Granular Matter (2015) 17:727–742
DOI 10.1007/s10035-015-0590-0

ORIGINAl PAPER

Pore shapes, volume distribution and orientations in monodisperse granular assemblies

Adnan Sufian¹ · Adrian R. Russell¹ · Andrew J. Whittle² · Mohammad Saadatfar³

Received: 25 February 2015 / Published online: 5 September 2015
© Springer-Verlag Berlin Heidelberg 2015

Abstract The complex mechanical behaviour of granular materials is commonly studied by considering the evolving particle contact network. An often overlooked feature is the influence of micro-scale geometric configuration of pores on the macroscopic response. This paper presents a series of tools to quantify the shape, volume distribution and orientation characteristics of the pore space. The proposed approach is compared against data extracted from physical and numerical experiments with monodisperse assemblies of spheres. Individual pores are represented by polyhedral pore unit cells obtained by combining the Delaunay tessellation with an algorithm for merging Delaunay cells based on the concept of maximal inscribed sphere, after Al-Raoush et al. (Soil Sci Soc Am J 67(6):1687–1700, 2003). A pore shape parameter is proposed that considers pore volume and surface, and is analytically related to the void ratio and the number of edges forming the polyhedral pore unit cell. The pore volume distribution is shown to be uniquely described by the analytical $k$-gamma distribution proposed by Aste and Di Matteo (Phys Rev E 77(2):021309, 2008). A pore orientation tensor is introduced to define the principal orientation of individual pore units. This is subsequently used to define a global orientation tensor that reveals an isotropic pore network for the reference monodisperse assemblies. The global orientation tensor is analytically expressed in terms of the parameters defining the pore volume distribution.

Keywords Pore characterisation · Pore geometry · Volume distribution · Orientation tensor

1 Introduction

Granular materials exhibit complex mechanical behaviour due to interactions of discrete particles. Understanding this mechanical behaviour is of great importance to many engineering applications, including soil behaviour, chemical processes and manufacturing [49]. Several studies [27,31,33,35,48] have established that loads are primarily transmitted through a sub-network of strong force chains that align with the direction of the imposed major principal stress. Force chains are braced against buckling by the surrounding weaker contacts. This bi-modal system evolves with applied stress and has been characterised by the anisotropy of the particle contact network. However, the micro-scale geometric pore features in granular materials have received limited attention even though deformation of pores is a major contributor to strain [14] and the pore geometry influences fluid flow, water retention and internal erosion. Consequently, characterising the pore space is an essential step in gaining a more complete understanding of granular media and this paper provides new insights, particularly on shape, volume distribution and orientation of pores in assemblies of monodisperse spheres.

The pore space in granular materials comprising impenetrable particles is almost entirely interconnected [28,47]. This makes the definition of individual pores (referred to as pore units in this paper) somewhat obscure. While a con-

---

1 School of Civil and Environmental Engineering, The University of New South Wales, Sydney, NSW 2052, Australia
2 Department of Civil and Environmental Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, United States of America
3 Department of Applied Mathematics, Research School of Physics and Engineering, The Australian National University, Canberra, ACT 0200, Australia
clusive definition of a pore unit is difficult, Dullien [13] suggested that a pore unit can be defined as a region in the pore space bounded by the surface of adjacent particles and planes of local minima, which are referred to as pore constrictions. This definition facilitates the network model of the pore space and allows for the calculation of shape, volume and orientation associated with each pore unit.

A few studies have presented quantitative characterisations of these pore features. Reboul et al. [36] presented a statistical description of pore volumes, by defining pore units using the modified Delaunay tessellation introduced by Al-Raoush et al. [1]. Kang et al. [21] extended the application of the modified Delaunay tessellation by considering the evolution of pore sizes in the numerical simulation of a direct shear test. Aste and Di Matteo [4] and Aste et al. [5] utilised the framework of granular statistical mechanics [15] to demonstrate that a unique distribution of Voronoi cell volumes can be described analytically by a modified gamma distribution function.

The shape of pore units is highly irregular even in assemblies of monodisperse spheres. Prior studies have described pore shape qualitatively [19,28] or approximated the pore unit with simple geometric objects. Ordonez-Miranda and Alvarado-Gil [30] described pores as spheroids with a defined aspect ratio, while Li and Li [25] defined pore shape as the ratio of the half-radii of an ellipse approximation of pore units in the 2D void cell system.

Orientation can be characterised by spherical harmonic distribution functions [10,34] or fabric tensors [29], as is commonly applied to the evolving contact network. However, there has been limited application of these concepts to assess orientation characteristics of pores. Konishi and Naruse [23] presented a 2D void tensor allowing for the determination of the principal orientation of individual pores, which can subsequently be implemented in a mean void tensor to describe a collection of pores. Shire et al. [44] presented a fabric tensor which specifically considered pore constrictions to explore stress-induced anisotropy in numerical simulation of elemental shear tests, where the orientation of pore constrictions was related to the force chain network.

By defining pore units using the modified Delaunay tessellation proposed by Al-Raoush et al. [1], this paper presents new quantitative tools to assess shape, volume distribution and orientation of pores in granular materials. Shape is defined after Russell [38] by considering the actual geometry of pore units. It is demonstrated that the shape parameter can be analytically expressed as a function of local void ratio and local edge numbers of the polyhedral pore units, both of which are easily interpreted. This paper also explores the applicability of the $k$-gamma distribution function [4,5] to describe the volume distribution of pore units formed by the modified Delaunay tessellation. Further, a novel pore orientation tensor is proposed, which is applicable at the micro-scale to define the orientation of pore units and also at the macro-scale to explore anisotropy of the granular assembly.

The proposed functions for pore shape, volume distribution and orientation are evaluated using data extracted from physical and numerical experiments of monodisperse assemblies of spheres listed in Table 1. The E-D dataset has been obtained from physical experiments and comprise disordered assemblies of hard, spherical, acrylic beads (with slight polydispersity of approximately 3 %), formed by pouring the beads into a container, where the position of the particles have been determined through X-ray computed tomography (refer to [6]). The N-RLP and N-GL datasets have been developed by numerical simulations. Assemblies in these datasets are formed by isotropically compressing a non-interacting cloud of particles to a mechanically stable jammed state at a desired density. A Hertz-Mindlin contact interaction model was employed in these simulations and the sample was bound in a periodic box. These datasets were developed to investigate the random loose packing (N-RLP) and granular line (N-GL) boundary of the phase diagram for jammed matter in [45].

