Jamming of Deformable Polygons

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There are two main classes of physics-based models for two-dimensional cellular materials: packings of repulsive disks and the vertex model. These models have several disadvantages. For example, disk interactions are typically a function of particle overlap, yet the model assumes that the disks remain circular during overlap. The shapes of the cells can vary in the vertex model, however, the packing fraction is fixed at $\phi = 1$. Here, we describe the deformable particle model (DPM), where each particle is a polygon composed of a large number of vertices. The total energy includes three terms: two quadratic terms to penalize deviations from the preferred particle area $a_0$ and perimeter $p_0$ and a repulsive interaction between DPM polygons that penalizes overlaps. We performed simulations to study the onset of jamming in packings of DPM polygons as a function of asphericity, $A = p^2/4\pi a_0$. We show that the packing fraction at jamming onset $\phi_A(A)$ grows with increasing $A$, reaching confluence at $A \approx 1.16$. $A^*$ corresponds to the value at which DPM polygons completely fill the cells obtained from a surface-Voronoi tessellation. Further, we show that DPM polygons develop invaginations for $A > A^*$ with excess perimeter that grows linearly with $A - A^*$. We confirm that packings of DPM polygons are solid-like over the full range of $A$ by showing that the shear modulus is nonzero.

There are many physical systems that can be modeled as packings of discrete, deformable particles, including cell monolayers, developing embryos, foams, and emulsions \textsuperscript{1-6}. A spectrum of models with varying degrees of complexity have been employed to study these systems. Perhaps the simplest model involves packings of disk-shaped particles that interact via purely repulsive forces \textsuperscript{7-10}. The power of this model is its simplicity and the ability to study a wide range of packing fractions from below jamming, where particles are not in contact, to jamming onset, where nearly all particles are at contact, to above jamming, where the particles are over-compressed. However, in this model, forces between particles are generated via particle overlaps, and the particles remain spherical during overlap, which is unphysical. In contrast, the vertex model \textsuperscript{11,12} in two spatial dimensions (2D) employs deformable polygons (with a relatively small number of vertices, but different polygonal shapes), with no particle overlaps, to study the structural and mechanical properties of cell monolayers. However, the vertex model only considers confluent systems with packing fraction $\phi = 1$, and thus it cannot describe inter-cellular space.

Disk-packing models allow us to study the onset of jamming of 2D cellular materials as a function of packing fraction, whereas, the vertex model allows us to study the onset of jamming as a function of the particle shape, e.g. the asphericity, $A = p^2/4\pi a$, where $p$ and $a$ are the perimeter and area of the particles \textsuperscript{13,14}. In this letter, we introduce the deformable particle model (DPM), which enables us to vary both the packing fraction of the system and particle shape. In 2D, the DPM is a polygon with a large number of vertices, which enables the modeling of particle deformation. The total energy of a collection of DPM polygons includes three terms. Two quadratic terms for each polygon to penalize deviations from the preferred area and perimeter and a purely repulsive contact interaction between pairs of deformable polygons to penalize particle overlaps.

We performed numerical simulations to study the onset of jamming in packings of deformable polygons and found several key results. First, we show that the packing fraction at jamming onset $\phi_I(A)$ increases with $A$, starting at $\phi_I \approx 0.81$ or $\approx 0.88$ for rigid, monodisperse disks ($A = 1$), depending on the roughness of the particles, and reaching $\phi_I = 1$ for $A \geq A^*$, where $A^* \approx 1.16$. We find similar results for $\phi_I(A)$ in jammed packings of bidisperse deformable polygons, except $\phi_I(A = 1)$ is different. We show that $A^*$ corresponds to the value at which the DPM polygons completely fill the cells ob-
tained from Voronoi tessellation. Further, for \( A > A^* \), the deformable polygons develop invaginations, which grow with \( A - A^* \). We show that the distributions of Voronoi polygon areas for jammed DPM packings follow \( k \)-gamma distributions for all \( A \), which is a hallmark of jamming in systems composed of rigid particles. By calculating the static shear modulus \( \mathcal{G} \), we confirm that packings of deformable polygons are jammed for all \( A \). The DPM in 2D can be used to study the growth and evolution of cell monolayers and can be extended to three spatial dimensions to study collective cell motion and packing in tissues and tumors.

