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Voronoi Polygons and Polyhedra

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A new algorithm for the calculation of Voronoi polytopes in 2D and 3D Euclidean space is described. Some results for random nuclei with reciprocal boundary conditions in 2D and 3D are discussed in relation to previous findings. In 2D the number of sides distribution is identified as being close to $\Gamma(3.5; 21)$. Kiang's conjectures for the distributions of areas and volumes for polygonal and polyhedral tessellations respectively, are supported: the challenge of deriving his Γ-distributions beyond 1D still stands. © 1993 Academic Press, Inc.

1. INTRODUCTION

With respect to nuclei a unique polytope encloses all parts of space closer to a given nucleus than to any other nucleus. Such a polytope, often named after Voronoi [34] or Dirichlet [14] is necessarily convex. The Voronoi polyhedra for certain regular arrays of nuclei are familiar as Wigner–Seitz [37] cells but limited statistics of Voronoi polytopes for irregular distributions of nuclei were studied mathematically in the pioneering work of Meijering [23].

Barrett and Mackay [6] distinguish between "exact" and "statistical" algorithms: in the former the geometrical features are themselves explicitly computed; in the latter, test points are selected and to which nucleus each "belongs" is determined. Kiang's program [20] being statistical yielded only areas of polygons and volumes of polyhedra.

Kiang conjectured that the generalized formula

$$\Gamma(\lambda; \alpha) = \frac{\lambda(\lambda x)^{\alpha-1} \exp(-\lambda x)}{\Gamma(\alpha)} \qquad (1)$$

(wherein the two parameters, λ and α, are equal) applies and is $\Gamma(4; 4)$ for the areas of 2D Voronoi polygons and $\Gamma(6; 6)$ for the volumes of 3D Voronoi polyhedra. This is derived from his demonstration that the distribution of lengths of 1D Voronoi polytopes for random nuclei on a line in $\Gamma(2; 2)$. Kiang's conjecture for dimensions higher than one has been disputed by others (below) but recent results [24] support Kiang. However, it is said [36] that Kiang revised his value for the two parameters in 2D, but in the context of sparser data than presented here.

Our 2D and 3D programs for the present results are "exact" and we compute actual tessellations rather than repeatedly computing a single Voronoi polygon for a "central" nucleus, which has been done in some investigations, e.g., Crain [13], Andrade and Fortes [1]. Moreover, our programs invoke the reciprocal boundary condition, or not, as desired, which is explained below.

The program for 2D used here (referred to as VORONOI in the text [24]) tolerates vertices of >3-hedral valency should they arise. The program was readily extended to 3D (referred to as VOR3D in the text) to obtain statistics, including of plane sections (Moore [24]). The Voronoi programs outlined by Angell and Moore [2] and by Angell [3] have different algorithms: that described by Angell and Moore [4] is quite different, computing a 2D slice of an N-dimensional "weighted" Voronoi tessellation.

Other exact 3D programs exist, notably that of Finney [15] in connection with Bernal's well-known researches upon the structure of liquids [7–10] yielding statistics upon Voronoi polyhedra for nuclei corresponding to the centres of co-equal balls packed randomly. For 3D: chronologically there are algorithms (not necessarily "exact") in Refs. [27, 20, 10, 15, 21, 28, 12, 17, 22, 11, 35, 30, 32, 5, 26, 18, 31, 6], but it is remarkable how little numerical data upon random Voronoi polyhedra has been published.

2. THE ALGORITHM

The term "vertex" is here reserved for any point in a 2D or 3D tessellation where the apices of its component polygons or polyhedra meet. The term "apex" refers to a "corner" of a single polygon or polyhedron.

In 2D, to find the Voronoi polygon of each nucleus the Voronoi "supra-polygon"—the region of the same shape as the Voronoi polygon but of twice its linear dimensions (Fig. 1), is constructed. Each nucleus $\mathbf{p}_i$ ($i = 1, ..., N$) is taken in turn as the "target nucleus" forming the temporary origin

