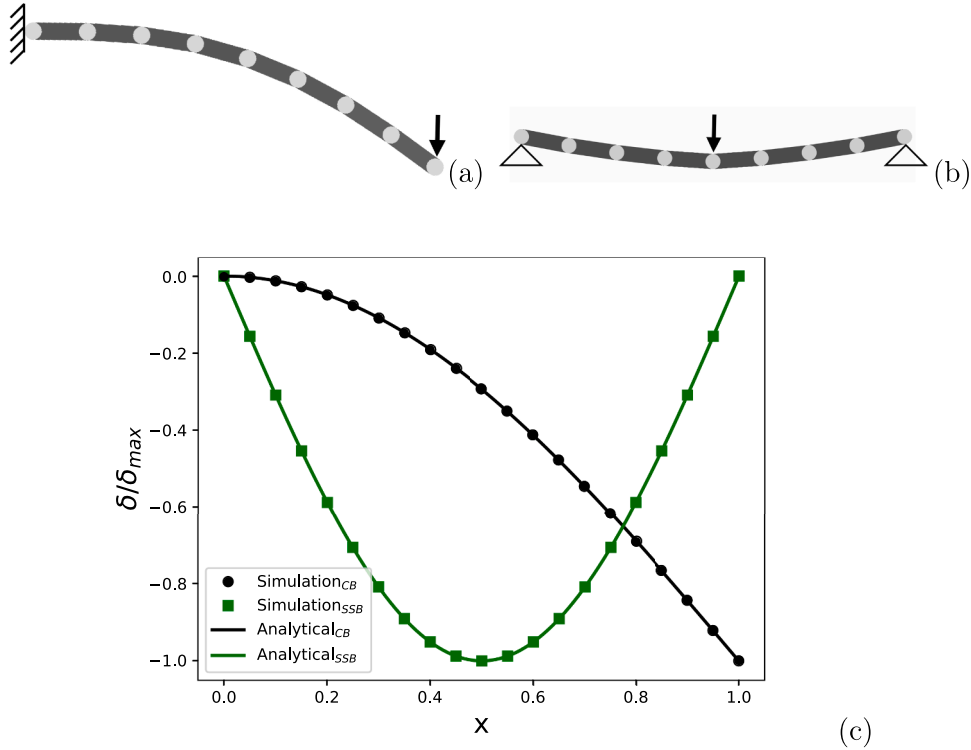


Fig. 8. (a) Simulated cantilever beam with 8 elements, (b) simulated simple support beam with 8 elements, and (c) normalized vertical deflection δ/δ_{max} as a function of the location x along the beam for cantilever beam (CB) and simple support beam (SSB) with 20 elements. The solid lines are the analytical expressions (15) and (17). The arrows indicate the location of the external force.

This expression is based on the consideration that the moment M_b at a vertex is equivalent to the bending moment of a continuous beam at the location of the vertex. Note that the bending stress over the cross section is given by $\sigma_b = \frac{M_b y}{I_c}$, where $I_c = h^3 \ell / 12$ is the centroidal moment of inertia of the beam's cross section and y is the distance from the beam's axis [40].

For the plastic thresholds F_s^Y and M_b^Y , we assume that they are related to the material tensile plastic stress σ^Y through the following rela-

tions:

$$F_s^Y = h s \sigma^Y, \tag{13}$$

and

$$M_b^Y = \frac{4 I_c}{h} \sigma^Y. \tag{14}$$

The latter assumes that the angular plastic threshold is reached when the largest shear stress $\sigma_s = \frac{M_b h}{4 I_c}$ in the section of the beam is equal to the plastic stress threshold σ^Y .

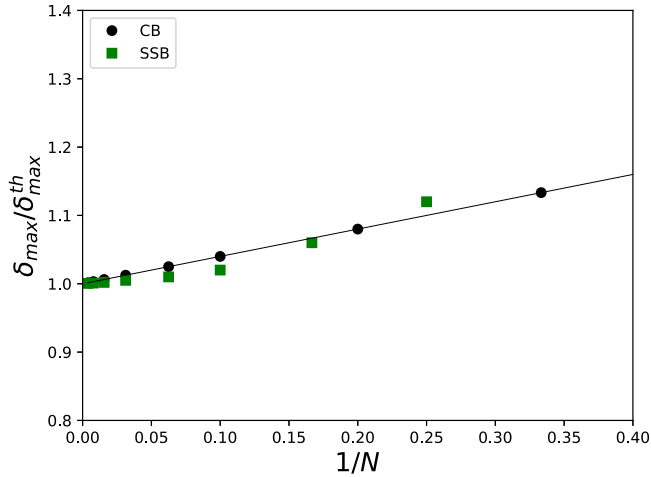


Fig. 9. The ratio of the maximum deflection δ_{max} of cantilever beam and simple support beam to its theoretical value δ_{max}^{th} as a function of the inverse of the number of nodes N .

To verify the code and the calibration of the values of k_s and k_b , we simulated the elastic behavior of a cantilever beam (CB) under the action of a force F applied at its free end and a simply supported beam (SSB) under the action of a force F applied at its center for an increasing number of nodes. The analytical expression for the normalized elastic deflection in the CB case is [40]:

$$\frac{\delta^{CB}(x)}{\delta_{max}^{CB}} = \frac{1}{2} \left(\frac{x}{L} \right)^2 \left(3 - \frac{x}{L} \right), \quad (15)$$

where L is the length of the cantilever, and the origin of the x -coordinate is the left fixed end of the beam. The maximum elastic deflection occurs at the free end of the cantilever and is given by:

$$\delta_{max}^{CB} = \frac{F L^3}{3 E I_c}. \quad (16)$$

The analytical expression for elastic deflection in the case of SSB is:

$$\frac{\delta^{SSB}(x)}{\delta_{max}^{SSB}} = \frac{16}{5} \frac{x}{L} \left\{ 1 - 2 \left(\frac{x}{L} \right)^2 + \left(\frac{x}{L} \right)^3 \right\}, \quad (17)$$

with the maximum deflection at the center of the beam given by:

$$\delta_{max}^{SSB} = \frac{5F L^3}{768 E I_c}. \quad (18)$$

Fig. 8(a) and (b) display the equilibrium shapes of the two beams simulated with 9 nodes, using the expressions (11) and (12) to set the values of k_s and k_b . The vertical deflections δ , normalized by the maximum deflection δ_{max} , are shown in Fig. 8(b) with 21 nodes, alongside the analytical solutions (15) and (17). Despite the low number of nodes, the normalized vertical deflections are reproduced with high precision for both CB and SSB.

Fig. 9 shows the ratio of δ_{max} to its theoretical values δ_{max}^{th} (standing respectively for δ_{max}^{CB} and δ_{max}^{SSB}) as a function of $1/N$. This ratio is slightly above 1, indicating that the maximum deflection is over-estimated by simulations. However, as the number of nodes increases and $1/N$ tends to zero, the ratio converges to 1 as a nearly linear function of $1/N$. Hence, the numerical solution approaches its analytical value as the number of nodes increases, and the value in the continuum limit can be predicted by extrapolation. This behavior is a consequence of finite resolution in simulations, which affects the strain field, and is therefore independent of the method used [41].

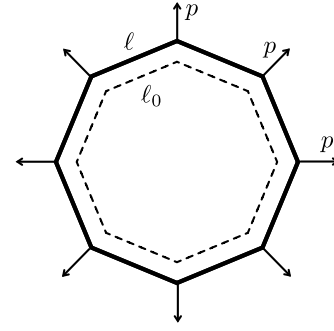


Fig. 10. A particle composed of N mass points (nodes) and subjected to internal pressure p .

5. Diametral compression of a core-shell particle

5.1. Dimensionless parameters

Let us consider a core-shell particle as a regular polygone of radius R_0 and composed of N mass points. The particle shape tends to a circle with increasing N . The deformation of this particle under general loading depends on the values of the stiffness parameters k_s , k_b , K_Ω , and M_b^Y . From these four elastic parameters we can define three dimensionless parameters, which are expected to fully control the range of all possible behaviors of the particle. The bending stiffness k_b can be compared to the stretch stiffness k_s via the distance ℓ between mass points. The corresponding stiffness ratio ξ is

$$\xi = \frac{k_b}{k_s \ell^2} = \frac{1}{12} \left(\frac{h}{\ell} \right)^2, \quad (19)$$

where Eqs. (11) and (12) are used.

The second dimensionless parameter η can be defined by comparing K_Ω with the effective stiffness $K_{\partial\Omega}$ induced by shell elements:

$$\eta = \frac{K_\Omega}{K_{\partial\Omega}}. \quad (20)$$

This parameter represents the core-to-shell stiffness ratio. For $\eta = 0$, a circular particle behaves as an elastic ring, while for $\eta \gg 1$, its behavior is expected to be closer to that of a solid elastic particle.

