Estimate for the fractal dimension of the Apollonian gasket in $d$ dimensions

R. S. Farr
Unilever R&D, Olivier van Noortlaan 120, AT3133, Vlaardingen, The Netherlands and the London Institute for Mathematical Sciences, 22 S. Audley St., Mayfair, London, UK

E. Griffiths
(Dated: June 9, 2010)

We adapt a recent theory for the random close packing of polydisperse spheres in three dimensions [R. S. Farr and R. D. Groot, J. Chem. Phys. 131 244104 (2009)] in order to predict the Hausdorff dimension $d_A$ of the Apollonian gasket in dimensions 2 and above. Our approximate results agree with published values in 2 and 3 dimensions to within 0.05% and 0.6% respectively, and we provide predictions for dimensions 4 to 8.

PACS numbers: 05.45.Df, 61.43.Gt, 61.43.Hv

Leibniz [1] first suggested that a plane area can be completely covered with discs, in an approximately self-similar manner, through a construction which involves starting with three equal touching discs, and then repeatedly adding the largest possible disc which touches three neighbours, but does not overlap with any disc already in the packing. The result is illustrated in figure 1. According to Pappus of Alexandria, the problem of finding such osculating circles was first studied by Apollonius of Perga, in whose honour this ‘Apollonian packing’ is named. A similar construction can be envisaged for spheres (where each added sphere touches four neighbours [2]). In higher dimensions, a construction based upon iterating the analogue of Soddy’s formula [3] or applying iterated inversions [4] to hyperspheres will lead to overlaps [5]. Therefore in this paper we use the term ‘Apollonian packing’ to refer to an ‘osculatory packing’ [2], which starts from $d+1$ equal, touching hyperspheres at the vertices of a regular $d$–simplex, and where repeatedly, the largest possible $d$-dimensional hypersphere is added to the existing packing that does not overlap any already present. The added hypersphere touches $d+1$ others at this stage (although this fact is not needed for the subsequent argument).

Apollonian networks [6], which are graphs derived from Apollonian packings, have been suggested as models for real-world networks, such as social networks and hierarchical road systems [7]. In these contexts, networks based on Apollonian packings with any dimension, including $d > 3$ may be of practical relevance [8].

In lower dimensions ($d = 2, 3$), the physical significance of Apollonian packings is that they can be used as idealized models of high density granular materials, for example in high strength concrete [9]. Furthermore, related constructions, such as space-filling bearings in two [10] and three [11] dimensions, and random space filling bearings [12] have been proposed as simplified models for the geometry of turbulence [13] or the broken material near a geological fault. Random Apollonian packings of shapes other than hyperspheres have also been studied [14]. In all these cases, the method of adding spheres is modified so that it is no longer the largest possible non-overlapping sphere which is added at each stage; for example in the case of bearings an additional constraint is needed to ensure a bichromatic colouring [11]. These modifications all have the effect of reducing the rapidity with which the packing approaches a volume fraction of unity as spheres are added and also alter the fractal dimension of their residual sets. In recent work on random bearings [15] the fractal dimension can even be varied continuously by choice of parameters.

The residual set or ‘Apollonian gasket’ of such structures is of practical relevance, since its surface area and volume (for the 3d case) are related to solvent adsorption and permeability to flow through the packing. These geometrical properties of the residual set are finite, provided the packing contains only spheres larger than a certain cutoff diameter. However, in the limit where spheres of arbitrarily small size are included, the residual set is frac-
tal in nature, and its Hausdorff dimension captures the essential geometric information \[4\].

Recent high-precision calculations have shown that in 2d, the dimension of the Apollonian gasket is \(d_{A,2} \approx 1.30568\) \[1\], while in 3d, it is \(d_{A,3} \approx 2.4739465\) \[2\].

Since the Apollonian packing is a special kind of sphere packing in three dimensions, then it is interesting to investigate whether the recent approximate theory for the volume fraction of random close packings of polydisperse spheres, presented in Ref. \[17\] may shed some light on this problem also. The hope is that the essential geometric features of sphere packings captured in Ref. \[17\] might apply to non-random cases also.

In the theory of Ref. \[17\], we start with a known distribution of sphere diameters \(P_{dd}(D)\), where \(P_{dd}(D)\) is the number fraction of the spheres with diameters in the range \((D, D + dD)\), and we ask what is the maximum random packing density which can be obtained?