For the DPM, each "particle" is a collection of \( N_v \) vertices that form an \( N_v \)-sided deformable polygon. (See Fig. 1.) Each polygon has \( N_v \) edges that are indexed by \( i = 1, \ldots, N_v \). To ensure that each particle remains a polygon, adjacent vertices are connected via linear springs, each with spring constant \( k_l \) and equilibrium length \( l_0 = p_0/N_v \), where \( p_0 \) is the preferred perimeter of the polygon. For reference, the asphericity for a rigid (regular) polygon with \( N_v \) vertices is \( \mathcal{A}_v = N_v \tan(\pi/N_v)/\pi \), which reduces to \( \mathcal{A}_v = 1 \) in the \( N_v \to \infty \) limit.

The total energy, \( U \), for the DPM also includes a quadratic term that penalizes deviations of the polygon area \( a \) from the reference value \( a_0 \), which models particle elasticity. In addition, we include a pairwise, purely repulsive interaction energy, \( U_{\text{int}} \), to prevent overlaps between polygons. The total energy for \( N \) deformable polygons is therefore

\[
U = \sum_{m=1}^{N} \sum_{i=1}^{N_v} \frac{k_l}{2} (l_{mi} - l_0)^2 + \sum_{m=1}^{N} \frac{k_a}{2} (a_m - a_0)^2 \quad (1)
\]

\[+ U_{\text{int}},\]

where \( l_{mi} \) is the length of the \( i \)th edge of polygon \( m \) and \( k_a \) is the spring constant for the quadratic term in area, which is proportional to the polygon’s compressibility.

We implement two methods for calculating the repulsive interactions between deformable polygons. For the rough surface method, we fix disks with diameter \( \delta = l_0 = 1 \) at each polygon vertex (Fig. 1 (a) and (b)). In this case, the repulsive interactions are obtained by summing up repulsive linear spring interactions between overlapping disks on contacting polygons:

\[
U_{\text{int}} = \sum_{m=1}^{N} \sum_{n>m}^{N} \sum_{j=1}^{N_v} \sum_{k=1}^{N_v} \frac{k_r}{2} (\delta - |\mathbf{v}_{mj} - \mathbf{v}_{nk}|)^2 \quad (2)
\]

\[\times \Theta(\delta - |\mathbf{v}_{mj} - \mathbf{v}_{nk}|),\]

where \( k_r \) gives the strength of the repulsive interactions, \( \mathbf{v}_{mj} \) is the position of the \( j \)th vertex in polygon \( m \) and \( \Theta(\cdot) \) is the Heaviside step function. We also implemented a smooth surface method by modeling the polygon edges as circulo-lines (i.e. the collection of points that are a fixed distance from a line) with width \( \delta \) [10]. (See Fig. 1 (c) and (d).) In this method, we again use Eq. 2 for the repulsive interactions between polygons, except the overlap \( \delta - |\mathbf{v}_{mj} - \mathbf{v}_{nk}| \) is replaced by \( \delta - d_{\text{min}} \), where \( d_{\text{min}} \) is minimum distance between the line segments \( l_{mj} \) and \( l_{nk} \) on contacting polygons \( m \) and \( n \). We set the ratio \( k_l k_0/k_a = 10 \) and \( k_l/k_a = 1 \); other values of these parameters yield similar results near jamming onset. Energies will be measured in units of \( k_b l_0^3 \).

We study systems containing from \( N = 64 \) to 1000 deformable polygons. To generate static packings, we place the polygons with random locations and orientations in a square box with periodic boundary conditions and \( \phi = 0.2 \). We successively compress the system isotropically using small packing fraction increments \( d\phi < 10^{-4} \) and minimizing the total potential energy after each compression step using over-damped molecular dynamics simulations until the kinetic energy per particle \( K/N < 10^{-20} \). We use bisection with compression and decompression to identify jamming onset, where the total energy per particle satisfies \( 0 < U/N < 10^{-16} \).