An estimation of $K_{\partial\Omega}$ can be obtained by considering a circular particle subjected to an external isotropic pressure p , as shown in Fig. 10. The application of this pressure leads to the variation of the radius from R_0 to R , the variation $\Delta V = V - V_0$ of the volume, and the variation of the length between two mass points from ℓ_0 to ℓ . Since the central angle $2\pi/N$ between two adjacent mass points does not change, we have

$$\frac{\Delta V}{V_0} = \frac{\ell + \ell_0}{\ell_0} \frac{\Delta \ell}{\ell_0}. \quad (21)$$

The pressure is isotropically distributed on the midpoints of the segments. Hence, the force acting at each vertex is

$$f = p \ell s \cos \left(\frac{\pi}{N} \right). \quad (22)$$

This force is balanced by the extensional force $g = k_s \Delta \ell$ acting between the mass points, such that

$$2g \sin \left(\frac{\pi}{N} \right) = f. \quad (23)$$

As a result, according to Eq. (21), we have

$$p = \frac{2k_s}{s} \tan \left(\frac{\pi}{N} \right) \frac{\Delta \ell}{\ell_0} = \frac{2k_s}{s} \frac{\ell_0}{\ell + \ell_0} \tan \left(\frac{\pi}{N} \right) \frac{\Delta V}{V_0}, \quad (24)$$

implying

$$K_{\partial\Omega} = \frac{2k_s}{s} \frac{\ell_0}{\ell + \ell_0} \tan \left(\frac{\pi}{N} \right) \simeq \frac{k_s}{s} \tan \left(\frac{\pi}{N} \right) = \frac{2\pi}{Ns} \frac{Eh}{1 - \nu^2} \quad (25)$$

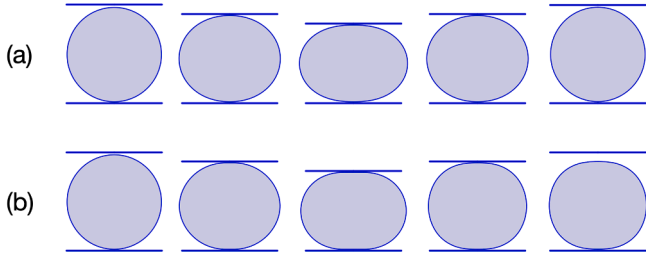


Fig. 11. Evolution of particle shape during the compression and decompression of a circular particle between two flat walls for a large value of the stiffness ratio $\eta = \infty$ in the purely elastic case (a) and for a small elastic limit ratio γ (b).

The latter approximation correspond to the value of $K_{\partial\Omega}$ in the initial state with $\ell \simeq \ell_0$. This expression allows us to calculate the core-to-shell stiffness ratio η from its definition (20).

The third dimensionless parameter can be defined by comparing the elastic limit M^Y to the characteristic moment of the particle

$$M^* = \frac{EI_c}{(1 - \nu^2)R}, \quad (26)$$

which represents the elastic energy of an elastic sheet of length $2\pi R$ that is curved to a cylinder of radius R . We therefore define the following elastic limit ratio characterizing the shell plasticity:

$$\gamma = \frac{M^Y}{M^*}. \quad (27)$$

As γ increases from zero, the shell behavior varies from a floppy membrane-like to a solid elastic behavior.

As an illustration, let us consider the diametral quasi-static compression-decompression cycle of a single circular particle between two flat and parallel walls, varying the elastic and plastic parameters of the particle. The strain rate is kept sufficiently low to ensure complete relaxation after each strain increment. The walls are modeled as rigid bars represented by open cells with node reference angles equal to 0 and with high values of k_b and k_s compared to those of the particle.

Fig. 11 shows the evolution of the particle shape with a high value of the stiffness ratio η in the purely elastic case ($\gamma = \infty$) and in the case of a finite elastic limit γ where the particle undergoes plastic deformation. The maximum vertical strain is $\varepsilon = 1 - b/b_0 = 0.35$, where b is the distance between the two walls and $b_0 = 2R$ is its initial value. In the purely elastic case, the particle deforms nearly as a flattening ellipse, with a minor axis length b perpendicular to the walls and a major axis length a parallel to the walls. Initially, the contacts with the walls are point contacts but develop a small flat contact area as deformation continues. During unloading, the particle fully recovers its initial circular shape. In the case with a small elastic limit, the particle rapidly reaches the plastic deformation regime during compression, resulting in a larger contact area with the walls compared to the purely elastic case. We also see that the particle does not fully recover its initial shape after unloading as a result of the cumulative plastic deformation of the shell. In the following, we compare the particle deformation in the elastic and plastic cases with analytical expressions.

5.2. Elastic ring

At the beginning of compression, the particle flattens but remains rounded. As the strain increases, the shape evolves to resemble a rounded-cap rectangle or a stadium-like shape, characterized by two parallel flat sides in contact with the walls and two lateral semi-circular sides [42]. The evolution of the particle aspect ratio a/b_0 as a function of b can be predicted for these two shapes under the assumption that the perimeter remains constant. For the elliptical shape, the relationship between a and b is given by the following implicit equation [42]:

$$2b_0 = 3(a + b) - \sqrt{(a + 3b)(3a + b)}. \quad (28)$$

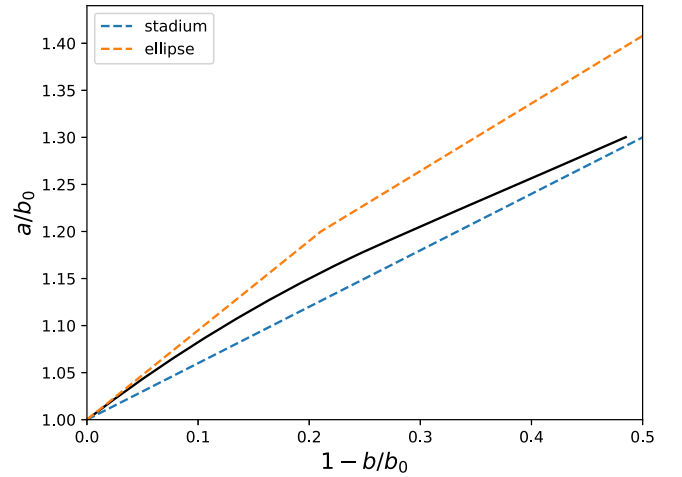


Fig. 12. Evolution of the major axis length a normalized by the initial value b_0 of the minor axis length as a function of axial strain $1 - b/b_0$ during diametral compression of an elastic ring ($\eta = 0$) from numerical simulation (black line) and from two models assuming either elliptic (red line) or stadium-like (blue) particle shape with constant perimeter. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

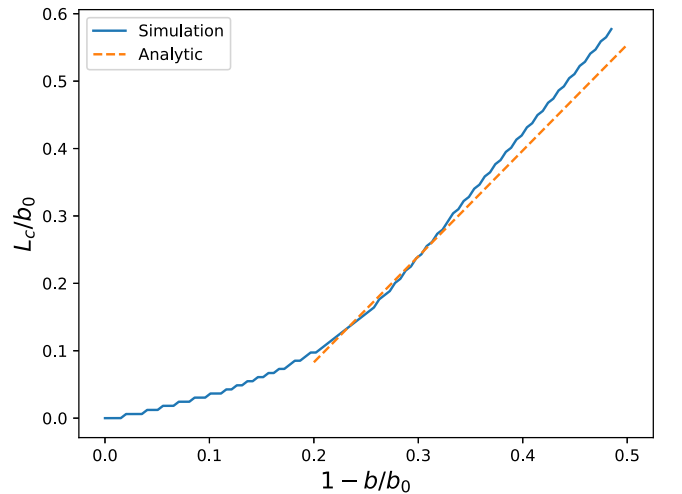


Fig. 13. Evolution of the contact length L_c normalized by the initial diameter b_0 as a function of axial strain during diametral compression of an elastic ring ($\eta = 0$). The slope of the dashed line is $\pi/2$.

In the case of the stadium-like shape, the aspect ratio a/b_0 is expressed as:

$$\frac{a}{b_0} = 1 + \left(\frac{\pi}{2} - 1\right) \left(1 - \frac{b}{b_0}\right). \quad (29)$$

These equations provide a simple way to describe the deformation behavior of the particle as it is compressed.

The analytical ratio a/b_0 is plotted as a function of $\varepsilon = 1 - b/b_0$ in Fig. 12 for the two shapes discussed earlier, based on Eqs. (28) and (29), as well as from numerical simulations with $\eta = 0$ (elastic ring). As expected, the simulated evolution of a/b_0 falls between the two shapes, resembling an ellipse at low ε values and transitioning toward a stadium-like shape at higher values. Fig. 13 illustrates the corresponding evolution of the normalized contact length L_c/b_0 . This contact length increases nonlinearly with vertical strain but shifts to a linear trend beyond $\varepsilon \simeq 0.3$. The linear behavior in the second regime aligns with the shape transition from ellipse to stadium-like. For a stadium-like shape

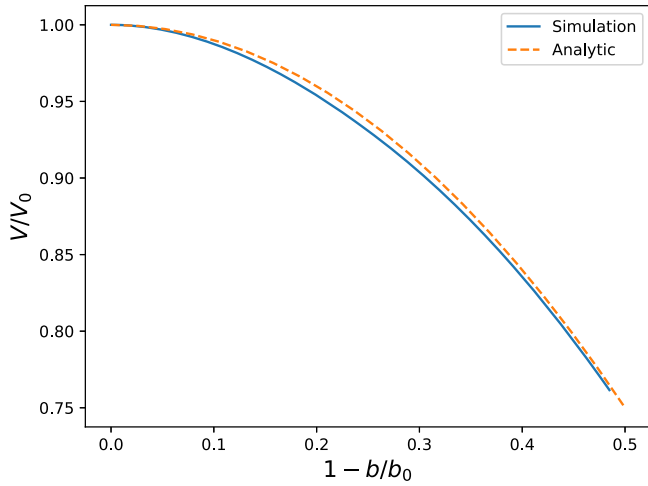


Fig. 14. Evolution of the normalized volume of an elastic ring ($\eta = 0$) as a function of axial strain during diametral compression.

