On the shapes of natural sand grains

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[1] Digitized outlines of sand grains from a dozen locations, including deserts, beaches, and seaboards, have been acquired using an optical microscope linked to a desktop computer. Fourier analysis of the outlines returns the normalized power spectrum of each sample, averaged over several hundred grains. Regardless of the origin of the samples, these power spectra all exhibit essentially the same inverse power law dependence on the harmonic number, \( n \), varying as \( n^{-10/3} \) for \( 2 \leq n \leq 20 \). This “universal” spectrum provides the basis of a numerical technique for synthesizing the irregular outline of a sand grain: The outline is represented as a random pulse train in which identically shaped microasperities, with normally distributed amplitudes, are randomly superimposed on the perimeter of a circle. By identifying the spectrum of the microasperities with the observed inverse power law dependence derived from the optical images, the synthetic outlines are constrained to show the same statistical properties as the outlines of the real grains. The synthesized and real outlines are qualitatively similar in that visually, it is difficult to distinguish between them. The new numerical technique for synthesizing irregular outlines of sand grains has potential for investigating the random packing of realistically rough particles through computer simulation.


1. Introduction

[2] Since the early efforts of Wentworth [1919, 1922] and Vadell [1936] to quantify the shapes of rocks and pebbles, several techniques have been developed for characterizing the morphology of irregular particles, including sand grains. Perhaps the crudest measure of particle shape is the ratio of the major linear axes of the two- or three-dimensional outline [Sneed and Folk, 1958; Bluck, 1967; King and Buckley, 1968; Pittman and Ovenshine, 1968]. More sophisticated techniques include the use of the fractal dimension [Orford and Whalley, 1987], but by far the most widespread method is an expansion of the radius of the two-dimensional projected outline as an orthonormal series, most commonly a Fourier series [Ehrlich and Weinberg, 1970; Boon and Hennig, 1982; Clark, 1987; Diepenbroek et al., 1992; Drevin, 2006].

[3] In this paper, the Fourier series technique is applied to images of sand grains produced by an optical microscope linked to a desktop computer. An algorithm returns a digitized, two-dimensional outline of each grain, identifies the centroid, and, with the centroid as the origin, generates the radius, \( r \), as a function of the polar angle, \( \theta \). A standard fast Fourier transform program then returns the Fourier coefficients for \( r(\theta) \), which, in effect, represent the shape spectrum of the grain. The Fourier analysis is repeated for several hundred sand grains, all taken from the same population, and the resultant spectra are ensemble-averaged, yielding a smoothed shape spectrum for the sand sample under consideration.

[4] The resolution of the optical microscope limits the Fourier series of the measured grain shapes to about 20 harmonics. Over this range, the ensemble-averaged shape spectra of a dozen different sand samples, collected from deserts, sand dunes, beaches, seaboards and an estuary, all display remarkably similar characteristics, which would seem to impose a limitation on the utility of the Fourier technique as a discriminator of particle provenance or weathering history. A notable feature, common to all the sand grain shape spectra presented in this article, is an inverse power law dependence on the harmonic number, \( n \): the power spectra vary as \( n^{-5r} \), where \( s \approx 5/3 \), over the range of harmonics from \( n = 2 \) to \( n = 20 \). A sample of manufactured glass beads, which are nominally spherical and of uniform size, was used as a control, to provide a measure of the noise floor of the optical imaging system. The glass bead spectrum falls well below the sand grain spectra over most of the range \( n \leq 20 \).

[5] On the basis of the uniformity of the ensemble-averaged sand grain spectra, a statistical model is developed in the paper for synthesizing the two-dimensional outlines of individual sand grains. In essence, the model relies on a random pulse train [Buckingham, 1983] argument in which microscopic asperities with random, normally distributed amplitudes are placed at random positions around the circumference of a circle. The outlines of the synthetic grains have the same spectral properties as, and visually
show a strong resemblance to, the outlines of the optical images of actual sand grains.

2. Grain Shape Analysis

2.1. Optical Images

[6] As listed in Table 1, the materials investigated in this study include marine and estuarine sediments, beach sands and weathered, terrigenous desert sands. The sample labeled “SAX99, Gulf of Mexico” was collected from the seabed during the Office of Naval Research–supported SAX99 experiment off Fort Walton Beach, northern Gulf of Mexico [Richardson et al., 2001]. In most of the samples listed in Table 1, the grains were quartz or coral, some with an admixture of volcanic rock, and all had a unimodal size distribution with the mean radius ranging from 20 to 250 μm.

