Gapped Gapless Packing Structures

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Abstract

The assumption of a gapless packing structure has previously been used to obtain the density and partial coordination numbers of a random mixture of hard spheres in the maximally dense regime. Here we extend the notion of a gapless packing structure to allow for the determination of the characteristics of a packing away from maximal density, by adding an appropriate number of void spherical elements. A gapless packing is then considered in which the void and solid spherical elements are supposed to be indistinguishable except for the purposes of calculating packing fraction and coordination number. We utilize the notion of specific volume to generate a one parameter family of void distributions to obtain a set of coupled integral equations which are solved numerically.

Mono-disperse and bi-disperse packings are investigated for packing fractions ranging from $\rho = 0.26$ to 0.78. Results are shown to be comparable to experiments and the effect of varying packing fraction on coordination numbers is shown to be invariant with respect to number distribution. A linear relationship between coordination number and packing fraction is elucidated for moderate to low packing fractions. Maximum and minimum random packing fractions are also discussed.

Key words: random packing, hard sphere, packing fraction, poly-disperse

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1 Introduction

Granular materials are of widespread interest. Processes ranging from mixing to combustion are sensitive to particle number distribution, packing fraction, and partial coordination numbers. Granular systems, however, are very complex. Indeed, even idealized systems such as disk and sphere packings have eluded a satisfactory analytic theory.

Here we model a granular system as a random poly-disperse packing of hard spheres. This is a disordered packing in which incompressible spheres of various radii are mixed. Typically for such a packing the relative number of spheres at a given radius is known, and the packing fraction (i.e. the percent of the volume taken up by the spheres) is easily determined. However, the number and types of contacts between various spheres (given by partial coordination numbers), are difficult to characterize.

The gapless packing assumption, originally developed by Wise [1], Hogendijk [2] and later Dodds [3], has yielded some promising results in this area. This method assumes that every point in the packing lies within a tetrahedron which is defined by four spheres in mutual contact. By considering the properties of each tetrahedral unit along with the probability of finding and forming that unit we can calculate the average properties of the packing. Unfortunately, because the packing is assumed to be gapless, this analytic theory is only applicable at theoretical maximum densities. In fact, this method overestimates both coordination number and maximal packing fraction. In [3] Dodds calculated a coordination number of 13.4 for a gapless mono-disperse packing. However, due to geometrical considerations no more than 12 spheres of equal radius can be packed around a similarly sized sphere. Additionally, Dodds method predicted a maximum theoretical density for a mono-disperse packing of $\rho = 0.7796$ which is considerably larger than the accepted maximum packing fraction of $\rho = 0.7405$ associated with the face centered cubic structure (FCC). Thus, in a realistic packing there must be gaps.

Many attempts have been made to extend the method of gapless packing to realistic or arbitrary packing fractions. In [4] a fudge factor of 0.13 was used to adjust the experimentally unreachable packing fractions determined by Dodds to values which are consistent with mono-disperse random dense packing experiments where ρ varies between 0.63 and 0.66. While this elucidates the effect of number distribution on volume fraction it renders the coordination number calculations meaningless. A more promising adaptation to arbitrary packing fraction was recently proposed in [5] where each spherical element was associated with the convex polyhedron obtained by radical tessellation or navigation map. Faces of these polygons corresponded to near neighbors and thus segment the packing into tetrahedron. To determine the properties of these tetrahedron, mean distances to near neighbors are approximated heuristically. This allows for the determination of the mean number (and type) of near neighbor spheres but does not yield true coordination numbers for spheres which are actually in contact.

Here we propose an extension of the gapless packing assumption to arbitrary packing fraction, which allows for the calculation of partial coordination numbers. We assume that any packing structure can be transformed into a gapless Dodds network through the addition of the appropriate number of non-overlapping void or gap spheres of various sizes (see Fig. 1). We approximate the void number distribution using probabilistic arguments and a notion similar to specific volume. A one parameter family of distributions is formulated as a function of the given number distribution of solid elements as well as a target volume fraction. This family is collapsed to a single distribution by applying the method of Dodds to the combined number distribution of void and solid spherical elements and then matching the resulting volume fraction to the target value.

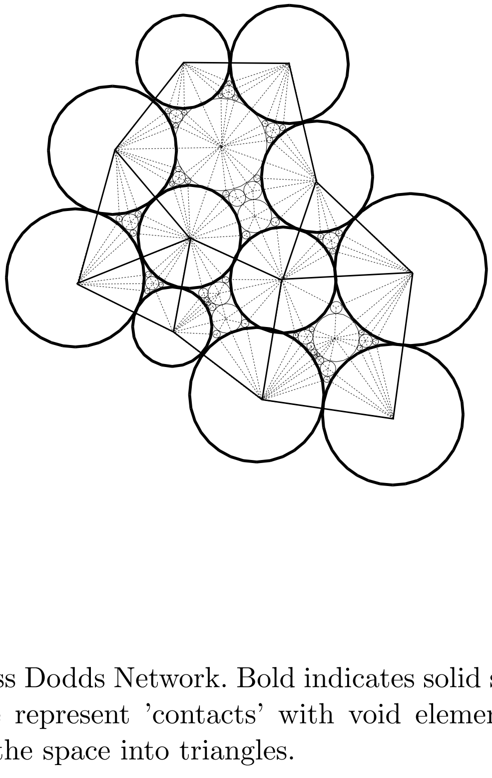

Fig. 1. Gapped Gapless Dodds Network. Bold indicates solid spherical elements and contacts. Dashed line represent 'contacts' with void elements. This construction completely segments the space into triangles.

