

# Identification and analysis of 3D pores in packed particulate materials

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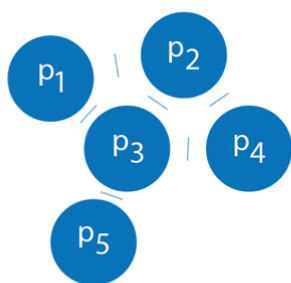
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authors and unedited

## Supplementary Information for

### Identification and analysis of 3D-pores in packed particulate materials

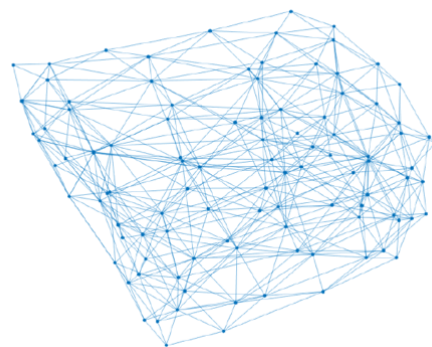
#### Supplementary Figures

**a**



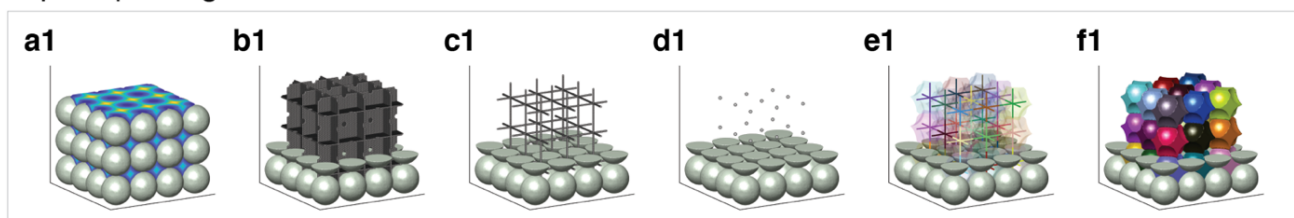
|                | p <sub>1</sub> | p <sub>2</sub> | p <sub>3</sub> | p <sub>4</sub> | p <sub>5</sub> |
|----------------|----------------|----------------|----------------|----------------|----------------|
| p <sub>1</sub> | 0              | 1              | 1              | 0              | 0              |
| p <sub>2</sub> | 1              | 0              | 1              | 1              | 0              |
| p <sub>3</sub> | 1              | 1              | 0              | 1              | 1              |
| p <sub>4</sub> | 0              | 1              | 1              | 0              | 0              |
| p <sub>5</sub> | 0              | 0              | 1              | 0              | 0              |

**b**

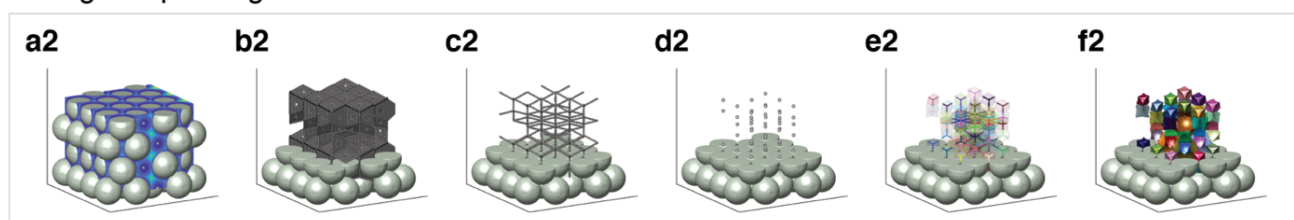


**Supplementary Figure 1 | Information about particle connectivity can be stored in an adjacency matrix and visually represented by a neighboring-particle graph. a,** We demonstrate using a 2D example: for a set of particles,  $p_1, \dots, p_5$ , we indicate that a pair of particles are neighbors, i.e., share a medial axis ridge (blue line), by inputting a 1 at the corresponding locations of the adjacency matrix (right). The adjacency matrix serves as a quick look-up table for particle connectivity. **b,** Particle configuration can be represented by a graph, where nodes represent the particles and edges represent 2D-ridges that exist between neighboring particles. The sample neighboring-particle graph represents a random packing of monodisperse 130  $\mu\text{m}$  diameter spherical, rigid particles in a 600 x 600 x 600  $\mu\text{m}^3$  container.

## Square packing



## Hexagonal packing



**Supplementary Figure 2 | LOVAMAP methodology outputs for square packing and hexagonal packing.** **a1,2**, Heatmap representation of the Euclidean distance transform (EDT) computed on the void space. **b1,2**, 2D-ridges, which lie between neighboring particles. **c1,2**, 1D-ridges, which lie at the intersection of 2D-ridges. **d1,2**, Peaks, which lie at the intersection of 1D-ridges. **e1,2**, Void space 3D-pore backbones with transparent pore. **f1,2**, Void space 3D-pores. For square packing, we are showing both interior and surface pores; for hexagonal packing, we are only showing interior 3D-pores.

a)

3D-pore volume (pL)

square:  $y = (8(\frac{x}{2})^3 - (\frac{4}{3})\pi(\frac{x}{2})^3) / 1.0e-6$

NRMSE: 2.011e-4

hexagonal:  $y = (\frac{4}{3}(\frac{x}{2})^3 - \frac{4}{3}(3\arccos(\frac{1}{3}) - \pi)(\frac{x}{2})^3) / 1.0e-6$

NRMSE: 0.04279

$y = (5.026e-8)x^3 + (2.010e-5)x^2 - (1.540e-3)x + 0.03603$

R<sup>2</sup>: 0.9990

b)

# 3D-pores · pL<sup>-1</sup>

40 & 100:  $y = (-2.949e-2)*x + 0.02902$  R<sup>2</sup>: 0.9960

50 & 100:  $y = (-1.247e-2)*x + 0.01261$  R<sup>2</sup>: 0.9938

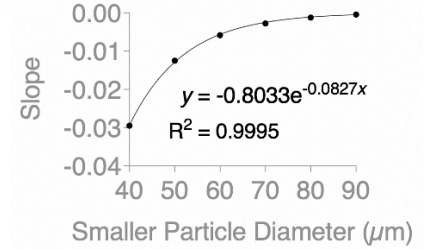
60 & 100:  $y = (-5.826e-3)*x + 0.006271$  R<sup>2</sup>: 0.9871

70 & 100:  $y = (-2.748e-3)*x + 0.003345$  R<sup>2</sup>: 0.9836

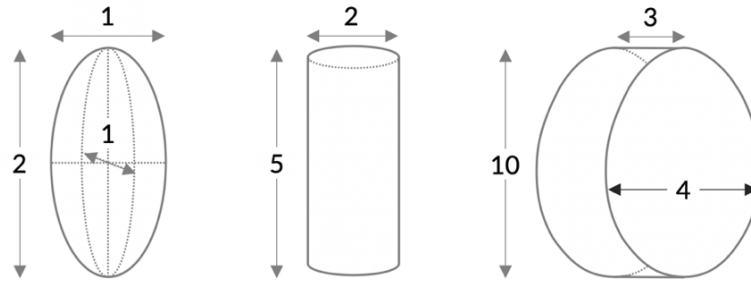
80 & 100:  $y = (-1.223e-3)*x + 0.001876$  R<sup>2</sup>: 0.9502