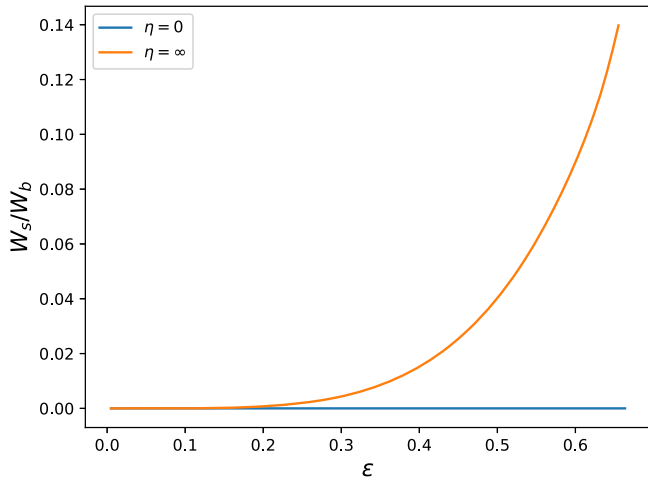


Fig. 15. The ratio of extensional energy W_s to bending energy W_b for two values of the stiffness ratio η as a function of axial strain.

with constant perimeter, it can be shown that

$$\frac{L_c}{b_0} = \frac{\pi}{2} \left(1 - \frac{b}{b_0} \right). \quad (30)$$

A straight line with a slope of $\pi/2$ is plotted in Fig. 13, demonstrating that the slope observed in simulations during the second regime is very close to this value. A similar relation can be derived for the evolution of the volume V of the stadium-like shape under the constant perimeter assumption:

$$\frac{V}{V_0} = 1 - \left(1 - \frac{b}{b_0} \right)^2. \quad (31)$$

As shown in Fig. 14, this relation is in excellent agreement with the volume evolution of an elastic ring from the onset of compression through to large strains.

The assumption of a constant perimeter is physically justified by the lower energy cost of bending as compared to stretching in the case $\eta = 0$. In our simulations, we find the ratio of the total stretching energy W_s to the bending energy W_b is negligibly small for $\eta = 0$ but increases with deformation for large values of η as shown in Fig. 15. Note that the ratio W_s/W_b is proportional to the ratio $k_s/k_b \propto h^{-2}$ and tends to infinity as h vanishes.

It is also interesting to compare the energy costs for the faceting of the particle against the walls and for a uniform deformation of the

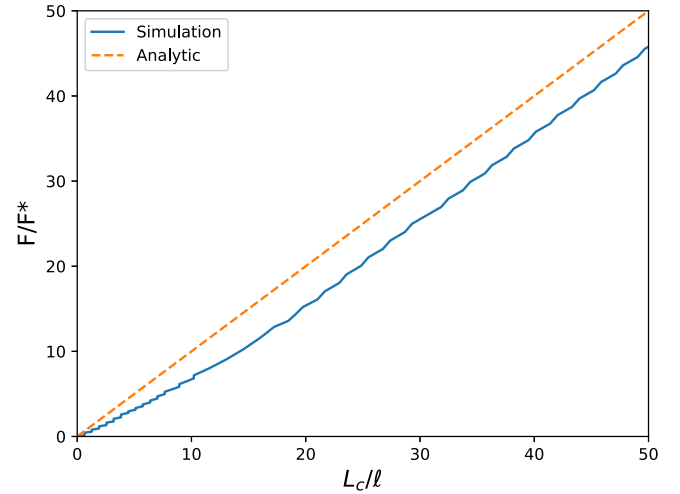


Fig. 16. The total wall-particle normal force F normalized by the characteristic force F^* for $\eta = 0$ as a function of the contact length L_c during diametral compression of an elastic ring from simulations (full line) and from the approximate analytical expression (33) (dashed line).

particle. The first deformation mechanism is local in the sense that it takes place only at the contact with the two walls while the curvature remains equal to the initial curvature everywhere else. The second mechanism involves a slight decrease or increase of the curvature at all points of the shell. The total energy stored in the two contacts of length L_c with the two walls is $W_{contact} = (k_b/2)(2L_c/R_0^2)$ since the curvature changes from $1/R_0$ to 0 and the range of deformation is $2L_c$. Alternatively, if the same amount of deformation was uniformly distributed on the shell, the change of curvature would be $\pm L_c/R_0^2$ and therefore the total energy stored in the shell would be $W_{uniform} = (k_b/2)(L_c/R_0^2)^2(2\pi R_0)$. The latter involves a multiplication by the total perimeter $2\pi R_0$ in order to obtain the total energy. Requiring $W_{contact} < W_{uniform}$ implies $L_c/b_0 > 1/2\pi \approx 0.16$. This means that the uniform deformation mode is energetically more favorable at low strains, but faceting becomes more favorable (with lower energy cost) when the contact length exceeds $0.16b_0$. This is consistent with Fig. 13, which shows that the contact length increases indeed much faster beyond $\epsilon \approx 0.25$ corresponding to $L_c \approx 0.16b_0$.

Another important variable is the total force F exerted by the wall on the particle. For an elastic ring, the vertical force F'_k acting on each vertex of the particle by the wall creates a local moment $F'_k \ell$ relative to the two neighboring vertices $k-1$ and $k+1$. This moment is balanced by the torque M'_k resulting from the change $\Delta\theta'_k$ in the vertex angle. Initially, the angles are $\pi - 2\pi/N$, but due to compression, the angles at the vertices in contact with the wall tend to π because the interface in the contact zone between the wall and the particle is flat. Therefore, $\Delta\theta'_k = 2\pi/N$, leading to $M'_k = 2\pi k_b/N$. The equilibrium of each vertex in the contact zone implies $M'_k = 2\pi k_b/N = F'_k \ell$, which, together with Eq. (12), leads to $F'_k = F^*$ with

$$F^* = \frac{k_b}{R} = \frac{EI_c}{(1-\nu^2)R\ell}. \quad (32)$$

This force is the characteristic elastic force of the particle. Since F'_k is independent of the vertex position k in the contact zone, the total contact force is the number N' of nodes on the contact line multiplied by F^* . Therefore, for $N' = L_c/\ell$, we have

$$\frac{F}{F^*} = \frac{L_c}{\ell}. \quad (33)$$

The derivation of this expression does not depend on the particle shape, suggesting that during diametral compression, Eq. (33) is valid in both small-strain and large-strain regimes.

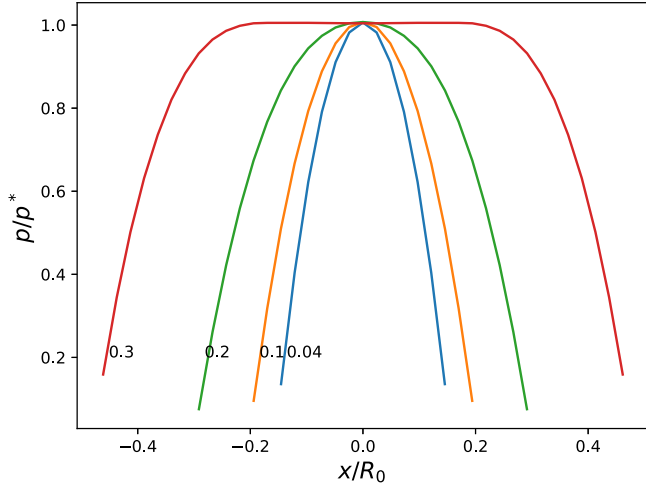


Fig. 17. Local pressure p normalized by the characteristic pressure p^* (see text) in the contact zone as a function of nodal position x normalized by the initial particle radius R during diametral compression. The numbers indicate the vertical deformation $1 - b/b_0$. The origin of x is the middle of the contact zone.

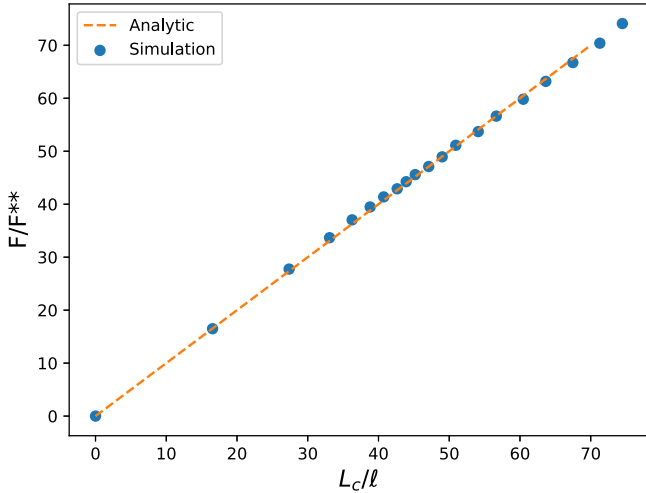


Fig. 18. The total wall-particle normal force F normalized by the plastic force threshold F^{**} for $\eta = 0$ as a function of the contact length L_c during diametral compression of a plastic ring from simulations (full line) and from the approximate analytical expression (36) (dashed line).