2 A Variation on the Method of Dodds

In his paper [3] Dodds showed that, given a discrete set of sphere radii r_i and the number of such spheres in the packing N_i, the assumption of gapless packing allows for a complete characterization of the packing. What follows is a brief review of the gapless packing method of Dodds, with our simplified derivation and more direct calculation of mean coordination numbers.

Under the assumption of a gapless packing every point in the packing is assumed to lie inside a tetrahedron, the vertices of which lie at the centers of 4 spheres in mutual contact. Since the packing is random, we say that various tetrahedrons are formed by random combinations of four spheres. Using the notation of [5] we define p_{ijkl} as the probability of forming a tetrahedron with spheres of radii r_i, r_j, r_k, r_l at ordered vertices 1,2,3,4. If p_i is supposed to be the probability that a sphere of radius r_i is located at a particular vertex of a given tetrahedron and p_i is supposed to be independent of p_j for all $i \neq j$ (by virtue of the packing being random) then we conclude

$$p_{ijkl} = p_i p_j p_k p_l \tag{1}$$

For reasons which will become apparent we define M^4 as the total number of tetrahedra in the system, and let $x_i = Mp_i$. Therefore the total number of tetrahedra is given by

$$M^4 = \left(\sum_i Mp_i\right)^4 = \left(\sum_i x_i\right)^4 \tag{2}$$

and the total number of tetrahedra of various types is given by the appropriate term of the expansion of the right hand side.

We now appeal to a principle of conservations of species to relate the given number distribution N_i to the frequency of tetrahedral participation x_i. Since each sphere participates in multiple tetrahedra it is clear that only a fraction of a given sphere lies within in a given tetrahedron. That fraction is given by the intersection the sphere and the tetrahedron (see Fig. 2). We define A^i_{jkl} as $(4\pi)^{-1}$ times the solid angle which corresponds to the intersection of a sphere of radius r_i and a tetrahedron composed of spheres of radii r_i, r_j, r_k, r_l. Thus the total volume of spheres of radius r_i is given by

$$\frac{4}{3}\pi N_i r_i^3 = 4x_i \sum_{jkl} x_j x_k x_l \frac{4}{3}\pi A^i_{jkl} r_i^3 \tag{3}$$

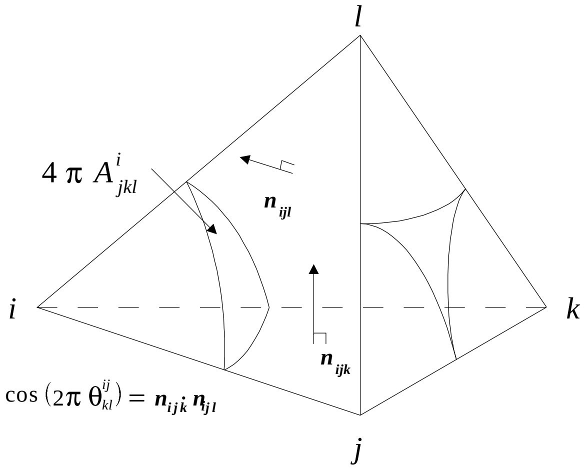

Fig. 2. Solid and Dihedral angles

With the exception of a normalization factor $4M^3$ this is identical to the formulation of Dodds. As we shall see the selection of the correct normalization factor greatly simplifies the calculation of partial coordination numbers. If there are n sphere types in our distribution, Eq. [3] represents a system of n non-linear equations for unknowns (x_i, $i = 1..n$), which can be solved numerically.

Of interest is the relative number of types of contacts between spheres. Total coordination number C_i is defined as the average number of particles which the average particle of radius r_i touches. Similarly, partial coordination numbers C_{ij} are defined as the average number of particles of radius r_j which the average particle of radius r_i touches. Thus

$$C_i = \sum_j C_{ij} \tag{4}$$

$$N_i C_{ij} = N_j C_{ji} \tag{5}$$

To calculate partial coordination numbers we observe that there is a one to one correspondence between the contacts and the segments of straight lines that connect the centers of touching spheres. These segments are edges of the tetrahedra that form the packing. However, because each segment associated with a contact serves as an edge for several tetrahedra there is not a one-to-one correspondence between tetrahedron edges and contacts. We therefore weight the edge of each tetrahedron by the dihedral angle between the two faces which make up that edge. For example, if every tetrahedra with edge ij has dihedral angle equal to $2\pi/4$ then a segment which connects spheres of radius r_i and r_j would participate in four tetrahedra. Thus to obtain the number of contacts we would calculate the number of tetrahedron with edge ij and then divide by four. This results from the fact that the total dihedral angle around any given segment ij must equal 2π. Therefore since the total number of contacts of type ij is given by $N_i C_{ij}$ the total dihedral angle associated with ij segments is given by