[7] An optical microscope with a data link to a desktop computer was used to create high-contrast, digital images, each showing, typically, 5 to 10 grains. The contrast was achieved by spreading the grains on a highly reflective background and illuminating them from above. This technique returns dark grain shapes, near silhouettes, against a bright background, which is ideal for the subsequent outlining procedure. As examples of the high-contrast technique, Figure 1 shows images of all the sand grain samples listed in Table 1. Each such image was taken as the microscope systematically scanned the ensemble of grains; and the number of grains analyzed per sample was chosen to satisfy the convergence criterion of Kennedy and Mazzullo [1991].

[8] Once captured, each image was processed using an automated routine written as an M-file in MATLAB. The background of the image was removed using a contrast threshold, which was adjusted manually to a level that depended on the grain material and the intensity of the overhead illumination. With the contrast set appropriately, the pixels of the image that fell below the threshold accurately depicted the grain shapes. The perimeter of each grain was then traced and saved as a set of x − y coordinates, with several hundred points used to represent the outline. In certain cases, a square boxcar filter was used to smooth the image prior to tracing the grain perimeter, although care was taken to ensure that the spatial size of the filter, which varied from sample to sample, was less than 1% of the size of any geometric measurements made at a later stage of the analysis. This small-scale smoothing not only facilitated the perimeter-tracing algorithm but also removed any reentrant angles, that is, angles associated with the outline folding back upon itself. As an example of the 2-D grain shapes obtained from the perimeter-tracing procedure, an image of sand grains from Imperial Beach, California, is shown in Figure 2a with the associated outlines depicted in Figure 2b.

[9] From the coordinates of its outline, several simple geometric features of a grain may be quantified, including the perimeter, which was calculated directly. In addition, a standard least squares fitting procedure returned the circle of equivalent area, from which the mean radius was obtained, and also the best fitting ellipse, which yielded the eccentricity of the grain. Finally, in order to proceed with a Fourier analysis of the grain shape, the x − y coordinates of the outline were expressed in terms of a polar coordinate system with its origin at the centroid. This procedure returned the radius, r, as a function of polar angle, θ, the latter measured from an arbitrarily chosen point on the outline. The technique used to identify the centroid is discussed below.

2.2. Fourier Analysis of the Grain Shape

[10] Since the work of Schwarz and Shane [1969] in the late 1960s, Fourier decomposition has become a standard technique for analyzing grain shapes [Drevin, 2006; Ehrlich et al., 1980, 1987; Rosler et al., 1987]. Symmetry dictates that the radial function r(θ) be periodic with a period of 2π, allowing r(θ) to be expanded in the bilateral Fourier series

\[
r(\theta) = \sum_{n=-\infty}^{\infty} R_n e^{in\theta},
\]

where \( R_n \) is the complex amplitude of the nth harmonic and \( i = \sqrt{-1} \). As illustrated by Ehrlich et al. [1987, Figure 1], the harmonics represent the contributions of geometrical, lobate forms to the overall shape of the outline: the zeroth harmonic represents the circle of equivalent area, the first harmonic a circle with the origin on its circumference, the second a figure of eight, the third a trefoil, the fourth a quatrefoil, and so on. Note that, as r(θ) is real,

\[
R_n = R_{-n}^*.
\]
where the asterisk denotes complex conjugation. It follows from equation (2) that $R_0$ is real, representing the mean radius of the individual grain. A standard inversion argument, invoking the orthogonality of the exponential basis functions in equation (1), leads to the following integral expression for $R_n$:

$$R_n = \frac{1}{2\pi} \int_{-\pi}^{\pi} r(\theta) e^{-in\theta} d\theta,$$

(3)

where, from the limits on the integral, it may be inferred that $r(\theta)$ is defined in the angular interval $-\pi < \theta < \pi$.

[11] It is implicit in the Fourier expansion of equation (1) that the radius is a single-valued function of the polar angle, $\theta$. This well-known limitation prohibits the use of the Fourier technique on a grain with reentrant angles, that is, angles which are associated with the outline doubling back on itself, thus giving rise to multivalued radii. After small-scale smoothing was applied, the number of grains showing such behavior was not significant, below the 0.5% level, in each of the sand samples listed in Table 1. Moreover, none of the samples exhibited significantly more or less occurrences of multivalued behavior than any of the others.

[12] As a brief aside, in the event that an outline were to possess pronounced reentrant angles, as in the cases reported by Bowman et al. [2001], a variant of the Fourier series technique, suggested by Clark [1987] and referred to by Thomas et al. [1995] as Fourier descriptors, could provide an alternative method for the classification of particle shape. The Fourier descriptors approach is not subject to the limitation that the radius be single valued, relying, in essence, on a representation of the particle outline in the complex plane. Although the Fourier descriptors technique can handle more complicated shapes than the Fourier series representation, it is not required for the sand samples currently under discussion.