Fig. 16 shows F/F^* for an elastic ring as a function of L_c/ℓ . The simulation data are close to the expected affine relation in both regimes, though with a slightly lower slope in the first regime. The simulated forces are consistently below the predicted values because the model assumes the contact line is flat and that all forces at all nodes in the contact area reach their maximum value F^* . An example of the pressure profile along the contact line is shown in Fig. 17 at four different instants of compression. The pressures p are calculated by dividing the contact force on segments of length ℓ by $s\ell$. The pressures are normalized by the characteristic pressure $p^* = F^*/(s\ell)$. We see that the pressure is not constant across the entire contact zone. Initially, the largest pressure p^* is only reached at the center of the contact zone, with a parabolic force profile around it. At larger strains, a long plateau of constant pressure p^* forms, but the pressure decreases on both sides of this plateau over several nodes, explaining the lower contact force compared to the prediction of Eq. (33).

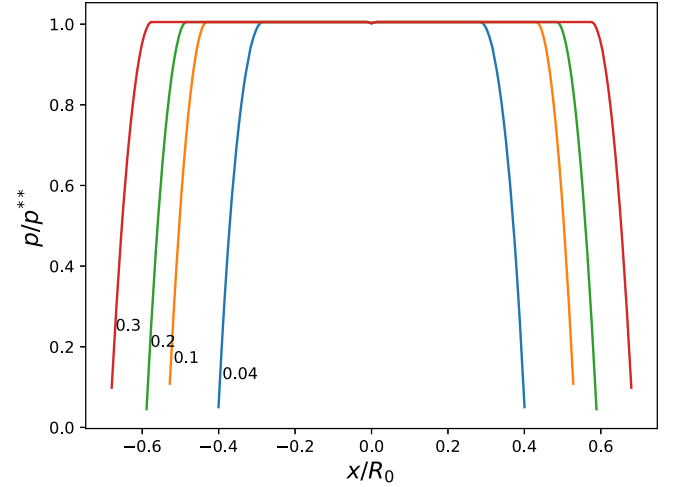


Fig. 19. Local pressure p normalized by the characteristic pressure p^{**} (see text) in the contact zone as a function of nodal position x normalized by the initial particle radius R during diametral compression for $M^Y/M^* = 5 \times 10^{-5}$. The numbers indicate the vertical deformation $1 - b/b_0$. The origin of x is the center of the contact zone.

5.3. Plastic ring

Let us now consider the ring ($\eta = 0$) with a finite plastic threshold M^Y . This threshold must be compared with the elastic characteristic torque M^* defined from Eq. (32) as follows:

$$M^* = F^* \ell = \frac{EI_c}{(1 - \nu^2)R}. \quad (34)$$

The amount of plastic deformation of a particle depends on the ratio M^Y/M^* . For illustration, we focus on an example where the plastic threshold is reached at very low strains. Simulations of diametral compression were conducted for $M^Y/M^* = 5 \times 10^{-5}$. At such a low plastic threshold, it can be assumed that all vertices in the contact zone between the particle and the driving wall are at the plastic threshold. Following the same reasoning as in the case of the elastic ring, all forces are expected to equal the plastic force threshold:

$$F^{**} = \frac{M^Y}{\ell}. \quad (35)$$

Consequently, as in Eq. (33), the total contact force F is given by

$$\frac{F}{F^{**}} = \frac{L_c}{\ell}. \quad (36)$$

Eq. (36) shows excellent agreement with the simulation data, as illustrated in Fig. 18, without distinguishing between low- and large-strain regimes. The pressure profile along the contact line is displayed in Fig. 19 at four different instants of compression. The pressure is normalized by the characteristic pressure $p^{**} = F^{**}/(s\ell)$. A broad pressure plateau emerges from the beginning of diametral compression, with a steep pressure drop on both sides of this plateau. This indicates that the assumption of a flat contact area holds better in the plastic case, which explains the excellent agreement of the simulation data with Eq. (36).

Fig. 20 displays the particle volume as a function of diametral strain $\varepsilon = 1 - b/b_0$. In the plastic case, the volume reduction slightly exceeds that of the elastic ring in the initial regime, but they coincide at larger strains. The key difference is that the plastic ring retains its distorted shape upon unloading, while the elastic ring recovers its original circular shape.

5.4. Influence of core stiffness

The presence of a nonzero core stiffness K_Ω leads to an internal pressure p that arises from volume changes. This pressure exerts a radial

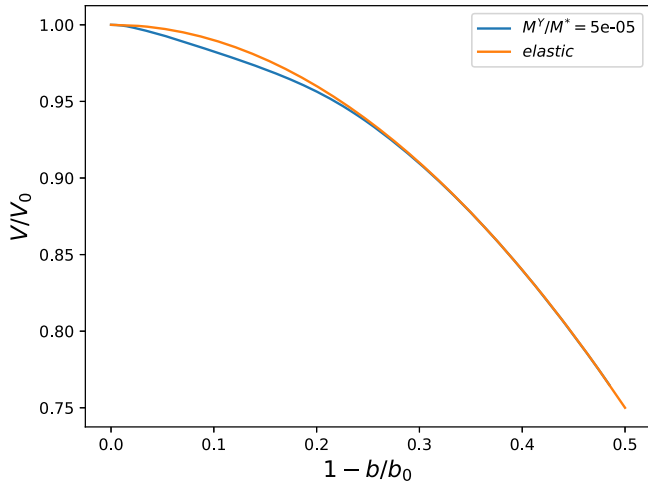


Fig. 20. Evolution of the normalized volume of a ring ($\eta = 0$) as a function of diametral strain during diametral compression for a plastic ring with $M^Y/M^* = 5 \times 10^{-5}$ as compared with that of an elastic ring.

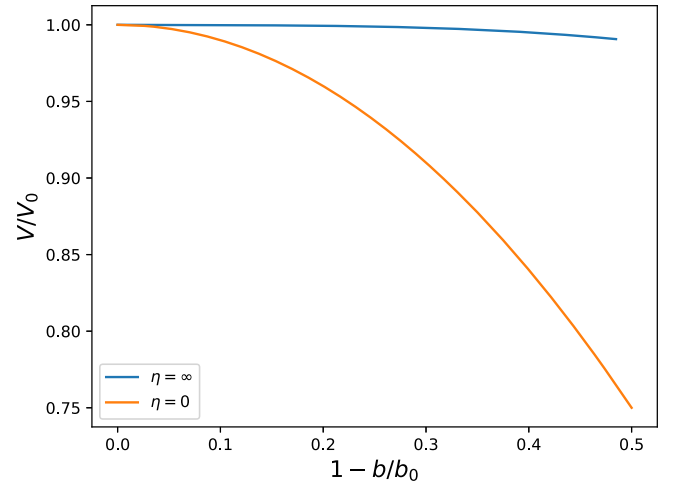


Fig. 22. The volume of an elastic ring as a function of diametral strain $1 - b/b_0$ for $\eta = 0$ (without core stiffness) and for $\eta = \infty$ (with high core stiffness).

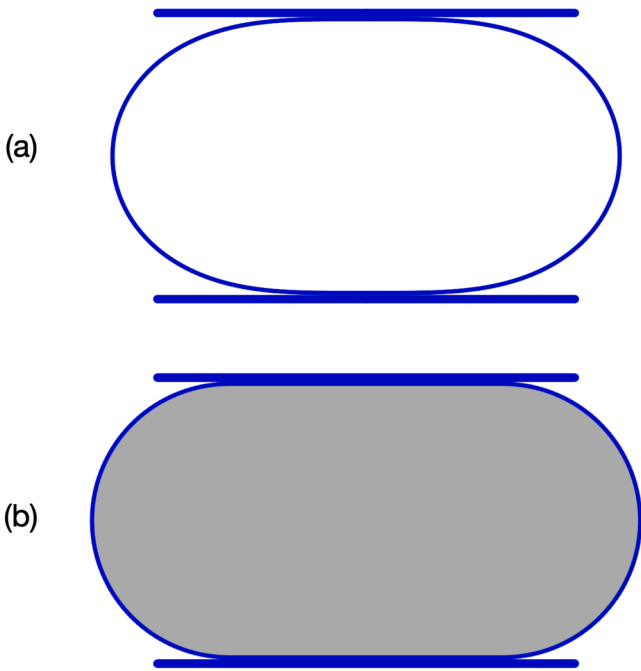


Fig. 21. The shape of an elastic ring at diametral strain $1 - b/b_0 = 0.3$ for $\eta = 0$ (without core stiffness) (a) and for $\eta = \infty$ (with high core stiffness) (b).

force $F_{in} = ps\ell$ on each element, which tends to increase the angles between elements, especially at the vertices in contact with the wall. We focus here on a very large value $\eta \simeq 10^5$, denoted as $\eta = \infty$ in the figures.

