27/28th International Conference
ENGINEERING MECHANICS 2022
Milovy, Czech Republic, May 9 –12, 2022
Paper **#113,** pp. 405–408, doi: 10.21495/51-2-405

LDPM STRUCTURE ENHANCEMENT WITH VORONOI PARTICLES

Vozáb J. [*]**, Vorel J.** [**]

Abstract: *More accurate models to describe the response of particulate polymers and other similar materials, such as concrete, at failure are demanded. Therefore, this paper briefly describes the influence of underlying structure in numerical modelling. The standard distribution of particles in the model is briefly described. This paper discusses the possibility of using Voronoi non-circular particles in the LDPM. A semilinear method to describe non-spherical particles in space is discussed and investigated in terms of computational complexity.*

Keywords: Polymers, Concrete, LDPM, Voronoi, Structure.

1. Introduction

The requirements for optimal building design and rehabilitation are strongly pronounced in the nowadays industry. As one of the most widely used materials, concrete is still under investigation (Ghobarah, 2001; Wen, 2001). Different polymers are typically utilized for rehabilitation, and thus, their properties and interaction with concrete are also widely studied (Abali et al., 2020). From the engineering point of view, the accurate response prediction of these types of materials is one of the essential elements and can be decisive for an efficient and safe design. In this paper, we focus on the Lattice Discrete Particle Model (LDPM) (Cusatis et al., 2011b,a) to capture the particle distribution, size and material properties together with the ability to simulate thermosets on the scale of application.

2. Structure

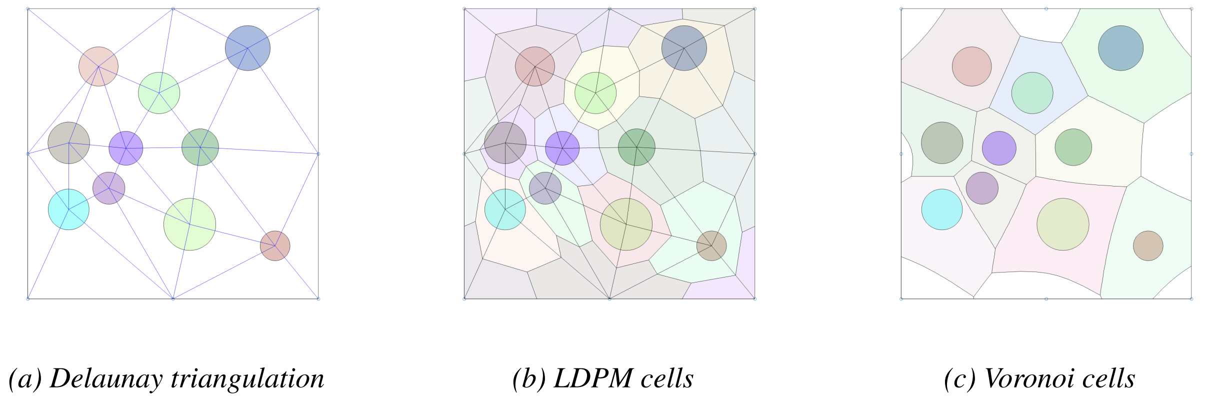
Since the LDPM is a discrete model, the underlying particles distribution, size, shape, and orientation may crucially influence the prediction (Yan et al., 2021). Composite materials such as particulate polymers or concrete can be seen as heterogeneous materials composed of grains of different shapes and sizes (fractions) bonded together by the matrix phase. However, still the most common approach is to neglect the heterogeneity and consider the materials as homogeneous. The material can be then simulated using the standard finite element method.

A more complex approach is to simulate the material structure as in the LDPM (Cusatis et al., 2011b). The simplest method of this approach is to generate spherical particles with a radius according to the grain size curve and place them randomly in the volume. The example of this structure is shown in Fig.1b. Note that the images of the structures are rendered in 2D to make the subtle differences between the structures apparent. The generated particles are used to form tetrahedrons (the most primitive polytope in space) using Delaunai triangulation, as shown in Fig.1a. The tetrahedrons are then split into parts that belong to each grain. All these parts of the tetrahedrons belonging to a single grain are then combined to form the resulting particle defined by the complex polyhedron (Cusatis et al., 2011b). However, these particles have the disadvantages of being difficult to construct and of being restricted to spherical particles only. At the same time, inappropriate placement of the particles can create undesirable fragments in the material structure.

