Deposition of general ellipsoidal particles

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We present a systematic overview of granular deposits composed of ellipsoidal particles with different particle shapes and size polydispersities. We study the density and anisotropy of such deposits as functions of small to moderate size polydispersity and two shape parameters that fully describe the shape of a general ellipsoid. Our results show that, while shape influences significantly the macroscopic properties of the deposits, polydispersity in the studied range plays apparently a secondary role. The density attains a maximum for a particular family of nonsymmetrical ellipsoids, larger than the density observed for prolate or oblate ellipsoids. As for anisotropy measures, the contact forces are increasingly preferred along the vertical direction as the shape of the particles deviates from a sphere. The deposits are constructed by means of a molecular dynamics method, where the contact forces are efficiently and accurately computed. The main results are discussed in the light of applications for porous media models and sedimentation processes.

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I. INTRODUCTION

The granular character of many processes in nature has motivated the study of granular packings since Kepler’s time [1]. One such process is the deposition of particles subject to gravity [2], which underlies the formation of sandstones and ceramics, and, in general, the emergence of porous materials. Modeling porous media [4,5] in a realistic way is important, for instance, to understand permeability of soils for petroleum engineering or in material sciences.

However, a model for grain deposition should incorporate two ingredients not always easy to combine. First, empirical studies [6] show that the shape of grains significantly deviates from the sphere with a small to moderate polydispersity in their sizes. Until recently most computational studies dealt with round particles for simplicity, in solving specific problems such as obtaining the optimal packing [7,8], constructing space-filling configurations [9–11], or studying elongated shapes [3]. Some progress was recently made in addressing the influence of particle shape on the macroscopic observables of the agglomerate, focusing on ellipsoidal particles [12,13] and even in more general shapes [14,15], without accounting for the size polydispersity.

Second, deposition processes are fundamentally sequential and therefore should be modeled through sequential procedures. The procedure introduced by Donev et al. [12,13] for jammed configurations captures some of the general features observed in granular deposits, such as their density and average coordination number, although it is based on a nonsequential procedure. However, deposition under gravity does not generally lead to a jammed state. Recently, some sequential procedures have been carried out in two-dimensional deposits of monodisperse elongated particles [2,3].

In this paper we focus on three-dimensional polydisperse deposits of general ellipsoids and study how macroscopic properties of such deposits depend on the shape and size polydispersity of particles. We show that the density and coordination number of deposits behave similarly to what is observed in jammed systems. However, in contrast with randomly constructed jammed systems, the deposits become strongly anisotropic when the shape of the particles deviates from the sphere. Furthermore, we find that introducing small to moderate polydispersities has minor effects.

To this end, we develop an efficient algorithm for the calculation of the interaction forces at all contact points within a three-dimensional deposits of polydisperse ellipsoids and use it in a molecular dynamics [16,17] method to perform our simulations. Further, we introduce two shape parameters which describe any ellipsoid, enabling a systematic study of the role of particle shape in granular deposits.

The outline of the paper is as follows. In Sec. II we describe the algorithm for calculating the contact forces between colliding ellipsoids with arbitrary size and shape, as well as the simulation setup. In Sec. III the control parameters describing the polydispersity in the size and the shape of a general ellipsoid are introduced. In Sec. IV the variations of macroscopic observables taken from the entire deposit are studied as functions of the control parameters. We focus on the density, coordination number, and anisotropy of the deposits. A discussion and conclusions are given in Sec. V.

II. MODELING THE CONTACT FORCES BETWEEN ELLIPSOIDAL PARTICLES

When dealing with large systems, calculating the interparticle forces is by far the most time-consuming part of the computations. This is due to the fact that, in general, every particle can interact with every other one. In granular materials, however, the interparticle forces are short ranged, making techniques such as the Verlet-list and linked-cell algorithms indispensable in reducing the computation time. These techniques are employed to eliminate the redundant calculations for pairs which are too far apart to have any interaction [16].
In time-driven molecular dynamics (MD) methods for granular materials the system is evolved for one time step, allowing the particles to overlap. Then normal repulsion forces on the particles are calculated as a function of the amount of overlapping, which is defined usually by a line segment. Here we refer to this line segment as the contact vector (see Fig. 1).