Fig. 21 illustrates the shape of an elastic ring at a vertical strain of $1 - b/b_0 = 0.3$ for two cases: $\eta = 0$ (no core stiffness) and $\eta = \infty$. As expected, the contact area is significantly larger for $\eta = \infty$. In contrast to the $\eta = 0$ case, as shown in Fig. 22, the volume change for $\eta = \infty$ is minimal and does not follow the expression (31) for a stadium-like shape. The typical evolution of a stadium-like shape involves a reduction in the radius of the circular sides and an increase in contact length. However, the internal pressure development hinders the increase in curvature. As a result, the contact area increases more rapidly, while the curvature of the sides increases more slowly compared to the $\eta = 0$ case. Indeed, Fig. 23 shows that the growth rate of L_c is approximately 2.1, exceeding the $\pi/2$ value expected for a stadium-like shape. Consequently, the effect

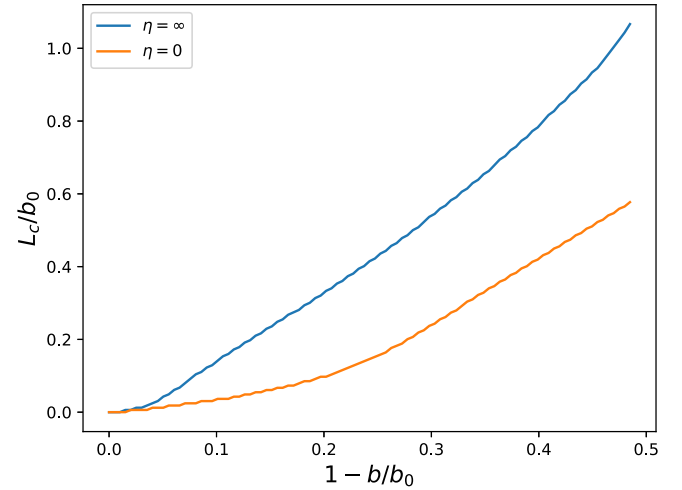


Fig. 23. The normalized contact length L_c of an elastic ring as a function of diametral strain $1 - b/b_0$ for $\eta = 0$ (without core stiffness) and for $\eta = \infty$ (with high core stiffness).

of core pressure or core stiffness is to facilitate extensive contacts with the walls (and other particles) without a significant change in volume.

The total force F acting on the contact line is the sum of the internal force F_{in} due to pressure p and the characteristic elastic force F^* at each node, multiplied by the number of nodes L_c/ℓ :

$$\frac{F}{F^*} = \left(1 + \frac{ps\ell}{F^*}\right) \frac{L_c}{\ell}. \quad (37)$$

The significance of the additional term, compared to Eq. (33), depends on p , which is a function of the volume change. Fig. 24 illustrates F as a function of L_c for both $\eta = 0$ and $\eta = \infty$. As expected, for a given L_c/ℓ , the contact force is higher in the $\eta = \infty$ case, with the difference increasing as volume change and contact length increase.

The pressure distribution along the contact line, shown in Fig. 25, reveals that the force plateau extends over nearly the entire contact area, with sharp drops at both ends of the plateau. Unlike the plastic case, the plateau level rises with diametral compression due to the increasing internal pressure. Hence, Eq. (37) provides an accurate estimate of the force. If p remains constant, F is a linear function of L_c . However, if the volume change linearly depends on diametral strain, p will also vary linearly with L_c , causing F to increase quadratically, similar to a solid cylinder of Young's modulus E and Poisson's ratio ν . For such a solid

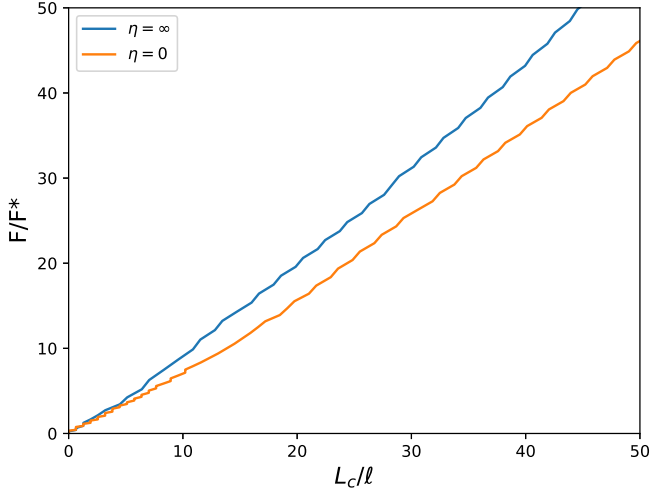


Fig. 24. The normalized contact force as a function of contact length L_c during diametral compression of an elastic ring as a function of vertical strain $1 - b/b_0$ for $\eta = 0$ (without core stiffness) and for $\eta = \infty$ (with high core stiffness).

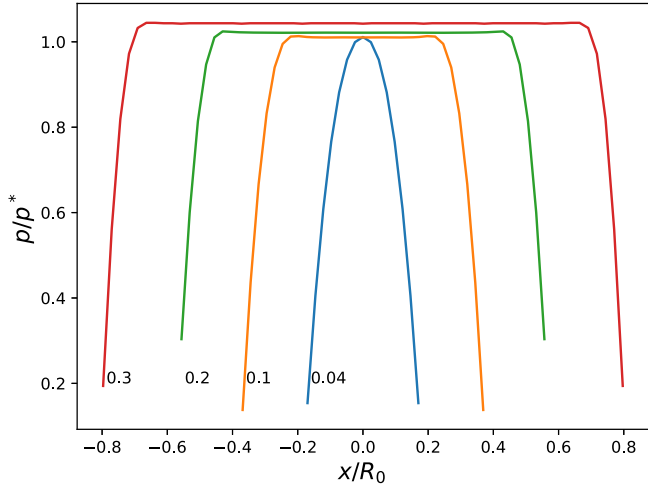


Fig. 25. Local pressure p normalized by the characteristic pressure p^* (see text) in the contact zone as a function of nodal position x normalized by the initial particle radius R during diametral compression of an elastic ring for $\eta = \infty$ (with high core stiffness). The numbers indicate the diametral deformation $1 - b/b_0$. The origin of x is the middle of the contact zone.

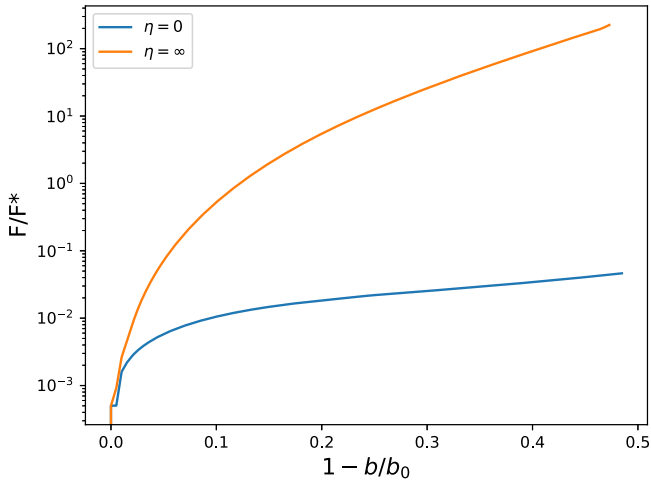


Fig. 26. The normalized contact force as a function of diametral strain $\varepsilon = 1 - b/b_0$ for $\eta = 0$ (without core stiffness) and for $\eta = \infty$ (with high core stiffness).

cylinder, the analytical expression of L_c as a function of F is given by [43]:

$$L_c = \left\{ 2F \frac{R}{\pi s} \frac{1 - \nu^2}{E} \right\}^{1/2}. \quad (38)$$

It is important to note that the volume change at small strains (below 10%) is negligible, and the particle behaves like an elastic ring without core pressure, with the contact force increasing linearly with contact area. This behavior is clearly observed in Fig. 24 at low values of L_c/ℓ . In plant cells, the hydrostatic turgor pressure plays a similar role with respect to cell walls as core pressure does in our model with respect to shell elements. The incompressibility of the liquid prevents significant volume change, so the turgor pressure primarily facilitates the faceting of cell walls during interactions [44,45].

Fig. 26 shows the normalized vertical force F/F^* as a function of the diametral strain $\varepsilon = 1 - b/b_0$ for $\eta = 0$ and $\eta = \infty$. In both cases, the force increases rapidly (faster than exponential) with ε at the beginning of compression, but asymptotically tends to a linear form for $\eta = 0$ and a nearly exponential form for $\eta = \infty$. This indicates that the volumetric strain decreases almost exponentially with strain. This decrease is small for $\eta = \infty$, as observed in Fig. 22, but its effect is amplified by the high value of the core stiffness.

6. Uniaxial compaction of an assembly of soft disks

In this section, we present simulations of the uniaxial compaction of an assembly of soft frictionless circular particles. The particles are initially allowed to fall into a rectangular box under their own weight. After the sample reaches static equilibrium, gravity is removed, and the top wall is moved downward at a constant velocity. The simulation involves 500 particles with an average radius R and a standard deviation $\Delta R/R = 0.15$.

Fig. 27 shows snapshots of the uniaxial compaction process up to a cumulative vertical strain $\varepsilon = \ln(H/H_0) \simeq 0.3$, where H is the current sample height and H_0 is the height at the first point of contact between the top wall and the top layer of particles as seen in Fig. 27(a). During compaction, the void ratio e , defined as the ratio of the total volume V_p of the pore space between particles to the total volume V_s of particles, decreases due to three factors: 1) particle rearrangements, 2) particle volume reduction, and 3) particle shape change. The extent to which each factor contributes to pore reduction depends on the elasto-plastic parameters M^Y and η .