![Fig. 1: Schematic of deformable polygons with \( N_v = 34 \) vertices (with the position of the \( j \)th vertex in the \( m \)th polygon given by \( \mathbf{v}_{mj} \)), area \( a \), and perimeter \( p \). \( l_{mj} = p/N_v \) is the line segment between vertices \( j \) and \( j+1 \) in polygon \( m \). We implemented two methods for modeling edges of deformable polygons. In (a) and (b), we show the rough surface method, where we fix the centers of disks with diameter \( \delta \) at polygon vertices. In (c) and (d), we show the smooth surface method, where we model polygon edges as circulo-lines with width \( \delta \). \( d_{\text{min}} \) is minimum distance between line segments \( l_{mj} \) and \( l_{nk} \).](image)
the smooth surface method. The results obtained near $A = 1$ are similar to previous results for jammed packings of monodisperse, frictionless ($\phi_J \approx 0.88-0.89$ [17]) and frictional disks ($\phi_J \approx 0.8$ [18]). For $A/A_v > 1.02$, $\phi_J/\phi_{\text{max}}$ possess similar dependence on $A$ for the two surface roughness methods. We also find similar results for jammed packings of bidisperse polygons (half large with $N_v = 17$ and half small with $N_v = 12$ and perimeter ratio $r = 1.4$). As shown in Fig. 2 (b), the jammed packings become confluent with $\phi_J \approx 1$ for $A > A^* \approx 1.16$ in the large $N_v$ limit.

FIG. 2: (a) Packing fraction at jamming onset $\phi_J$ (normalized by the maximum packing fraction, $\phi_{\text{max}}$, for each surface roughness model), (b) the deviation of $\phi_J$ from the confluent value, $1 - \phi_J$, (c) coordination number $z$, and (d) average friction coefficient $\mu$ (for the rough surface model) for static packings of $N = 64$ deformable polygons as a function of asphericity $A$. In (a) and (c), $A$ is normalized by the area $A_v$ of a regular polygon with $N_v$ vertices. For monodisperse systems with the smooth surface model, $N_v = 12$ (squares), while $N_v = 12$ (circles), 24 (triangles), and 34 (stars) for monodisperse systems with the rough surface model. Bidisperse systems (exes) have $N_v = 17$ (12) for the large (small) polygons, using the rough surface model. The vertical dashed lines in (a) and (b) indicate $A = A^* \approx 1.16$ at which jammed packings become confluent in the large $N_v$ limit. In (a), we also show $\phi_J/\phi_{\text{max}} \approx 0.81$ (with $\phi_{\text{max}} = 1$) for $N = 64$ monodisperse, frictional discs using the Cundall-Strack friction model with $\mu = 0.65$ (filled diamond). In (c), the dashed line indicates $z(A/A_v) = z(1) + z_0(A/A_v - 1)^\beta$, where $z(1) \approx 3.3$ was obtained from the Cundall-Strack model with $\mu = 0.65$, $z_0 \approx 3.9$, and $\beta \approx 0.25$.

In Fig. 2 (c), we show the interparticle coordination number $z$ versus $A/A_v$ for $N = 64$ deformable polygons for both surface roughness models. Near $A/A_v = 1$, the smooth roughness model yields packings with $z \approx 4$ (where rattler polygons with fewer than 2 interparticle contacts are not included). This result is consistent with isostatic packings [19] of frictionless, monodisperse and bidisperse disks. In contrast, $z < 4$ near $A/A_v = 1$ using the rough surface model, which is consistent with studies of packings of frictional disks [20][21]. For both surface roughness models, $z(A/A_v) - z(1)$ increases as a power-law in $A/A_v - 1$. We find that $z = 5.8 \pm 0.1$ at confluence when $A = A^*$. In contrast, prior work has suggested that $z = 5$ is the isostatic contact number for the vertex model [13].