The contact vector between two ellipsoids can be defined in more than one way. The common method, introduced by Perram and Wertheim [18] and developed by others [13,19,20], is based on finding two points, one on the surface of each ellipsoid, by minimizing a potential through a variational problem with one geometric constraint. The two points obtained can be used to define the contact vector. However, the contact vector defined in this way is not necessarily normal to the surface of the particles, particularly when the particles are strongly asymmetrical, leading to nonphysical motions of the particles. Furthermore, the Herzian contact law is based on the assumption that the overlapping vector is normal to the particles.

An alternative method consists in finding two points on the surfaces of the ellipsoids at which the corresponding surface normals point exactly in opposite directions. Consequently, the vector connecting these two points is normal to the surfaces of the ellipsoids at the contact point. These new points are used to define a new contact vector. Although it is not generally possible to define a contact force is exerted on a vector which is along the gradients of both ellipsoids at the contact point. These new points are used to define a new contact vector (see Fig. 1), a new direction is calculated by averaging the gradients of both ellipsoids at the contact point. These new points are used to define a new contact vector (see Fig. 1).

To retain computational efficiency, we use the former method and introduce an additional step for correcting the direction of the contact vector.

The geometric potential of the ellipsoid $A$ is defined as

$$f_A(X) = (X - X_A)^T A (X - X_A),$$

where $A$ is a $3 \times 3$ matrix encoding the shape and orientation of the ellipsoid, and $X$ and $X_A$ are the Cartesian coordinates of a point on the surface and the centroid of the ellipsoid, respectively. The equation $f_A(X) = 1$ describes the surface of ellipsoid $A$. Considering a pair of ellipsoids $A$ and $B$, we find two minimum points $X_m^{(A)}$ and $X_m^{(B)}$ on the surfaces of $A$ and $B$ by minimizing $f_B$ and $f_A$, respectively. These points are shown schematically in Fig. 1. To obtain the minima of $f_A(X)$ subject to the constraint of being on the surface of ellipsoid $B$ we minimize the following auxiliary potential:

$$f(X) = (X - X_A)^T A (X - X_A)$$

$$\times \lambda [(X - X_B)^T B (X - X_B) - 1],$$

where $\lambda$ is the Lagrange multiplier associated with the constraint. Setting to zero the gradient of this function with respect to $X$,

$$\nabla f(X) = A (X_m - X_A) + \lambda B (X_m - X_B) = 0,$$

we obtain an equation for optimum points $X_m$ for $A$:

$$X_m = (A + \lambda B)^{-1} (A X_A + \lambda B X_B).$$

To derive an equation for $\lambda$ we left-multiply Eq. (3) by $(X_m - X_B)^T$ and use the fact that $X_m$ lies on $B$ and that the gradients of the potential functions of the ellipsoids at minimum points are in opposite directions:

$$\lambda = |(X_m - X_B)^T A (X_m - X_A)|.$$

Equations (4) and (5) can be solved iteratively to find $X_m^{(A)}$ and $X_m^{(B)}$ up to the desired precision. The second point $X_m^{(B)}$ can be found similarly.

The contact point $X_c$ where a contact force is exerted on both ellipsoids is defined as the midpoint between $X_m^{(A)}$ and $X_m^{(B)}$. The contact vector for ellipsoid $A$ is defined as $\xi_A = X_m^{(A)} - X_m^{(B)}$ and for ellipsoid $B$ as $\xi_B = X_m^{(A)} - X_m^{(B)}$ (see Fig. 1). Although Eq. (4) involves inversion of a $3 \times 3$ matrix, finding the minima can be very efficient if the initial points are chosen properly. Good approximations for the minima are the minima from the last time step or, if the ellipsoids were disjoint in the last time step, the closest points on the surfaces of the ellipsoids which are known from the collision detection procedure described later in this section. These points are then used as initial points, reducing the number of iterations significantly.