[13] Returning to the Fourier series in equation (1), the unilateral amplitude spectrum of a single grain is given by the modulus of the Fourier coefficients:

$$S_n = 2|R_n|, \quad n \geq 1,$$

(4)

where the factor of 2 arises from the folding of the negative harmonics onto the positive $n$ axis. For $n = 0$, the factor of 2 is absent and the amplitude spectrum is equal to $R_0$. If the Fourier series in equation (1) had been expressed as a sum of cosine and sine terms with real amplitudes $A_n$ and $B_n$, respectively, then it is readily shown that the amplitude spectrum, $S_n$ in equation (4), is identically equal to $\sqrt{A_n^2 + B_n^2}$. For a sample of grains from the same population, the mean amplitude spectrum is

$$\bar{S}_n = 2\overline{|R_n|}, \quad n \geq 1,$$

(5)

where the overbar denotes an ensemble average taken over the sample. Again, for $n = 0$, the factor of 2 is absent and the ensemble-averaged amplitude spectrum is equal to $\overline{R_0}$.

2.3. Centroid

[14] Before proceeding with a discussion of the grain shape data, one more issue needs to be addressed, namely the choice of origin for the polar coordinate system of an individual grain. Wherever it is placed, the origin should facilitate a comparison of the spectra from different grains and, indeed, different populations of grains. As discussed by
a number of authors [Boon and Hennigar, 1982; Schwarz and Shane, 1969; Full and Ehrlich, 1982], the geometric center or centroid of the outline is the appropriate origin of the polar coordinate system. Since the radius of the circle represented by the first harmonic is the offset of the origin from the centroid, the first harmonic, $R_1$, is identically zero when the origin and the centroid are coincident.

Several iterative procedures for determining the centroid have been proposed in the literature [Ehrlich and Weinberg, 1970; Boon and Hennigar, 1982], including the Evans method described by Full and Ehrlich [1982]. An iterative algorithm, but relatively simple, was also the basis of the search procedure used in identifying the centroids of the sands listed in Table 1. The criterion used to locate the centroid is that the amplitude of the first Fourier harmonic should converge to some suitably small number.

Figure 2. Quartz sand grains from Imperial Beach, California: (a) optical image and (b) associated outlines used for shape analysis.

The initial estimate of the centroid, $(x_0, y_0)$, was taken as the center of the circle obtained from a least squares fit to the outline of a grain. Then the $x - y$ coordinates of the outline were converted to $r(\theta)$, with $(x_0, y_0)$ as the origin of the polar coordinate system. After upsampling $r(\theta)$ and interpolating over 1028 points spaced at equal angular intervals, $\Delta \theta$, the amplitude of the first Fourier harmonic was evaluated. The calculation was then repeated at eight points surrounding the original estimate of the centroid, $(x_0 \pm \delta, y_0 \mp \delta), (x_0 \pm \delta, y_0) \text{ and } (x_0, y_0 \pm \delta)$, and the point returning the smallest value of the first Fourier harmonic was chosen as the new origin, $(x_0, y_0)$. This procedure was repeated until convergence was achieved. Initially, the size of the search grid, defined by $\delta$, was chosen arbitrarily as half the size of the pixels in the image and this was reduced by half when a minimum was found. The iteration was terminated when the value of the first Fourier harmonic, relative to $R_0$, fell
below \(10^{-9}\), a criterion which is more stringent than that specified by Full and Ehrlich [1982].

3. Measured Amplitude Spectra

[17] The amplitude spectra of the 12 sand samples listed in Table 1, normalized to the mean radius of the sample, \(R_0\), and computed according to equation (5), are plotted on log-log axes in Figure 3. Also shown in the figure is the normalized amplitude spectrum of a sample of Sil-rock glass beads, which provides an indication of the noise floor of the optical imaging system. As illustrated by the image in Figure 4, the Sil-rock beads have excellent roundness, with radii specified by the manufacturer as uniform to within 3%. It is evident that over the first 20 harmonics, the sand grain spectra lie above the resolution limit of the imaging system.

[18] A striking feature of the normalized sand spectra in Figure 3 is the degree of similarity between them. Owing to the normalization, they have all collapsed onto essentially the same curve, which exhibits a uniform negative slope, indicative of an inverse power law dependence on the harmonic number, \(n\). Accordingly, the amplitude spectra may be represented by the simple expression

\[
S_n = \alpha R_0 n^{-s}, \quad n \geq 2,
\]

where the index \(s = 5/3\) is representative of the spectral slope of all the samples. As for the value of the dimensionless scaling constant, a reasonable estimate for most of the spectra in Figure 3 is \(\alpha \approx 0.57\).