$$2\pi N_i C_{ij} = 12\, x_i\, x_j \sum_{kl} x_k\, x_l\, 2\pi \theta^{ij}_{kl} \tag{6}$$

where θ^{ij}_{kl} is $(2\pi)^{-1}$ times the dihedral angle along edge ij in a tetrahedron composed of spheres of radii r_i, r_j, r_k, r_l, and $12\, x_i\, x_j\, x_k\, x_l$ is the number of such tetrahedral edges (see Fig. 2). Note that the prefactor of 12 is derived differently for the two cases $i \neq j$ and $i = j$. None-the-less we find

$$\begin{aligned} C_{ij} &= \tfrac{12}{N_i}\, x_i\, x_j \textstyle\sum_{kl} x_k\, x_l\, \theta^{ij}_{kl} \\ C_i &= 3\bar{\theta}^i / \bar{A}^i \end{aligned} \tag{7}$$

where $\bar{\theta}^i = M^{-3} \sum_{jkl} x_j x_k x_l \theta^{ij}_{kl}$ and $\bar{A}^i = M^{-3} \sum_{jkl} x_j x_k x_l A^i_{jkl}$ are the average dihedral and solid angle fractions associated with a sphere of radius r_i.

Similarly, the packing fraction of a gapless packing network is given by the ratio of the total volume taken up by spherical elements and the total volume taken up by the associated tetrahedron

$$\rho = \frac{\sum_i \frac{4}{3}\pi N^s_i r^3_i}{\sum_{ijkl} x_i x_j x_k x_l V_{ijkl}} \tag{8}$$

where V_{ijkl} is the volume of a tetrahedron associated with spheres of radii r_i, r_j, r_k, r_l. This formulation is slightly different from that used in Dodds original paper, where a volume fraction associated with each tetrahedron was calculated, and then this quantity was averaged over the various tetrahedra. We believe that this calculation is more accurate, as the Dodds calculation is thought to overestimate the contribution of smaller tetrahedra [6].

3 Void Number Distribution

It should be clear that the gapless method of Dodds, requires only a given number distribution of solid spherical elements (N_i). For a Dodds-like calculation in a gapped gapless packing, we consider the void and solid elements to be indistinguishable. Thus if we have a void number distribution N^g_i, in addition to a given solid number distribution N^s_i we simply let $N_i = N^s_i + N^g_i$

and apply the method of Dodds to determine the characteristics of a packing away from maximal packing fraction.

Since we are considering random media, it seems appropriate to consider a probabilistic approach for the determination of such a void number distribution. Both void and solid spherical elements are non-intersecting so that the density function associated with the probability of finding such an element is given by

$$P_r[R_{s,g} = r] = \frac{1}{V}\frac{4}{3}\pi N_{s,g}(r)\, r^3 \tag{9}$$

where V is the total volume of the sample under consideration (henceforth normalized to $\frac{4}{3}\pi$) and the subscript s, g is intended to indicate that this holds for both solid and gap spheres. Note, that we now use $N_{s,g}(r)$ to represent *continuous* number distributions analogous to $N_i^{s,g}$ in the discrete case.

Now suppose that the probability $P_r[R_g > R]$ of finding a gap of radius $R_g > R]$ is proportional to the probability that a randomly selected point is outside every spherical region of radius $(R + r)$ associated with each sphere in the packing. The extended spheres of radius $(R + r)$ which surround each spherical element most certainly intersect, and thus no probabilistic relationship as simple as Eq. [9] exists. After [7], [8] we use the notion of specific volume to approximate the volume of truncated annular regions which are mutually exclusive. More specifically, we associated every point in the packing with the sphere which is nearest that point. The volume of the sphere and its neighborhood comprise the specific volume associated with that sphere. Generically, we let the function $V_a(R, r, \lambda)$ give the fraction of the annulus of width R which contributes to the specific volume around each sphere of radius r. Here λ is some density dependent parameter.