The overlap vector calculated in this way, however, is not necessarily normal to the ellipsoids at the contact point. In fact, the normal directions to $A$ and $B$ at points $X_m^{(A)}$ and $X_m^{(B)}$ deviate significantly from each other when the particles are strongly aspherical. To overcome this problem we introduce an additional step for correcting the contact vector, as described next.

If the calculated contact vectors deviate more than a given amount from the gradients of the ellipsoids’ potential at the contact point $X_c$, a new direction is calculated by averaging the gradients at $X_c$. Then, two new points are calculated from the intersection of the line along this direction passing through the contact point. These new points are used to define a new contact vector. Although it is not generally possible to define a vector which is along the gradients of both ellipsoids at the contact point, this approximation gives satisfactory results in terms of energy conservation.

Having described the procedure for calculating the contact of two colliding ellipsoids, we next need an efficient way to determine when two previously disjoint ellipsoids collide. To this end, we use the technique proposed by Wang et al. [22] which is described briefly as follows.

FIG. 1. (Color online) Sketch of the contact vector $\xi$ used to define the normal repulsive force between two overlapping ellipsoids $A$ and $B$. The contact point is chosen to be $X_c$ after proper derivation of points $X_m^{(A)}$ and $X_m^{(B)}$ at the surfaces of the ellipsoids (see text). The full procedure is sketched in Fig. 2.
In homogeneous coordinates the equation for the surface of a general ellipsoid is given by

\[ A : X^T \tilde{A} X = 0, \]  

where \( X \) is any point on the surface of the ellipsoid and \( \tilde{A} \) is the \( 4 \times 4 \) matrix of the affine transformation which transforms the unit sphere centered at the origin into the ellipsoid.

Given two ellipsoids \( A : X^T \tilde{A} X = 0 \) and \( B : X^T \tilde{B} X = 0 \), their characteristic equation is defined as \( f(v) = \text{det}(v \tilde{A} + \tilde{B}) \), whose roots are the eigenvalues of the matrix \( -\tilde{A}^{-1} \tilde{B} \). Furthermore, it can be shown [22] that (i) \( f(v) = 0 \) has at least two negative roots, (ii) \( f(v) = 0 \) has two distinct positive roots if and only if the two ellipsoids are disjoint, and (iii) \( f(v) = 0 \) has a positive double root if and only if the two ellipsoids are externally touching. Therefore, by examining the eigenvalues of \( -\tilde{A}^{-1} \tilde{B} \) one can determine if two ellipsoids collide.

When the ellipsoids are disjoint, the corresponding eigenvectors give the coordinates of the four vertices \( V_i, i = 1, \ldots, 4 \), of a tetrahedron which is self-polar for both ellipsoids \( A \) and \( B \) [23], i.e., \( V_i^T \tilde{A} V_j = V_i^T \tilde{B} V_j = 0, \forall i \neq j \). Two of the vertices lie outside both ellipsoids (external vertices), while the other two are contained inside the ellipsoids, one in each (internal vertices). In this case, a set of separation planes can be defined using three points exterior to both ellipsoids, two of them being the external vertices and the other a point on the line segment connecting the internal vertices. We choose the third point as the midpoint between the surfaces of two ellipsoids on this line segment.

Having the separation plane between the two disjoint ellipsoids, in the subsequent time step we check if the ellipsoids intersect that plane. If not, the ellipsoids are still disjoint and the procedure stops. This helps to eliminate the need for checking for collision between the ellipsoids which is more computationally expensive. Only when any of the ellipsoids intersects the separation plane is it necessary to check again for collision between the ellipsoids. If the ellipsoids turn out to be still disjoint, their separation plane and closest points are updated to be used in the next time step. If the ellipsoids do collide the contact vector is calculated and saved to be used for the calculation of the contact force.

As described in Ref. [22], the efficiency gain through the employment of separation planes is highest for dilute systems where the rate of collisions between particles is low. This is the case for the early stages in our simulations. However, in later stages the particles are most of the time in contact and thus the overhead of calculating the separation planes becomes larger than the efficiency gain. Therefore, this procedure is turned off for late stages.