90 & 100:  $y = (-4.115e-4)*x + 0.001105$  R<sup>2</sup>: 0.7084

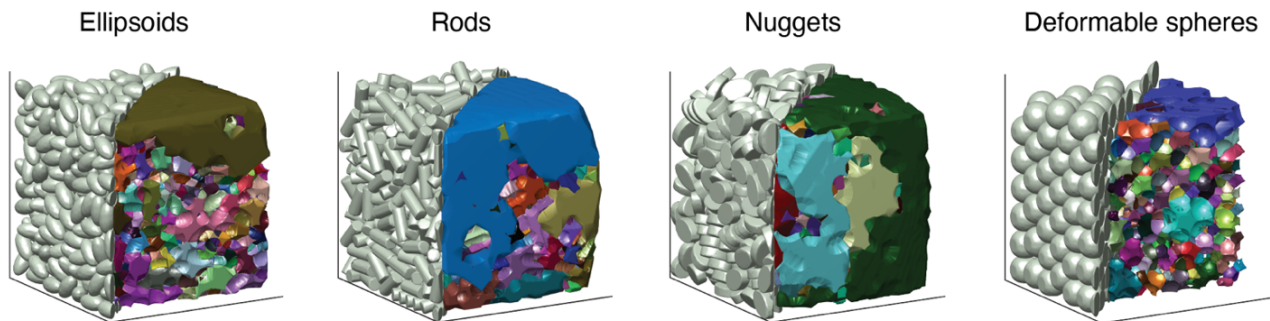
c)



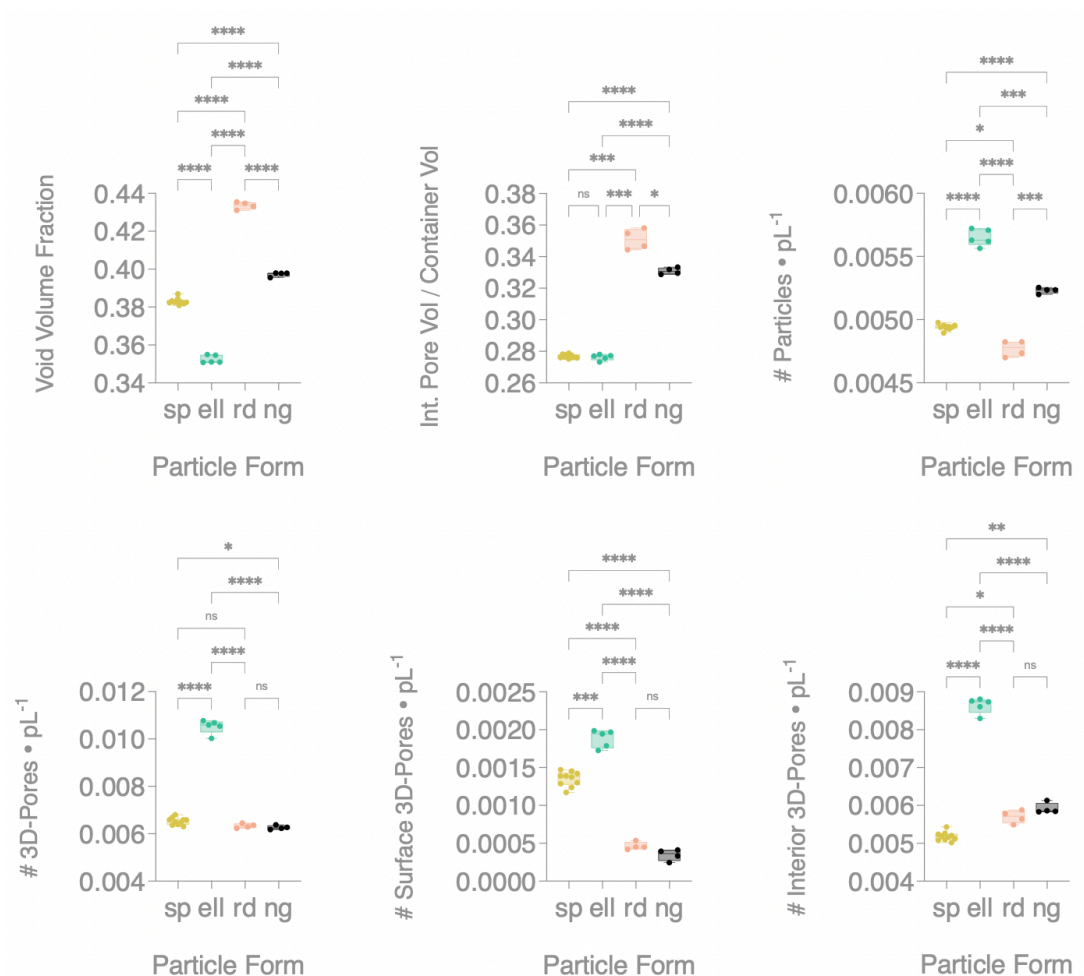
**Supplementary Figure 3 | Error to predicted and fitted curves.** **a**, For square packing of spheres, we report the closed-form expression for 3D-pore volume scaled to picoliters (pL), then use this expression to compute the root mean squared error normalized by the mean (NRMSE) for LOVAMAP outputs. For hexagonal packing, we derive an expression that closely approximates 3D-pore volume of the smaller pore and report NRMSE for LOVAMAP outputs; for the larger pore, we fit a third-degree polynomial to LOVAMAP outputs using least squares (reporting R-squared). For all equations,  $x$  = particle diameter of sphere (μm),  $y$  = 3D-pore volume (pL). **b**, For binary mixtures of two different sphere sizes, we fit a linear equation to the number of 3D-pores (per pL) using least squares (reporting R-squared).  $x$  = Proportion of Larger Particle,  $y$  = # of 3D-pores per pL. **c**, The slopes of the linear equations in (b) are plotted as a function of the smaller particle diameter and fit to an exponential curve ( $R^2 = 0.9995$ ).



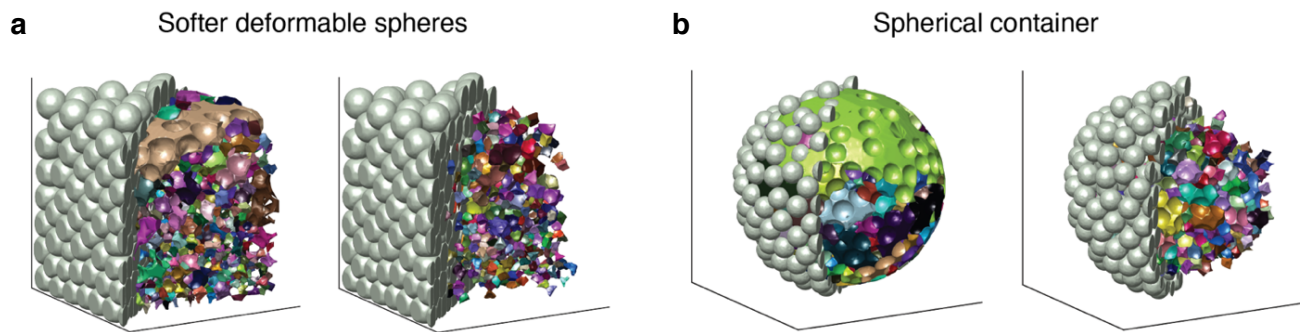
**Supplementary Figure 4 | Relative dimensions for non-spherical particles.** For ellipsoids (prolate spheroids), rods (cylinders), and nuggets (egg-like shape), we adjust particle size to match the volume of equivalent spheres while holding the above ratios constant.