Just as the probability of finding a solid or void spherical element is given by the probability that a randomly selected point X in the packing falls into a sphere of that type, the probability of finding a gap of radius $R_g \geq R$ is related to $N_s(r)$ by

$$\begin{aligned} &P_r[R_g > R] \propto \\ &\qquad P_r[X \text{ not within } R \text{ units of any solid element in the packing}] \\ &\qquad\qquad = 1 - \int_0^\infty N_s(r)[r^3 + V_a(R, r, \lambda)]\, dr \end{aligned} \tag{10}$$

Note that we continue to normalize total volume $V = \frac{4}{3}\pi$ so that the number distribution is related to the packing fraction by

$$\rho = \int_0^\infty N_s(r)\, r^3\, dr \tag{11}$$

Clearly, setting Eq. [10] equals to zero and solving for R gives the maximum void radius. In principle, we could consider a void of slightly smaller radius and ask how many such voids could we add to the packing before the probability of finding another void of that radius or larger equals zero. Recalling that void spheres are also assumed to be non-intersecting, we say that we have added a sufficient number of gaps of radius R once the probability of finding another void sphere of that radius or larger equals zero. Thus the right side of Eq. [10] is adjusted to include the presence of void of radii $R_g > R$ and set equal to zero to yield an integral equation which relates the unknown $N_g(r)$ to the given solid sphere number distribution $N_s(r)$.

$$\int_R^{R_{\max}} \left[N_g(r)r^3 + N_g(r)V_a(R,r,\lambda)\right] dr = 1 - \rho - \int_0^\infty N_s(r)V_a(R,r,\lambda)\, dr \tag{12}$$

This integral equation (and the parameter λ) provides a packing fraction (ρ) dependent one parameter family of solutions for the number distribution of void spheres.

3.1 FFA Distribution

Of course, it is not clear what form the function V_a should take. Naively we may assume that it is simply be proportional to the volume of the spherical annulus, with (as yet unknown) proportionality constant λ. Then Eq. [12] yields the fixed fraction annular (FFA) distribution given by

$$\int_R^{R_{\max}} N_g(r)r^3 + \lambda N_g(r)((R+r)^3 - r^3)\, dr = 1 - \rho - \int_0^\infty \lambda N_s(r)((R+r)^3 - r^3)\, dr \tag{13}$$

where $R_{\max}$ is the maximal void sphere radius. Asymptotic analysis of such a simple form for V_a leads to $N_g(R) \propto R^{-3}$ as $R \to 0$, consistent with Aste's result for a disordered covering [9].

3.2 SSC Distribution

For the purposes of comparison we also consider a slightly more complex form of V_a. By assuming that all contacts occur between spheres of similar radius we obtain the self-same contact (SSC) distribution. The derivation, though lengthy, is a straightforeword analysis of the geometry of sphere contacts.

$$\begin{aligned}
V_a(R,r,\lambda) &= r^3\tfrac{3\bar{C}-4}{(\bar{C}-2)^2} && \delta \geq 1\\
&= R^3(1-\tfrac{\bar{C}}{2}) + 3R^2r(1-\tfrac{\bar{C}}{4}) + 3r^2R && \delta \leq 1\\
\delta &= \tfrac{\bar{C}}{2}(1-\tfrac{r}{R+r})\\
\bar{C} &= \bar{C}_\infty + \lambda \textstyle\int_R^\infty N_g(r)dr
\end{aligned} \tag{14}$$

$\bar{C}$ is intended to represent the average number of contacts per sphere in the mixture, and $\bar{C}_\infty$ is derived by assuming that void spheres of all radii have a non-negative probability of occurrence. Indeed, the $\bar{C}_\infty$ as a function of packing fraction is itself a decent approximation for the coordination number in the mono-disperse case. In this case the free parameter λ is associated with the rate at which average number of contacts changes with the addition of new void sphere. In principle, λ may be negative as the average number of contacts is expected to approach 6 as the radius of void spheres tends to zero [9].

We also note that the SSC distribution closely corresponds to an exponential distribution in volume for the probability of finding a radius R void region, i.e. $N_g(R)R^3 = (1-\rho)3\lambda R^2 e^{-\lambda R^3}$ (see Fig. 3).

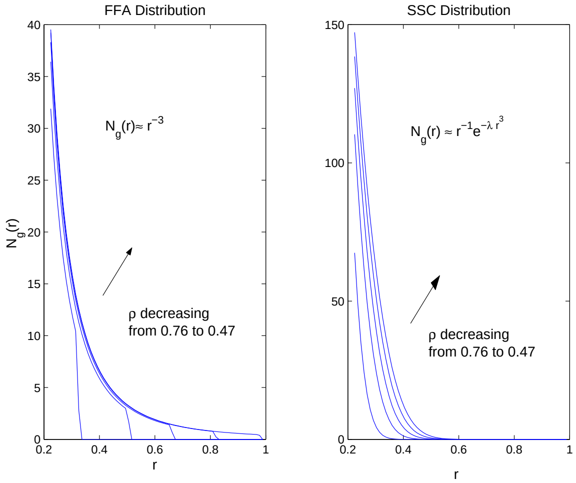

Fig. 3. Void number distribution at various packing fractions. Note that the FFA distribution is broader and transitions sharply at the maximal void radius.

It should be clear that the function V_a can be made arbitrarily complex to account for the more subtle influences of topology and geometry. In fact it can be more strongly coupled to the equation of Dodds by including dependence upon partial coordination numbers similar to [5]. Regardless, once a gap number distribution has been formulated we can apply the method of Dodds to determine the parameter λ.