Each dataset comprises several assemblies and Table 1 summarises the number of particles in a Representative Element Volume, $N_{REV}$, and the corresponding void ratio, $\epsilon_{REV}$. Void ratio ($\epsilon$) is defined as the ratio of pore volume to solid volume, and is related to the packing density ($\rho$) by the expression $\rho = 1/(1 + \epsilon)$. Void ratio is the preferred state parameter as this study focuses on the geometric characteristics of pores. All assemblies considered in this study fall within the amorphous regime for packing of monodisperse spheres. It is assumed that all assemblies comprise rigid particles (with the assumption of small contact deformation) and the static assemblies are at mechanical equilibrium.

### 2 Tessellation of pore space

The complex pore space morphology in granular materials can be described by a network model comprising pore bodies connected via pore constrictions [8,9,26,37]. Several methods [7,20,25,41] have been proposed to tessellate the pore space of granular materials containing non-overlapping particles.

In this study, pore units are defined using the modified Delaunay tessellation proposed by Al-Raoush et al. [1], where individual Delaunay cells are merged according to

---

1. N-RLP and N-GL datasets available online at [http://lisg1.engr.ccny.cuny.edu/~makse/soft_data.html](http://lisg1.engr.ccny.cuny.edu/~makse/soft_data.html).
a certain criteria to form pore units. This method is selected because it is able to capture a larger variation in pore sizes, and hence, is able to distinguish between large highly connected pore bodies and small compact pores. It also readily allows for the calculation of geometric properties of pore bodies. The modified Delaunay tessellation shares some similarities with the method described in Sastry et al. [39, 40], where a dual Voronoi-Delaunay tessellation is considered in identifying pores. Both these methods define pore bodies as a union of Delaunay cells, thereby allowing for large size variations to be captured. However, Sastry et al. [39, 40] consider a hard sphere liquid model, where the exclusion spheres are allowed to overlap, effectively creating disconnected pores. In granular assemblies of non-overlapping particles, the pore space is interconnected and as such the modified Delaunay tessellation is preferred.

The classical Delaunay tessellation has been frequently used to delineate the pore space [2, 14, 18, 36, 37, 50, 51]. However, pore units derived from single Delaunay cells have a limited size range due to nearest neighbour constraints and large pore bodies are not defined, as noted by Al-Raoush et al. [1]. Single Delaunay cells have exactly four faces and thus the pore units considered in this study. The pore units are identified as polyhedral cells which can have convex and concave geometries. Merging of Delaunay cells is based on the identification of the maximal inscribed sphere contained within the pore space for each Delaunay cell and is readily determined analytically. However, a local optimisation is required when the inscribed sphere is not completely located within the pore space. The local optimisation procedure is outlined in Appendix 1.

Al-Raoush et al. [1] modifies this initial tessellation by introducing the concept of merging Delaunay cells to form tetrahedral Delaunay cells. It is important to note that the Delaunay tessellation can exhibit issues in regards to triangulation close to sample boundaries, resulting in the formation of degenerate tetrahedrons and avoids creating planarity on the REV boundaries. This ensured that no tetrahedral units were discounted from the analyses. However, all datasets included a degenerate simplex involving four near coplanar particles forming a flat Delaunay cell.

Table 1 Datasets used for validation of pore characterisation

| Dataset E-D | Dataset N-GL | Dataset N-RLP |
|-------------|--------------|--------------|
| Assembly    | $N_{REV}$   | $\epsilon_{REV}$ | Assembly    | $N_{REV}$   | $\epsilon_{REV}$ | Assembly    | $N_{REV}$   | $\epsilon_{REV}$ |
| p1v         | 2353         | 0.6606       | m1g         | 5091         | 0.8137       | m1l         | 5111         | 0.5640       |
| p2v         | 2066         | 0.6528       | m2g         | 5011         | 0.7840       | m2l         | 5116         | 0.5640       |
| p3v         | 2184         | 0.6683       | m3g         | 5012         | 0.7406       | m3l         | 5113         | 0.5830       |
| p4v         | 2347         | 0.6667       | m4g         | 5011         | 0.6980       | m4l         | 5101         | 0.6563       |
| p5v         | 2277         | 0.6838       | m5g         | 5012         | 0.6833       | m5l         | 5107         | 0.7887       |
| p6v         | 2632         | 0.6787       | m6g         | 5110         | 0.6689       | m6l         | 5098         | 0.6979       |
| p7v         | 1933         | 0.6709       | m7g         | 5111         | 0.5782       | m7l         | 5110         | 0.7338       |
| p8v         | 1729         | 0.6556       | m8g         | 5018         | 0.5756       | m8l         | 5099         | 0.6130       |
| p9v         | 1821         | 0.6708       | m9g         | 5093         | 0.5723       | m9l         | 5103         | 0.7609       |
| p10v        | 1936         | 0.6762       | m10g        | 5099         | 0.5699       | m10l        | 5129         | 0.6328       |
| p11v        | 2028         | 0.6845       | m11g        | 5091         | 0.6130       | m11l        | 5091         | 0.8100       |
| p12v        | 2174         | 0.6801       | m12l        | 5101         | 0.6770       | m13l        | 5095         | 0.6043       |
|             |              |              | m14l        | 5099         | 0.8159       | m15l        | 5099         | 0.8175       |
are illustrated in Fig. 1. This study employs the criterion shown in Fig. 1b. Appendix 2 presents additional analysis of the alternate merging criteria shown in Fig. 1a. This additional analysis suggests that while the choice of the merging criteria can influence micro-scale features, broader macroscopic characteristics discussed in this paper are not greatly influenced by the choice of the merging criteria. It should be noted that an inscribed sphere can overlap with multiple other inscribed spheres and this results in the formation of large pore units. Further, the degenerate cases of flat Delaunay cells were found to merge with adjacent Delaunay cells to form larger pore units. These flat Delaunay cells typically contained large inscribed spheres, which resulted in merging with neighbouring Delaunay cells. This ensured that no local arrangements were discarded from the analysis.