Fig. 28 shows the vertical stress σ as a function of the vertical strain ε during both the loading (downward movement of the top wall) and unloading (upward movement of the top wall) phases. The data is presented for four distinct sets of parameter values: 1) $\eta = 0$ and a high value of the relative plastic threshold M^Y/M^* (elastic particles without core stiffness), 2) $\eta = 1$ and high M^Y/M^* (elastic particles and low core stiffness), 3) $\eta = \infty$ and high M^Y/M^* (elastic particles and high core stiffness), and 4) $\eta = 0$ and very low value of M^Y/M^* (plastic particles without core stiffness). The initial configuration at $H = H_0$ is the same for all the four simulations. The stresses are normalized by the characteristic stress

$$\sigma^* = \frac{F^*}{2Rs}. \quad (39)$$

For purely elastic particles (high M^Y/M^*), σ/σ^* increases in a strongly nonlinear manner with ε during loading. Upon unloading, the stress decreases along a path that is close to but slightly below the loading path, indicating a residual strain. This residual strain suggests that due to particle rearrangements, the sample ends up in a slightly more compact state than initially, while the particles regain their original circular shape. The residual strain is smaller for higher values of η . This collective granular plasticity is typically observed in granular materials composed of rigid particles. In contrast, for plastic deformable particles (with a very low M^Y/M^*), the particles undergo irreversible deformation during loading, and σ/σ^* decreases until a significant residual strain

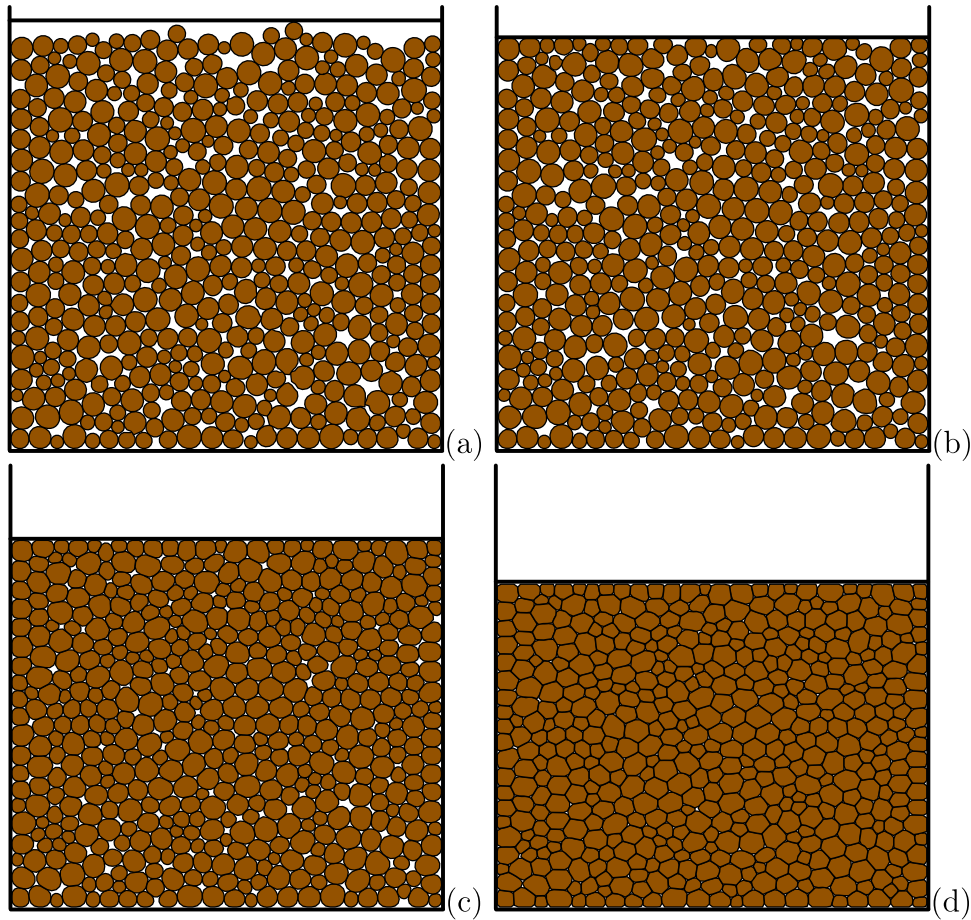


Fig. 27. Snapshots of the uniaxial compaction of an assembly of 500 soft core-shell particles.

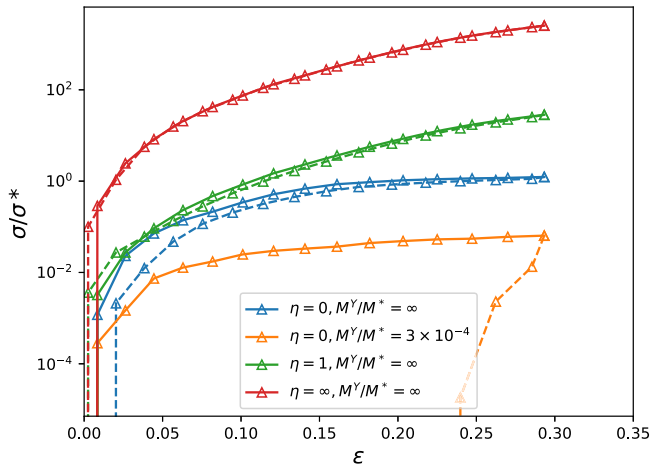


Fig. 28. Vertical stress σ normalized by the characteristic stress σ^* (see text) during uniaxial compaction (full lines) and decompaction (dashed lines) of an assembly of soft particles for four sets of parameter values: 1) $\eta = 0$ and a high value of the relative plastic threshold M^Y/M^* , 2) $\eta = 1$ and high M^Y/M^* , 3) $\eta = \infty$ and high M^Y/M^* , and 4) $\eta = 0$ and low value of M^Y/M^* .

is reached. Here, the plastic behavior is primarily attributed to the intrinsic plasticity of the particles rather than their rearrangement. The observed increase in σ/σ^* with increasing η reflects the corresponding rise in particle bulk stiffness.

Fig. 29(a) displays the relationship between the void ratio e and the normalized stress σ/σ^* for the same parameter sets discussed in Fig. 28. For a total cumulative compaction $\epsilon = 0.3$, the void ratio e decreases from 0.22 to 0.1 for $\eta = 0$ in the elastic case, to 0.04 for $\eta = \infty$ in the elastic case, and to 0.06 for $\eta = 0$ in the plastic case. These variations in e correspond to changes in particle shapes under stress. During unloading, e increases across all elastic cases and follows a trajectory close to that during loading. When the vertical strain returns to zero, e remains slightly lower than the initial value e_0 , indicating that despite the particles' fully elastic behavior, there is a small residual compaction due to particle rearrangements. In the case of plastic rings, where M^Y/M^* is low, the change in particle shape is irreversible, leading to a slight increase in e due to elastic restitution. However, e retains a low value after full unloading, attributed to both particle plastic deformation and particle rearrangements.

The void ratio e decreases as a function of σ/σ^* initially in a nonlinear manner but, at higher stresses, follows a logarithmic function over two decades:

$$e = e_0 - C \log_{10} \left(\frac{\sigma}{\sigma^*} \right), \quad (40)$$

where C represents the compressibility index. This compaction law is well documented for clays, although its microscopic origins are not fully understood [46]. In our simulations, the value of C is approximately 0.07 for elastic particles, regardless of the stiffness ratio η . However, for plastic particles, C is higher, reflecting their increased deformability.

The volume-change behavior of granular materials is typically described using the void ratio e or the packing fraction $\Phi = 1/(1 + e)$. This variable is sufficient when the total particle volume is conserved during compaction or flow. However, when particles undergo volume changes,

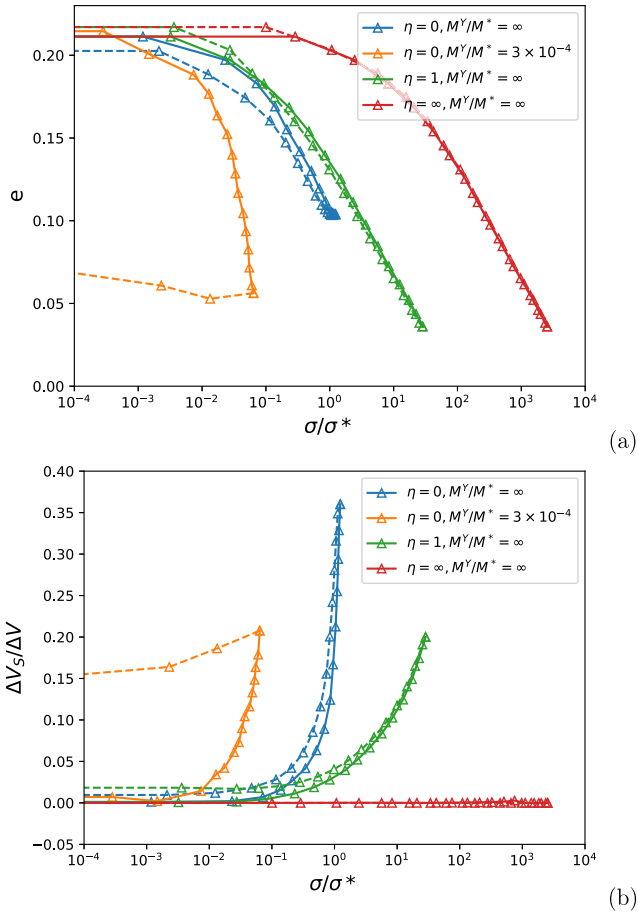


Fig. 29. Void ratio e (a) and relative particle volume variation $\Delta V_s/\Delta V$ (b) as a function of the normalized stress σ/σ^* for the same four parameter sets as in Fig. 28. The solid and dashed lines represent the loading and unloading paths, respectively.

it is necessary to consider also the ratio $\Delta V_s/\Delta V$, where ΔV_s represents the cumulative change in particle volume from its initial state, and ΔV denotes the cumulative volume change of the entire sample. This ratio quantifies the contribution of particle volume change to the overall compaction.