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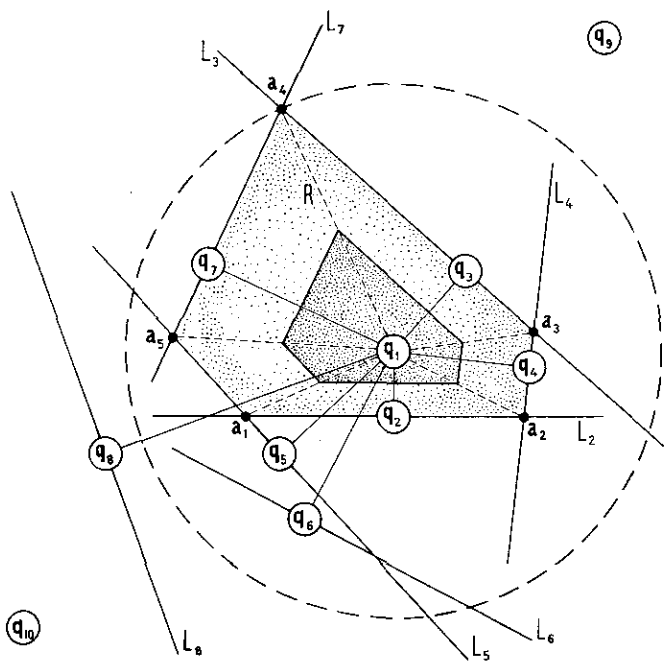

FIG. 1. The Voronoi suprapolygon (lightly stippled) of nucleus $\mathbf{p}_i = \mathbf{q}_1$ due to nuclei $\mathbf{q}_2, \mathbf{q}_3, \ldots$. Its apices are $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_5$ and its "radius" is R. The corresponding Voronoi polygon is heavily stippled.

of the vector co-ordinate system. A strategy is applied so that nuclei outside the immediate vicinity of the target nucleus $\mathbf{p}_i$ are not considered unless necessary. The less remote nuclei $\mathbf{q}_j$ ($j = 2, 3, \ldots, j = 1$ is the target nucleus $\mathbf{p}_i$) are chosen in increasing distance from the target nucleus and through each the line L_j is calculated perpendicular to the line joining $\mathbf{q}_j$ to the origin. The supra-polygon of $\mathbf{q}_1$ is then the area surrounding the origin which is not itself intersected by the lines L_j.

By first defining an initial triangle so large as certainly to contain the supra-polygon, the lines $L_2, L_3, \ldots$ are taken in sequence to lop pieces off the progressively more lopped polygon, until eventually the "radius" of the latter (the maximum distance from the origin to each of the apices) becomes less than the distance of the next line L_j from the origin. The remaining lines L_k $(k \geqslant j)$ cannot intersect this polygon; whence it must be the required Voronoi supra-polygon.

The line L_j is defined by the vector $\mathbf{q}_j = (q_x, q_y)$. The polygon is defined by the apices $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \ldots, \mathbf{a}_c$ (anti-clockwise about the origin), where $\mathbf{a}_c = \mathbf{a}_1$ closes the polygon. Since the slope of the line L_j is $-q_x/q_y$, the equation of L_j can be given in the functional form

$$f(x, y) \equiv q_x^2 + q_y^2 - xq_x - yq_y = 0. \tag{2}$$

The apices $\mathbf{a}_t$ ($t = 2, 3, \ldots, c$) of the polygon are considered in turn. If $f(\mathbf{a}_t) \geqslant 0$ then $\mathbf{a}_t$ remains as an apex of the polygon, whereas if $f(\mathbf{a}_t) < 0$ then this apex will be lopped off. When the sign of $f(\mathbf{a}_t)$ is not the same as the sign of $f(\mathbf{a}_{t-1})$ then L_j intersects the side of the polygon which joins the apices $\mathbf{a}_{t-1}$ and $\mathbf{a}_t$. This intersection (which will be a new apex in the lopped polygon) is located at

$$\mathbf{a}_t + \mu(\mathbf{a}_{t-1} - \mathbf{a}_t), \tag{3}$$

where

$$\mu = \frac{f(\mathbf{a}_t)}{(\mathbf{a}_{t-1} - \mathbf{a}_t) \cdot \mathbf{q}_j}. \tag{4}$$

For gathering statistical data, the tessellations (2D and 3D) had 1000 nuclei each. Pseudo-random numbers, distributed with an equal probability over the interval 0 to 1, represented the co-ordinates of the nuclei in a unit square or cube.

The strategy to reduce the number of nuclei considered with respect to the target nucleus, is briefly as follows:

The unit square is divided into 50×50 integer boxes and the nuclei are categorised accordingly. First, the integer box in which the target nucleus lies is identified. All nuclei lying in the same integer box as the target nucleus, plus those lying in the eight adjacent integer boxes, are recovered. But only those within a disc centered on the target nucleus and of radius equal to the side length of an integer box are sorted into ascending distance from the target nucleus. These nuclei are then taken in this sequence for calculation of their lines L_j during the polygon lopping.