As mentioned previously, the modified Delaunay tessellation provides a better characterisation of the pore space compared to the classical Delaunay tessellation. This is broadly shown in the statistics of Figs. 2 and 3. Figure 2a shows an increasing number of pore units with increasing density (that is, decreasing void ratio) for the datasets in Table 1. In dense assemblies, there is a lower probability of encountering large pore units containing many Delaunay cells. In fact, pore units in dense assemblies are more likely to be composed of only a few Delaunay cells, and this leads to an increase in the number of pore units with density. This is also reflected in the percentage of unmerged pore units, \( N_{\text{unm}}(\%) \), in Fig. 2b. This indicates that the percentage of tetrahedral pore units (that is, the smallest geometrically achievable pore unit) increases with density. Figure 3 shows the distribution of the number of Delaunay cells forming a pore unit and demonstrates that the modified Delaunay tessellation is capable of capturing large variations in pore sizes. This distribution monotonically decays and this agrees with the intuitive notion that there exist many small pores and fewer larger pores in a mechanically stable system.

### 3 Geometric characteristics and pore shape

Tessellation of the pore space allows for the determination of geometric properties of individual Delaunay cells and pore units. There are three fundamental geometric properties of
The surface area of this sector forms a spherical triangle, as shown in Fig. 4b. The area of a spherical triangle corresponding to the $i$\textsuperscript{th} particle in the Delaunay cell is given by $S_{p,i} = r_{p,i}^2 (A + B + C - \pi)$, where $r_{p,i}$ is the radius of the $i$\textsuperscript{th} particle and $A$, $B$, $C$ are the angles of the spherical triangle. $A$, $B$, $C$ are calculated by considering the dihedral angles $a$, $b$, $c$ in Fig. 4b and applying spherical trigonometry. The total pore surface area is then simply $S_p = \sum_{i=1}^{4} S_{p,i}$. Further, each particle sector forms a pyramid with base given by the spherical triangle and hence the volume of each particle sector is given by $V_{s,i} = \frac{1}{3} S_{p,i} r_{p,i}$ and the total solid volume of the Delaunay cell is $V_s = \sum_{i=1}^{4} V_{s,i}$. The total pore volume in a Delaunay cell is simply $V_p = V_{cell} - V_s$.

The calculation of $V_s$, $V_p$ and $S_p$ for pore units is straightforward, as these properties are determined by summing the respective geometric properties for each Delaunay cell forming the merged pore unit. This is an advantage of initially employing a Delaunay tessellation to the pore space.

Using the geometric properties calculated above, the shape of individual pore units can be characterised by the dimensionless pore shape parameter, $F$, defined by \cite{38}:

$$F = \frac{A_p}{\Gamma_p}$$

where $A_p$ is a dimensionless pore volume parameter determined from $V_p = A_p d_{eq}^3$ and $\Gamma_p$ is a dimensionless pore surface area parameter determined from $S_p = \Gamma_p d_{eq}^2$. The characteristic pore size ($d_{eq}$) is defined as the diameter of an equivalent sphere with volume $V_p$. $F$ can also be thought of as a dimensionless ratio of pore surface area to volume.

It is worth noting that Speedy \cite{46} and Sastry et al. \cite{40} consider a similar ratio of average volume and surface area in providing an expression for the equation of state for equilibrium hard sphere liquids. In Russell \cite{38}, a macroscopically averaged value of $F$ is considered in the characterisation of water retention in soils. In this paper, we extend these concepts from a micro-scale perspective by defining $F$ as a function of local geometry (void ratio) and local topology (polyhedral edge numbers) for each individual pore unit.

An interesting result is presented in Russell \cite{38}, where it is suggested that for systems of equal sized spheres, the dimensionless shape parameter can be related to local void ratio ($\epsilon$) by Eq. 2.

$$F = \frac{1}{6} \epsilon^{2/3}$$

The void ratio is defined as the ratio of pore volume to solid particle volume, $\epsilon = \frac{V_p}{V_s}$. Equation 2 was derived by considering the unit cells presented in Graton and Fraser \cite{19}. These unit cells considered only monodisperse particles and
were defined in such a way that there was exactly one whole particle per cell. The expression in Eq. 2 loses its generality for different definitions of a unit cell. Therefore, a generalised expression is developed relating \( F \) to void ratio for any definition of a pore unit cell for both monodisperse systems (Sect. 3.1) and polydisperse systems (Sect. 3.2). The expression for monodisperse systems is extended in Sect. 3.3 by incorporating a local topological property.

3.1 Relationship for monodisperse particles

Consider the pore unit shown in Fig. 4a. The pore volume is given by \( V_p = \frac{\pi}{6} d_{eq}^3 \), and by setting \( d_{eq} = d_p \), it can be shown that \( A_p = \frac{2}{3} S_p \). This relation is still applicable for polydisperse systems.

Equating surface area of particles, \( S_p \), and surface area of pores, \( S_p \), allows for the inclusion of local void ratio into the formulation. Note that the particle sectors in Fig. 4a may not necessarily form a single sphere. Therefore, \( N_p \) is given by \( N_p = \frac{\sum V_i}{\pi d_{eq}^2} \), where the summation is over all particle sectors. Consequently, the surface area of particles is given by \( S_p = N_p \pi d_{eq}^2 \). As \( S_p = S_p \) and using the definition \( S_p = \Gamma_p d_{eq}^2 \), an expression for \( \Gamma_p \) is derived.

\[
\Gamma_p = \frac{N_p \pi}{d_{eq}} (d_{eq}^2 - d_p)^2
\]

Using the definition of void ratio, \( \epsilon = \frac{V_v}{V_p} \), it can be shown that:

\[
\left( \frac{d_{eq}}{d_p} \right)^2 = (\epsilon N_p)^{2/3}
\]

Substituting Eq. 4 into Eq. 3 gives:

\[
\Gamma_p = \frac{\pi N_p^{1/3}}{\epsilon^{2/3}}
\]

Therefore from Eq. 5, the dimensionless shape parameter, \( F \), can be defined as:

\[
F = \frac{A_p}{\Gamma_p} = \frac{1}{6} N_p^{-1/3} \epsilon^{2/3}
\]

It should be noted that the expression in Eq. 6 reflects the choice of the characteristic pore size \( d_p = d_{eq} \).