4 Gapped Gapless Packing

As the void distribution function is not a discrete function, the method of Dodds must be adjusted. Additionally, the presence of void spheres means that not all contacts are contacts between solid elements. Finally, the parameter λ must also be determined in order to complete the system. We therefore, couple Eq. [12] with the integral form of [3] to obtain the following system

$$\int_R^\infty \left[N_g(r)r^3 + N_g(r)V_a(R,r,\lambda)\right]\,dr = 1-\rho-\int_0^\infty N_s(r)V_a(R,r,\lambda)\,dr \quad (15)$$

$$N_s(r)+N_g(r) = 4\,x(r)\int\!\!\int\!\!\int A(r,s,t,u)\,x(s)\,x(t)\,x(u)\,ds\,dt\,du \quad (16)$$

where integrals without limits indicate that we integrate over all sphere radii. These equations determine $x(r)$ and $N_g(r)$ as a function of the parameter λ. However, Eq. [15] assumed that the total volume of the sample had been normalized to $\frac{4}{3}\pi$. Thus the total volume of the sample given by the continuous form of 8 yields the scalar equation

$$\frac{4}{3}\pi = \int\!\!\int\!\!\int\!\!\int V_{\text{tet}}(r,s,t,u)\,x(r)\,x(s)\,x(t)\,x(u)\,dr\,ds\,dt\,du \quad (17)$$

which is required to complete the system and determine the parameter λ. Thus given a target packing fraction ρ and the appropriately normalized solid sphere number distribution, $N_s(r)$ in Eq. [11], we can obtain partial coordination numbers given by the continuous form of Eq. [7]

$$\begin{aligned}(N_s(r)+N_g(r))\,C(r,s)&\\ &= \frac{N_s(s)}{N_s(s)+N_g(s)}\,x(r)\,x(s)\int\!\!\int x(t)\,x(u)\,\theta(r,s,t,u)\,dt\,du \quad (18)\end{aligned}$$

Note that the expected relationship, $N_s(r)C(r,s) = N_s(s)C(s,r)$, is maintained.

Unfortunately, the gapless packing assumption comes with restrictions on the range of sphere radii which can be considered. Specifically, we must limit ourselves to the consideration of particle radii which lead to well formed tetrahedra. In [3] a well formed tetrahedron was defined as a tetrahedron in which four spheres are in mutual contact, i.e. the smallest sphere must not be so small that it could fit through the gap formed by the contact with the larger three. This leads to a restriction which limits the ratio of the smallest to largest radii of $2\sqrt{3}/3 - 1 \approx 0.1547$. However, this allows part of the smaller sphere to extend through the opposing face of the tetrahedron, which violates the assumption that the entire packing can be segmented into tetrahedron which contain the local properties of the mixture. To prevent this we can use the slightly more stringent ratio restriction of 1/6. However, in a gapped gapless packing we must acknowledge that a tetrahedron composed of unit spheres surrounds a gap of radius $\sqrt{3/2} - 1 \approx 0.22$. These voids are uncounted in a straightforward application of the gapless packing, and though we may add a kissing sphere term to Eq. [16], for simplicity here we simply use this most stringent radius restriction.

5 Results

The above equations were solved numerically to obtain coordination numbers as a function of packing fraction for various number distributions of solid spheres. All calculations approximated the continuous void distribution with a discrete distribution which included no less than 70 void spheres evenly spaced between minimum and maximum allowable radii. Tests for numerical convergence indicated that solving the integral equations at higher resolution (1000 particles) alters void distributions by less than 1% using the L_1 norm.

5.1 The Mono-Disperse Case

We initially verified the model by a thorough analysis of the mono-disperse case, in which a single solid sphere of unit radius was considered, along with 70 gap spheres. Densities between 0.26 and the gapless maximum density of 0.7796 were inspected. As previously noted, it is known that this maximum theoretical density is unrealistically large. The gapped gapless method yields a contact number of 12 at $\rho \approx 0.735$, in agreement with the density associated with the body centered cubic structure.

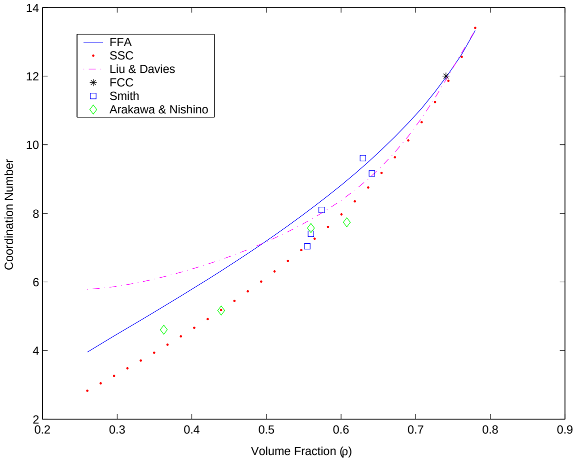

Fig. 4. Mean coordination number with comparisons to experimental results as well as the mono-disperse analytic approximation of Liu and Davies. The $*$ indicates the packing fraction and coordination number associated with the face centered cubic packing structure.

