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X-Ray Computed Microtomography and Spherical Harmonic Analysis were used to create 3D Analytical Mathematical Models of Random Star-Shaped Particles

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Abstract

To compute any physical quantity for a random particle, the mathematical shape of the particle must be known. The mathematics for regular particles like spheres and ellipsoids is simple. Mathematically characterising the shape of random particles with realistic shapes had not been done previously. However, since around the year 2002, a method that combines X-ray computed tomography and spherical harmonic analysis has been developed to give analytical, differentiable mathematical functions for the three-dimensional shape of star-shape particles, which are a broad class of particles covering most industrial particles of interest, ranging from micrometre scale to millimetre scale particles.

Keywords: X-ray • Spherical • Harmonic • Tomography

Introduction

Random-shaped particles play an important role in many scientific and industrial applications. "Random shape" can refer to particles that are close to being spherical but have a random degree of shape perturbation, or collections of ellipsoids with a random distribution of semi-axes, or truly random particles, such as crushed gravel or sand, with shapes that are very far from spheres or ellipsoids. In the majority of these cases, the particle's actual shape is critical to the properties under consideration. Examples include particle packing in a bed, the effect of inclusions on the rheological properties of suspensions, the effect of inclusions embedded in a solid on composite properties, and light scattering from a particle [1].

Because the volume and surface points of regular particles are known analytically, exact calculations such as light scattering or any integral over the surface and volume can be performed. For example, if the origin is the centre of a sphere, the surface can be specified by the function r(h, /)=R, where h and / are the spherical polar angles and R is the radius of the sphere, and r(h, /) 6 R specifies both the volume and the surface. The goal of this review is to briefly describe how to generate explicit, mathematical functions that can be differentiated at least twice and that analytically specify the surface and volume of a large class of random threedimensional (3D) particles. This means that any calculation that can be performed on geometrically regular particles can also be performed on this class of random shape particles, known as star-shape particles.

The X-ray CT/SH method can measure a large number of particles in a single sample, but it is a slower process than optical methods like laser diffraction. As a result, it was interesting to see if new particles with the same shape statistics as the original sample could be generated based on a sample of particles that had already been characterised with X-ray CT/SH. A statistical method was developed to accomplish this, and subsequent research discovered that on the order of 1000 original particles were required to generate new particles that qualitatively looked like the original particles and had similar shape statistics [2].

Literature Review

In the part-proc.f programme, a particle with some internal porosity or a few internal non-particle voxels generated during the thresholding process is examined, and these voxels are converted back into particle voxels. There are no holes in the particle now. A star-shaped object with no holes can be analytically described by the function r(h, /), which was introduced in Section 1 of this review, where r(h, /) is the distance from the origin taken inside the particle in the kernel (see above), in the (h, /) direction. The standard spherical polar coordinate system is used, with h representing the angle from the positive z-axis and / representing the angle from the positive x-axis, which is assumed to be positive in this case.

Following the application of a threshold, the slices are stacked using a programme that reads in each image and converts it to ascii (tiff2array.c). This is a straightforward but critical step in converting image data into a data structure that can be processed by subsequent particle generation programmes. The end result is a 3D array with integer values for each phase. This procedure can be modified so that image stacking and ascii conversion are performed first, followed by 3D thresholding. When an interior scan is made with an artificial circular boundary in each image, a slightly different procedure (tiff2pgm2mic.f) is used to generate the asci image stack [3].

To extract the particles, special software written in Fortran 77 was created (part-proc.f. The software searches for voxels with a specific phase number, which indicates the presence of a particle. After locating a particle, all voxels with the same label that are connected to the first voxel are identified using a burning algorithm. When no more such voxels are discovered, the collection of voxels discovered is referred to as a particle. During this process, an indicator is activated if one of the voxels makes contact with a surface, either of the images or, if there is a third phase surrounding the cylinder of real data, contacting this third phase.

Discussion

In some ways, this technique creates a "point cloud" on the surface of

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a given particle. There are other methods in the literature for generating a differentiable, single mathematical function that fits the point cloud. Radial basis functions are a popular mathematical method that has been applied to macroscopic objects rather than microscopic powders. It is, however, applicable to non-star-shaped objects. Would broaden it beyond the spherical harmonic approach described in this article. The spherical harmonic approach, however, may be computationally simpler and faster when applied to thousands of small powder particles [4].

Using an earlier version of this contact algorithm, the Anm model was created, which randomly places SH particles into a unit cell using either fixed or periodic boundary conditions. Each particle is chosen at random from a given dataset and size range before being attempted placement in the unit cell without contacting any other particles. Cement, mortar, and concrete microstructures can be created in this manner. To fit this microstructure and compute properties, adaptive finite element meshes can be generated. The contact algorithm described above has been incorporated into the Anm model, as has the ability for each particle to have one or more uniform thickness interfacial zones around its surface [5].

Because most rock and sand for concrete, asphalt, and gravel bed support come from blasted and crushed rock, a study was conducted on blasted and crushed rock of a single type. According to standard sieve analysis, the size scale ranged from 60 mm to about 20 lm, a size range of 3000. The particles were classified as Small=0.0175-0.24 mm, Medium=0.24-3.29 mm, and Large=3.29-45.1 mm. In the width parameter, each size range covered about 1.1 decade [6].

A systematic study of ten Norwegian rock types crushed in a vertical shaft impact (VSI) crusher and airseparated into three size ranges: 0-20 lm, 20-63 lm, and 63-125 lm was conducted. Epoxy samples were created and scanned in an X-ray CT scanner. These SH methods were used to collect and analyse millions of particles. The findings will be presented in four articles that will be published. It was discovered that the VSI crusher produces more evenly distributed particles than conventional cone crushers [7].

Conclusion

The TSQUARE library can be linked to a driver programme to automatically calculate shape properties of multiple particles drawn from a single population and report individual results as well as population statistics. For instance, displays the mean and standard deviation of five shape characteristics calculated on 200 particles drawn from four different particle sources. According to the results, 200 particles were more than enough to compute a consistent and accurate average.Parameters of shape the table shows that the variation in any shape characteristic within one particle source is comparable to the variation in mean values from source to source.

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Conflict of Interest

There are no conflicts of interest by author.

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