3.2 Relationship for polydisperse particles

The derivation can be extended to assemblies of polydisperse spheres. As above, \( A_p = \frac{2}{3} S_p \). In polydisperse assemblies, the surface area of particles is given by:

\[
S_p = \sum_i \pi N_i d_i^2
\]

where \( d_i \) is the diameter of the \( i \)th particle and \( N_i \) is the equivalent number of spheres of diameter \( d_i \) that are included within the unit cell. Note that Eq. 7 does not place a limit on the number of particles forming a unit cell. This generality allows the expression to be used for either Delaunay cells or pore units. By equating \( S_p = S_p \), an expression for \( \Gamma_p \) is derived:

\[
\Gamma_p = \frac{\pi}{d_{eq}^2} \sum_i N_i d_i^2
\]

Using the definition of void ratio, it can be shown that the equivalent sphere diameter is:

\[
d_{eq}^2 = \epsilon^{2/3} \left( \sum_i N_i d_i^2 \right)^{2/3}
\]

By substituting Eq. 9 into Eq. 8, \( \Gamma_p \) for polydisperse assemblies is given by:

\[
\Gamma_p = \frac{\pi}{\epsilon^{2/3} \left( \sum_i N_i d_i^2 \right)^{2/3}} \sum_i N_i d_i^2
\]

Therefore, the pore shape parameter in polydisperse assemblies is given by:

\[
F = \frac{\epsilon^{2/3} \left( \sum_i N_i d_i^2 \right)^{2/3}}{6 \sum_i N_i d_i^2}
\]

It can be readily shown that Eq. 11 simplifies to Eq. 6 when \( d_i \) takes on the same value for all \( i \) (that is, for monodisperse assemblies).

3.3 Analytical relationship between shape parameter and geometry of Pore units

Equations 6 and 11 provide a relationship between the shape of pore units and a geometric property (void ratio). This section shows that the pore shape parameter, \( F \), can also be analytically related to the number of edges forming the polyhedral pore unit, \( N_e \), for assemblies of monodisperse spheres. The topological feature, \( N_e \), reflects the polyhedral shape of the pore unit in a manner which is not captured by \( N_p \) alone.

In the following derivation, the pore unit is assumed to be a regular polyhedron and can be one of three platonic solids; tetrahedron \( (N_e = 6) \), octahedron \( (N_e = 12) \) or icosahedron \( (N_e = 30) \). Specific expressions for platonic solids have been extracted from [11]. For regular polyhedrons, the Schläfli symbol is given by \( \{p, q\} \), where \( p \) refers to the number of edges composing each face and \( q \) defines the number of
faces forming a vertex of a regular polyhedron. For the three platonic solids mentioned above, \( p = 3 \). This is a reasonable choice since pore unit faces are unlikely to be composed of more than three edges (as this would require two adjacent faces of merged Delaunay cells to be coplanar). In a highly disordered assembly this condition is unlikely to occur.

For a regular polyhedron, \( N_p \) is related to the solid angle, \( \Omega \), and the number of vertices of the polyhedron, \( N_v \):

\[
N_p = \frac{N_v \Omega}{4\pi} \quad (12)
\]

From the Schlafli relationships for platonic solids, it is known that:

\[
N_v = \frac{2N_e}{q} \quad (13)
\]

The solid angle is given by:

\[
\Omega = q\theta - \pi(q - 2) \quad (14)
\]

Combining Eqs. 13 and 14 gives an expression for \( N_v\Omega \), where \( \theta \) is the dihedral angle.

\[
N_v\Omega = 2N_e \left[ \theta - \pi \left( \frac{q - 2}{q} \right) \right] \quad (15)
\]

\( q \) is determined by considering the following identity:

\[
q = \frac{2N_e p}{2p + N_e p - 2N_e} \quad (16)
\]

For the case \( p = 3 \), Eq. 16 simplifies to \( q = \frac{6N_e}{6 + N_e} \), and a simplified expression for \( \frac{q-2}{q} \) can be determined:

\[
\frac{q-2}{q} = \frac{2}{3} \left( \frac{N_e - 3}{N_e} \right) \quad (17)
\]

The dihedral angle for platonic solids is given by the solution to \( \sin \left( \frac{\theta}{2} \right) = \cos \left( \frac{\pi}{q} \right) / \sin \left( \frac{\pi}{p} \right) \):

\[
\theta = 2 \sin^{-1} \left\{ \frac{2 \cos \left( \frac{\pi(6+N_v)}{6N_e} \right)}{\sqrt{3}} \right\} \quad (18)
\]

Substituting Eqs. 17 and 18 into Eq. 15 provides an expression for \( N_p \) as a function of \( N_e \), as shown in Eq. 19.

\[
N_p = \frac{N_v \Omega}{4\pi} = \frac{N_e}{2\pi} \left[ 2 \sin^{-1} \left\{ \frac{2 \cos \left( \frac{\pi(6+N_v)}{6N_e} \right)}{\sqrt{3}} \right\} - \frac{2\pi}{3} \left( \frac{N_e - 3}{N_e} \right) \right] \quad (19)
\]

4 Pore volume distribution

Characterising the pore volume distribution in granular assemblies is essential in quantifying the highly complex geometric configuration of pores. In this study, the distri-

![Figure 5](image-url)
Distribution of pore unit volumes is described by the analytical $k$-gamma distribution function [4, 5].

$$f(V_p - V_{p, \text{min}} : k, \chi) = \frac{(V_p - V_{p, \text{min}})^{k-1}}{I(k) \chi^k} e^{-\frac{V_p - V_{p, \text{min}}}{\chi}}$$  \hspace{1cm} (21)

Equation 21 is a modified gamma distribution function in the variable $V_p - V_{p, \text{min}}$, with parameters $k$ and $\chi$, where $V_{p, \text{min}}$ is the theoretical minimum pore volume (for rigid particles). For Delaunay cells, $V_{p, \text{min}} = 0$ to account for the presence of flat tetrahedrons as discussed in Sect. 2. However, observations from the numerical analysis confirm that these degenerate Delaunay cells merge with adjacent tetrahedrons to form larger pore units. Consequently, the minimum pore volume for pore units is defined as the pore volume in a regular tetrahedron, where all edges contain contact points. This is given by Eq. 22, where $d_s$ is the particle diameter in a monodisperse assembly.