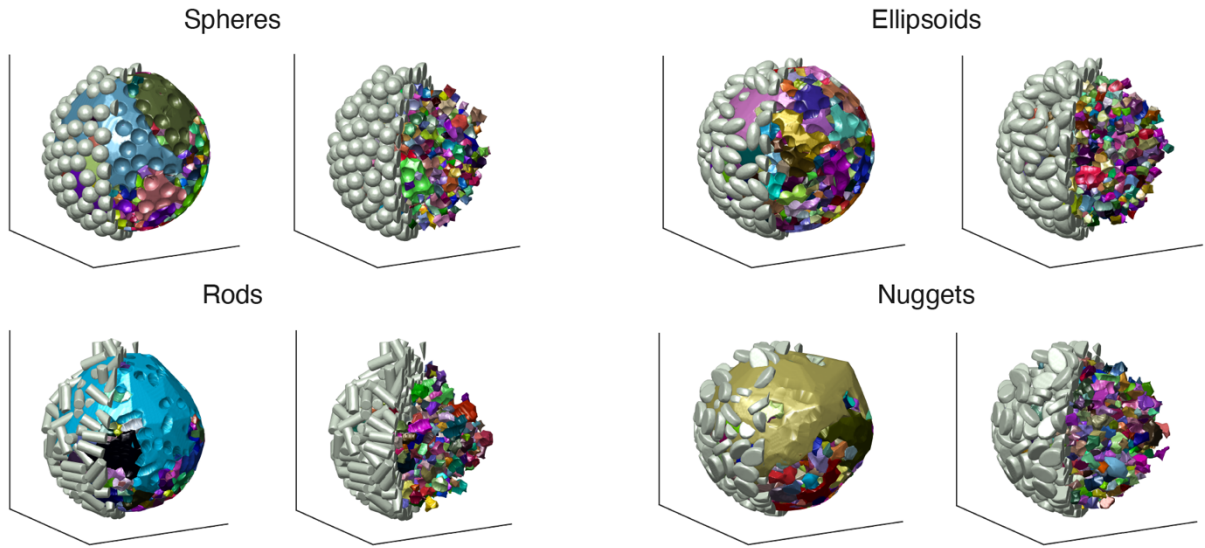
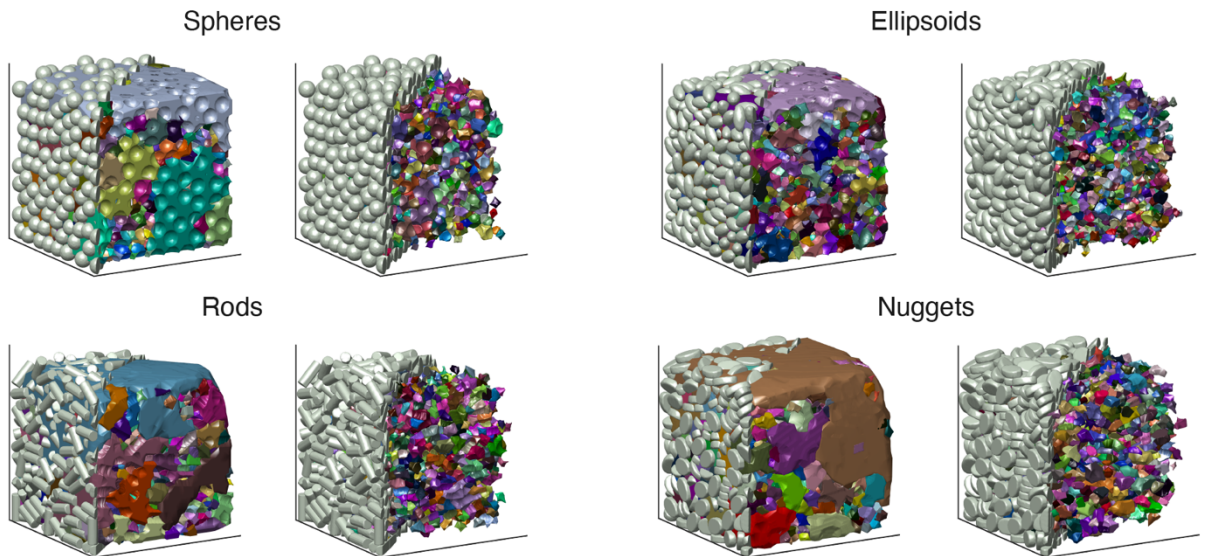
**Supplementary Figure 5 | LOVAMAP output of surface 3D-pores for monodisperse packed particles.** These images are the surface-pore counterparts to Figure 3E-H.



**Supplementary Figure 6 | LOVAMAP output comparisons for rigid spheres (sp), ellipsoids (ell), rods (rd), and nuggets (ng).** Reporting the void volume fraction, the cumulative interior 3D-pore volume normalized by container size, the number of particles per picoliter (pL), the total number of 3D-pores per pL (shown in Figure 3I, inset), the number of surface 3D-pores per pL (i.e., pores that extend to the exterior of the packing structure), and the number of interior 3D-pores per pL for each particle domain. Domains contain particles with volume equal to 113 pL (the volume of a 60  $\mu\text{m}$  diameter sphere).  $N = 10, 5, 4$ , and  $4$ , for spheres, ellipsoids, rods, and nuggets, respectively. Statistical analysis using Welch's ANOVA test (\*\*\*\*  $p$ -value =  $<0.0001$ ).