Fig. 4 shows the results for the two gap distribution functions. The SSC distribution is in excellent agreement with the analytic results of Liu and Davies [10, 11], who considered a radial basis function for the number distribution of particles at a given distance. A significant departure from their results occurs at lower densities where the Liu and Davies radial basis function is known to diverge.

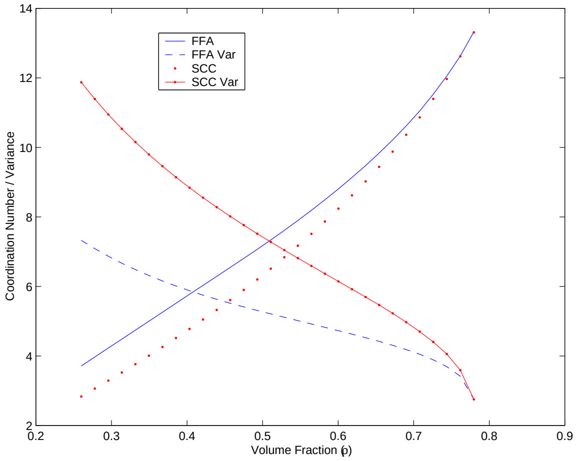

Fig. 5. Variance of coordination numbers of FFA and SCC. The broader void distribution of the FFA seems to yield more reasonable results.

The FFA distribution predicts higher coordination numbers than the SSC distribution and diverges from the results of Liu and Davies nearer to the maximum theoretical packing fraction. This demonstrates that a proper choice for V_a is critical and more work is necessary in this area. None-the-less both distribution functions are comparable to the experimental results of Smith et al. [12] and Arakawa and Nishino [13]. Another benefit of this method is indicated in Fig. 5 in which the coordination number variances are plotted. These variances demonstrate the expected monotonically decreasing behavior, and are sufficiently high in magnitude to indicate that, even at lower packing fractions, it is not unreasonable to see the formation of perfect or nearly perfect tetrahedra. Additionally, we estimate that in the gapped gapless model the probability that a sphere is locally hanging free in space, while non-zero, is quite small (≤ 0.01 at $\rho = 0.26$).

5.2 Maximum/Minimum packing fraction

We define the minimum packing fraction as the value for which the average total coordination number for every sphere is at least 4 (the minimum number of contacts needed for local stability of the packing). Clearly the two distributions predict quite different minimal packing numbers. (FFA: $\rho = 0.26$; SSC: $\rho = 0.36$). The broader distribution associated with FFA may give more accurate results, but again, more work is needed.

The determination of maximum density in a random packing is more difficult. Recall that a kissing sphere term was neglected in Eq. [16]. This term is absent when $r_{\rm min} = 0.22$ and negligible when the packing fraction is moderate to small for $r_{\rm min} = 1/6$. Near the maximum theoretical packing fraction this is no longer the case. Therefore, to avoid over counting these intra-tetrahedral spheres an additional term is added to Eq. [16]. We define $R_k(s, t, u, v)$ as the radius of the kissing sphere which fits into a tetrahedron composed of spheres of radii s, t, u, v and simply note that for every tetrahedron of that type we find an additional void sphere of radius $r = R_k(s, t, u, v)$. Thus if $\delta(r)$ is the Dirac delta function Eq. [16] becomes

$$\begin{aligned} N_s(r) + N_g(r) = 4\,x(r) \int\int\int A(r, s, t, u)\, x(s)\, x(t)\, x(u)\, ds\, dt\, du \\ + \int\int\int\int \delta(r - R_k(s, t, u, v))\, x(s)\, x(t)\, x(u)\, x(v)\, ds\, dt\, du\, dv \end{aligned} \tag{19}$$

To be completely rigorous we should also count void spheres which correspond to the kissing sphere and each of the three combinations of spheres of radii s, t, u, v, and so on. However, the radius of these secondary kissing spheres is demonstrably less than $r_{min} = 1/6$.

Regardless, the addition of this term renders the system unsolvable for all packing fractions larger than a critical value which is dependent on the void distribution function. This is because high density packings require very specific void distributions. In particular, the face centered cubic structure requires that the void distribution be given by a sum of delta functions. This implies that the void distributions necessary to achieve packing fractions above this critical value are not random. Since in a random packing the voids must also be randomly distributed we say that no random packing exists beyond this value. For the FFA distribution the critical packing fraction occurs at $\rho_{\max} \approx 0.66$, while for the SSC distribution determine $\rho_{\max} \approx 0.69$. Both are reasonable upper bounds on random packing density, though the FFA distribution is clearly in better agreement with experiments.