Figure 2 shows the flowchart of the complete procedure which is performed for all potentially overlapping pairs of ellipsoids. It is worth noting that, to further speed up the procedure, only the pairs whose spherical envelopes intersect are evaluated.

The contact force can be decomposed into normal and tangential forces. The tangential forces such as static and dynamical friction are generally derived from the normal force. For calculating the magnitude of the normal force we use the Hertzian model [16]:

\[ F_n \propto \xi^{3/2} + K \sqrt{\xi \frac{d\xi}{dt}}, \]  

with \( \xi = \|\vec{\xi}\| \) being the length of the contact vector between the particles and \( K \) being the dissipative constant depending on the material viscosity [24]. Since we are concerned only with the properties of the deposit at rest, we choose \( K \) sufficiently large for the deposit to relax rapidly. This relaxation is enhanced by including a tangential force \( \vec{F}_t = -\mu F_n \vec{v}_t/\|\vec{v}_t\| \), \( \mu \) being the dynamic friction coefficient and \( \vec{v}_t \) the relative tangent velocity of the particles.

Finally, the procedure described above is used in a MD simulation together with standard methods, namely, a prediction-correction integrator for solving the equations of motions, quaternions for describing the orientation of the particles, and a linked-cell algorithm to eliminate unnecessary collision detections. For details of the MD methods, see, e.g., Ref. [16] and references therein.

### III. Control Parameters for Size and Shape

The size and shape of the particles are the main parameters whose effects on the properties of the system are to be studied. In the following we explain how these are defined and chosen when preparing the samples. All samples considered here are cubic and the size of the sample is taken as the length unit (size \( L = 1 \)).
We define the size of an ellipsoidal particle as the radius of the sphere with the same volume, i.e., \( r = (abc)^{1/3} \) with \( a \), \( b \), and \( c \) being the three semi-axis radii of the ellipsoid. We refer to a sample as monodisperse in size when all its constituting particles have the same volume, i.e., the same size \( r \). To introduce size polydispersity we adopt the approach by Voivet et al. [25]: instead of directly choosing the size distribution \( n(r) \) of the particles, we consider the distribution of the total volume \( V(r) = \frac{2}{3} \pi n(r) r^3 \) of all particles with size \( r \).

We chose \( V(r) \) as

\[
V(r) = \begin{cases} 
     C \left( \frac{r-r_{\text{min}}}{r_{\text{max}}-r_{\text{min}}} \right)^{\alpha-1} & \text{if } r_{\text{min}} \leq r \leq r_{\text{max}}, \\
     0 & \text{otherwise},
\end{cases}
\]

where \( \alpha \) and \( \beta \) determine the shape of the distribution and \( C \) is the normalization factor. Figure 3 shows \( V(r) \) for different values of \( \alpha \) and \( \beta \) and the corresponding size distributions \( n(r) \) (inset). For \( \alpha = \beta = 3 \) this function takes a symmetric shape with a peak at \((r_{\text{min}} + r_{\text{max}})/2\). For the samples studied in this work we have chosen \( \alpha = \beta = 3 \), which corresponds to a distribution (solid line in Fig. 3) very close to a truncated Gaussian.

The width of the distribution is controlled by the polydispersity parameter \( \delta_r \), which is defined as [25]

\[
\delta_r = \frac{r_{\text{max}} - r_{\text{min}}}{r_{\text{max}} + r_{\text{min}}}.
\]

For \( \delta_r = 0 \) the particles are monodisperse while \( \delta_r = 1 \) corresponds to infinite polydispersity. Here, we consider small to moderate polydispersity, \( \delta_r \leq 0.6 \).

The shape of an ellipsoid is characterized by two parameters here defined as \( \eta = a/b \geq 1 \) and \( \zeta = b/c \geq 1 \), with \( a \geq b \geq c \). For prolate \((a > b = c)\) and oblate \((a = b > c)\) ellipsoids, the shape can be fully characterized by the aspect ratio \( a/c = \eta \zeta \). The particular case \( \eta = \zeta = 1 \) corresponds to the sphere. These shape parameters together with the size \( r \) fully specify any ellipsoid. Figure 4 shows examples of ellipsoids of equal size \( r \) for different values of \( \eta \) and \( \zeta \).