$$V_{p, \text{min}} = \left(\frac{1}{6\sqrt{2}} - \frac{\arccos \left(\frac{23}{27}\right)}{6}\right) d_s^3 \approx 0.02597 d_s^3$$  \hspace{1cm} (22)

The parameter $k$ can be determined analytically by:

$$k = \frac{\langle V_p \rangle - V_{p, \text{min}}}{\sigma^2}$$  \hspace{1cm} (23)

where $\langle V_p \rangle$ is the mean pore volume and $\sigma^2$ is the fluctuations in pore volume given by $\langle (V_p - V_{p, \text{min}})^2 \rangle - \langle V_p - V_{p, \text{min}} \rangle^2$. The parameter $\chi$ can also be defined analytically by:

$$\chi = \frac{\langle V_p \rangle - V_{p, \text{min}}}{k}$$  \hspace{1cm} (24)

While Aste and Di Matteo [4] and Aste et al. [5] validated the $k$-gamma distribution function by considering Voronoi cell volumes, Fig. 6 demonstrates that the analytical $k$-gamma distribution function accurately reflects the distribution of pore unit volumes. However, there is a small discrepancy at very small pore volumes, $V_p - V_{p, \text{min}} \approx 0$, which was also noted in [22]. The lack of an inflection point in the analytical solution shown in Fig. 6 suggests that the most probable configuration occurs when $V_p - V_{p, \text{min}} = 0$, but this is not supported by the numerical analysis. While granular systems have a tendency to approach the densest possible local configuration (that is, the configuration of minimum potential energy), the phenomenon of geometric frustration [17] prevents the majority of pore units attaining the theoretical minimum pore volume in disordered assemblies of monodisperse spheres. This is also reflected in the observation of polytetrahedral structures in Anikeenko and Medvedev [2], where it was demonstrated that there is a preference for the formation of irregular polytetrahedra comprising clusters of quasi-regular tetrahedrons that do not necessarily have the theoretical minimum pore volume. Hence, there is a lower limit above which the analytical expression in Eq. 21 can provide an accurate approximation of the pore volume distribution.

Aside from this minor discrepancy, uniqueness in the pore volume distribution is observed when plotted in the variable $V_p - V_{p, \text{min}} / \langle V_p \rangle - V_{p, \text{min}}$, as shown in Fig. 7. The collapsed distribution shown in Fig. 7b can be fitted analytically by the parameter $k = 0.6$.

Aste and Di Matteo [4] demonstrated that $\chi$ takes on physical meaning within the theoretical framework of granular statistical mechanics (proposed by [15]) as an equivalent granular temperature termed compactivity and reflects the macroscopic density of a static granular system [20]. This is illustrated in Fig. 8a which shows a linear relationship between $\chi$ and the macroscopic void ratio. The compactivity
χ decreases with decreasing void ratio, which agrees with the intuitive notion that for denser systems, the number of accessible configurations reduces, that is, larger pores are less probable in dense assemblies. The results also suggest a cut-off at the random close packing limit (ε = 0.56), which may signal the commencement of partial crystallisation within the assembly.

Equation 24 indicates that the quantity χk can be thought of as the mean free pore volume, ⟨V_p⟩ − V_{p, min}, and reflects how far the granular system is from the densest possible configuration. However, it is important to note that the configuration corresponding to ⟨V_p⟩ − V_{p, min} = 0 is not attainable, as this would require all pore units to be regular tetrahedrons and such a configuration cannot tile the pore space. Figure 8b shows there is also a linear relationship between χk and void ratio within the amorphous region with the mean free pore volume decreasing with decreasing void ratio.

The parameter k exhibits somewhat random fluctuations in a narrow range between 0.54 and 0.65, as illustrated in Fig. 8c. According to Aste and Di Matteo [4], k is an equivalent granular specific heat defined by $\frac{\partial \langle V_p \rangle}{\partial \chi}$. The linear relationship observed in Fig. 8a suggests $\Delta \chi \propto \Delta \epsilon$, and similarly, the linear relationship shown in Fig. 8b suggests $\Delta \langle V_p \rangle \propto \Delta \epsilon$. Hence, k is expected to be constant, where the observed fluctuations in Fig. 8c may result from deviations from the respective linear relationships. Indeed, k was observed to fluctuate in a small region around $k \approx 12$ for Voronoi cell volume distribution in disordered assemblies [4]. This suggests that k is an indicator of the method of tessellation employed in partitioning the pore space.
5 Orientation characteristics

The anisotropy of the pore network can be characterised by considering the orientation of pore units. A tensor (P) is introduced to define the principal orientation of individual pore units. Following the definition of a fabric tensor [29], P is defined as:

\[
P = \frac{1}{N} \sum_{m=1}^{N} n^m \otimes n^m = \begin{bmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{bmatrix}
\]  

(25)

where \(N\) is the number of vectors. In order to describe orientation of pore units, \(n^m\) is defined as the vector normal to each triangular face of the polyhedral pore unit cell and is scaled by the square root of the area of the corresponding triangular face (\(a^m\)):

\[
n^m = \sqrt{a^m} \hat{n}^m
\]  

(26)

where \(\hat{n}^m\) is the unit normal vector to the triangular face. \(n^m\) is therefore the projection of the surface area of each face to the corresponding coordinate axes. Components of the orientation tensor are given by:

\[
P_{ij} = \frac{1}{N} \sum_{m=1}^{N} a^m \hat{n}_i^m \hat{n}_j^m
\]  

(27)

\(P\) is a symmetric tensor and it can be readily shown that \(\text{tr} (P) = \langle a^m \rangle\), that is, \(\text{tr} (P)\) is the average surface area per triangular face. Further, the non-diagonal terms reflect the skew or distortion of the surface area of a pore unit within a particular plane. Hence, it is easy to see that when the principal axes coincide with the coordinate system, \(P\) will only contain diagonal terms, as there will be no skew in the surface area. Hence, it is convenient to decompose the orientation tensor into isotropic and anisotropic components:

\[
P = \kappa I + \kappa F
\]  

(28)

where \(\kappa\) is a scalar quantity, \(I\) is the isotropic tensor given by the identity tensor, and \(F\) is the anisotropic orientation tensor.