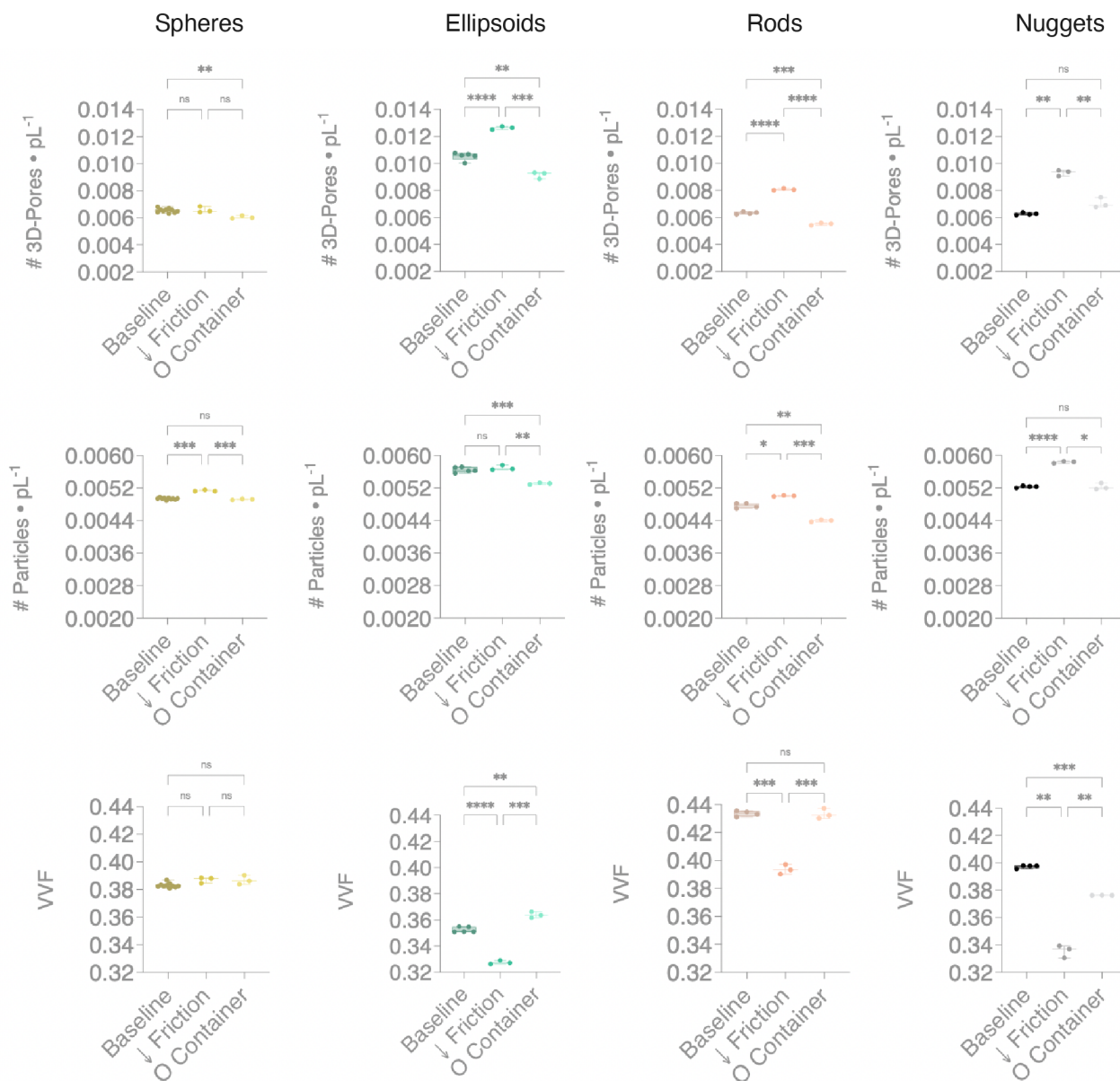


**Supplementary Figure 7 | Test datasets used as unbiased estimators.** **a**, Showing surface and interior 3D-pores for 100  $\mu\text{m}$  diameter 'softer' deformable spheres ( $\delta = 100$ ,  $\lambda = 400$ ,  $\mu = 50$ ) in a 600 x 600 x 600  $\mu\text{m}^3$  cubic container. **b**, Showing surface and interior 3D-pores for 60  $\mu\text{m}$  diameter rigid spheres in a 600  $\mu\text{m}$  diameter spherical container.

**a****Spherical Container****b****Lower Friction****c****NRMSE**

|            | Spherical Container |                 | Lower Friction |                 |
|------------|---------------------|-----------------|----------------|-----------------|
|            | # 3D-Pores          | Median Pore Vol | # 3D-Pores     | Median Pore Vol |
| Spheres    | 0.03731             | 0.00092         | 0.00910        | 0.00163         |
| Ellipsoids | 0.00456             | 0.05146         | 0.04816        | 0.09565         |
| Rods       | 0.01021             | 0.01561         | 0.01277        | 0.04061         |
| Nuggets    | 0.02234             | 0.09323         | 0.00042        | 0.13495         |

**Supplementary Figure 8 | Varying particle friction and container shape for rigid spheres (sp), ellipsoids (ell), rods (rd), and nuggets (ng).** **a**, Showing surface and interior 3D-pores for packed particle domains generated using friction parameter = 0.5, where default friction parameter = 1.0. **b**, Showing surface and interior 3D-pores for packed particle domains generated using a 600  $\mu\text{m}$  diameter spherical container. **c**, LOVAMAP output data for (a) and (b) are shown overlaying Equation 1 curve from Figure 2J. **d**, Reporting the root mean squared error normalized by the mean (NRMSE) for datapoints in (c), which confirms good fit. Domains contain particles with volume equal to 113 pL (the volume of a 60  $\mu\text{m}$  diameter sphere).

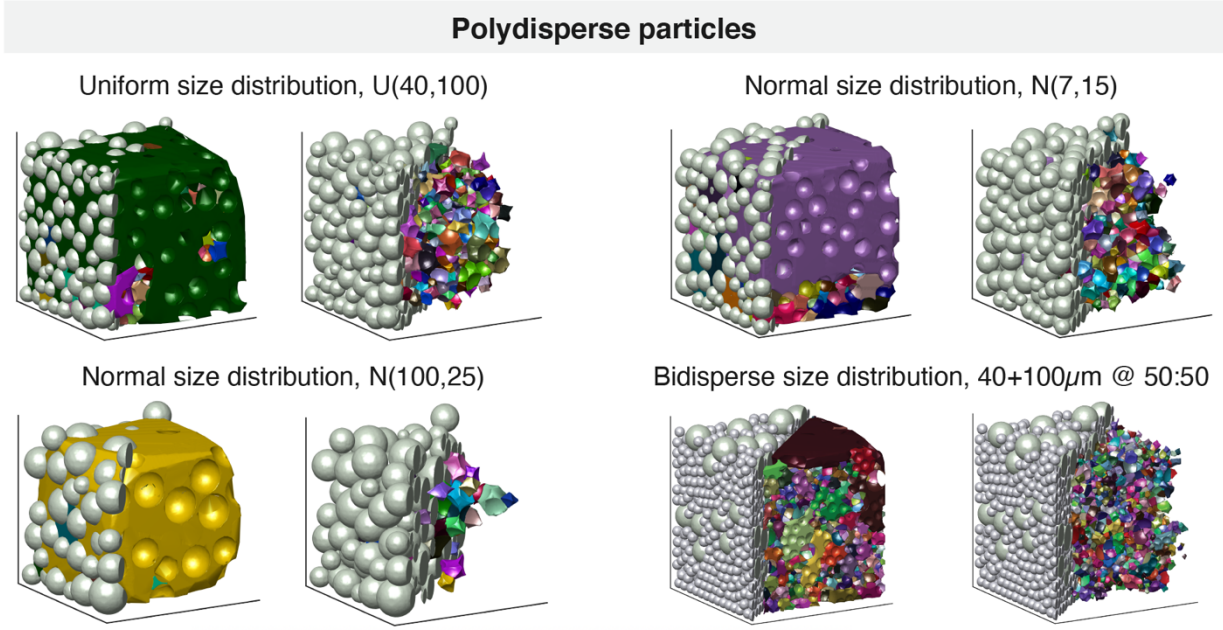


**Supplementary Figure 9 | LOVAMAP output comparisons for particle domains in Supp. Fig. 6**

**and 8.** Reporting the total number of 3D-pores per picoliter (pL), the number of particles per pL, and the void volume fraction (VVF) for Baseline domains (cubic container with default friction parameter = 1.0), ↓ Friction (cubic container with friction parameter = 0.5), and O Container (spherical container with default friction parameter = 1.0). As expected, lower friction generally leads to more particles and less VVF. Spherical particles are least sensitive to changes in friction and container shape. Data accompanies domain images in Supplementary Figure 8. Domains contain particles with volume equal

to 113 pL (the volume of a 60  $\mu\text{m}$  diameter sphere).  $N = 10, 5, 3,$  and  $3,$  for Baseline spheres, Baseline non-spheres,  $\downarrow$  Friction, and O Container groups, respectively. Statistical analysis using Welch's ANOVA test (\*\*\*\*  $p\text{-value} = <0.0001$ ).