5.3 The Bi-Disperse Case

The sheer utility of this approach is demonstrated by the relative ease with which it handles a poly-disperse packing. To examine the bi-disperse case, only the given number distribution function needs to be altered. Two cases are presented here. First, we consider a packing of two sphere radii in which the smaller sphere had a radius of two thirds that of the larger. Fig. 6 shows partial coordination numbers as a function of the volume fraction of smaller spheres at various packing fractions.

Fig. 7, however, demonstrates a weakness of this model. The self-same coordinations numbers C_{11} and C_{33} do not match at volume fractions of 0 and 1, depsite the fact that both correspond to the mono-disperse packings. Comparison to the mono-disperse case demonstrates that C_{33}, the self-same coordination number of the larger sphere, gives the correct result. This is expected since the limitation on the range of void radii means that in the limit as the number of larger particles goes to zero we do not obtain the same void distribution as the mono-disperse case. For example, when ρ is above some critical value, the monodisperse case with a sphere of radius 3, has a void distribution with radii ranging from 0.22×3 to 3. Similarly, in the monodisperse case for a sphere of radius 1, the void distribution has radii ranging from 0.22 to 1. However, in the bi-disperse case, as the number of particle of radius 3 goes to zero we are still restricted to considering void radii ranging from 0.22×3 to 3. Thus in the limit as the number of large particles goes to zero we do not obtain the range of potential void sphere radii associated with the mono-disperse case. Fortunately, this discrepancy is noticeable only when the smallest solid sphere is less than 1/2 the radius of the largest sphere.

5.4 The Volume Fraction Function

Figs. 8, 9, and 10 confirm the long standing belief that volume fraction only weakly influences coordination number ratios. Here we have plotted coordina-

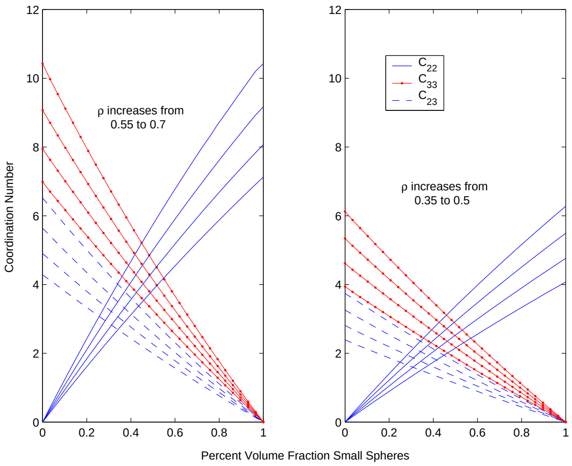

Fig. 6. C_{ij} gives coordination number between any sphere of radius r_i and a solid sphere of radius r_j. Here we see the effects of varying packing fraction as well as percent volume fraction smaller spheres, defined as $N_i^s r_i^3/\rho$.

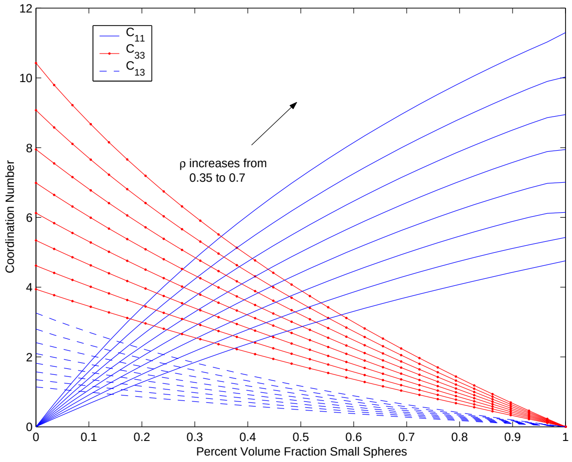

Fig. 7. Note $C_{11}(0) \neq C_{33}(1)$ implies dubious results for packing in which a significant amount of the mass is composed of smaller spheres.

tion numbers of the bi-disperse packings at various packing fractions normalized by the total average coordination number given by

$$C_{\text{tot}} = \frac{\int \int C(r,s) N_s(r)\, dr\, ds}{\int N_s(r)\, dr} \tag{20}$$

This implies that we can assume that partial coordination numbers can be suitably approximated by a function of the form

$$C(r,s) = f(\rho/\rho_{\text{max}}) \bar{C}(r, s, [\bar{N}_s]) \tag{21}$$

where f is solely a function of ρ normalized by the maximum gapless packing

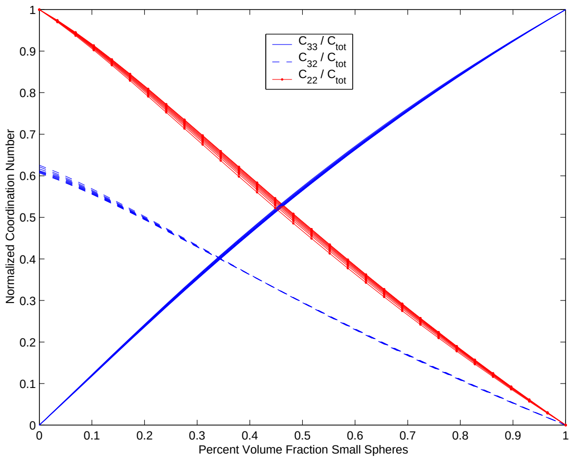

Fig. 8. Normalized coordination number C_{ij}/C_{tot} for ρ between 0.35 and 0.75.