Similarly to the size polydispersity, two additional parameters \( \delta_\eta \) and \( \delta_\zeta \) can be defined for the polydispersities in the shape of the particles. In this study we consider systems of monodisperse particles, describing each deposit by \( \eta \), \( \zeta \), and the size polydispersity \( \delta_r \).

In this work, all the deposits are generated by releasing particles with randomly chosen positions and orientations and letting them fall into an open box, under gravity along the vertical direction. The box is limited from below by a rigid wall (ground) and is periodic in \( x \) and \( y \) directions. In order...
IV. MACROSCOPIC PROPERTIES OF THE DEPOSIT

The macroscopic properties considered in our study are the packing density, the average coordination number, and the anisotropy.

A. Packing density and coordination number

Figure 6 shows the packing density in deposits of $N \sim 3000$ monodisperse ellipsoids as a function of the shape. When the shape deviates from spherical, i.e., when $\eta > 1$ or $\zeta > 1$, the density first increases rapidly; then it attains a maximum, and finally decreases slowly. From Fig. 6(a) one sees that typically, along lines of constant $\eta$ (or constant $\zeta$), the maximum is observed around $\eta = \zeta$. Further, along $\eta = \zeta$, that is where $b^2 = ac$, a global maximum is attained at $\eta = \zeta \approx 1.4$, as can be observed from Fig. 6(b) (solid line).

The observation of the existence of a global maximum at the diagonal $\eta = \zeta$, shown in Fig. 6(a), provides further evidence that there is an optimal shape of ellipsoid in constructing random dense packings of monodisperse particles. Previously, other authors addressed this point for particular shapes, showing similar results, e.g., in Refs. [13,14]. In these works a higher density is observed along $\eta = \zeta$, due to the authors’ method for generating the packings: instead of being generated via deposition, their samples are prepared to be in the jammed state using a generalized form of the Lubachevsky-Stillinger algorithm [26,27]. This method is generally more efficient in attaining high densities than the method of deposition even without including static friction (as is the case for our samples).

Figure 6(b) shows the density along three lines in the space of the shape parameters, namely, $\eta = 1, \zeta = 1$, and $\eta = \zeta$. In the main plot we choose the horizontal axis as $(a - c)/a = (\eta \zeta - 1)/(\eta \zeta)$, that is where $a/c$. Although the curves seem similar, we have found no scaling which could collapse all the curves to a single curve (we discuss this more below).

Figure 7(a) shows the average coordination number $Z$ as a function of the shape of the particles. For spheroidal particles, $Z$ increases gradually with the aspect ratio toward a maximum. For a general ellipsoid the coordination number attains a maximum higher than the maximum observed for spheroids ($\eta = 1$ or $\zeta = 1$), but decreases to values comparable to those of spheroids for larger $\eta$ and $\zeta$. This can be understood by considering the fact that for $\eta = \zeta \gg 1$, one of the semiaxis radii is significantly larger than the other two and therefore the particle can be regarded as a prolate ellipsoid. The effect of polydispersity is examined by comparing the result for three different values of $\delta_0$, as shown in the inset of Fig. 7(a). The results indicate that the coordination number seems to be insensitive to low to moderate size polydispersities. The same is observed for the density (not shown).

Figure 7(b) shows the average coordination per unit area, $\bar{Z}$. In order to make $\bar{Z}$ independent of the system size, it is multiplied by the surface area of a sphere of the same volume, $4\pi (abc)^{2/3}$. In this representation, one can see that there exists a globally optimum shape for $\eta = \zeta \sim 1.4$. This corresponds to the same shape for which the packing has the highest density. A simple intuitive interpretation is that higher densities result in more contacts per particle. However, a closer inspection reveals no one-to-one relation between $\bar{Z}$ and $\rho$, nor a monotonic one (not shown here). This relation is nontrivial and depends on the shape of the constituting particles.

