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Procedia Engineering 81 (2014) 2409 – 2414

Procedia Engineering

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11th International Conference on Technology of Plasticity, ICTP 2014, 19-24 October 2014, Nagoya Congress Center, Nagoya, Japan

Optimisation of size-controllable centroidal voronoi tessellation for FEM simulation of micro forming processes

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Abstract

Voronoi tessellation has been employed to characterise material features in Finite Element Method (FEM) simulation, however, a poor mesh quality of the voronoi tessellations causes problems in explicit dynamic simulation of forming processes. Although centroidal voronoi tessellation can partly improve the mesh quality by homogenisation of voronoi tessellations, small features, such as short edges and small facets, lead to an inferior mesh quality. Further, centroidal voronoi tessellation cannot represent all real micro structures of materials because of the almost equal tessellation shape and size. In this paper, a density function is applied to control the size and distribution of voronoi tessellations and then a Laplacian operator is employed to optimise the centroidal voronoi tessellations. After optimisation, the small features can be eliminated and the elements are quadrilateral in 2D and hexahedral in 3D cases. Moreover, the mesh quality is significantly higher than that of the mesh generated on the original voronoi or centroidal voronoi tessellation. This work is beneficial for explicit dynamic simulation of forming processes, such as micro deep drawing processes.

Selection and peer-review under responsibility of the Department of Materials Science and Engineering, Nagoya University

Keywords: Voronoi; Centroidal voronoi; Optimisation; Laplacian; FEM

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Selection and peer-review under responsibility of the Department of Materials Science and Engineering, Nagoya University
doi:10.1016/j.proeng.2014.10.342

1. Introduction

Due to the growth of the micro system industry in recent decades, especially in microelectronic mechanical systems (MEMS), micro forming processes have drawn increasing attention. For deep understanding and precise control of micro forming processes, the finite element method (FEM) has been adapted based on macro forming simulation. However, size effects, such as deviation of material properties at a micro scale from those at a macro scale, become considerable and hence cannot be ignored.

A precise description of material at a micro scale, instead of the normal material models utilised in the current FEM, is one solution to extend the FEM's application scope. Voronoi structures have been employed to characterise material properties at micro scale owing to the similarity between their geometrical features and material's micro structures (Lu et al., 2013). In a simulation model each voronoi tessellation denotes one grain with its own properties, and therefore, a material's properties can be expressed at a micro level and more precisely than those of normal material models. However, initial voronoi structure is far from actual material's micro structure and, moreover, it is almost impossible to generate mesh based on this voronoi structure. To overcome these obstacles, centroidal voronoi, where the generating point of each voronoi tessellation is at the corresponding mass centroid, has been introduced into the FEM (Fritzen et al., 2009; Lu et al., 2012). The centroidal voronoi smoothes the initial voronoi structure by homogenisation of each voronoi tessellation and limitation of small angles. Consequently, meshing on this simplified voronoi structure becomes feasible.

Nevertheless, the centroidal voronoi is not suitable for all materials' micro structures. For example, it is unsuitable for non-equiaxed crystalline materials. Furthermore, the centroidal voronoi cannot avoid small features, such as short edges and small facets, which cause significant mesh quality deterioration. In this paper, a mass density function, that adjusts voronoi tessellations' size and distribution, is applied in order to approximate real materials' micro structures. Given that forming processes simulation requires a high mesh quality, an optimisation program is developed based on size-controllable centroidal voronoi tessellations. This eliminates small features while maintaining the tessellations' size distribution.

Nomenclature

I_n	a set of positive integers
k	number of neighbours
p	a set of points
R^m	space of m dimensions
$V(p_i)$	voronoi tessellation of the i^{th} generator p_i
x	point's coordinates
x^*	centre of a point's all neighbours
x_i^*	mass centroid of a tessellation
ρ	mass density
Ω_i	a set of neighbours of the i^{th} point p_i

2. Centroidal voronoi tessellation

The voronoi tessellations are a special spatial partition where all points inside a voronoi tessellation are closer to their associated generating point than to any other generating points outside and there is no overlap between any two different voronoi tessellations. This geometrical character is comparable to the crystalline distribution of metals where each grain has their own region and there is not any overlap between them. Therefore, the voronoi tessellations are applied to represent the micro structure of materials. The definition of a voronoi tessellation is based on its geometrical features. Given a set of points p in a given space R^m, the voronoi tessellation is the region defined by Eq. (1).

$$V(p_i) = \left\{x \middle| \|x - p_i\| \le \|x - p_j\|, i \ne j, i, j \in I_n\right\}, \quad (1)$$

where $p = \{p_1, p_2, \cdots\cdots, p_n\} \subset R^m, (2 \le n \le \infty), p_i \ne p_j, i \ne j, i, j, \in I_n = \{1, \cdots\cdots, n\}$, x is a point in the space R^m, p_i and p_j are generating points of voronoi tessellations and I_n is the set of positive integers.

