Online Supplementary Material

A Granocentric model v2 master equations

Using the description of the model in Sec. 1.1, we derive the relationship between the three model control parameters and the probability distributions of neighbors and contacts. Recall that each time a neighbor is selected for a given central particle, it takes up a portion of the available solid angle, Ω^*, and that neighbors are selected until the sum of all filled solid angle is greater than Ω^*. The probability density function (pdf) for the amount of solid angle each neighbor fills, $\rho(\omega)$, depends on both the center particle and neighbor particle radius, as well as their surface-to-surface distance. Thus the distribution $\rho(\omega)$ inherently depends on the distribution of particle radii, as well as the model control parameters p and δ^*. Therefore, the probability distribution for the number of neighbors depends on all three model control parameters. In order to determine this distribution, we may write a master equation for $F_n(\Omega)$, the probability that after n neighboring particles have been selected, their total solid angle is less than Ω. By considering all possible solid angles for the next added particle, we obtain the master equation

$$F_{n+1}(\Omega) = \int_0^\Omega F_n(\Omega-\omega)\rho(\omega)d\omega \tag{1}$$

where $F_0(\Omega) = 1$. To relate this function to the probability that the central particle has exactly n neighbors, first recall that the last added neighbor is included into the neighbor shell only half the time. Also realize that neighbors are added until the last added neighbor causes the filled solid angle to increase above the threshold Ω^*; before adding the last neighbor the filled solid angle is less than Ω^*. Then, if the last neighbor is to be rejected from the shell of neighbors, there must be n neighbors that do not overfill Ω^*, but $n+1$ that do. This happens with probability $F_n(\Omega^*) - F_{n+1}(\Omega^*)$. Similarly, if the last neighbor is to be accepted, there must be $n-1$ neighbors that do not overfill Ω^*, but n that do. This occurs with probability $F_{n-1}(\Omega^*) - F_n(\Omega^*)$. Combining these we obtain the probability that there are exactly n neighbors as

$$P(N=n) = \frac{1}{2}\Big[F_{n-1}(\Omega^*) - F_{n+1}(\Omega^*)\Big]. \tag{2}$$

We follow a similar procedure to determine the joint probability for the number of neighbors and the number of contacts by creating a master equation for the function $G_n(\Omega, z)$, the probability that after adding n particles, z of which are contacting, the total filled solid angle is below Ω. The pdf for the amount of solid angle each neighbor fills, $\rho(\omega)$, can be divided between contacting and non-contacting neighbors as $\rho(\omega) = p\rho_z(\omega)+(1-p)\rho_n(\omega)$ where $\rho_z(\omega)$ is the conditional pdf for the solid angle of contacting neighbors and $\rho_n(\omega)$ is the conditional pdf for the solid angle of non-contacting neighbors. We obtain the master equation

$$\begin{aligned} G_{n+1}(\Omega, z) = p\int_0^\Omega G_n(\Omega-\omega, z-1)\rho_z(\omega)d\omega \\ + (1-p)\int_0^\Omega G_n(\Omega-\omega, z)\rho_n(\omega)d\omega, \end{aligned} \tag{3}$$

for $G_n(\Omega, z)$ by considering whether the next added neighbor is a contact (and increase z by one) or is not. We may write the joint distribution for n neighbors and z contacts by considering three cases: (1) the last added particle is not kept as a neighbor, (2) the last added neighbor is a non-contact and is kept, and (3) the last added neighbor is a contact and is kept. These possibilities are independent, and their respective probabilities can be added to obtain

$$P(N=n, Z=z) = \frac{1}{2}\Big(G^{(1)} + (1-p)G^{(2)} + pG^{(3)}\Big) \tag{4}$$

where

$$G^{(1)} = G_n(\Omega^*, z) - \int_0^{\Omega^*} G_n(\Omega^*-\omega, z)\rho(\omega)d\omega$$

$$G^{(2)} = G_{n-1}(\Omega^*, z) - \int_0^{\Omega^*} G_{n-1}(\Omega^*-\omega, z)\rho_n(\omega)d\omega$$

$$G^{(3)} = G_{n-1}(\Omega^*, z-1) - \int_0^{\Omega^*} G_{n-1}(\Omega^*-\omega, z-1)\rho_c(\omega)d\omega$$

are the probabilities of the three cases enumerated above.

B Algorithm: Selecting neighbors

This algorithm for model v2 takes advantage matrix manipulation to compute all simulations simultaneously and

eradicate as many loops as possible, thus enhancing the efficiency of the implementation of the model. Note that by moving steps 3 and 4 to after step 5, the algorithm can be used for generating cells of model v1.

1. Select the center particle's radius, R_c, from the prescribed distribution, $P_R(r)$, for all N_s Monte Carlo simulations.

2. Create an $N_s \times m$ matrix, $\mathcal{R}$, of potential neighboring particle radii, R_j, selected from $P_R(r)$, where m is greater than the maximum number of expected neighboring particles (we chose $m = 35$).

3. Create an $N_s \times m$ logical matrix, $\mathcal{C}$, for contacting particles. Each element is set to one with probability p, then the first $z_{\min}$ columns are set to one; these contacting particles ensure mechanical stability.