Taking the matrix inner product of Eq. 28 with \(I\) and setting \(\kappa \langle P : I \rangle = 0\), the result \(\langle P \rangle : I = \kappa \langle I : I \rangle\) is obtained from which an expression for the scalar quantity \(\kappa\) can be explicitly defined:

\[
\kappa = \frac{\text{tr} (P)}{3} = \frac{\langle a^m \rangle}{3}
\]  

(29)

Further, setting \(\kappa \langle F : I \rangle = 0\) places an additional constraint on the anisotropic orientation tensor; \(\text{tr} (F) = 0\). \(F\) is also a symmetric tensor and reflects the change in surface area of the polyhedral cell required to bring about isotropic orientation.

\(P\) can be regarded as an interface tensor and has been considered in the context of assessing cell shape anisotropy in cellular foams [24] and random sphere packs [42, 43]. This study goes beyond shape anisotropy and utilises \(P\) to determine principal orientation of individual pore units through an eigen-decomposition. An eigen-decomposition of the orientation tensor results in an eigenvalue matrix (\(\mathbb{D}\)) and an eigenvector matrix (\(\mathbb{V}\)), which can be interpreted to provide the principal axes of orientation of individual pore units. The eigenvalues (\(\lambda\)) are determined from the solution to \(f (\lambda) = \det (P - \lambda I) = 0\). This reveals an interesting relationship that \(\text{tr} (\mathbb{D}) = \langle a^m \rangle\), which suggest that the eigenvalues reflect the average surface area per triangular face projected in the principal directions. Consequently, the major, minor and intermediate axes of orientation are defined by the minimum, maximum and intermediate eigenvalues in \(\mathbb{D}\), respectively. Intuitively, the direction of maximum elongation corresponds to the minimum surface area projected in that direction, while the direction of minimum elongation corresponds to the maximum surface area. This approach to determining principal axes has been validated by comparison with a bounding ellipsoid approximation of pore units.

The formulation outlined above can be applied to define the major direction of orientation of all pore units forming an assembly. The vector defining the major direction of orientation can be expressed in terms of its azimuthal (\(\phi\)) and elevation angle (\(\beta\)). A lower hemisphere equal-angle stereographic projection can be used to display the distribution of pore unit orientations. This analysis has been conducted for all assemblies in the E-D, N-RLP and N-GL datasets (Table 1). Figure 9a shows a typical stereonet using a probability density contour. The stereonet suggests radial symmetry in pore orientation distribution, which is confirmed by the distribution of azimuthal angles shown in the rose diagram in Fig. 9b.

The distribution of elevation angles (\(\beta\)) for all assemblies in Table 1 is shown in Fig. 10. All assemblies have similar distribution in elevation angle, and coupled with the radial symmetry shown in Fig. 9 suggests that all assemblies have the same pore orientation distribution. Diambrta et al. [12] provided an expression for the cumulative distribution of orientation with an elevation angle within \(\pm \beta\) from the horizontal under axisymmetric conditions (Eq. 30).

\[
P (\beta) = \frac{1}{2 \beta} \int_{\beta}^{\beta} \rho (\alpha) \cos (\alpha) d \alpha
\]  

(30)

\(\rho (\alpha)\) is a generalised probability distribution function and reflects the concentration of pores with an elevation angle \(\alpha\) above the horizontal. \(\overline{\rho}\) represents the average concentration defined by \(\overline{\rho} = \frac{1}{V_p} \int \rho (\alpha) dV_p\). For isotropic distributions, \(\rho (\alpha) = \overline{\rho}\), and hence \(P (\beta) = \sin (\beta)\). This is compared to
Pore shapes, volume distribution and orientations in monodisperse granular assemblies

5.1 Global orientation tensor

Following [23], the principal orientation of individual pore units can be used to define a global orientation tensor \( P^M \), which determines the orientation characteristics for a set of pore units. For \( P^M \), \( n^m \) is defined as:

\[
n^m = \sqrt{V^m_p - V_{p,\text{min}}} \hat{n}_m^m
\]  

(31)

where \( V^m_p \) is the normalised pore volume, \( V_{p,\text{min}} \) is the normalised theoretical minimum pore volume and \( \hat{n}_m^m \) is the unit vector representing the major principal orientation of the pore unit (note that each pore unit comprises two complementary vectors). Using this definition, the elements of the \( P^M \) tensor are given by:

\[
P_{ij}^M = \frac{1}{2N} \sum_{m=1}^{2N} \left( V^m_p - V_{p,\text{min}} \right) \hat{n}_i^m \hat{n}_j^m
\]  

(32)

Therefore, it is apparent from Eq. 32 that \( P^M \) reflects the orientation distribution of pore volume in the sample, that is, what volume of the pore space is orientated in a given direction. Figure 9c shows a typical example of the computed elements of \( P^M \), which confirms the isotropic arrangement of pores, as the dominant terms are the leading diagonal elements, which are invariant to rotation of coordinate axis.

Interestingly, analytical expressions for the elements of the \( P^M \) tensor can be derived with assumptions relevant to the datasets considered in this study. Note that the scaling factor in Eq. 31 has been chosen in order to apply the pore volume distribution function in Eq. 21. Suppose the distribution of vectors representing the major axis of orientation of pore units is defined by \( E(n) \), which satisfies \( \int_{\Omega} E(n) \, d\Omega = 1 \), where \( \Omega \) is the solid angle. If it is assumed that the volume of a pore unit is independent of its orientation, then Eq. 32 can be expressed as:

\[
P_{ij}^M = \frac{1}{V_p} \int_{\Omega} \int E(\mathbf{n}) \, d\Omega \, d\mathbf{n}
\]  

(33)

where \( \mathbf{n} = \mathbf{n}_i^m \). This assumption is valid for the assemblies considered in this study due to the sample preparation process in both physical and numerical experiments. However, it is likely that there will be a relation between orientation and pore volume during shearing. The first term of
Eq. 33 can be alternatively expressed as:

\[ \Omega = \text{diagonal elements in the numerically calculated } P \]

\[ \text{implies that } \hat{E} \]

\[ \text{is shown by the dashed line (with slope } 1:1). \]

Further, the minimum and maximum diagonal elements in the numerically calculated \( P \) are shown by the + symbol to reflect the error between the numerical and analytical solution.