We also measured the effective friction coefficient $\mu_c = |F_{mn}^t|/|F_{mn}^r|$ at each contact $c$ between polygons $m$ and $n$ in static packings of deformable polygons using the rough surface model. $|F_{mn}^t|$ is the normal component (in the center-to-center direction) and $|F_{mn}^r|$ is the tangential component of the repulsive contact force. For each static packing, we find the maximum $\mu_c$ over all contacts and average it over at least 500 packings. The average maximum friction coefficient $\mu$ depends on the parameters $N_v$ and $l_0$ in the rigid polygon limit ($A = A_v$). For $N_v = 12$ and $l_0 = 1$, $\mu \approx 0.7$ for $A_{12} \approx 1.02$ and decreases as $N_v$ increases (and $A_v \rightarrow 1$). In Fig. 2 (d), we show that $\mu$ increases by an order of magnitude as $A$ increases from 1 to 1.25. We find similar increases for $\mu(A)$ when using different values of $N_v$, which change $\mu(A = 1)$. Despite the fact that the friction coefficient increases strongly with $A$ when using the rough surface model, both the smooth and rough surface models yield similar results for $\phi_J(A)$ and $z(A)$ at jamming onset and away from the rigid-disk limit. Thus, particle deformation weakens the influence of static friction on the structural properties of jammed packings of deformable particles.

To understand the value $A^* \approx 1.16$ above which static packings of deformable polygons are confluent, we calculate the free area as a function of $A$ using surface-Voronoi tessellation [22]. In Fig. 3 we show example jammed packings at three values of $A$ approaching $A^*$. At $A = 1.03$, well-below $A^*$, the deformable polygons are quasi-circular and there is a relatively large amount of free area. As $A$ increases, the “effective” sides of the deformable polygons straighten and fill the surface-Voronoi cells. When $A \sim A^*$, it is difficult to differentiate the DPM polygons from the surface-Voronoi cells. We find that the average number of effective sides for jammed DPM polygons is $N_v = 5.8 \pm 0.1$ at confluence.

Prior studies have shown that the areas of the Voronoi polygons for hard-disk configurations follow $k$-gamma distributions [15][23], which can be written as

$$P(x) = \frac{k^k}{(k-1)!}x^{k-1}\exp(-kx),$$

where $x = (a_t - a_{\text{min}})/(\langle a_t \rangle - a_{\text{min}})$, $a_t$ is the area of each Voronoi polygon, $a_{\text{min}}$ is the area of the smallest Voronoi polygon, $\langle a_t \rangle$ is an average over Voronoi polygons in a given system, and the parameter $k = (\langle a_t \rangle - a_{\text{min}})^2/\sigma_a^2$, where $\sigma_a^2$ is the variance of the distribution.
FIG. 3: Jammed packings of deformable polygons for the rough surface model with $N_v = 34$ and (a) $A = 1.03$, (b) 1.08, and (c) 1.16, near $A^*$. The polygonal cells (solid lines) surrounding each DPM are obtained from surface-Voronoi tessellations.

with $\sigma_a^2 = \langle (a_t - a_{\text{min}})^2 \rangle$, controls the width of the distribution. In Fig. 4 (a), we show that the distribution $P(x)$ for packings of deformable polygons resembles a $k$-gamma distribution with a $k$-value that depends on $A$. The inset shows that $k$ increases from 2 to $\approx 5$ as $A$ varies from 1 to 1.25. Prior studies have shown similar values for $k$ for Voronoi-tessellated hard-disk systems [23] ($k = 3.6$) and jammed bidisperse foams [4] ($k \approx 6$). We also note that recent studies of cell monolayers have shown that the cell shape anisotropies (ratio of the long and short axes) follow $k$-gamma distributions with $k \approx 2.5$ [24].

In Fig. 4 (b) and (c), we show calculations of the bulk and shear moduli for packings of deformable polygons (rough surface model with $N_v = 12$) as a function of $A$ for several system sizes. The bulk modulus $B$ is roughly independent of system size and grows strongly with $A$ (changing by more than two orders of magnitude) as the packings gain more neighbors. In contrast, at each $N$, the shear modulus $G$ increases only by a factor of 3 as $A$ increases from 1 to 1.25. As a result, the ratio $B/G$ varies from $10^4$ to $10^5$, indicating that the system is in the isotropic elastic limit, over this range of $A$ [25]. In the inset of Fig. 4(c), we show that even though packings of deformable polygons at jamming onset are solid-like with non-zero shear moduli $G > 0$ for any finite $N$, $G$ at jamming onset scales as $N^{-1}$ with increasing system size. Similar system-size scaling was found for the shear modulus of bidisperse disk packings at jamming onset [26]. Disks packings, as well as packings of deformable polygons, can be mechanically stable in the large system limit by adding a nonzero pressure.