4. Create an $N_s \times m$ matrix, $\mathcal{D}$, of surface-to-surface distances, δ_j, from the center particle: each element is chosen from the prescribed distribution and then scaled so that they have mean δ^*. Then, for each (i, j) where $\mathcal{C}_{ij} = 1$ the element $\mathcal{D}_{ij} = 0$ since this particle is contacting.

5. Calculate the $N_s \times m$ matrix $\mathcal{O}$, of solid angle shadowed on a unit sphere by each potential neighbor by first repeating the center particle radius, R_c, for each simulation across m columns, forming the $N_s \times m$ matrix $\mathcal{R}_c$. Then the solid angle matrix is

$$\mathcal{O} = 2\pi \left(1 - \frac{\sqrt{(\mathcal{R} + \mathcal{R}_c + \mathcal{D})^2 - \mathcal{R}^2}}{\mathcal{R} + \mathcal{R}_c + \mathcal{D}} \right) \qquad (5)$$

   where operations are carried out element-by-element within the matrices.

6. Compute the cumulative sum of matrix $\mathcal{O}$ across each row. The potential neighbors which are included as actual neighbors are those where this cumulative sum is less than Ω^*. Half the time, the next potential neighbor is also chosen. The actual neighbors are stored as a logical matrix, $\mathcal{N}$.

The number of neighbors in each simulation is the sum across the rows of matrix $\mathcal{N}$, while the number of contacts in each simulation is the sum across the rows of the matrix who's elements are $\mathcal{N}_{ij}\mathcal{C}_{ij}$.

When using this algorithm to generate the numbers of neighbors and contacts for the purpose of optimizing model parameters, we keep the bank of generated random sizes, $\mathcal{R}$, $\mathcal{R}_c$, and and distances $\mathcal{D}$. When changing δ^*, the distances are simply rescaled, and the solids angle matrix, $\mathcal{O}$, recalculated. Changing Ω^* simply changes the neighbors that are selected. In our Monte Carlo simulations, we controled the statistical error by generating up to 10^5 cell samples and checked convergence of the results.

C Algorithm: Computing volume

We present this algorithm for generating the cell volumes in model v2 from the view point of a single simulation, but note that it can be efficiently implemented with the matrices generated by Algorithm 1.

1. Determine the filled solid angle of the cell,

$$\Omega_{\text{tot}} = \sum_{j=1}^{m} \mathcal{N}_{ij}\mathcal{O}_{ij}.$$

   The remaining approximate physical solid angle not filled by neighboring particles is $4\pi - \Omega_{\text{tot}}$.

2. Distribute this remaining solid angle to each contacting neighbor ($\forall k : \mathcal{N}_{ik}\mathcal{C}_{ik} = 1$) proportionally to its solid angle $\mathcal{O}_{ik}$:

$$\Delta\omega_k = \mathcal{O}_{ik} \frac{4\pi - \Omega_{\text{tot}}}{\sum_{j=1}^{m} \mathcal{N}_{ij}\mathcal{C}_{ij}\mathcal{O}_{ij}}. \qquad (6)$$

   For the non-contacting neighbors no solid angle is added and $\Delta\omega_k = 0$.

3. For each potential neighbor ($k = 1$ to m) with radius $R = \mathcal{R}_{ik}$:

   - Calculate the angle of the cone defined by the newly determined solid angle shadowed:

$$\hat{\theta} = \cos^{-1}\left(1 - \frac{\mathcal{O}_{ik} + \Delta\omega_k}{2\pi} \right) \qquad (7)$$

   - Determine the location of the hyperbolic sheet cap defined by the navigation map[30] (i.e. the points equidistance from the surfaces of both neighbor and center spheres) in polar coordinates, (r, θ). Taking $\theta = 0$ to be the line connecting the centers of the center particle and the kth neighbor particle, we obtain the hyperbolic sheet's location,

$$r(\theta) = \frac{1}{2} \frac{R^2 + (R_c - R)^2}{R\cos\theta - (R_c - R)}, \qquad (8)$$

     by equating the boundary-to-surface distance for both the center particle and neighbor particle; its location is rotationally symmetric about $\theta = 0$.

- Integrate in spherical coordinates the volume from $r = 0$ to the cap defined by Eq. (8), over θ from the centerline of the cone ($\theta = 0$) to $\theta = \hat{\theta}_k$ defined in Eq. (7), and over ϕ from 0 to 2π to obtain

$$V_k = V(\hat{\theta}; R_c, R, \delta) = \frac{\pi(\delta + 2R_c)^3(\delta + 2R)}{24(\delta + R + R_c)} \times \left\{ \frac{(\delta + 2R)^2}{\left[R - R_c + (\delta + R + R_c)\cos\hat{\theta}\right]^2} - 1 \right\} \tag{9}$$

  where $\delta = \mathcal{D}_{ik}$ is the surface-to-surface distance.

4. Compute the total local cell volume by summing the volume contributions from each contributing neighbor:

$$V = \sum_{k=1}^{m} \mathcal{N}_{ik} V_k \tag{10}$$

   where V_k is computed using Eq. (9).