[19] The uniformity of the spectra in Figure 3 raises an interesting question: do other sand samples, apart from those in Table 1, show the “universal” spectral behavior described by equation (6). A few ensemble-averaged amplitude spectra of sand grains have appeared in the literature, although usually plotted on log-linear axes rather than the log-log axes used here. To facilitate a comparison with equation (6), several such log-linear plots [Clark, 1987, Figure 4; Ehrlich and Weinberg, 1970, Figure 5, profiles A–C] have been digitized and replotted on log-log axes in Figure 5. It is evident that these previously published spectra are indeed consistent with equation (6), thus reinforcing the implication of Figure 3 that the normalized spectra of natural sand grains are all essentially the same.

4. Power Spectrum, Correlation Function, and Roughness

[20] Although the amplitude spectrum is widely used as an expression of grain shape, a more useful representation is the power spectrum, since it can be related directly to the

Figure 3. Normalized amplitude spectra of the sands and glass beads listed in Table 1. The solid black line above the spectral data illustrates a power law that scales as \(n^{-5/3}\).

Figure 4. Optical image of Sil-rock glass beads, which were used as a control.
variance of the radial excursions about the mean [Boon and Hennigar, 1982]. The power spectrum is also the basis of a new theoretical technique, to be introduced later, for synthesizing grain outlines. Using a notation similar to that in equation (5), the power spectrum is

$$P_n = \frac{2}{C_0^2} |R_n|^2; \quad n \geq 1,$$

and, for \( n = 0 \), \( P_0 = \frac{R_0^2}{C_0^2} \). As in equation (5), the factor of 2 in equation (7) arises from folding the negative harmonics onto the positive \( n \) axis. Figure 6 shows the power spectra, normalized to \( R_0 \) and plotted on log-log axes, of the sands and glass beads listed in Table 1.

[21] As with the amplitude spectra in Figure 3, the normalized power spectra of the sands in Figure 6 all collapse onto essentially the same curve, which exhibits a uniform negative slope, again consistent with an inverse power law dependence on harmonic number, \( n \).

[22] To relate the power spectrum to the variance, the radial excursions about the mean on an individual grain are expressed as the Fourier series

$$u(\theta) = r(\theta) - R_0 = \sum_{n=-\infty}^{\infty} U_n e^{i n \theta},$$

from which it follows that

$$U_n = \frac{1}{2\pi} \int_{-\pi}^{\pi} u(\theta) e^{-i n \theta} d\theta.$$

Clearly, for \( |n| \geq 1 \), \( U_n \) and \( R_n \) are identical and, since \( u(\theta) \) is a zero-mean process, \( U_0 = 0 \). The autocorrelation function of \( u(\theta) \), averaged over a sample of grains from the same population, is

$$\phi(\tau) = \frac{1}{2\pi} \int_{-\pi}^{\pi} u(\theta) u(\theta + \tau) d\theta,$$

where, as before, the overbar denotes an ensemble average. From grain to grain, the complex amplitudes, \( U_n \), in equation (9) are independent random variables, and hence a
straightforward substitution of the Fourier series into equation (11) yields

\[ f(t) = \sum_{n=1}^{\infty} \frac{C_{01}}{j U_n} e^{j \omega_n t}, \tag{12} \]

from which the variance is

\[ \bar{\phi}(0) = 2 \sum_{n=2}^{\infty} |R_n|^2, \tag{13} \]

where \( R_n \) has been substituted for \( U_n \) and the negative harmonics have been folded onto the positive \( n \) axis. It is implicit in equation (13) that \( R_1 = 0 \); and, from equation (7), it is evident that the summation on the right of equation (13) is over the terms of the ensemble-averaged power spectrum of the grains in the sample.

[23] A convenient measure of grain shape, or roughness, denoted by \( \rho \), is the root-mean-square value of the radial excursions about the mean:

\[ \rho = \sqrt{\bar{\phi}(0)}. \tag{14} \]

For the sands listed in Table 1, the power spectrum is given by the inverse power law in equation (8), which, when substituted into equation (14), returns a roughness approximately equal to 17% of the root-mean-square value of \( R_0 \):

\[ \rho = \left( \frac{0.2 R_0^2}{\sum_{n=2}^{\infty} n^{-10/3}} \right)^{1/2} = 0.171 \sqrt{R_0}. \tag{15} \]

[24] Because the series in equation (15) converges rapidly, the first 20 or so spectral harmonics, namely those that fall above the noise floor limit of the optical imaging system, as shown in Figure 6, are sufficient to achieve a reasonable estimate of grain roughness. As a consequence of this rapid convergence, however, the roughness, as defined in equation (15), is dominated by the lower-order harmonics and thus contains little information about the finer-scale radial structure. Of course, this fine structure could be the key to the provenance or weathering of the grains, having been caused, perhaps, by scouring, fragmentation or other formation processes.