The procedure consists of several stages: First, \(P_{dd}(D)\) is converted into a number distribution of one dimensional rods \(P_{dd}(L)\), by imagining a random non-overlapping (but not necessarily close packed) distribution of spheres, passing a straight line through this distribution, and counting each portion of the line within a sphere to be a rod. The resulting distribution of rod lengths is given \[17\] by

\[
P_{dd}(L) = 2L \int_{0}^{\infty} P_{dd}(D) dD \int_{0}^{\infty} P_{dd}(D) dD.
\]

In order to simulate packing, we then imagine that this collection of rods interacts on a line through a hard pair potential which acts between each pair of rods \(L_i\) and \(L_j\) through

\[
V(h) = \begin{cases} 
\infty & \text{if } h < \min(fL_i, fL_j) \\
0 & \text{if } h \geq \min(fL_i, fL_j)
\end{cases}
\]

In Eq. \(2\), \(h\) is the closest approach of the two ends of the rods, \(f > 0\) is a free parameter in the theory (which we explain later), and the potential is able to reach through smaller rods which may be in the gap between the two rods under consideration.

Finally, we search over all orderings of the rods, and find the ordering which occupies the maximum length fraction on the line. This search can be accomplished by a simple greedy algorithm \[17\], and the final length fraction occupied by the rods is our estimate for the maximum random packing fraction of the spheres in 3d.

As described, the theory depends on a free parameter \(f\), which in Ref. \[17\] is fixed by ensuring that the predicted close packing density for monodisperse spheres matches the known random close packing density \(\phi_{RCP} \approx 0.6435\). With this calibration, \(f \approx 0.7654\) and the theory can be applied to arbitrary sphere size distributions.

For the further development of this paper, we require the generalization of this model to other dimensions. Therefore consider a polydisperse collection of \(d\)-dimensional hyperspheres, where \(P_{dd}(D) dD\) is the number fraction of hyperspheres with diameters in the range \((D, D + dD)\), and \(d \geq 2\). If we consider passing a straight line at random through a single hypersphere of diameter \(D\), then we will generate a collection of rods with a normalized length distribution given by

\[
\hat{P}_{dd}(L; D) = (d - 1)L D^{1 - d}(D^2 - L^2)^{(d - 3)}/2 \theta(D - L),
\]

where \(\theta(x)\) is the Heaviside step function.

The distribution of rod lengths generated from passing a line through a random distribution of \(d\) dimensional hyperspheres, will therefore be given by a convolution with \(P_{dd}\), but also taking into account that the collision cross section for the line with a hypersphere of diameter \(D\) scales as \(D^{d-1}\). The result is

\[
P_{dd}(x) \propto \int_{D = L}^{\infty} D^{d-1} P_{dd}(D) \hat{P}_{dd}(L; D) dD,
\]

which with the correct normalization (obtained by reversing the order of integration over \(D\) and \(L\), gives the appropriate generalization of Eq. \[11\], namely

\[
P_{dd}(L) = (d - 1) \int_{0}^{\infty} \frac{(D^2 - L^2)^{(d - 3)/2} P_{dd}(D) dD}{\int_{0}^{\infty} D^{d-1} P_{dd}(D) dD}.
\]

Now, consider the analogue of the Apollonian packing for rods on a line subject to the potential of Eq. \[2\]. This consists of starting with a set of equal large rods, and then placing the largest possible rods into the gaps between them, which do not require the large rods to move. This process is then repeated iteratively, as in figure \[1\].

In one unit cell of this structure, there is one rod of the longest length (which we take as unity), which leaves a gap of size \(f\) to be filled by the smaller rods. In choosing and placing these smaller rods, we need \(2^i\) rods of length \(f(1 + 2f)^{-1}\), then in the remaining gaps, which are of length \(f^2(1 + 2f)^{-1}\), we place \(2^i\) rods of length \(f^2(1 + 2f)^{-2}\). Repeating this process, we have at iteration number \(j\), \(2^j\) rods of length \(f^{j+1}(1 + 2f)^{-(j+1)}\).

This implies that asymptotically, as \(L \to 0\), the total number of rods of size greater than \(L\) behaves as

\[
\int_{L}^{\infty} P_{dd}(L') dL' \propto 1 + \sum_{i=0}^{j} 2^i,
\]

where \(L = f^{j+1}(1 + 2f)^{-(j+1)}\). Therefore

\[
\int_{L}^{\infty} P_{dd}(L') dL' \propto L^x \quad \text{where} \quad x = \frac{\ln 2}{\ln \left(\frac{1}{1 + 2f}\right)}.
\]
Now, the distribution $P_{dd}(L)$ in Eq. (7) has a corresponding distribution $P_{dd}(D)$ of hyperspheres, which from Eq. (3) is given asymptotically in the limit $D \to 0$ by

$$\int_D^\infty P_{dd}(D') dD' \propto D^y \quad \text{where} \quad y = x - d + 1. \quad (8)$$

We now link these results back to the dimension $d_A$ of the Apollonian gasket in $d$ dimensions in the following manner: According to Refs. [2, 18, 19], the cardinality of the set of spheres in an Apollonian packing, with curvature not exceeding $\kappa$, is given by

$$N(\kappa) \propto \kappa^{d_A}. \quad (9)$$

Combining Eqs. (7), (8) and (9), we therefore obtain our estimate for the Hausdorff dimension $d_A$ of the residual set of the packing:

$$d_A \approx -y = d - 1 - \frac{\ln 2}{\ln \left(\frac{f}{1 + 2f}\right)}, \quad (10)$$

where $f$ is the appropriate value for each dimension $d$ of space.