FIG. 4: (a) Distribution of areas $a_t$ of the surface-Voronoi tessellated polygons for 14 values of the asphericity from $A = 1.02$ (squares) to 1.25 (exes) for $N = 64$ monodisperse DPM polygons with $N_v = 12$ and the rough surface model. The distributions $P(x)$ are plotted against the rescaled variable $x = (a_t - a_{\text{min}})/(\langle a_t \rangle - a_{\text{min}})$, where $a_{\text{min}}$ is the minimum tessellated area for each packing. (inset) $P(x)$ resemble $k$-gamma distributions with $k$-values that depend on $A$. (b) Bulk $B$ and (c) shear $G$ moduli for jammed packings using the model in (a) versus $A$ for system sizes $N = 32$ (triangles), 64 (circles), 200 (squares), and 512 (stars). The inset to (c) shows the system-size scaling of $G$. The dashed lines have slope $-1$. 
FIG. 5: (a) Excess perimeter $\xi = p - p_{\text{conv}}$, where $p$ is the perimeter of the DPM and $p_{\text{conv}}$ is the perimeter of the convex hull of the DPM for packings of deformable polygons (rough surface model with $N_v = 34$) plotted versus the asphericity $A$. The vertical dashed line indicates $A^* \approx 1.16$ and the blue and green arrows indicate the values of $A$ for the packings in (b) and (c), respectively. The red and yellow solid lines represent the perimeters of the DPM and convex hull, respectively. The insets in (b) and (c) are close-ups of the regions of the packings indicated by the blue dashed boxes.

The coordination number and bulk and shear moduli vary continuously as $A$ increases above $A^*$. Other than being confluent for $A > A^*$, what is different about jammed packings of deformable polygons for $A$ above versus below $A^*$? In Fig. 5(a), we show the excess perimeter $\xi = p - p_{\text{conv}}$ for packings of deformable polygons, where $p_{\text{conv}}$ is the perimeter of the convex hull of each $N_v$-sided polygon. $p \approx p_{\text{conv}}$ (with $\xi = 0$) for $A < A^*$ as shown in Fig. 5(b). The excess perimeter becomes nonzero for $A > A^*$ when the deformable polygons buckle and develop invaginations [Fig. 5(c)]. Thus, jammed packings of deformable polygons at confluence are under tension for $A < A^*$ and are under compression for $A > A^*$.

In conclusion, we developed the DPM model, which can be used to study 2D cellular materials composed of deformable particles, including foams, emulsions, and cell monolayers, over a wide range of packing fraction, particle shape and deformability. By studying DPM packings, we showed that the packing fraction at jamming onset $\phi_J$ grows with particle asphericity $A$, reaching confluence at $A^* \approx 1.16$. $A^*$ coincides with the value of the asphericity at which the DPM polygons completely fill the cells from the surface-Voronoi tessellation of the DPM packings. We also calculated the bulk $B$ and shear $G$ moduli of the packings and show that they are solid-like above and below $A^*$. The ratio $B/G$ for the DPM packings is in the isotropic elastic limit. For $A > A^*$, we showed that DPM polygons possess invaginations that grow with $A - A^*$. Thus, at confluence, DPM packings are under compression for $A > A^*$ and under tension for $A < A^*$. In future studies, we will extend the DPM to three dimensions to investigate the structural and mechanical properties of tissues. Based on Voronoi tessellations of monodisperse sphere packings, we predict that jammed DPM packings in 3D will be confluent for $A_{3D} > A_{3D}^* \approx 1.18$, where $A_{3D} = s^{3/2}/6\sqrt{\pi}v$, and $s$ and $v$ are the surface area and volume of the 3D DPM particles, respectively.

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