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The effects of regularity on the geometrical properties of Voronoi tessellations

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HIGHLIGHTS

- Effect of regularity on the properties of a random 3D Voronoi tessellation.
- Statistical analysis of Voronoi tessellations using 10^6 cell generations.
- Probability distributions derived for geometric properties of the tessellations.
- A simple scheme for generating Voronoi tessellations with regularity control.
- Application of controlled Voronoi tessellations in micromechanics modelling.

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ABSTRACT

This study comprehensively quantifies the effects of regularity on the geometrical properties of a random three-dimensional Voronoi tessellation (VT), where regularity was defined as the ratio of the minimum seed distance to the seed distance of the correlated body-centred cubic lattice. A scheme to generate Voronoi tessellations with controlled regularity is proposed, which was used to simulate 10^6 cells for a series of regularities. The results were used to derive probability distributions for the properties of the tessellation, including faces and edges per cell, vertex and dihedral cell angles, cell areas and volumes, etc. An understanding of the relation between a simple, measurable parameter characterizing the degree of regularity of a Voronoi tessellation and its geometrical properties is essential in generating virtual microstructures that are statistically representative of reality; the statistical results are also relevant to all other applications involving random Voronoi tessellations. Finally, an application is presented of the proposed Voronoi tessellation generation scheme applied to micromechanical modelling of grain structures with defined regularities for crystal plasticity finite element analysis.

1. Introduction

The three-dimensional (3D) Voronoi tessellation (VT) geometric model [1] partitions space into convex polygons, or cells, which fill the available volume completely. The VT model and its variants have been applied in a wide range of science and engineering subjects [2,3], including crystallography [4], materials science [5,6], biology [7], geography [8],

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astronomy [9], management [10] and control [11]. These models have been found extremely useful in micromechanical modelling, e.g. in generating high fidelity virtual cellular structures for mechanics simulations [5,6], and grain structures for large-scale realistic micro-forming analyses [12,13].

Some micromechanical applications require exact microstructure representation using reconstructions based on e.g. Electron Backscatter Diffraction (EBSD) measurements [14]. The VT is employed where a statistically equivalent representation of a real grain structure is sufficient, which obviates the need for laborious and expensive experimental characterization; statistically equivalent representations also facilitate parametric studies to correlate features of the grain morphology to the mechanical behaviour. Other methods for generating statistically equivalent virtual grain structures exist, including the Monte Carlo (Potts) model [15], ellipsoid packing [16], cellular automata [17], phase field [18] and level set [19] methods. In some instances, these methods are coupled to kinetics equations to describe an evolving microstructure, e.g. static recrystallization [20].

The VT model can be interpreted as the product of the isotropic growth process from a spatial distribution of static seeds. The resulting structure is completely and unambiguously determined by the initial distribution of seeds. If seeds are entirely randomly generated, the resulting structure is a Poisson Voronoi tessellation. An important adaptation of the Voronoi tessellation is the 'hard-sphere' model, which introduces a *minimum exclusion distance* between adjacent seeds upon which the tessellation is based. This type of 'hard-sphere' model, along with the limiting case of a Poisson Voronoi tessellation for which the exclusion distance is zero, will be considered in this paper.

The geometric characteristics of three-dimensional Poisson Voronoi tessellations have been studied extensively. Meijering [4] derived theoretical results for several properties including the mean numbers of faces and edges per cell and the mean total surface area and edge length per cell, while Gilbert [21] enumerated the theoretical variances of the cell volume. Mason et al. [22] derived local relations to evaluate the number of faces of a grain in individual grain clusters. Meanwhile, Mahin et al. [23] and Andrade and Fortes [24] studied characteristics of such cells using computer simulation, the former considering planar sections through the tessellation and the latter considering the cell volume; in each case the simulations were based upon fewer than 10,000 cells. Using larger-scale simulations, Kumar et al. [25] simulated 358,000 Poisson Voronoi cells and examined the distributions of various properties including the numbers of faces and edges per cell and both total surface area and the volume per cell. In a subsequent study, Kumar and Kurtz [26] simulated 377,000 cells and derived distributions of the dihedral and bond angles (the angles between adjacent faces and edges, respectively), as well as the total edge length of a cell and of a cell face. Ferenc and Néda [27] studied the cell size distribution properties for two- and three-dimensional Poisson Voronoi tessellations, and proposed a simpler general form of distribution function, calibrated based on statistical results.

Naturally occurring Voronoi tessellations vary significantly in their 'degree' of regularity. The higher the minimum exclusion distance for a given number of points in a region, the greater will be the regularity of the corresponding Voronoi tessellation. Studies of Voronoi tessellations with non-zero exclusion distance, which may be regarded as packings of hard spheres, include those by Hanson [28] who considered the cell volume distribution. In addition, for such tessellations based upon sphere packing, Oger et al. [29] derived distributions for the number of faces per cell, the total surface area per cell and the volume per cell, as well as several metric properties for an f-faceted cell. Lucarini [30] examined the statistical properties of random 3D tessellations, which were produced by perturbing cubic lattices with a specified Gaussian noise to individual lattice points. The distribution features of the number of faces, the area and the volume have been reported for tessellations obtained with different strengths of white noise. In Ref. [31], Kumar and Kumaran studied the cell volume distributions of random Voronoi tessellations, and a parameter to evaluate a tessellation's regularity was proposed based on the statistical variation of the volume distribution. This was based on the fact that the more regular a tessellation is, the narrower its volume distribution. The value can only be determined by a statistical evaluation, not by a geometrical measurement.

This paper will build upon previous works in two dimensions [32], and 3D Voronoi tessellations with different degrees of regularity [5,6]. The main objective is an investigation of the relation between the topological and metric characteristics of a Voronoi tessellation and its 'degree of regularity', defined here by a parameter a. Previous statistical studies were limited to examinations of particular regularities; Kumar and Kurtz [26] and Oger et al. [29] focused mainly on Poisson ($\alpha = 0$) and delta ($\alpha \sim 0.7$) type Voronoi tessellations, respectively. This study also goes beyond previous studies by examining 10^6 cells. The statistical results can be of importance for every application involving random Voronoi tessellations. In order to demonstrate the potential application, three dimensional crystal plasticity finite element (CPFE) models were built, where virtual grain structures are generated with controlled regularities using the proposed scheme.

2. Method of analysis

2.1. The seeds

Firstly, N points are generated in a central cube that has a volume V_0 and periodic boundary conditions. A Cartesian coordinate system is chosen, and points are placed in the cube by deriving x, y and z coordinates independently from pseudo-random numbers[1] generated evenly between zero and one. Once the first point has been placed, subsequent points are

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[1] The 'rand()' library function on the Silicon Graphics IRIX6.5 platform is used here.