**a**



**b**

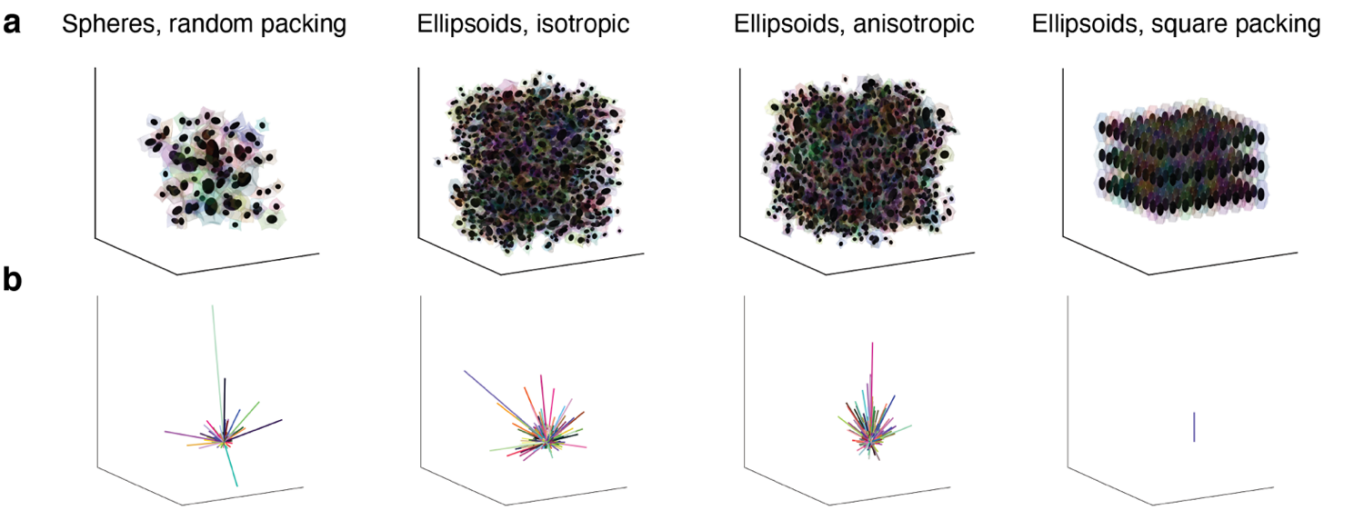
**NRMSE**

|             | # 3D-Pores | Median Pore Vol |
|-------------|------------|-----------------|
| U(40,100)   | 0.04348    | 0.00650         |
| N(70,15)    | 0.00498    | 0.00259         |
| N(100,5)    | 0.11062    | 0.08511         |
| N(100,20)   | 0.25292    | 0.01578         |
| N(100,25)   | 0.30726    | 0.01695         |
| B(40,50:50) | 0.01749    | 0.63499         |
| B(50,70:30) | 0.00274    | 0.40328         |
| B(80,50:50) | 0.12536    | 0.04924         |

**Supplementary Figure 10 | Varying particle size distribution.** **a**, Showing surface and interior 3D-pores for packed particle domains generated using friction parameter = 0.5, where default friction parameter = 1.0. **b**, Showing surface and interior 3D-pores for packed particle domains generated using a 600 μm diameter spherical container. **c**, LOVAMAP output data for (a) and (b) are shown overlaying Equation 1 curve from Figure 2J. **d**, Reporting the root mean squared error normalized by the mean (NRMSE) for datapoints in (c), which confirms good fit. Domains contain particles with volume equal to 113 pL (the volume of a 60 μm diameter sphere).

|          | Rigid |        |      | Semi-soft |        |      | Soft |        |      |
|----------|-------|--------|------|-----------|--------|------|------|--------|------|
|          | min   | median | max  | min       | median | max  | min  | median | max  |
| 2D-pores | 4.92  | 25.2   | 220  | 4.51      | 16.0   | 124  | 4.51 | 14.2   | 67.7 |
| 3D-pores | 21.5  | 30.7   | 98.7 | 8.00      | 21.5   | 58.0 | 5.66 | 14.4   | 56.0 |

**Supplementary Figure 11 | Comparing 2D-pore vs. 3D-pore diameters ( $\mu\text{m}$ ) for rigid, semi-soft, and soft 100  $\mu\text{m}$  diameter spherical particle domains.** Approximating pore diameter using 2D z-slice data produces smaller median 2D-pore diameters and a wider range in values (min, max) compared to LOVAMAP 3D-pore diameters. This trend is more apparent for stiffer particles. See **Methods** section “Surface of the particle packing: segmenting into 2D surface pores” for how we generate 2D-pores.

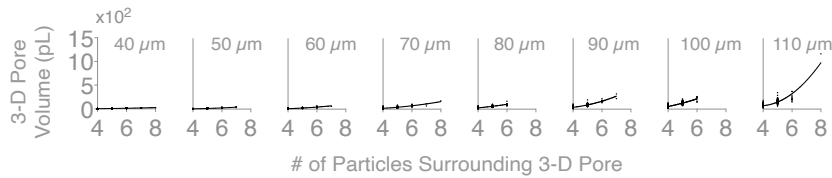


**Supplementary Figure 12 | PCA ellipsoid images of particle domains with ranging particle orientation.** **a**, PCA ellipsoids of interior 3D-pores shown for corresponding particle domains in Figure 4C. **b**, Major axes vectors of the PCA ellipsoids in (a), scaled by their respective eigenvalues and translated to a common point.

|                     |                                   |               |
|---------------------|-----------------------------------|---------------|
| 40 $\mu\text{m}$ :  | $y = 0.08129x^2 + 5.013x - 20.91$ | $R^2: 0.9606$ |
| 50 $\mu\text{m}$ :  | $y = 0.2085x^2 + 8.907x - 37.28$  | $R^2: 0.9648$ |
| 60 $\mu\text{m}$ :  | $y = 0.4412x^2 + 13.68x - 57.07$  | $R^2: 0.9639$ |
| 70 $\mu\text{m}$ :  | $y = 0.5517x^2 + 24.40x - 100.5$  | $R^2: 0.9686$ |
| 80 $\mu\text{m}$ :  | $y = 0.9912x^2 + 34.31x - 140.9$  | $R^2: 0.9655$ |
| 90 $\mu\text{m}$ :  | $y = 2.058x^2 + 37.27x - 157.4$   | $R^2: 0.9625$ |
| 100 $\mu\text{m}$ : | $y = 2.272x^2 + 60.90x - 247.7$   | $R^2: 0.9569$ |
| 110 $\mu\text{m}$ : | $y = 3.101x^2 + 74.83x - 301.5$   | $R^2: 0.9727$ |

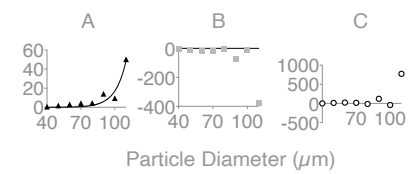
**Supplementary Figure 13 | Quadratic fit using least squares for LOVAMAP 3D-pore volumes plotted by number of surrounding particles.** Ranging particle diameter from 40  $\mu\text{m}$  to 110  $\mu\text{m}$ . Accompanies Figure 5F.