If the algorithm still has not terminated by virtue of the next nucleus being more distant from the origin than the radius of the lopped polygon, then the square annulus of more remote integer boxes is brought into play. The radius of the disc is expanded accordingly and the nuclei within it are sorted into ascending distance from the target nucleus. Included in this sorting are the nuclei in the previous square annulus of integer boxes that lay outside the previous disc. Eventually the algorithm must terminate and the supra-polygon is reduced linearly by a half to become the Voronoi polygon. The above processes were also implemented in 3D [24]. In both 2D and 3D, when the RBC (reciprocal boundary condition) is required, appropriate integer boxes were translated. The latter results in the top edge of the tessellation matching its bottom edge, and the left-hand edge of the tessellation matching its right-hand edge. With the RBC applied, translated replicas of the 2D or 3D tessellation would themselves tessellate Euclidean 2D or 3D space, respectively.

For 3D, each apex of a polyhedron is tested to see if any lie on the far side of the lopping plane with respect to the target nucleus. If so, each of its facets, dealt with in any order, are categorised as follows:

Type 1. The single entirely new facet existing in the lopping plane.

Type 2. An old facet entirely on the far side of the lopping plane from the origin which will be completely lost.

Type 3. An old facet intersected by the lopping plane and modified accordingly (in the manner of the lopping of an individual polygon in the 2D algorithm—i.e., handedness of touring its apices is maintained).

Type 4. An old facet entirely on the same side of the lopping plane as the origin remaining as part of the new polyhedron.

3. RESULTS

Although we have obtained the distributions of a variety of measures of the Voronoi polytopes of random dispersions of nuclei in both 2D and 3D (with RBC), attention is here primarily confined to the measure that is 2D area and 3D volume. Some discussion of the measure that is 2D number of sides is given here because of its relevance in testing both the present, and previous, algorithms (see Table I). Throughout, s is the standard deviation of observed values.

3.1. *2-Dimensions.* For 100 runs of VORONOI (with RBC) for 1000 nuclei each, Fig. 2 shows the distribution of the number of sides per Voronoi polygon; Fig. 3a shows the distribution of the areas of these polygons.

3.2. *3-Dimensions.* For 50 runs of VOR3D (with RBC) for 1000 random nuclei each, Fig. 4a shows the distribution of the volumes of the Voronoi polyhedra.

4. DISCUSSION OF RESULTS FOR 2-DIMENSIONS

4.1. *Distribution of number of sides of the polygons.* The present data (Table I) is virtually identical to that obtained by Crain [13] and by Hinde and Miles [19] with respect to percentages, but the latter investigations lost some sides: whereas a finite three-hedral tessellation obeying the RBC has mean number of sides exactly six the proof of which is trivial [24]. The best two-parameter Γ-distributions [24] for integer and half-integer values of λ and α are given in Figs. 2a and b.

4.2. *Distribution of areas.* Kiang's [20] $\Gamma(4; 4)$ is superimposed in Fig. 3. Not only does Moran [25] believe

TABLE I

Comparison between Present Data on Number of Sides of Random Voronoi Polygons and Those of Crain and of Hinde and Miles

Number of sides	Crain '78		Hinde and Miles '80		Present study	
3	628	1.1%	22628	1.1%	1134	1.1%
4	6145	10.8%	214246	10.7%	10587	10.6%
5	14783	25.9%	518251	25.9%	26099	26.1%
6	16825	29.5%	588812	29.4%	29329	29.3%
7	11306	19.8%	398266	19.9%	19976	20.0%
8	5105	9.0%	180322	9.0%	9012	9.0%
9	1686	3.0%	59062	3.0%	2972	3.0%
10	428	0.8%	14858	0.7%	721	0.7%
11	81	0.1%	2984	0.2%	148	0.2%
12	10	<0.1%	493	<0.1%	19	<0.1%
13	3	<0.1%	68	<0.1%	3	<0.1%
14	0	—	10	<0.1%	0	—
⩾15	0	—	0	—	0	—
Total number of sides	341,815		11,999,335		600,000	
Total number of polygons	57,000		2,000,000		100,000	
Mean number of sides per polygon	5.99675		5.99967		6	
Sides lost	185		665		None	