[25] A fine-scale roughness could be defined using a formulation similar to that in equation (15) but with the summation taken over a selected range of harmonic numbers. In order to be representative of the fine detail that may be associated with the history of the grains, this range would necessarily extend above \( n = 20 \), taking it into a region where the universal inverse power law representation of the spectrum in equation (8) is of uncertain validity. Presumably, if the fine-scale structure were actually representative of grain provenance, then equation (8) should be expected to fail above some critical harmonic number, beyond which the spectrum would vary from sample to sample. If this were found to be the case, say from high-resolution scanning electron microscope (SEM) images [Marshall, 1987; Reed et al., 2002], then perhaps the history of the grains could be inferred from the fine-scale structure in the outlines.

5. Grain Synthesis

[26] The universal spectral representation of grain shape in equation (8) suggests that some feature exists that is common to the outlines of the sand samples listed in Table 1, but one which is so subtle that it is not immediately obvious from a visual inspection of the outlines themselves. To investigate such a possibility, it is postulated that the outline of a grain is a stochastic curve that can be represented as a random pulse train, an idea that is drawn from time series analysis [Buckingham, 1983]: a stochastic process, such as...
noise from an amplifier, is represented as a summation of independent, Poisson-distributed pulses of identical shape. For white noise, with a flat, indefinitely broad spectrum, such a pulse train takes the form of a random sequence of delta functions. This serves to illustrate a general property of random pulse trains: the spectrum of the stochastic process itself is the same, to within a scaling constant, as the spectrum of any one of the deterministic pulses within the pulse train.

[27] In the case of a sand grain, the “pulses” may be conceptualized as microasperities, which are superimposed at random positions on the perimeter of a circle of radius \( R_0 \).

Let each microasperity be represented by a pulse shape function, \( f(\theta) \), which, in view of equation (8), is clearly not a delta function. Then, the radial excursions about the mean may be expressed as a random sequence of terms constituting the random pulse train:

\[
u(\theta) = \sum_{k=1}^{K} a_k f(\theta - \theta_k), \tag{16}\]

where \( a_k \) and \( \theta_k \), respectively, are the amplitude and angular position of the \( k \)th pulse, and \( K \) is the number of microasperities in the interval \(-\pi < \theta < \pi\). The \( \theta_k \) are uniformly distributed in the interval \(-\pi < \theta < \pi\), with probability density \( 1/2\pi \), and the \( a_k \) are normally distributed about zero. The amplitude, \( a_k \), and position, \( \theta_k \), of the \( k \)th pulse are independent and, since the pulses themselves are independent, the \( a_k \) are pairwise-independent, that is \( a_k a_m = 0 \) for \( k \neq m \). In order to synthesize a grain outline, the problem now is to determine the pulse shape function, \( f(\theta) \).

[28] Since \( \nu(\theta) \) is periodic over the interval \(-\pi < \theta < \pi\), it follows from an inspection of equation (16) that \( f(\theta) \) must also be periodic over the same interval. Furthermore, \( f(\theta) \) is taken to be an even function of \( \theta \) because, on average over a large number of microasperities, \( f(\theta) \) can show no preferred asymmetry between positive and negative angles. Under these conditions, the Fourier transform of \( \nu(\theta) \) is

\[
U_n = \frac{1}{2\pi} \sum_{k=1}^{K} a_k \int_{-\pi}^{\pi} f(\theta - \theta_k) e^{-i\nu \theta} \, d\theta \tag{17}
\]

where

\[
F_n = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(\theta) e^{-i\nu \theta} \, d\theta \tag{18}
\]

is the Fourier transform of the deterministic pulse shape function, \( f(\theta) \). The final expression in equation (17) is obtained by making the substitution \( \nu' = \theta - \theta_k \) and invoking the periodicity of \( f(\theta) \) over the interval \(-\pi < \theta < \pi\). After averaging over a large number of grains, all possessing exactly \( K \) microasperities, the unilateral power spectrum of the radial fluctuations, from equation (17), is

\[
F_n = \frac{1}{2} |U_n|^2 = \frac{1}{2} |F_n|^2 \sum_{k=1}^{K} a_k a_m e^{-i\nu(k - m)} \tag{19}
\]

where

\[
\nu = \frac{K}{2\pi} \tag{20a}
\]

is the mean number of microasperities per radian and

\[
a^2 = \frac{1}{K} \sum_{k=1}^{K} a_k^2 \tag{20b}
\]

is the mean square value of the pulse amplitudes, \( a_k \).