**a** Over-segmentation: Monodisperse spheres



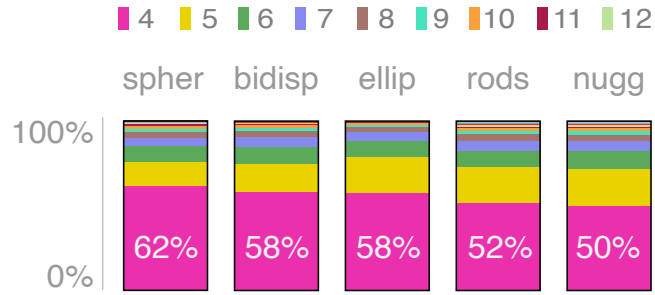
|                     |                                     |               |
|---------------------|-------------------------------------|---------------|
| 40 $\mu\text{m}$ :  | $y = 0.6494x^2 - 1.788x - 0.005339$ | $R^2: 0.8576$ |
| 50 $\mu\text{m}$ :  | $y = 1.871x^2 - 8.965x + 12.19$     | $R^2: 0.8514$ |
| 60 $\mu\text{m}$ :  | $y = 3.184x^2 - 15.13x + 20.59$     | $R^2: 0.8274$ |
| 70 $\mu\text{m}$ :  | $y = 4.301x^2 - 16.30x + 14.99$     | $R^2: 0.7495$ |
| 80 $\mu\text{m}$ :  | $y = 4.493x^2 - 7.445x - 14.27$     | $R^2: 0.7558$ |
| 90 $\mu\text{m}$ :  | $y = 14.13x^2 - 76.63x + 120$       | $R^2: 0.8004$ |
| 100 $\mu\text{m}$ : | $y = 9.509x^2 - 13.49x - 43.09$     | $R^2: 0.7480$ |
| 110 $\mu\text{m}$ : | $y = 50.33x^2 - 376.5x + 774.2$     | $R^2: 0.7719$ |

**b** Quadratic fit:  $y = Ax^2 + Bx + C$



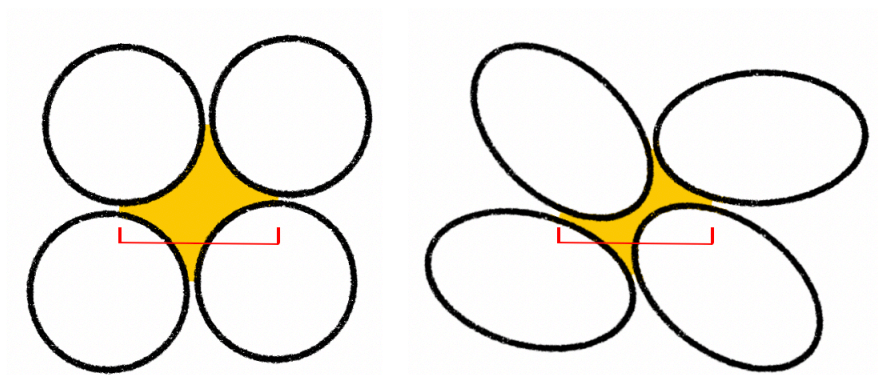
|                                 |                |
|---------------------------------|----------------|
| $A = 0.0004353e^{0.1057\delta}$ | $R^2: 0.9174$  |
| $B$ , unstable parameters       | $R^2: -0.2894$ |
| $C$ , nonconvergence            |                |

**Supplementary Figure 14 | Over-segmentation outputs of 3D-pore volume plotted by number of surrounding particles.** **a**, Ranging particle diameter from 40  $\mu\text{m}$  to 110  $\mu\text{m}$ . 3D-pores derived from over-segmentation are surrounded by no more than eight particles (compare to LOVAMAP outputs in Figure 5F). Quadratic curves using least squares show worse fits ( $R^2$ ) relative to LOVAMAP data shown in Supplementary Figure 13. **b**, Coefficients of quadratic curves in (a) do not all follow exponential trends as in Figure 5G for LOVAMAP outputs.  $\delta$  = spherical particle diameter ( $\mu\text{m}$ ). Parameters for B were unstable and therefore were not returned; an exponential fit for C did not converge and therefore parameters were not returned.



### Supplementary Figure 15 | 3D-pore population percentage by number of surrounding particles.

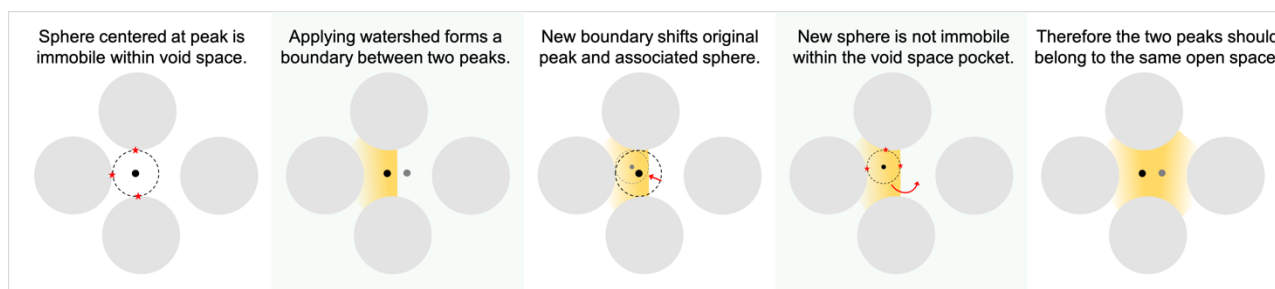
These plots show the proportion of 3D-pore types in different particle domains, where pore types are organized by the number of particles surrounding them (indicated by color legend at top). Key: (spher) spheres, (bidisp) bidisperse spheres, (ellip) ellipsoids, (nugg) nuggets. Showing cumulative pore data from  $N = 5$  domains.



**Supplementary Figure 16 | Pore volume vs. longest end-to-end length.** Compared to spheres, non-spherical-particle forms offer more opportunity for inward protrusion, which reduces pore volume while maintaining comparable longest length.