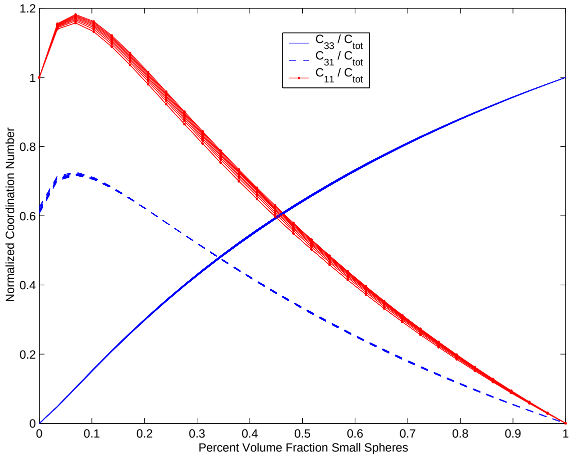

Fig. 9. Normalized coordination number C_{ij}/C_{tot} for ρ between 0.35 and 0.75.

fraction $\rho_{\max}$ associated the number distribution $\bar{N}_s$. The function $\bar{C}$ is the coordination number associated with the truly gapless Dodds network.

Fig. 11 plots the volume fraction function f for twenty randomly chosen polydisperse number distributions $\bar{N}_s(r)$ with solid spherical particles ranging in radius from 1/2 to 1. This function while independent of solid sphere number distribution, is clearly dependent upon the selection of the void distribution function. However, $f(\eta) \approx \sqrt{3}/2\eta$ is a good approximation for packing fractions in the experimentally achievable range.

6 Conclusions

We have extended the gapless packing method of Dodds to arbitrary packing fractions in a manner which allows for the calculation of true partial coordi-

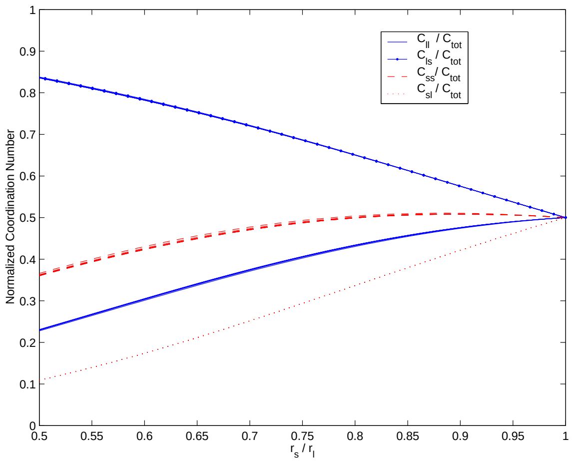

Fig. 10. Normalized coordination numbers $C_{ij}(\rho, r_l/r_s)/C_{tot}(\rho, r_l/r_s)$ for ρ between 0.35 and 0.75

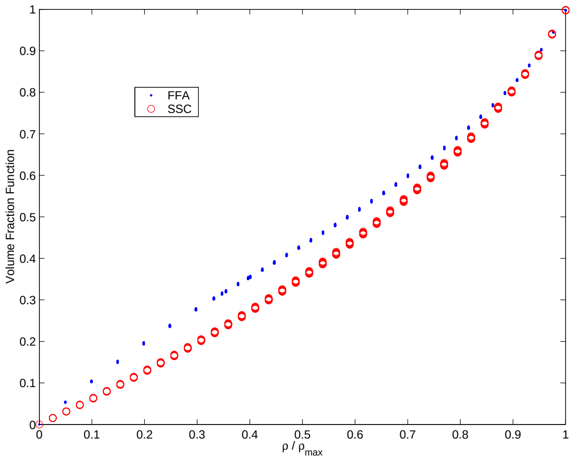

Fig. 11. The folume fraction function $f(\rho/\rho_{\max})$ as obtained normalizing partial coordination numbers $C_{ij}(\rho, [N_s])$ by the coordination number at maximal gapless density. Forty randomly selected poly-disperse solid sphere number distributions are plotted.

nation numbers of poly-disperse packings. We elucidated a linear relationship between packing fraction and coordination number for moderate packing fractions, and argued that large coordination number variances indicate that local jamming structures are most likely formed by spheres which locally organize into triangles or tetrahedra. Additionally, we rationalized that the experimentally determined maximum packing fraction of a random dense packing is related to 'randomness' of the void distribution, i.e. void distributions must have a great deal of structure at higher packing fractions. Furthermore, we numerically confirmed the assertion that coordination number ratios are unaffected by changes in packing fraction, and also demonstrated that the effects of varying packing fraction are independent of the number distribution of particles.

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