A further averaging over all values of \( K \) returns an identical expression to equation (19) for the spectrum of the fluctuations but with \( \nu \) interpreted as an ensemble average over all possible values of \( K \). It is evident from the steps preceding it that the final result in equation (19) has been derived using the conditions that \( a_k \) and \( \theta_k \) are independent and the \( \theta_k \) are pair-wise independent.

[29] The final expression for the power spectrum in equation (19) is analogous to Carson’s theorem [Buckingham, 1983] in time series analysis. In effect, Carson’s theorem states that the spectrum of the stochastic process, that is, the radial fluctuations about the mean in the case of sand grains, is the same, to within a scaling constant, as the spectrum of the pulse shape function. Since the power spectrum of the radial fluctuations is known from equation (8), Carson’s theorem provides a means of recovering the pulse shape function, \( f(\theta) \).

[30] On comparing the theoretical spectrum in equation (19) with the empirical expression in equation (8), the power spectrum of the pulse shape function may be identified as

\[
|F_n|^2 = \begin{cases} |n|^{-2s} & \text{for } |n| \geq 2, \\ 0 & \text{otherwise} \end{cases} \tag{21a}
\]

where \( s = 5/3 \). If \( \phi_n \) is the phase of \( F_n \), it follows that, for \( |n| \geq 2 \),

\[
F_n = |n|^{-s} e^{i\phi_n}, \tag{21b}
\]

where, for \( f(\theta) \) to be real,

\[
\phi_n = -\phi_{-n}. \tag{21c}
\]

The pulse shape function, \( f(\theta) \), may now be constructed from the Fourier series

\[
f(\theta) = \sum_{n=-\infty}^{\infty} F(n) e^{in\theta} = \sum_{n=2}^{\infty} n^{-s} \cos(n\theta + \phi_n) \tag{22}
\]

\[
= 2 \sum_{n=2}^{\infty} n^{-s} \{ \cos(n\theta) \cos(\phi_n) - \sin(n\theta) \sin(\phi_n) \}
\]

Since \( f(\theta) \) is constrained to be an even function of \( \theta \), the second term in parenthesis, which is odd with respect to \( \theta \), must be zero. This can occur only if the phase, \( \phi_n \), is zero or \( \pi \). (Strictly, \( \phi_n \) could be any multiple of \( \pi \), but it is clear
from equation (22) that all such multiples are equivalent either to zero or \( \pi \). Under this condition, the Fourier series for \( f(\theta) \) reduces to

\[
f(\theta) = 2 \sum_{n=2}^{\infty} n^{-2} \cos(n\theta) \cos(\phi_n),
\]

which is indeed even in \( \theta \).

[31] To proceed further, it is necessary to examine the possible choices for the phases \( \phi_n \). The simplest option is to set \( \phi_n = 0 \) for all \( n \geq 2 \), which allows a further reduction in the Fourier series in equation (23) to the form

\[
f(\theta) = 2 \sum_{n=2}^{\infty} n^{-2} \cos(n\theta).
\]

Another possibility is to set \( \phi_n = \pi \) for all \( n \), which yields exactly the same series for \( f(\theta) \) as in equation (24) but with a negative sign preceding the factor of 2 on the right side. Statistically, this change of sign makes no difference to the grain shapes returned by the random pulse train expression in equation (17), because all it achieves, in effect, is a change in the sign of the random pulse amplitudes, \( a_k \). But the distribution of the pulse amplitudes is symmetrical about zero and remains unchanged under a reversal of sign of the \( a_k \). It follows that the formulation of \( f(\theta) \) in equation (24) is valid not only for \( \phi_n = 0 \) but also for \( \phi_n = \pi \), in both cases for all \( n \geq 2 \).

[32] A third choice is to set \( \phi_n = n\pi \), which, from equation (22) returns the following Fourier series for \( f(\theta) \):

\[
f(\theta) = 2 \sum_{n=2}^{\infty} n^{-2} \cos(n(\theta + \pi)).
\]

All this has achieved is a shift in the origin of the polar angle from \( \theta = 0 \) to \( \theta = -\pi \). But the origin of \( \theta \) is arbitrarily chosen anyway and, statistically, has no influence on the shapes of the grains returned by the random pulse train expression in equation (17). In this sense, the condition \( \phi_n = n\pi \) is no different from \( \phi_n = 0 \), the implication being that the former is covered by equation (24) as a descriptor of grain shape.