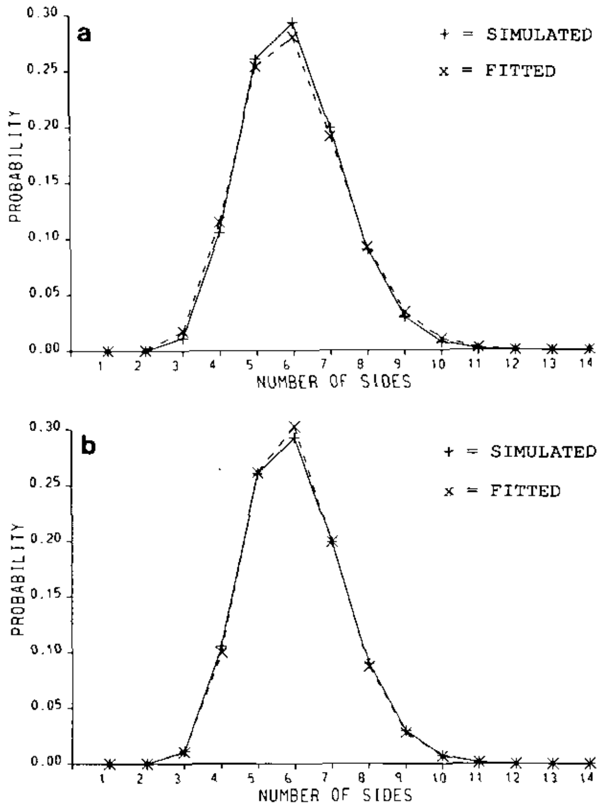

FIG. 2. The present results (mean = 6, $s^2 = 1.77492$) for distribution of number of sides of the 100,000 random Voronoi polygons: (a) with $\Gamma(3; 18)$ fitted (mean = 6, $s^2 = 2$); (b) with $\Gamma(3.5; 21)$ fitted (mean = 6, $s^2 = 1.71429$).

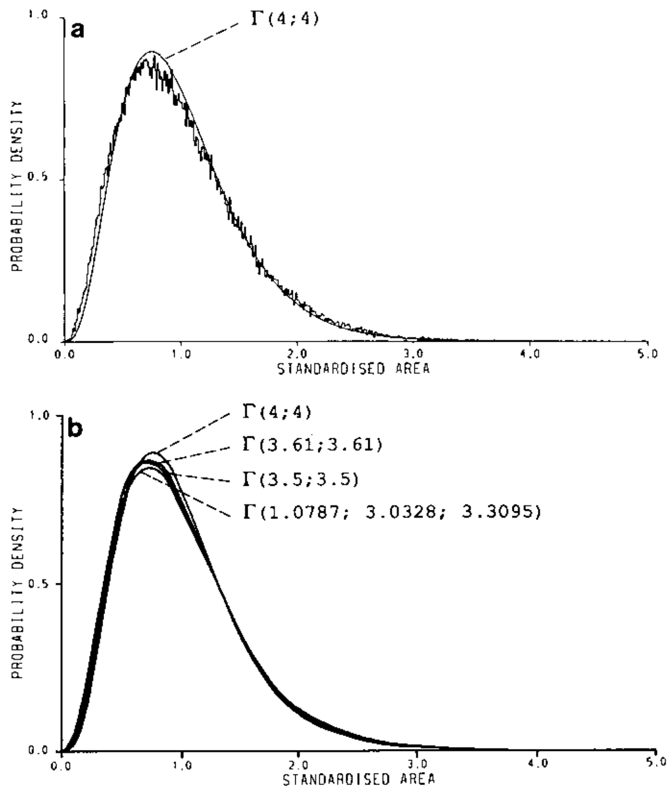

FIG. 3. Standardised distribution of areas of 100,000 polygons (class interval 0.01) mean = 1.00000, $s = 0.53048$: (a) with Kiang's $\Gamma(4;4)$ superimposed; (b) some other Γ-distributions for comparison (see text).

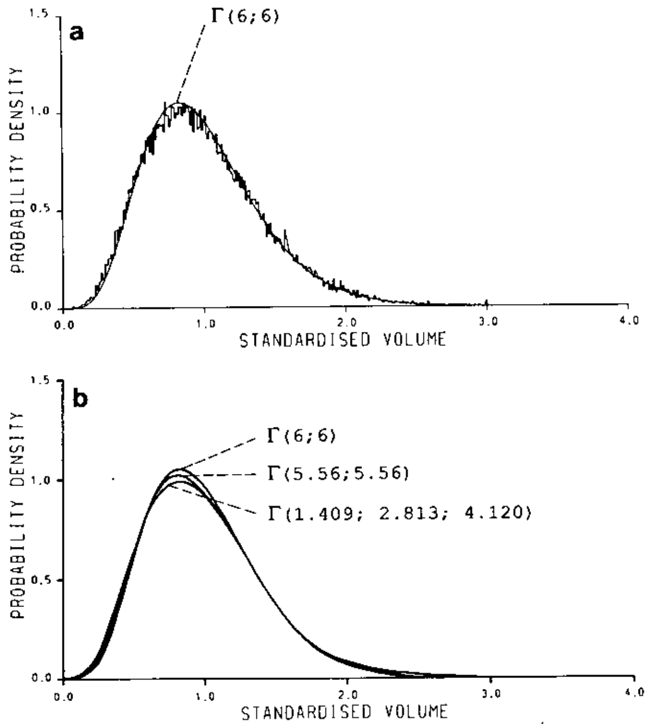

FIG. 4. Standardised distribution of volumes for the 50,000 random Voronoi polyhedra (class interval 0.01) mean = 0.99994, $s = 0.41899$: (a) with Kiang's $\Gamma(6;6)$ superimposed; (b) some other Γ-distributions for comparison (see text).