Fig. 29(b) shows $\Delta V_s/\Delta V$ as a function of σ/σ^* . For $\eta = \infty$, ΔV_s is negligible. However, as η decreases, $\Delta V_s/\Delta V$ increases significantly, reaching a peak value of 0.37 for $\eta = 0$ when $\sigma \approx \sigma^*$ (corresponding to $\epsilon = 0.3$). This means that at this point, particle volume change accounts for 37% of the total sample volume change ΔV . The remainder of the volume change is due to changes in the pore volume ΔV_p , resulting from particle shape alterations and, to a lesser extent, particle rearrangements. This high volume change is consistent with the significant particle volume change observed during diametral compression of elastic rings.

In the case of plastic particles, the volume change contribution at $\epsilon = 0.3$ is lower, with $\Delta V_s/\Delta V \approx 0.22$. This is because plasticity allows particles to change shape more easily than volume. Snapshots of the samples at $\epsilon = 0.3$ (just before unloading) are shown in Fig. 30, along with color-coded levels indicating the elastic energies W^i of particles i , normalized by the average elastic energy per particle $\langle W \rangle$. In all cases, the elastic energy distribution is inhomogeneous and closely related to particle shapes. For elastic particles without core stiffness (Fig. 30(a)), there is a large number of rounded-shaped particles with low energy, alongside elongated, stadium-like particles with high energies, often forming locally ordered groups. In contrast, elastic particles with high core stiffness (Fig. 30(b)) deform into polygonal shapes that efficiently

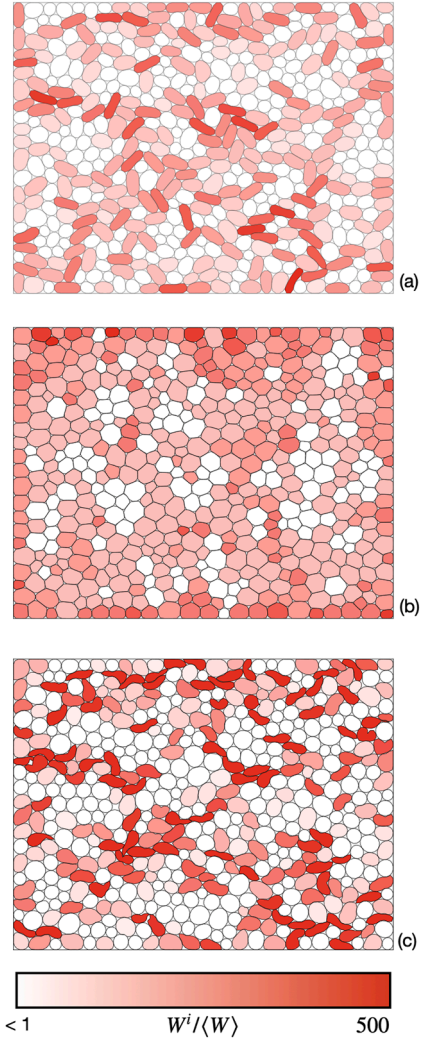


Fig. 30. Snapshots of the compacted samples for a cumulative vertical deformation of $\epsilon = 0.3$ with (a) $\eta = 0$ and a high value of the relative plastic threshold M^Y/M^* (elastic particles without core stiffness), (b) $\eta = \infty$ and high M^Y/M^* (elastic particles and high core stiffness), and (c) $\eta = 0$ and very low value of M^Y/M^* (plastic particles without core stiffness). Color levels represent the normalized elastic energies of the particles for the energies above the average energy per particle. Particles of elastic energy below the average are in white.

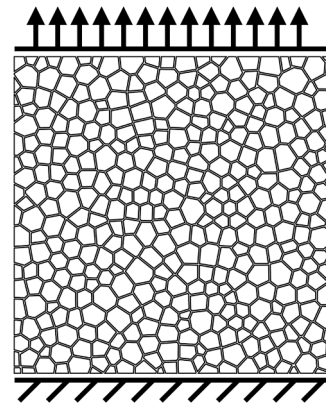


Fig. 31. A cohesive cellular tissue subjected to axial extension. The bottom wall is immobile.

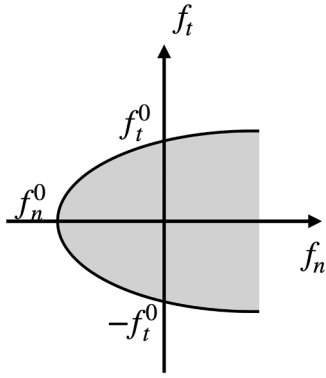


Fig. 32. The yield criterion at the interface between two cells; see Eq. (41).

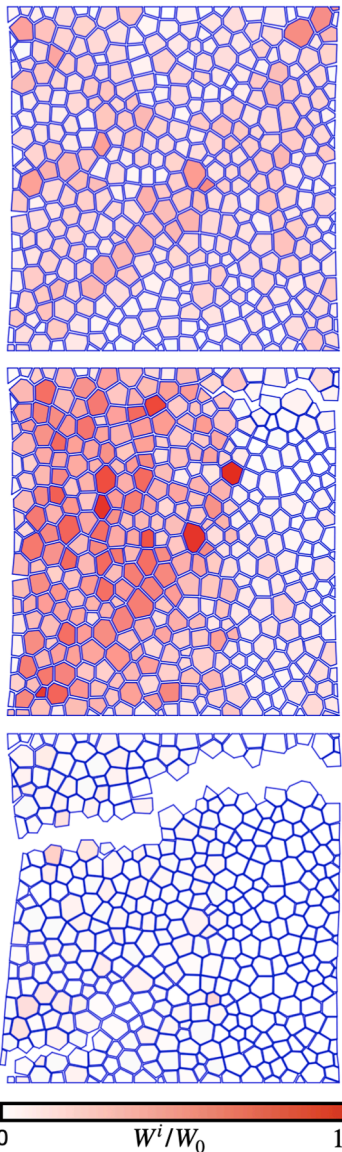


Fig. 33. Three snapshots of the tensile loading of a cellular tissue. The color levels are proportional to the elastic energies of the cells normalized by the fracture energy W_0 of a single normal cohesive link.

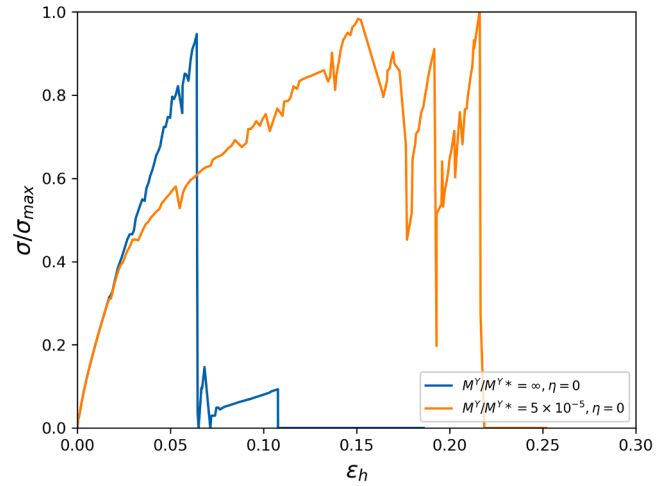


Fig. 34. Vertical stress normalized by the peak stress σ_{\max} versus vertical strain ϵ_h for an elastic ring (large value M^Y/M^* and $\eta = 0$) and a plastic ring (small value of M^Y/M^* and $\eta = 0$).

fill space, similar to observations in MPM simulations of solid disks [22,37]. This polygonal structure arises from the ability of elastic rings with isotropic core stiffness to create large surface areas. For plastic particles (Fig. 30(c)), many particles maintain an elliptical shape, while others are strongly distorted due to their plasticity, which allows them to better conform to their local environment. The efficient filling of pore space in Fig. 30(b) and (c), with void ratios $e \approx 0.04$ and $e \approx 0.06$, respectively, results from two distinct mechanisms: the creation of flat interfaces in Fig. 30(b) and the adaptation of particle shapes to the pore space in Fig. 30(c). Notably, the void ratio is also higher in regions with elliptical particles as compared with the initial configuration of circular particles since even slight deviations from circular or spherical shape can significantly increase the void ratio [47,48].