The double integral in Eq. 33 is the mean free pore volume, \( \langle V_p \rangle - V_{p, \text{min}} \), which from Eq. 24 is given by \( \chi k \). Further, the isotropic arrangement demonstrated in Figs. 9 and 10 implies that \( E(\hat{n}) = \frac{1}{12 \pi} \). In spherical coordinates, a unit vector is given by \( \hat{n} = \left( \hat{n}_1, \hat{n}_2, \hat{n}_3 \right) = \left( \cos(\phi) \sin(\beta), \sin(\phi) \sin(\beta), \cos(\beta) \right) \)

and the relationship \( d\Omega = \sin(\beta) \) d\( \beta \) d\( \phi \) holds. Therefore, Eq. 33 can be alternatively expressed as:

\[ P_{ij}^M = \frac{\chi k}{4\pi} \int_0^\pi \int_0^{2\pi} \hat{n}_i \hat{n}_j \sin(\beta) \) d\( \beta \) d\( \phi \]

Equation 34 can be easily solved and hence the analytical solution to \( P^M \) is given by:

\[ P^M = \frac{\chi k}{3} \]

Figure 11 demonstrates that the analytical solution in Eq. 35 accurately reflects the numerically determined global orientation tensor and confirms the isotropic orientation of the pore network.

### 6 Conclusion

A set of parameters have been presented to quantify the micro-scale pore features in granular assemblies. The proposed approach is evaluated using data extracted from physical and numerical experiments for monodisperse assemblies of spheres. Individual pore units were defined using the modified Delaunay tessellation proposed by Al-Raoush et al. [1], which readily allowed for the calculation of geometric properties of pore units.

A pore shape parameter \( (F) \) was derived and found to be a function of void ratio and the number of edges forming the pore unit. This analytical expression agreed well with the numerically interpreted properties of all datasets.

The pore volume distribution was found to be uniquely defined by the analytical \( k \)-gamma distribution function, where \( \chi \) corresponds to the compactivity and \( \chi k \) corresponds to the mean free pore volume. Both show a linear relationship with void ratio. The parameter \( k \) exhibited small random fluctuations around a constant value and is thought to provide an indication of the method of tessellation employed to partition the pore space. Even though this study considered pore space geometry and implemented a tessellation vastly different from Aste and Di Matteo [4] and Aste et al. [5], the \( k \)-gamma distribution still remained applicable and was able to accurately describe pore volume distribution.

The principal orientation of individual pore units is defined by the orientation tensor, \( P \) (Eq. 27). The distribution of the major principal orientation suggests that the pore network in all of the reference assemblies (Table 1) are isotropically oriented. The global orientation tensor, \( P^M \) (Eq. 32), incorporates vectors defined by the major principal orientation of individual pore units scaled by the pore volume. For assemblies of monodisperse spherical particles, an analytical expression for the global orientation tensor was derived in terms of the mean free pore volume \( (\chi k) \) and shown to agree well with values derived from physical and numerical experiments.

This paper focused on jammed amorphous monodisperse systems of non-overlapping spheres. An interesting avenue for future research is to assess the validity of the findings in this study with related systems, including hard sphere liquids, crystalline assemblies and partially crystalline amorphous systems. The partially crystalline amorphous assemblies are of particular interest to determine if there exist any distinct changes in pore space characteristics beyond the random close packing limit and also to assess the influence of crystalline configurations on the mechanical response of granular materials, as suggested by O’Sullivan et al. [32]. While this study explored micro-scale features in static granular assemblies, the long term goal of this research is to explore how these pore space features evolve under different load paths and whether the pore space can provide a better understanding of the complex mechanical response of granular materials.

### Acknowledgments

A.S. thanks A.J.W. and Massachusetts Institute of Technology for hosting him from August 2014 to May 2015. A.R.R.
Pore shapes, volume distribution and orientations in monodisperse granular assemblies

thanks M.S. and The Australian National University for hosting him during the first half of 2014 to start this work, and The University of New South Wales for granting him leave through the Special Studies Program.

**Funding** This study was funded by the Australian Research Council (Grant number DP150104123).

**Appendix 1: Local optimisation to inscribed sphere**

An iterative local optimisation procedure is required when the analytically determined inscribed sphere for a Delaunay cell (the initial solution) intersects adjacent particles, and is therefore not contained within the pore space. This is particularly prevalent for polydisperse assemblies and was only required for the E-D dataset in this paper. Particles intersected by the initial solution and those forming the Delaunay cell are referred to as constraining particles (Fig. 12a). For computational efficiency, only constraining particles located within two diametric shells from the reference Delaunay cell are considered in subsequent calculations. A combinatorics approach is implemented to define all possible configurations of four constraining particles. There are \( n \choose 4 \) configurations, where \( n \) is the number of constraining particles and the inscribed sphere for each combination is determined (Fig. 12b). Only inscribed spheres that do not intersect the constraining particles are retained, where the largest retained inscribed sphere is the maximal inscribed sphere (Fig. 12c). If additional iterations are required (as is the case in Fig. 12c), additional constraining particles are considered and the combinatoric approach is implemented again to converge upon the maximal inscribed sphere located completely within the pore space. While this process does not completely disassociate the inscribed sphere from the Delaunay cell, it qualitatively produces the same results in Al-Raoush et al. [1]. It should be noted that while Fig. 12 illustrates a convex configuration, solution to non-convex configurations are non-trivial and require an additional tun-

![Fig. 12](image-url) A 2D local configuration of five polydisperse particles (comprising three Delaunay cells). a The inscribed sphere (the initial solution) to the Delaunay cell formed by particles 2, 3, 4 is shown to intersect particle 1, and consequently local optimisation must be undertaken. The constraining particles are 1, 2, 3, 4. b There are \( n \choose 4 \) = 4 combinations and the inscribed sphere for each combination is illustrated. c Only two combinations have inscribed spheres that do not intersect the constraining particles. These solutions are retained and the largest of the retained solution is highlighted. Note that the high-lighted inscribed sphere is still not completely within the pore space, as it intersects particle 5. Hence, a subsequent iteration is required with constraining particles 1, 2, 3, 4, 5. d The retained solutions for the subsequent iteration is shown and the maximal inscribed sphere contained completely within the pore space is highlighted. It is worth noting that the solution to the remaining two Delaunay cells also converges to the same local maxima.