Kiang's conjecture mistaken, but Sibson [29] states that "No explicit form for the area distribution is known, for example—the conjecture that it is a gamma distribution has been shown to be false by numerical methods." Sibson does not detail the latter, nor does he cite the source of the conjecture in question. Presumably it is that of Kiang [20] and the numerical methods are those of Gilbert [16]. Gilbert arrived mathematically at 0.280 for the variance of random Voronoi polygons. In the present results $s^2 = 0.28141$—and yet $\Gamma(4;4)$ fits remarkably well (Fig. 3a) and no sides were lost.

According to Weaire, Kermode, and Wejchert [36], in 1984 Kiang revised his conjecture to become $\Gamma(3.5;3.5)$, but they found $\Gamma(3.58;3.58)$, $\Gamma(3.63;3.63)$, and $\Gamma(3.61;3.61)$ to fit their simulations better (with the latter fitting best). $\Gamma(3.5;3.5)$ is a better fit, but the other curves yield only very small differences, Fig. 3b. However, once a departure from $\Gamma(4;4)$ is made, the physical power of Kiang's conjecture, or why a two-parameter Γ-distribution should be fitted at all, is lost (and one must wonder why the volume distribution is so close to $\Gamma(6;6)$ if Kiang's conjecture does not have some considerable measure of truth about it).

Recently Tanemura [33] announced Kiang's conjecture to be false on the grounds that the three-parameter Γ-distribution fits better for 2D areas and 3D volumes. For areas he cites values for the three parameters (1.0787, 3.0328, and 3.3095, respectively) which were some of the trios of values which Hinde and Miles [19] fitted to their data. However, this curve (Fig. 3b) seems little different from the curve due to Kiang's two-parameter Γ-distribution using the value 3.61 due to Weaire, Kermode, and Wejchert [36]. Again there is no theoretical reason to support the values used.

5. DISCUSSION OF RESULTS FOR 3-DIMENSIONS

5.1. *Distribution of volumes of polyhedra.* Figure 4 has Kiang's $\Gamma(6;6)$ superimposed. The fit is excellent. This despite Moran [25] having said of Kiang's conjectural $\Gamma(6;6)$: "However Gilbert had obtained exact expressions for the variances which show that this conjecture cannot be true." However Gilbert's variance for volume is 0.180 and the variance for the present results—which fits Kiang's conjecture—is also 0.180 (to three significant figures). Andrade and Fortes [1] fit $\Gamma(5.56;5.56)$ (Fig. 4b). However, their class interval was 10 times coarser and for < 1000 polyhedra—an unspecified number of their tessellations lacked the RBC and peripheral polyhedra were ignored.

On one hand, Andrade and Fortes [1] regard the Voronoi volumes as being "well described" by Kiang's distribution but in which $\Gamma(5.56;5.56)$ is substituted for $\Gamma(6;6)$; on the other hand (equally recently) Tanemura [33] dismisses Kiang's conjecture (Section 2). He fits a three-parameter Γ-distribution, with values 1.409, 2.813, and 4.120 (Fig. 4b), respectively, referring to data in the press by Tanemura, Ogawa, and Ogita. However, their only data so far available are the mean values for numbers of facets, for number of apices, and for surface areas for an uncertain number of polyhedra [33]. To two places of decimals these agree with Meijering's values, but the distribution of volumes is not given.

6. CONCLUSIONS

6.1. *Random nuclei dispersed in 2D.* The greatest number of sides of any Voronoi polygon that occurred was 14, the mode is 6. The distribution of number of sides is here found to follow $\Gamma(3.5;21)$ closely. The work of Kiang is strongly supported and the mathematical challenge of deriving $\Gamma(4;4)$ for the area distribution remains.

6.2. *Random nuclei dispersed in 3D.* All the mean values obtained during the present computer simulations agree very closely with the values obtained mathematically by Meijering. Kiang's $\Gamma(6;6)$ curve for volume distribution is supported and the mathematical challenge of deriving it theoretically, stands.

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