These voronoi tessellations are determined by the points called generators. If the generators' information is not available for a given material, randomly distributed points can be utilised as the generators. However, the voronoi structure will be chaotic, as shown in Fig. 1, and far from real materials' micro structure. For this kind of voronoi structure, it is almost impossible to generate mesh for FEM simulation.

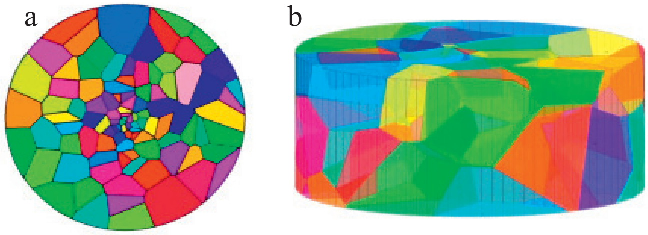

Fig. 1. Initial voronoi generated from randomly distributed generators in (a) 2D case and (b) 3D case.

For the sake of mesh generation, a centroidal voronoi where the generator coincides with the mass centroid of corresponding voronoi tessellation is employed. This simplifies the voronoi structure through homogenisation of all voronoi tessellations. This smoothing process boosts the similarities in both the shape and size of each tessellation. Consequently, the mesh can be generated with degenerated mesh elements, such as triangular and tetrahedral. The basic method applied in the authors' program to calculate centroidal voronoi tessellation is the Lloyd's method, which can be expressed as Fig. 2 (Du et al., 1999). The first step is generating initial voronoi tessellations with a set of points, than calculating the centroids of each voronoi tessellation following Eq. (2) and replacing the generators with these centroids. The next step is to generate new voronoi tessellations with the new generators and to check convergence criteria. These two steps are repeated until the criteria are satisfied.

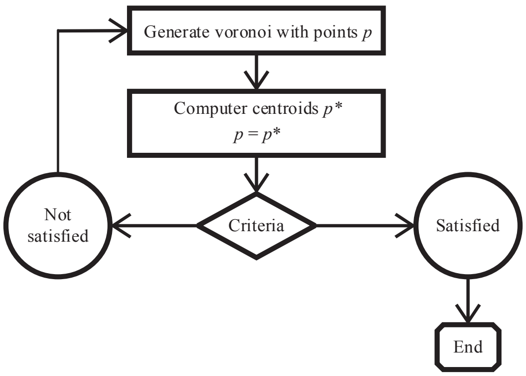

Fig. 2. Flow diagram of Lloyd's method.

$$x_i^* = \frac{\int_{V(p_i)} \rho(x) x dx}{\int_{V(p_i)} \rho(x) dx}, \tag{2}$$

where x_i^* is the mass centroid of the i^{th} voronoi tessellation, ρ is mass density and $V(p_i)$ is the voronoi tessellation of the i^{th} point p_i.

Although the centroidal voronoi tessellation meets the requirements for mesh generation, the centroidal voronoi structure can only represent equiaxed crystalline materials with almost equal grain shape and size. However, by choosing a proper mass density function, voronoi tessellations with different sizes can be obtained. For simplicity and ease of observation, Fig. 3 illustrates the centroidal voronoi with three different mass density functions in 2D. As shown in Fig. 3 (b) and (c), grains with different sizes can be obtained and the grain distribution is controlled by the density function. If a mass density function is carefully chosen, the centroidal voronoi tessellations can be seen to be analogous to materials' micro structures from a statistical viewpoint. For example, grains in fully annealed metals are equiaxed and can be represented by the centroid voronoi with a constant density, as shown in Fig. 3 (a).