7. Fracture of cellular tissues

To further demonstrate the applicability of soft particle dynamics, we consider the simulation of fracture in cellular tissues subjected to simple tension. Fig. 31 shows an example of a cellular tissue fixed at the bottom and subjected to vertical extension by moving the top wall. The cellular configuration is created using a Laguerre-Voronoi tessellation of a granular packing with small size polydispersity. The cells are then transformed into sphero-polygons with a small Minkowski radius r . The tissue's mechanical integrity is maintained by normal and tangential cohesive forces between the vertices of adjacent cells. For two neighboring vertices at the ends of the interface between adjacent cells, the initial distance is set to r . From this reference state, we define the normal displacement u_n and tangential displacement u_t , corresponding to normal and tangential forces f_n and f_t , respectively. The normal displacement u_n is perpendicular to the common interface, while the tangential displacement u_t is parallel to it.

We assume linear force-displacement relationships for both normal and tangential forces, such that $f_n = k_n u_n$ and $f_t = k_t u_t$, where k_n and k_t represent the normal and tangential stiffness coefficients of the interface, respectively. The sign convention used defines compressive forces and inward displacements as positive.

We define a fracture criterion based on a local yield function defined as:

$$\zeta = \frac{f_n}{f_n^0} + \left| \frac{f_t}{f_t^0} \right|^\alpha - 1, \tag{41}$$

where α is a model parameter, $f_n^0 < 0$ is the tensile normal force threshold in the absence of shear, and $f_t^0 > 0$ is the tangential force threshold

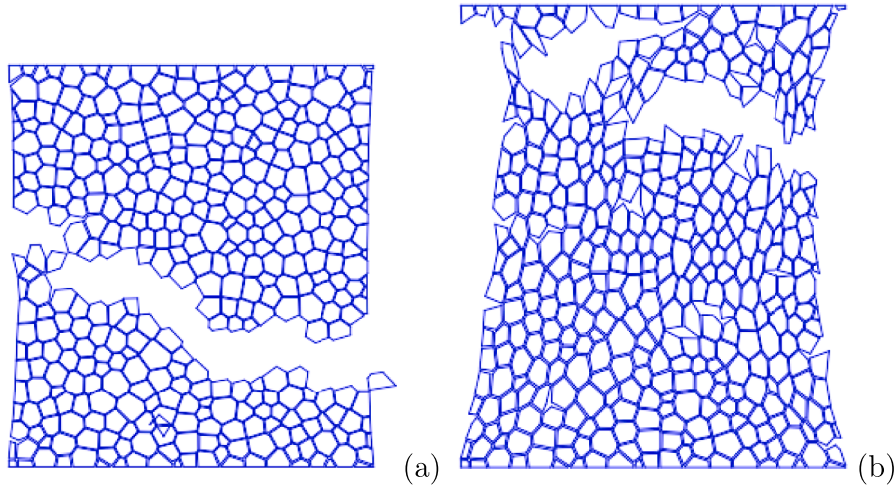


Fig. 35. Snapshots of the elastic (a) and plastic (b) cellular tissues fractured under tensile loading.

at zero normal force. This criterion is illustrated in Fig. 32 for $\alpha = 2$. Inside the yield surface ($\zeta < 0$), displacements follow elastic force laws. A link between two vertices breaks when $\zeta = 0$ is reached, signifying the onset of fracture. According to this equation, mode I fracture (normal displacement) occurs only under tension while in compression ($f_n > 0$), a link can break only due to shear.

For our simulations, we set $\alpha = 2$, as used in previous studies [49]. When links between cells break, the cohesive connection is lost irreversibly, and the interaction changes to a frictional contact with a coefficient of friction $\mu = 0.3$. We also set $k_t = 0.1k_n$. Fig. 33 shows three snapshots of a tissue undergoing tensile loading, along with the elastic energy distributions of the cells. The energy values are normalized by the fracture energy $W_0 = (f_n^0)^2 / 2k_n$ of a single normal cohesive bond. The first cracks typically appear near the boundaries, but only one crack propagates across the tissue, following a rough intercellular path.

In Fig. 34, we observe the vertical stress as a function of vertical strain for both elastic and plastic particles for $\eta = 0$. The elastic case exhibits brittle behavior: the stress increases with strain until reaching a peak, followed by a sharp drop. Cracking events manifest as fluctuations in the stress before fracture. In contrast, the plastic case shows initial elastic deformation followed by a prolonged plastic phase, characterized by stress drops of increasing magnitude. Snapshots of the fracture path (Fig. 35) reveal elongated cells and an irregular fracture path in the plastic case at failure.

8. Conclusion

In this paper, we introduced a Soft Particle Dynamics (SPD) model for simulating the dynamics of collections of soft core-shell particles such as granular materials composed of deformable particles and biological tissues. To accommodate large particle deformations, the particle surface is represented by a shell of mass points interacting through linear and angular stiffness, as well as a core stiffness. The model incorporates also frictional contact interactions between particles, shape plasticity, cohesive links, and fracture mechanics. Unlike continuum approaches, our SPD approach extends the Discrete Element Method (DEM) to include shape degrees of freedom.

We showed that the model parameters can be mapped to material properties such as the elastic and plastic moduli of a beam or a circular particle. For verification and validation, we compared the elastic deformation of beams under point loads and the compression of particles between two walls with theoretical or semi-theoretical predictions. These behaviors were analyzed using dimensionless variables to understand the influence of parameters such as core stiffness and shell plastic threshold on the particle deformation.

When applied to the uniaxial compaction of a collection of deformable circular particles, our numerical method effectively captures different mechanisms underlying the compaction process based on the values of model parameters. The particles adapt their shapes to fill pore spaces through elongation and flat edge-to-edge contacts, or by conforming to the shape of the pore space. The compaction process was observed to follow a logarithmic consolidation law, similar to that seen in clays. We also applied the model to cellular tissues by simulating tensile fracture in cellular tissues modeled as bonded polygonal cells.

Although the two-dimensional SPD, as formulated in this paper, does not precisely replicate the mechanical behavior of solid cylindrical particles – such as the force-surface area relationship in diametral compression – due to the degrees of freedom being limited to the particle periphery, it closely approximates the behavior of solid particles when high core stiffness is present. This leads to minimal volume change and the development of large contact areas with walls. The use of an isotropic pressure or stiffness is obviously a simplification and is only convenient for core-shell particles with a liquid core of weak viscosity as in living cells. However, the model can easily be extended to include a viscous term (e.g., $\Delta p = K_\Omega \Delta \varepsilon_v + \eta_\Omega \Delta \dot{\varepsilon}_v$), or incorporate a perfect gas law ($p\Omega \propto T$), or even account for shear resistance within the cell, effectively treating the core as a solid phase material rather than a fluid or gas. Such extensions would allow for a more nuanced representation of the interactions between core and the shell structure, particularly in systems where viscous dissipation or thermal effects play a significant role. The method is also particularly well-suited for simulating plant tissues and vesicles, with the control of core stiffness, internal pressure, or particle volume. Similar to the DEM, the computational cost of SPD simulations depends on the total number of particles, as well as the number of nodes per particle, which determines the accuracy of particle shape representation and its deformation.

Extending the SPD method to three dimensions is straightforward: mass points are distributed across each particle surface, with their interactions parameterized using linear elements connecting these vertices. As in 2D, the contact forces can be mapped to the neighboring mass points, mirroring conventional interpolation in finite element techniques. Contact detection between core-shells relies on the distances between vertices of a shell and the surface elements of another shell. This approach is, in fact, fully compatible with spheropolyhedra (so-called *R*-shapes), as demonstrated in several studies using the software Rockable [<https://github.com/richefeu/rockable>] [50,51]. The primary challenge in 3D lies in accurately modeling wall resistance to flexion, particularly when accounting for irreversible bending deformations.

The SPD model offers significant potential for efficient numerical simulations of deformable particle systems. It readily enables in-depth

studies of the mechanical behavior and rheology of complex granular assemblies composed of soft particles of arbitrary shape and size distributions without significant computational overhead. Indeed, particle shape is a key factor in real granular materials and its effect on the elasto-plastic behavior has been recently at focus of numerous studies [50–55]. Therefore, an interesting issue is how assemblies of soft particles of various shapes evolve during compaction and shear, on the one hand, and how their deformability affects the stress-strain behavior, on the other hand.

We are currently undertaking an extensive parametric study on the compaction of granular materials composed of core-shell particles, exploring a wide range of model parameters. The findings from this study will be detailed in an upcoming paper. While this paper primarily addressed examples of nearly homogeneous cellular structures, we have also conducted an in-depth investigation into the fracture behavior of disordered cellular tissues, with results to be presented in future work.

CRedit authorship contribution statement

Yohann Trivino: Writing – review & editing, Writing – original draft, Visualization, Software, Methodology, Investigation, Formal analysis, Conceptualization; **Vincent Richefeu:** Writing – review & editing, Writing – original draft, Software, Investigation, Formal analysis, Conceptualization; **Farhang Radjai:** Writing – review & editing, Writing – original draft, Supervision, Software, Investigation, Funding acquisition, Formal analysis, Conceptualization; **Komlanvi Lampoh:** Writing – review & editing, Writing – original draft, Supervision, Software, Methodology, Formal analysis, Conceptualization; **Jean-Yves Delenne:** Writing – review & editing, Writing – original draft, Supervision, Software, Methodology, Funding acquisition, Formal analysis, Conceptualization.

Data availability

Data will be made available on request.

Declaration of interests

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

Regarding the PhD Funding of Yohann Trivino - Yohann Trivino reports financial support was provided by National Research Institute for Agriculture Food and Environment TRANSFORM Department. Yohann Trivino reports financial support was provided by University of Montpellier. If there are other authors, they declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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