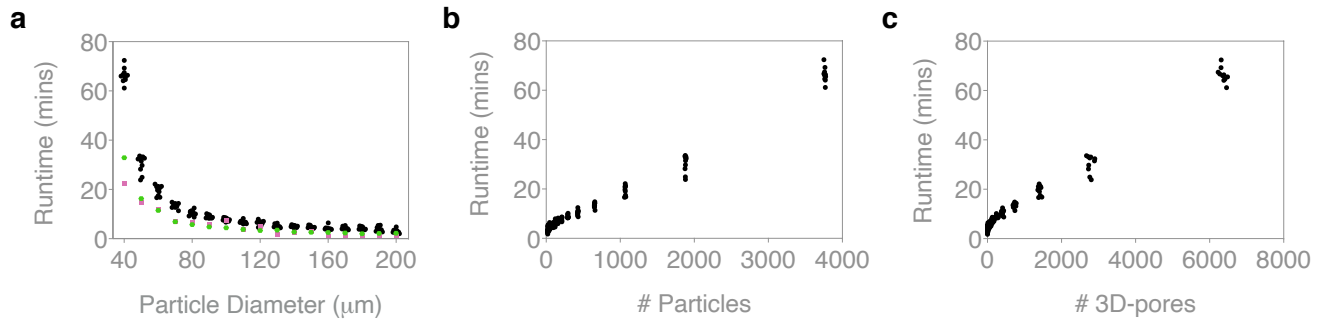
|                                 | Spheres | Ellipsoids | Rods  | Nuggets |
|---------------------------------|---------|------------|-------|---------|
| Longest Length / Avg. Int. Diam | 2.604   | 2.773      | 3.05  | 3.142   |
| PCA 1 / PCA 3                   | 1.448   | 1.565      | 1.765 | 1.770   |

**Supplementary Figure 17 | Median values for aspect ratio data.** (top) Aspect ratio computed as longest end-to-end length divided by the average internal diameter of 3D-pores. (bottom) Aspect ratio computed as PCA ellipsoid axis 1 divided by PCA ellipsoid axis 3. Both measurements of aspect ratio support the notion that packing of spherical particles produces less oblong 3D-pores relative to the other particle types. Accompanies Fig. 6E. See **Methods** section “**Computing Descriptors**” for additional detail of metrics.



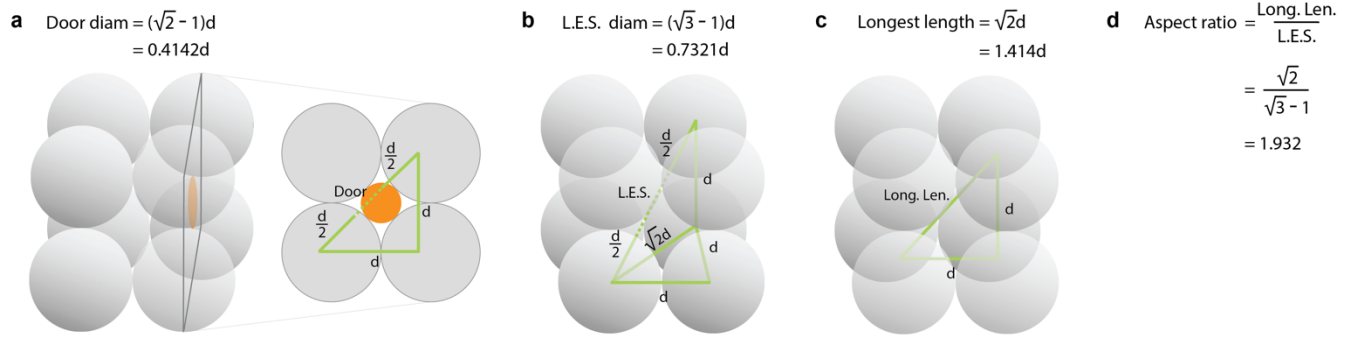
**Supplementary Figure 18 | Rationale for associating two peaks as part of the same pore.**

Accompanies ‘alternative explanation’ discussed in **Methods** section “**Associating peaks that belong to the same open space.**”



### Supplementary Figure 19 | Runtimes for packed particle analysis of monodisperse spheres

using LOVAMAP. **a**, Runtimes by particle diameter, where each data point represents a simulated particle domain comprising monodisperse, rigid, spherical particles in random packing (black;  $N = 10$  per size range), square packing (pink), or hexagonal packing (green). The number of voxels for each domain is kept within a range of  $2.9 - 3.4 \times 10^7$ . We see an expected inverse relationship between particle size and runtime. **b**, Runtimes by number of particles in a given domain containing monodisperse, rigid particles. As expected, runtimes increase as the number of particles increase. **c**, Runtimes by number of void space 3D-pores produced by LOVAMAP during segmentation of monodisperse, rigid, packed particles. Runtimes increase as the number of 3D-pores increases, which correlates with (b). All runtimes include LOVAMAP processes, as well as initial data transformation into 'labeled particle domains' from sphere data. Machine specifications: Intel Core i7-6800K (3.4 GHz) with 64 GB of RAM.



### Supplementary Figure 20 | Deriving descriptor measurements for square packing domains to

**validate LOVAMAP outputs.** **a**, (left) In square packing of spheres, the smallest door (orange circle) corresponds to the largest enclosed circle in 2D square packing of circles. The diameter of the largest enclosed circle (dotted green line) is 41.4% of  $d$ , where  $d$  is the diameter of the particles. For square packing of 100  $\mu\text{m}$  diameter particles, LOVAMAP returns a value of 42.9% for smallest door diameter, which is in good agreement with the analytical results. **b**, The largest enclosed sphere (L.E.S.) diameter (green dotted line; 3D-pore and L.E.S. not shown) is 73.2% of  $d$ . For square packing of 100  $\mu\text{m}$  diameter particles, LOVAMAP returns a value of 71.7% for largest enclosed sphere diameter, which is also in good agreement. Discrepancies between numerical and analytical results are attributed to the discretization of simulated data that depends on mesh size. **c**, The longest end-to-end length of a 3D-pore (Long. Len.) within square packing (see Figure 3A for example pores) is 141% of  $d$ . For square packing of 100  $\mu\text{m}$  diameter particles, LOVAMAP returns a value of 125% for longest length. The discrepancy is related to mesh size; namely, the mesh size may not be able to resolve the existence of void space voxels directly between touching particles. For this reason, the longest distance computed in LOVAMAP may be less than the true value. **d**, For our aspect ratio metric that is computed using longest end-to-end length and L.E.S., square packing of spheres has an aspect ratio of 1.93. LOVAMAP returns a value of 1.75. The discrepancy is due to discrepancy for both metrics described in (b) and (c).