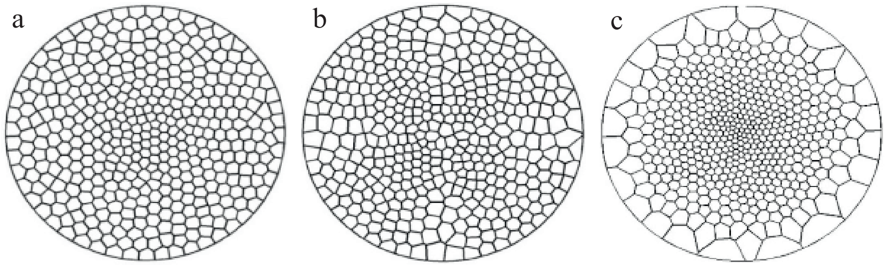

Fig. 3. Centroidal voronoi with different mass densities: (a) $\rho = 1$; (b) $\rho = \sin(\pi x) \times \sin(\pi y)$; (c) $\rho = e^{-20(x^2+y^2)}$.

3. Optimisation of centroidal voronoi tessellation

Due to significant deformation, a high mesh quality is an essential prerequisite for explicit dynamic simulation of micro forming processes (Sieger et al., 2010). Considering efficiency and accuracy, complete integral mesh elements are preferable to the degenerated mesh units. Generally, small features in the geometry will lead to degenerate meshes, such as triangulation meshes, being dominant and the mesh quality being poor. Therefore, an optimisation method is necessary to eliminate small features in the centroidal voronoi tessellations, while maintaining the size and distribution of tessellations. It is difficult to optimise voronoi tessellations directly as each voronoi tessellation is a polyhedron. A feasible approach to optimisation is to adjust Delaunay triangulations, the dual of voronoi tessellations. That is because that the vertexes of the voronoi tessellations are the circumcircle centres of the Delaunay triangulations and the vertex of each triangulation is the generator of one voronoi tessellation. Therefore, smoothing the Delaunay triangulations with a trend towards equilateral triangulations can effectively adjust the distance between two circumcircle centres of the neighbouring triangulations, and consequently elongate the short edges of the voronoi tessellations. Furthermore, small area facets in voronoi tessellations are eliminated because of the disappearance of short edges, the fundamentals of a facet.

A flow diagram explaining the optimisation process is shown in Fig. 4. The optimisation algorithm applied in this research is the Laplacian calculator as shown in Eq. (3). The basic idea of the Laplacian calculator is to move one point to the centre of all its neighbours (Chen, 2004,;Chen and Holst, 2011). In this study, as the centroidal voronoi tessellations are clipped to a special shape to model a deformed part, the boundary points are fixed and only inside points are traversed by the Laplacian calculator. Once satisfied with the termination criteria, the loop of the Laplacian traversal is ended. After the centroidal voronoi smoothing, the distribution of the fixed boundary points is acceptable, thus, it is suitable to maintain these boundary points.

$$x^* = \frac{1}{k} \sum_{x_j \in \Omega_i, x_j \neq x_i} x_j \ , \tag{3}$$

where x^* is the centre of the i^{th} point p_i's all neighbours, k is the number of neighbours and x_i and x_j are generators of the centroidal voronoi tessellations.

After optimisation the mesh on the voronoi tessellations is quadrilateral in 2D and hexahedral in 3D cases and the mesh quality is significantly higher than that of normal centroidal voronoi tessellations. Furthermore, this optimisation does not significantly change the size and distribution of the centroidal voronoi tessellations. Fig. 5 displays a comparison between the centroidal voronoi tessellations before and after optimisation, where there are 500 generators in a circle with radius of 0.8mm and the density function is $\rho = e^{-20(x^2+y^2)}$. From their partial enlarged views, ultra short edges can be found in the centroidal voronoi tessellations without optimisation while these short edges are enlarged after optimisation. An edge ratio which is the ratio of maximum to minimum edge length is chosen as an index of voronoi tessellation quality. The closer the edge ratio value is to one, the better the voronoi tessellations. Fig. 6(a) and (b) demonstrate the edge ratio distribution of the voronoi tessellations before and after optimisation. The key geometrical data are selected and listed in Table 1.

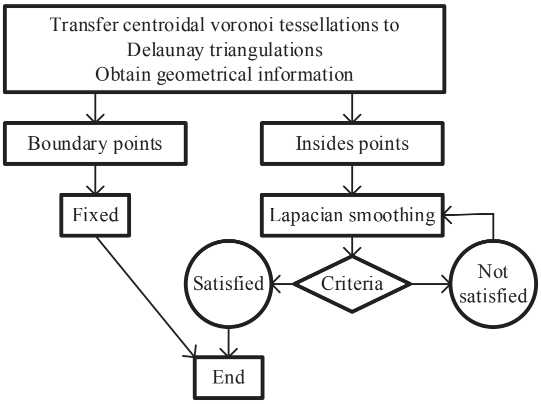

Fig. 4. Optimisation process.