[33] Finally, consider the possibility that each of the phases \( \phi_n \), \( n = 2, 3, 4, \ldots \), takes a value that is either zero or \( \pi \), forming an arbitrary sequence that may be stochastic or deterministic. Under the constraints of the random-pulse-train formulation, this sequence would have to be identical for each and every microasperity contributing to the outline of a grain, since all the microasperities are postulated to have the same shape function, \( f(\theta) \). Moreover, the same sequence of phases would also have to be representative of all the grains in the same population, since all exhibit the same statistical properties. From a physical point of view, it is difficult to imagine a grain formation or weathering process that would give rise to such a universal sequence of phases, especially as there is no obvious reason why any one sequence, either random or deterministic, should be favored over any other. The unavoidable conclusion is that no such sequence of phases is appropriate to the random-pulse-train formulation of sand grain outlines.

[34] Having pursued this process of elimination, it is evident that a reasonable choice for the phases is the first of those investigated above, namely \( \phi_n = 0 \) for all \( n \geq 2 \). The associated expression for the pulse shape function, \( f(\theta) \), is given by equation (24), which, through the equivalence of various choices for the phases, has more generality than would appear at first sight.

[35] To evaluate the infinite series for \( f(\theta) \) in equation (24), the summation is truncated after \( N \) terms, where \( N \) is a finite number:

\[
f(\theta) \approx 2 \sum_{n=2}^{N} n^{-2} \cos(n\theta).
\]

Since the series converges quite rapidly, the truncation introduces little loss of precision provided that \( N \) is of order 10 or greater. By taking \( N = 20 \), corresponding to the number of Fourier harmonics available from the optical imaging technique, the symmetrical pulse shape function illustrated in Figure 7a is obtained. By increasing the number of terms in the sum to \( N = 200 \), representing essentially full convergence, the “exact” pulse shape function is found to take the form shown in Figure 7b. Both curves in Figure 7 exhibit a pronounced central peak, which is slightly higher and sharper for the exact case with the higher number of terms in the sum. As discussed below, the net effect of the differences between the two curves in Figure 7 is the appearance of fine structure in the synthetic outlines generated with \( N = 200 \), which is absent when \( N = 20 \).

[36] With \( f(\theta) \) known from equation (26), the shape of a sand grain may now be synthesized using the random-pulse-train formulation in equation (16). A MATLAB algorithm has been written which performs the following procedure. To begin, a value of \( K \) in the region of several hundred is selected arbitrarily, and the mean square value of the pulse amplitudes, \( \bar{a}^2 \), is obtained by equating the empirical and theoretical power spectra in equations (8) and (19), respectively:

\[
\bar{a}^2 = \frac{\beta R_0^2}{4\pi\nu}.
\]

A random number generator is then used to produce a set of pulse amplitudes, \( a_k \), and a corresponding set of uniformly distributed angles, \( \theta_k \). The \( a_k \) are distributed normally about zero with a variance equal to \( \bar{a}^2 \), as given by equation (27). Once these two sets of random numbers have been created, the random pulse train summation in equation (17) is evaluated and added to the radius \( R_0 \) to return a grain outline, that is, the radius as a function of angular position, \( \theta \). Each such realization of an outline has a unique shape, since the sets of random numbers representing the pulse amplitudes and angular positions change each time the computer code is executed.

[37] Several examples of grain outlines, computed using the MATLAB grain synthesis algorithm, are shown in Figure 8. The values of the parameters used in the computation are: \( K = 1000 \), corresponding to \( \nu = 159.15 \); \( R_0 = 100 \mu m \); \( \beta = 0.2 \); \( N = 20 \); and, from equation (26), \( \bar{a}^2 = 1 \mu m^2 \). With these parameters, the roughness of the synthetic grains is \( \rho = 17.1 \mu m \), as evaluated from equation (15). Incidentally, it is easily demonstrated that the qualitative
appearance of the outlines returned by the code is insensitive to the precise value chosen for \( K \), provided that \( K \) is about 100 or greater.

For comparison with the synthetic grains, the outlines of actual grains, obtained using the optical imaging technique described earlier, are also shown in Figure 8. To remove pixelation noise, the outlines from the images were Fourier transformed and then reconstructed using just the first 20 harmonics, making them commensurate with the synthetic outlines in Figure 8. The synthetic and actual outlines have identical statistical properties and, visually, the similarity of the computed to the measured outlines is quite evident.