Supplementary Table

| Particle Diameter<br>( $\mu\text{m}$ )<br>(of equivalent<br>sphere) | Square<br>Packing | Hexagonal<br>Packing | Spheres            | Semi-Soft<br>Spheres | Soft Spheres<br>(test a) | Spheres in<br>Spherical<br>Container<br>(test b) |  |  |  |  |
|---------------------------------------------------------------------|-------------------|----------------------|--------------------|----------------------|--------------------------|--------------------------------------------------|--|--|--|--|
| 40                                                                  | 0.47              | 0.26                 | $0.38 \pm 0.00075$ |                      |                          |                                                  |  |  |  |  |
| 50                                                                  | 0.47              | 0.26                 | $0.38 \pm 0.0015$  | 0.29                 |                          |                                                  |  |  |  |  |
| 60                                                                  | 0.47              | 0.26                 | $0.38 \pm 0.0017$  |                      |                          | $0.39 \pm 0.0025$                                |  |  |  |  |
| 70                                                                  | 0.47              | 0.26                 | $0.39 \pm 0.0023$  | $0.25 \pm 0.0037$    |                          |                                                  |  |  |  |  |
| 80                                                                  | 0.48              | 0.25                 | $0.39 \pm 0.0034$  |                      |                          |                                                  |  |  |  |  |
| 90                                                                  | 0.47              | 0.25                 | $0.39 \pm 0.0043$  |                      |                          |                                                  |  |  |  |  |
| 100                                                                 | 0.47              | 0.25                 | $0.39 \pm 0.0081$  | $0.23 \pm 0.0036$    | $0.12 \pm 0.0032$        |                                                  |  |  |  |  |
| 110                                                                 | 0.47              | 0.26                 | $0.39 \pm 0.0058$  |                      |                          |                                                  |  |  |  |  |
| 120                                                                 | 0.48              | 0.25                 | $0.39 \pm 0.013$   |                      |                          |                                                  |  |  |  |  |
| 130                                                                 | 0.47              | 0.27                 | $0.39 \pm 0.011$   | $0.23 \pm 0.0069$    |                          |                                                  |  |  |  |  |
| 140                                                                 | 0.48              | 0.25                 | $0.40 \pm 0.012$   |                      |                          |                                                  |  |  |  |  |
| 150                                                                 | 0.47              | 0.25                 | $0.41 \pm 0.020$   |                      |                          |                                                  |  |  |  |  |

| Particle Diameter<br>( $\mu\text{m}$ )<br>(of equivalent<br>sphere) | Ellipsoids        | Ellipsoids in<br>Spherical<br>Container | Isotropic<br>Ellipsoids | Anisotropic<br>Ellipsoids | Square<br>Packing<br>Ellipsoids | Rods              | Rods in<br>Spherical<br>Container | Nuggets           | Nuggets in<br>Spherical<br>Container |
|---------------------------------------------------------------------|-------------------|-----------------------------------------|-------------------------|---------------------------|---------------------------------|-------------------|-----------------------------------|-------------------|--------------------------------------|
| 60                                                                  | $0.35 \pm 0.0021$ | $0.36 \pm 0.004$                        | $0.35 \pm 0.00092$      | 0.36                      | 0.48                            | $0.43 \pm 0.0020$ | $0.36 \pm 0.0029$                 | $0.40 \pm 0.0012$ | $0.38 \pm 0.0028$                    |
| 70                                                                  | $0.35 \pm 0.0026$ |                                         |                         |                           |                                 | $0.44 \pm 0.0056$ |                                   |                   |                                      |
| 80                                                                  | $0.35 \pm 0.0017$ |                                         |                         |                           |                                 | $0.45 \pm 0.0080$ |                                   | $0.41 \pm 0.0051$ |                                      |
| 90                                                                  | $0.36 \pm 0.0017$ |                                         |                         |                           |                                 | $0.45 \pm 0.0039$ |                                   |                   |                                      |
| 100                                                                 | $0.36 \pm 0.0023$ |                                         |                         |                           |                                 | $0.46 \pm 0.0075$ |                                   | $0.41 \pm 0.0057$ |                                      |
| 110                                                                 | $0.36 \pm 0.0051$ |                                         |                         |                           |                                 | $0.46 \pm 0.0099$ |                                   |                   |                                      |
| 120                                                                 | $0.36 \pm 0.0069$ |                                         |                         |                           |                                 | $0.47 \pm 0.013$  |                                   | $0.42 \pm 0.0046$ |                                      |

| Percentage of<br>Smaller Particle | 40 + 100 $\mu\text{m}$ | 50 + 100 $\mu\text{m}$ | 60 + 100 $\mu\text{m}$ | 70 + 100 $\mu\text{m}$ |
|-----------------------------------|------------------------|------------------------|------------------------|------------------------|
| 10%                               | $0.36 \pm 0.0063$      | $0.37 \pm 0.0054$      | $0.38 \pm 0.0043$      | $0.38 \pm 0.0062$      |
| 20%                               | $0.34 \pm 0.0054$      | $0.36 \pm 0.0056$      | $0.37 \pm 0.0037$      | $0.38 \pm 0.0039$      |
| 30%                               | $0.33 \pm 0.0046$      | $0.35 \pm 0.0036$      | $0.37 \pm 0.0051$      | $0.38 \pm 0.0063$      |
| 40%                               | $0.33 \pm 0.0049$      | $0.35 \pm 0.0038$      | $0.37 \pm 0.0035$      | $0.38 \pm 0.0043$      |
| 50%                               | $0.34 \pm 0.0052$      | $0.36 \pm 0.0028$      | $0.37 \pm 0.0039$      | $0.38 \pm 0.0032$      |
| 60%                               | $0.35 \pm 0.0041$      | $0.36 \pm 0.0044$      | $0.37 \pm 0.0041$      | $0.38 \pm 0.0029$      |
| 70%                               | $0.35 \pm 0.0031$      | $0.36 \pm 0.0059$      | $0.38 \pm 0.0033$      | $0.38 \pm 0.0017$      |
| 80%                               | $0.36 \pm 0.0035$      | $0.37 \pm 0.0050$      | $0.38 \pm 0.0052$      | $0.38 \pm 0.0049$      |
| 90%                               | $0.37 \pm 0.0013$      | $0.37 \pm 0.0016$      | $0.38 \pm 0.0035$      | $0.38 \pm 0.0038$      |

Supplementary Table 1 | Void volume fraction (VVF) of monodisperse particle domains.

Reporting mean and standard deviation of VVF for particle domain types. Particles are contained within a 600 x 600 x 600  $\mu\text{m}^3$  container unless otherwise stated. Spherical containers are 600  $\mu\text{m}$  in diameter.

Supplementary Notes

1. A Johnson-Mehl tessellation begins with points that expand at differing rates to form cells, while a set-Voronoi tessellation begins with the boundaries of sets of points and expands outward at a constant rate. Both terms have been used to refer to tessellations with non-linear boundaries.

2. Other metrics of distance include city-block/Manhattan (grassfire transform) and chessboard distance<sup>65, 71</sup>.
3. Experimental datasets comprise the following monodisperse packed particle domains: spheres (40, 50, 60, 70, 80, 90, 100, 110  $\mu\text{m}$  diameter), ellipsoids (60, 63, 70, 80, 90, 100, 110, 120  $\mu\text{m}$  diameter), rods (60, 62, 70, 80, 90, 100, 110, 120  $\mu\text{m}$  diameter), nuggets (60, 66, 80, 100, 120  $\mu\text{m}$  diameter), and deformable spheres (50, 70, 100, 130  $\mu\text{m}$  diameter). For non-spherical particles, groups refer to particle volumes that are equal to spheres with the listed diameters.