Figures 6 and 7 show that there is no simple parameter such as $\eta \zeta = a/c$ controlling the behavior of the density $\rho$ and the average coordination number $Z$. As can be seen from the contour lines, such a parameter would have a complex form with a nontrivial dependence on $b$. In fact, for a given aspect ratio $a/c$ the maximum values for $\rho$ and $Z$ are obtained when $b$ takes a value equal to the geometric mean of $a$ and $c$, i.e.,
with the positive vertical direction. Therefore, we will consider only the angle 

\[ \delta r \]

coordination number is plotted as a function of the shape parameters \( \eta \) and \( \zeta \), for different polydispersities \( \delta r \) [see Eq. (9)]. (b) The average coordination number \( Z \) of particles per unit area, \( \bar{\delta} \). In order to make \( \bar{\delta} \) independent of the system size, it is multiplied by the surface area of a sphere of the same volume, \( 4\pi(abc)^{3/2} \).

\[ b = \sqrt{ac}. \]

Again, these maxima are much higher than for the limiting cases when \( b = a \) or \( b = c \), indicating that the middle semiaxis \( b \) plays an important role.

**B. Anisotropy**

To study the anisotropy of the deposits we investigate the orientational order of the contact vectors and the principal directions of the ellipsoids by calculating their angular distributions. In general two angles are needed to specify the orientation of a vector in three-dimensional space, namely, one azimuthal angle and another angle with the vertical direction. Since the samples are periodic in the \( x \) and \( y \) directions, they are by construction homogeneous and isotropic in the \( x-y \) plane. This is also observed in our results (not shown here for the sake of brevity). Therefore, we will consider only the angle with the positive vertical direction.

Figure 8(a) shows the distribution of the contact normal angles \( \theta c \) for different values of the shape parameters \( \eta = \zeta \) with \( \delta r = 0 \). The vertical axis \( P(\Omega(\theta c)) \) represents the probability density of contact normal vectors within the solid angle \( \Omega(\theta c) \) at an angle \( \theta c \) with the \( z \) axis. We note that \( P(\Omega(\theta c)) \) is, by construction, symmetric with respect to \( \theta c \rightarrow \theta c + \pi/2 \), since for each contact normal of a particle there is a contact normal with opposite direction from the other particle with which it is in contact.

The results show that for deposits of spheres \( P(\Omega(\theta c)) \) is independent of \( \theta c \), and consequently the configuration of the contacts is isotropic and has no preferred direction. However, as the shape of the particles deviates from a sphere the number of side contacts between particles, i.e., the number of contacts on the horizontal plane, decreases and the contact normals line up along the vertical direction. This is seen in Fig. 8(a) and (its polar representation) Fig. 8(b), which show that for every shape (except the sphere) there is a minimum at \( \delta c = \pi/2 \) which corresponds to the number of contacts on the \((x, y)\) plane, while there is a maximum around \( \delta c = 0 \) (the vertical direction). The minimum at \( \delta c = \pi/2 \) together with the maximum at \( \delta c = 0 \) get more pronounced when \( \eta \) and \( \zeta \) are increased. This means that for larger values of \( \eta \) and \( \zeta \) which correspond to higher asphericities the particles tend to lie horizontally, to minimize the potential energy during deposition. Consequently most of the contacts will occur with the particles beneath and above. This can have a dramatic effect on the force chains and the response of the sample under shear or compression. Such a study is, however, beyond the scope of the current work.

Figure 8(c) shows a comparison of the angular distribution of contact normals for deposits with \( \eta = 6, \zeta = 1.8 \), with different polydispersities \( \delta r \). It is clear that the polydispersity has a minor effect.

To study the anisotropy of the orientation of the particles we do a similar analysis for the principal directions of each
ellipsoid. Figure 9 shows the probability distribution of the angle $\theta_0$ between the direction along the largest semiaxis $a$ of the particle and the vertical direction together with (b) its polar representation. Each curve corresponds to different values of the shape parameters.