If an extended range of harmonics were used in equation (26) to compute \( f(\theta) \), the resultant grain outlines would be expected to show more fine structure than those obtained using a smaller number of terms. This is exemplified in Figure 9, which shows two synthetic outlines that were generated using the parameter values listed above, except that in one case the upper limit on the summation for \( f(\theta) \) in equation (26) was set at \( N = 20 \) (Figure 9a) and in the other \( N = 200 \) (Figure 9b), corresponding to the pulse shape functions in Figures 7a and 7b, respectively. Identical sets of random amplitudes, \( a_k \), and angular positions, \( \theta_k \), were used in the two cases. It is apparent that a fine structure is present in the grain outline generated with the exact pulse shape function \( (N = 200) \) which is not visible when the summation for \( f(\theta) \) is truncated at \( N = 20 \). Although not a large effect, the appearance of fine structure as more terms are included in the Fourier sum for \( f(\theta) \) leaves open the possibility that, in practice, if deviations from the \( n^{-1/3} \) spectral power law

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**Figure 7.** Pulse shape function, as evaluated from the Fourier series in equation (26), taking the upper limit on the summation as (a) \( N = 20 \) and (b) \( N = 200 \).
were to occur above $n = 20$, then such departures could contain information about grain provenance or weathering.

6. Concluding Remarks

[40] The shapes of sand grains collected from a number of environments, including deserts, beaches and seabeds, have been examined using a digital optical microscope to create high-contrast images. An algorithm written in MATLAB was used to produce a two-dimensional outline of each grain, to identify the centroid, and to return the radius, $r$, as a function of the polar angle, $\theta$. The amplitude spectra and power spectra, averaged over a large number of grains from the same population, were obtained from the Fourier transform of the $r(\theta)$ coordinates. One important effect of the averaging is to suppress any bias that may be present in the 2-D projection of an individual grain. Such a bias could occur if its asymmetrical shape were to influence the orientation of a grain under the microscope.

[41] When normalized to the variance of the mean radius, the power spectra of all the sand samples exhibit essentially the same inverse power law dependence on the harmonic number $n$, varying as $\beta n^{-10/3}$, where the dimensionless scaling constant is $\beta \approx 0.2$. For the 12 sand samples investigated, this universal form for the power spectrum of the grain outlines holds for harmonic numbers up to $n = 20$.

[42] On the basis of this universal power spectrum, a mathematical technique is introduced for synthesizing the irregular outlines of individual sand grains. In effect, an outline is constructed by superimposing microasperities, identical in shape but with normally distributed amplitudes, at random positions around the perimeter of a circle. This random arrangement of microasperities may be represented as a random pulse train, a formulation that returns synthetic outlines with identical statistical properties to those of actual sand grains. Moreover, the computed and actual outlines are qualitatively so similar that, visually, they are difficult to distinguish from one another.

[43] It is well known, from the work of Hamilton [1970, 1972] and Richardson and colleagues [Richardson et al., 1991a, 1991b; Richardson and Briggs, 1996; Richardson,
1997], that the porosity of marine sediments tends to increase with decreasing grain size. Such behavior is not exhibited by smooth uniform spheres, which form packing structures, either regular or random, showing a porosity that is independent of particle size. In the case of sediments, Hamilton [1987] has proposed that the observed variation of porosity with grain size is associated with the irregular shapes of the particles; and, based on this idea, Buckingham [1997] has developed a simple mathematical model in which the porosity is expressed as a function of the mean radius of the grains and the root-mean-square excursions about the mean radius, the latter representing the roughness of the grain.

[44] Although Buckingham’s model fits the data sets of Hamilton and Richardson reasonably well, indicating that particle roughness almost certainly plays an important role in controlling the porosity of sediments, it still remains true that the packing structure of irregular particles such as sand grains is poorly understood. The numerical technique that has been introduced in this article for constructing highly irregular, synthetic outlines of sand grains provides a basis for investigating the random packing of realistically rough particles through computer simulation. Such an approach has the potential for providing new insights into the relationship between porosity and grain size that is observed in marine sediments.

[45] As presented in this article, the random-pulse-train synthesis of grain shapes is limited to two-dimensional projections of the particles. Extending the random-pulse-train argument to three dimensions on the basis of a spherical harmonic expansion is actually quite straightforward; provided that the assumption of similar grain statistics holds for all orientations. Such an assumption seems plausible but requires verification, which could be achieved from three-dimensional images of sand grains. Although the imaging and analysis of hundreds of grains in 3-D, necessary for statistical averaging, is a daunting task, it is perhaps the appropriate way forward.

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References
Full, E., and R. Ehrlich (1982), New approaches for location of centroids of quartz grain outlines to increase homology between Fourier amplitude spectra, Math. Geol., 14, 43–45, doi:10.1007/BF01037446.
Pittman, E. D., and A. T. Ovenshine (1968), Pebble morphology in the Merced River (California), Sediment. Geol., 2, 125–140.

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