![Fig. 13](image-url) Comparison of the analytical expression for the shape parameter and numerical data extracted from m1l assembly in the N-RLPA dataset.

![Fig. 14](image-url) The \( k \)-gamma distribution function is able to accurately describe the pore volume distribution for pore units defined using the alternate merging criteria. A typical assembly (m1l in the N-RLPA dataset) is shown.
Fig. 15  a Cumulative distribution for all assemblies in the N-RLPA analysis. b Rescaled distribution collapses on to a single curve, demonstrating that uniqueness is maintained when applying the alternate merging criteria. This curve can be described by the parameter $k = 0.6$

Appendix 2: Analysis for alternate merging criteria

In the main body of this paper, pore units were defined using the merging criteria shown in Fig. 1b. It was acknowledged that the choice of the merging criteria is somewhat arbitrary, and can influence micro-scale observations. Indeed, Al-Raoush et al. [1] demonstrated that applying the merging criteria shown in Fig. 1a will result in the observation of a greater number of small pores. To assess the impact of the merging criteria on the broader macroscopic characteristics discussed in this paper, additional analysis was conducted using the criteria shown in Fig. 1a. This additional analysis was only conducted for the N-RLP dataset, and for comparison this additional analysis will be referred to by N-RLPA.

The key findings of this additional analysis are summarised below:

1. The analytical expression relating pore shape to local void ratio and local edge numbers in Eq. 20 continues to reasonably describe the numerical data in the N-RLPA analysis. This is illustrated in Fig. 13 for a typical assembly. It is acknowledged that there is some scatter for $N_e = 6$, associated with the increase number of small pores associated with the alternate merging criteria.
2. The $k$-gamma distribution function accurately reflects the volume distribution of pore units defined using the alternate merging criteria for all assemblies in the N-RLPA dataset. A typical case is shown in Fig. 14, while Fig. 15 demonstrates that uniqueness is still maintained as all distributions collapse to a single curve.

3. Figure 16 compares variations in the $k$-gamma distribution parameters for the N-RLPA analysis against that shown in Fig. 8. Figure 16c illustrates that the merging criteria has minimal influence on $k$, but affects the variation in $\chi$ (Fig. 16a) and $\chi k$ (Fig. 16b). The lower values observed for $\chi$ and $\chi k$ reflects the observation of a greater number of small pores when applying the alternate merging criteria. This result was anticipated as more stringent merging requirements will reduce the number of accessible configurations, that is, the alternate merging criteria will reduce the probability of encountering larger pores. Nevertheless, the linear relationship with void ratio outlined in Sect. 4 is maintained for both $\chi$ and $\chi k$.

4. Irrespective of the merging criteria, the pore orientation tensor, $\mathbf{P}$, can be applied to identify the major principal orientation of each pore units. In a similar manner to Fig. 10, the distribution of elevation angles for all assemblies in the N-RLPA dataset is shown in Fig. 17a. An isotropic distribution is still maintained for the pore units defined using the alternate merging criteria. Further, the analytical expression for the global orientation tensor in Eq. 35 is still applicable to the N-RLPA analysis as demonstrated in Fig. 17b. While the magnitude of $P_{ij}^M$ is affected by the choice of the merging criteria, the observation of isotropic directional distribution of pore volume is maintained.

These additional analysis suggests that choice of the merging criteria does not broadly influence the macroscopic observations detailed in this paper. It is acknowledged that it would be useful to identify pore characteristics as a function of this criteria, and this presents an interesting area of future research.

References

1. Al-Raoush, R., Thompson, K., Willson, C.S.: Comparison of network generation techniques for unconsolidated porous media. Soil Sci. Soc. Am. J. 67(6), 1687–1700 (2003)
2. Anikeenko, A.V., Medvedev, N.N.: Polytetrahedral nature of the dense disordered packings of hard spheres. Phys. Rev. Lett. 98(23), 235504 (2007)
3. Anikeenko, A.V., Medvedev, N.N., Aste, T.: Structural and entropic insights into the nature of the random-close-packing limit. Phys. Rev. E 77(3), 031101 (2008)
4. Aste, T., Di Matteo, T.: Emergence of Gamma distributions in granular materials and packing models. Phys. Rev. E 77(2), 021309 (2008)
5. Aste, T., Di Matteo, T., Saadatfar, M., Senden, T.J., Schröter, M., Swinney, H.L.: An invariant distribution in static granular media. Europhys. Lett. (EPL) 79(2), 24003 (2007). doi: 10.1209/0295-5075/79/24003
6. Aste, T., Saadatfar, M., Senden, T.J.: Geometrical structure of disordered sphere packings. Phys. Rev. E 71(6), 061,302 (2005). doi: 10.1103/PhysRevE.71.061302
7. Bagi, K.: Stress and strain in granular assemblies. Mech. Mater. 22(3), 165–177 (1996)
8. Bakke, S., Oren, P.E.: 3-D Pore-scale modelling of sandstone and flow simulations in the pore network. Soc. Pet. Eng. J. 2, 136–149 (1997)
9. Bryant, S.L., King, P.R., Mellor, D.W.: Network model evaluation of permeability and spatial correlation in real random sphere packing. Transp. Porous Media 1(1), 53–70 (1993)
10. Chang, C.S., Yin, Z.: Micromechanical modeling for inherent anisotropy in granular materials. J. Eng. Mech. 136(7), 830–839 (2010)
11. Coxeter, H.S.M.: Regular Polytopes, 3rd edn. Dover Publication, Inc., New York (1973)
12. Diambra, A., Russell, A.R., Ibraim, E., Muir Wood, D.: Determination of fibre orientation distribution in reinforced sands. Geotechnique 57(7), 623–628 (2007)