The results above can also be obtained through the standard approach of computing eigenvectors of the fabric tensor of the particles. For a particle $A$, the fabric tensor $F^A$ is defined by [29]

$$F_{ij}^A = \sum_{c \in C^A} \frac{\ell_i^A e_j^A \cdot \ell_j^A e_i^A}{|e_i^A e_j^A|^2},$$

where $C^A$ is the set of contacts of particle $A$ and $\ell_i^A e_j^A (i, j = 1, 2, 3)$ are the components of the so-called branch vector joining the centroid of ellipsoid $A$ to a contact $c$. Defined in this way, the fabric tensor describes the local configuration of contacts between the particles.

Except for spherical particles, the branch vector corresponding to a contact is generally different from the normal vector at that contact. Therefore, the fabric tensor can be alternatively defined based on contact normals, as has been done in previous work [29,30]. In this case, the definition is the same as Eq. (10) except that $\ell$ denotes the contact normal.

In Fig. 10 we give the polar plot of the probability distributions of the orientation of the eigenvectors corresponding to the largest and smallest eigenvalues of fabric tensors based on both branch vectors [Figs. 10(a) and 10(c)] and normal vectors [Figs. 10(b) and 10(d)]. The angles of orientation are denoted by $\theta_b$ for branch vectors and $\theta_c$ for contact vectors and are, similarly, taken relative to the positive $z$ direction. Different curves correspond to different shapes.

As can be seen from Fig. 10, the two definitions of the fabric tensors lead to eigenvectors which are perpendicular to each other, i.e., $\langle \theta_b \rangle = \langle \theta_c \rangle + \pi/2$. This qualitatively reflects the previous results for contact normals and orientations. Additionally, the probability distributions of the eigenvectors corresponding to the smallest eigenvalues indicate vertical orientation of the smallest semiaxis. Consequently, not only does the largest semiaxis tend to lie in the horizontal plane but so does the second largest one.

In short, the results of Figs. 8–10 reflect the principle of minimum energy under the gravitational field controlling the deposition process: while the major semiaxis $a$ tends to align horizontally, the minor semiaxis $c$ tends to align along the vertical direction.
We quantify the degree of orientational alignment using a scalar order parameter defined as [31,32]

\[ S = \frac{3}{2} \left( \cos 2\left( \theta - \frac{\pi}{2} \right) \right) - \frac{1}{2}, \tag{11} \]

where \( \theta \) is the angle between the largest semiaxis of the particles and the vertical axis, and the average is taken over all the particles in the sample. This quantity becomes zero when the particles are randomly oriented and 1 when all particles lie in the horizontal plane.

The order parameter \( S \) is shown in Fig. 11(a) as a function of both shape parameters separately. Here one sees typically isolines of constant \( S \) given approximately by \( \eta \propto 1/\zeta \) which indicates that \( S \) depends almost exclusively on the product \( \eta \zeta \).

Figure 11(b) puts this dependency in evidence. In accordance with the previous results, Fig. 11 shows that as the shape of the particles deviates from a sphere anisotropy emerges in the sample, increasing rapidly as \( \eta \zeta = a/c \).

V. CONCLUSIONS

In this work, we studied systematically the static properties of deposits composed of ellipsoidal particles of different size and shape, focusing on their density and anisotropy. To this end, we developed an efficient molecular dynamics method for simulation of ellipsoidal particles which we used to generate deposits of such particles under gravity.

For monosized particles, the density increases rapidly as the shape of the particles deviates from a sphere, reaching, for particular values of the shape parameters, a maximum significantly higher than the one observed in random close packing of spheres. Further increase in the shape parameters, that is, further deviation from a sphere, causes the density to decrease slowly.

We also studied the anisotropy of such deposits and showed that as the shape of the particles deviates from a sphere stronger anisotropies are observed. Such anisotropies appear due to gravity and are absent in systems without gravity.

In the case of polydisperse particles the density takes higher values with qualitatively similar behavior. We observed that small to moderate polydispersities in the sizes of the particles has almost no effect on the anisotropic behavior of the system.

The densities observed in the deposits are generally lower than the ones obtained through procedures for optimal packings. Thus, as expected, deposition is not an ideal process for achieving the largest densities. Porous media and media formed through deposition processes also present densities much lower than the optimal one. Such observations point toward the possibility of using deposition of ellipsoids as a proper procedure for modeling porous media. This is the subject of future work.

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