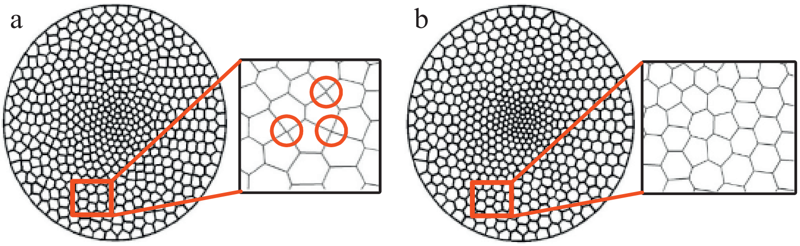

Fig. 5. Centroidal voronoi tessellations before (a) and after (b) optimisation.

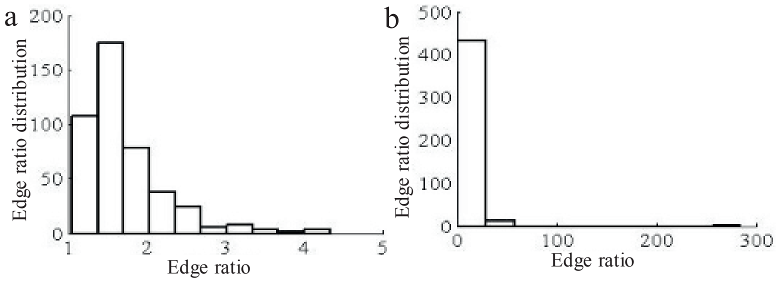

Fig. 6. Edge ratio distribution of voronoi tessellations (a) before and (b) after optimisation.

Table 1. Geometrical data of the centroidal voronoi tessellations before and after optimisation.

Comparing items	Before optimisation	After optimisation
Average edge ratio	5.5291	1.7256
Maximum edge ratio	284.6862	4.3361

The average edge ratio of the centroidal voronoi tessellations decreases from 5.53 to 1.7 after optimisation and the maximum edge ratio drops significantly from 284.7 before optimisation to 4.3 after optimisation. These results indicate that this optimisation can effectively eliminate short features in the voronoi tessellations.

After optimisation the geometry information is exported to an ANSYS command file which can be executed directly in the ANSYS environment. With exactly the same meshing methods, mesh is generated on the centroidal voronoi tessellations before and after optimisation respectively. Table 2 lists this mesh information. In terms of element quantity, the optimised centroidal voronoi tessellations need fewer mesh elements than the centroidal voronoi tessellations without optimisation. Moreover, the mesh qualities of these two voronoi tessellations are quite different. Element quality, which is the ratio of element area to edge length, and Skewness, which is an index of distortion is chosen to indicate mesh quality. For the element quality, a closer value to 1 is better, while as to the Skewness, a smaller value is better. The lowest element quality of the optimised centroidal voronoi tessellations is about 0.46, while that of the original centroidal voronoi tessellations is less than 0.02. The largest Skewness also validates that mesh quality of the optimised voronoi tessellations is higher as its maximum Skewness is smaller than that of the voronoi tessellations without the Laplacian optimisation.

Table 2. Mesh qualities of centroidal voronoi tessellations before and after optimisation.

State	Number of elements	Minimum element quality	Maximum Skewness
Before optimisation	35372	0.018	0.739
After optimisation	34535	0.455	0.555

4. Conclusions

This research provides an efficient method of optimising the centroidal voronoi tessellations for mesh generation. With a proper mass density function, special tessellation sizes and their distribution can be obtained and it is statistically similar to real materials' micro structures. Further, high quality mesh can be generated based on the optimised centroidal voronoi as small features in the voronoi tessellations are eliminated. The presented method offers access to precise simulation of micro forming processes, such as micro deep drawing.

Acknowledgements

The research is supported by the CSC scholarship (201206160011) from the China Scholarships Council and the International Postgraduate Tuition Award (IPTA) from the University of Wollongong. The study also obtained ARC funding support (FT120100432), and funding support from the State Key Laboratory of Rolling and Automation, Northeastern University, China.

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