To complete the calculation, we need a value for the free parameter $f$ in the theory. This will be done (as in the analysis of random close packing [17]) by calibrating the theory for the monodisperse case. To obtain the rod distribution corresponding to monodisperse hyperspheres, we use a collection of $n = 50\,000$ rods sampled uniformly from the distribution of Eq. (3). To do this, we take equal points on the inverse function of the integral of Eq. (3), so that our rod lengths are given by

$$L_i = D \left[1 - \left(\frac{i - 1}{2n}\right)^2/(d-1)^{1/2}\right], \quad (11)$$

where $i = 1 \ldots n$.

Applying the greedy one-dimensional packing algorithm described in Ref. [17], we calculate numerically the packing density of monodisperse hyperspheres as a function of the parameter $f$, for each dimension $d$ of space. The resulting curves for $d = 2$ to 6 are shown in figure 3.

In order to apply the packing theory, we need the value of $f$ for each dimension $d$. When applying the theory to random close packing in 3d, the calibration used was to ensure that the prediction for random close packing of monodisperse spheres was correct [17].

For the Apollonian packing each hypersphere is added in such a way as to optimally fill the remaining available space, and so the local geometry of packing will always be as efficient as possible. In order to capture this property, we choose $f$ to give the maximum possible local packing fraction of equal hyperspheres. This corresponds to placing equal osculating hyperspheres at the vertices of a regular $d$-simplex, and calculating the volume fraction occupied inside the simplex. We refer to this packing fraction as $\phi_{\text{simp}}$, and it is illustrated for the cases $d = 2$ and 3 in figure 4. An alternative argument for this choice, is that we are calibrating $f$ by using the true packing fraction of the first few hyperspheres in the Apollonian packing. In general, these will be of different sizes, but by taking the first $d + 1$, we again only need to consider equal spheres at the vertices of a simplex.

In 2d, this construction gives the same area fraction as a hexagonal packing, so $\phi_{\text{simp}} = \pi/(2\sqrt{3}) \approx 0.9069$. In three dimensions, we find $\phi_{\text{simp}} = 3\sqrt{2}\left[\cos^{-1}(1/3) - \pi/3\right] \approx 0.7796$, which is higher than can be achieved for any global packing of spheres in 3d (this limit is $\phi_{\text{ccc}} = \pi/\sqrt{18} \approx 0.74$, achieved for the face centred cubic or hexagonal close packed arrangement [20]).

For higher dimensions, we calculate the simplex packing fraction using a Monte-Carlo integration, noting that if one vertex of a regular simplex lies at the origin of $d$-dimensional Cartesian coordinates, then the other vertices can be chosen at the positions $\{\mathbf{s}^i\}$ where

$$s_i^j = \left(2d + 4 + 4\sqrt{1 + d}\right)^{-1/2} \left[1 + \sqrt{1 + d}\right] \delta_{ij} + 1. \quad (12)$$

A point $\mathbf{p}$ chosen randomly (and uniformly) in $(0, 1)^d$ can
TABLE I: Predictions for the Hausdorff dimension of the Apollonian gasket in d dimensions. The close packing density of spheres with centres at the vertices of a regular d-simplex is $\phi_{\text{simpl}}$. The corresponding value of f from the packing theory is shown, along with the predicted Hausdorff dimension $d^{\text{pred}}_A$, and the actual Hausdorff dimension $d^{\text{act}}_A$ if known [2][10].

| d  | $\phi_{\text{simpl}}$ | f          | $d^{\text{pred}}_A$ | $d^{\text{act}}_A$ |
|----|-------------------------|------------|----------------------|-------------------|
| 2  | 0.966900                | 0.131025   | 1.3606               | 1.3057            |
| 3  | 0.779636                | 0.394834   | 2.4586               | 2.4739            |
| 4  | 0.6478                  | 0.7864     | 3.5848               | -                 |
| 5  | 0.5257                  | 1.325      | 4.6840               | -                 |
| 6  | 0.4195                  | 2.047      | 5.7603               | -                 |
| 7  | 0.330                   | 3.02       | 6.8189               | -                 |
| 8  | 0.255                   | 4.35       | 7.864                | -                 |

be expanded as $p = \sum_j q_j s_j$, where $q_j = \sum_i t^i_j p_i$ and

$$t^i_j = \frac{(2d + 4 + 4\sqrt{1 + d})^{1/2}}{1 + \sqrt{1 + d}} \left[ \delta_{ij} - \frac{1}{1 + d + \sqrt{1 + d}} \right].$$

The point $p$ lies within the simplex if all the $q_j$’s are positive, and their sum does not exceed unity. We denote the volume of this simplex by $V_{\text{simpl}}$, which can thus be obtained by a Monte-Carlo integration, or from the analytic expression $V_{\text{simpl}} = 2^{-d/2} \sqrt{(1 + d)/d!}$. Furthermore, consider the volume $V_{\text{sph}}$ of that portion of a unit radius hypersphere lying within a large regular d-simplex, when the hypersphere has its centre at one of the vertices of the simplex. The point $p$ lies within this volume if all the $q_j$’s are positive, and $\sum_j (q_j)^2 < 1$. Again, this allows us to calculate $V_{\text{sph}}$ stochastically.

From these two quantities, the maximum packing fraction in a simplex is given by

$$\phi_{\text{simpl}} = (d + 1)V_{\text{sph}}/(2^dV_{\text{simpl}}),$$

which is shown in Table II alongside the predicted values of $d_A$ [from Eq. (10)] and the actual values (where known).

From Table II we see that the predictions from this model in 2 and 3 dimensions agree with the known values to within 0.05% and 0.6% respectively, and predictions for higher values of $d$ may be readily obtained.

In conclusion, the packing theory of Ref. [17], which was designed to abstract the essential geometric features of random close packing, also appears to contain enough information to predict important features of the hierarchical Apollonian packing. The extension of these arguments to more general Apollonian-type packings (such as space filling bearings [11] or random Apollonian packings [14]) will require further work, because the objects inserted into the packing are no longer maximal, which implies that both Eq. (7) and the calibration of $f$ will need to be modified. Nevertheless, we hope that further study of this or related theories will lead to more insights and further analytical results on both packings and granular materials.

Acknowledgments

Fig. I was supplied by the user ‘Time3000’ on the ‘Wikimedia Commons’ webproject.

[1] G. W. Leibniz and B. Look, The Leibniz - Des Bosses correspondence Yale University Press (2007).
[2] M. Borkovec, W. de Paris and R. Piekert, Fractals 2(4) 521-526 (1994).
[3] F. Soddy, Nature 139, 77-79 (1937).
[4] B. B. Mandelbrot, The Fractal Geometry of Nature (W. H. Freeman & Co., New York, 1982).
[5] H. Morall, J. Phys. A: Math. Gen. 27 7785-7791 (1994).
[6] J. P. K. Doye and C. P. Massen, Phys. Rev. E 71(1) 016128 (2005).
[7] J. S. Andrade, H. J. Herrmann, R. F. S. Andrade and L. da Silva, Phys. Rev. Lett. 94(1) 018702 (2005).
[8] Z. Z. Zhang, F. Comellas, G. Fertin and L. Rong, J. of Phys. A 39(8) 1811-1818 (2006).
[9] H. J. Herrmann, R. M. Baram and M. Wackenhut, Brazilian J. Phys. 33(3) 591-593 (2003).
[10] S. S. Manna and T. Vicsek, J. Stat. Phys. 64(3/4) 525-539 (1991).
[11] R. Mahmoody Baram, H. J. Herrmann and N. Rivier, Phys. Rev. Lett. 92(4) 044301 (2004).
[12] R. Mahmoody Baram and H. J. Herrmann, Phys. Rev. Lett. 95, 224303 (2005).
[13] G. Bachelor, Theory of homogeneous turbulence, Cambridge University Press, 1982.
[14] G. W. Delaney, S. Hutzler and T. Aste, Phys. Rev. Lett. 101, 120602 (2008).
[15] P. G. Lind, R. M. Baram and H. J. Herrmann, Phys. Rev. E 77, 021304 (2008).
[16] S. S. Manna and H. J. Herrmann, J. Phys. A: Math. Gen. 24, L481-L490 (1991).
[17] R. S. Farr and R. D. Groot, J. Chem. Phys. 131 244104 (2009).
[18] D. W. Boyd, Mathematika 20, 170-174 (1973).
[19] D. W. Boyd, Math. Comp. 39(159), 249-254 (1982).
[20] T. C. Hales, Annals of Mathematics 162(3) 1065-1185 (2005).