---

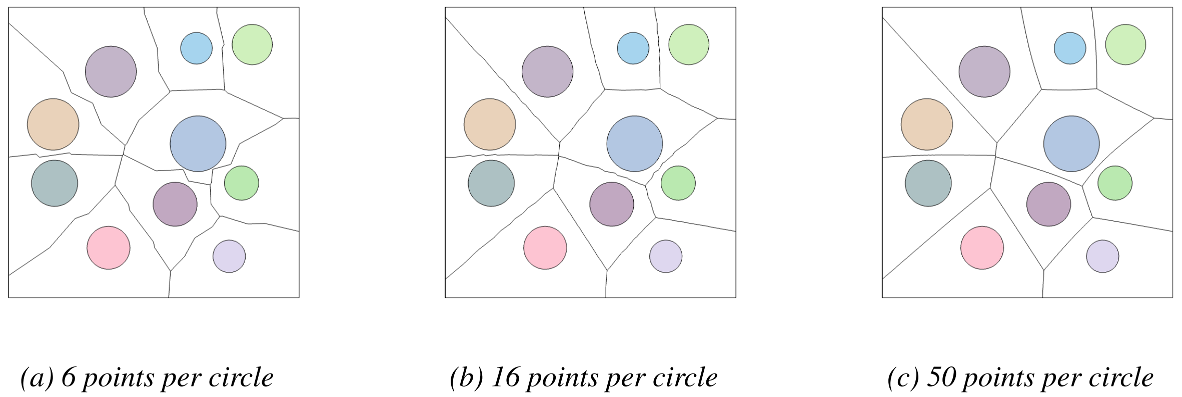
[*] Ing. Jan Vozáb: Faculty of Civil Engineering, Czech Technical University in Prague, 16629 Praha 6, Czech Republic; jan.vozabc@cvut.cz

[**] doc. Ing. Jan Vorel, Ph.D.: Faculty of Civil Engineering, Czech Technical University in Prague, 16629 Praha 6, Czech Republic; jan.vorel@fsv.cvut.cz



(a) Delaunay triangulation (b) LDPM cells (c) Voronoi cells

Fig. 1: Comparison of LDPM and Voronoi cells for set of circular particles.



(a) 6 points per circle (b) 16 points per circle (c) 50 points per circle

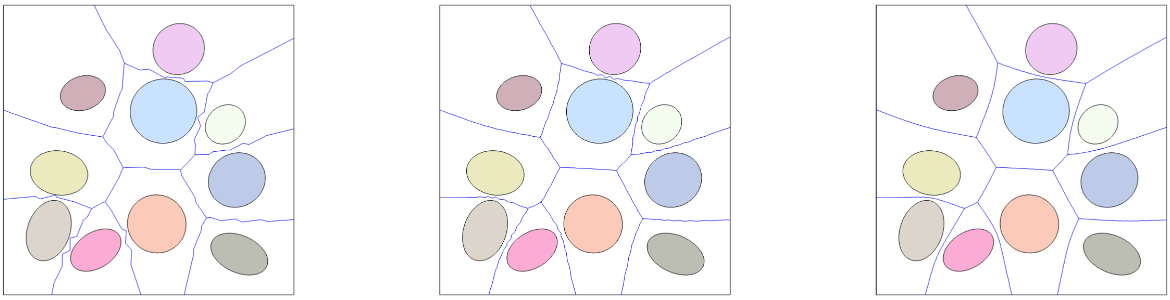
Fig. 2: Voronoi tessellation formed from circular particles.

3. Voronoi tessellations

In this paper, we explore the possibility of using tessellation of Voronoi cells for the LDPM model. Voronoi cells are particles where their boundary represents half of the distance between the particles from which tessellation occurs (Du et al., 1999). The boundaries are represented by straight lines for points in 2D and by planes for points in 3D. For more complex particles, Voronoi cells become more complicated. In the plane, the simplest planar particles are circles. In the case of congruent radii, the boundary is a straight line. If the radii are different, the boundary becomes a curve. If we consider more complex particles, such as ellipses, the boundary becomes even more complicated.

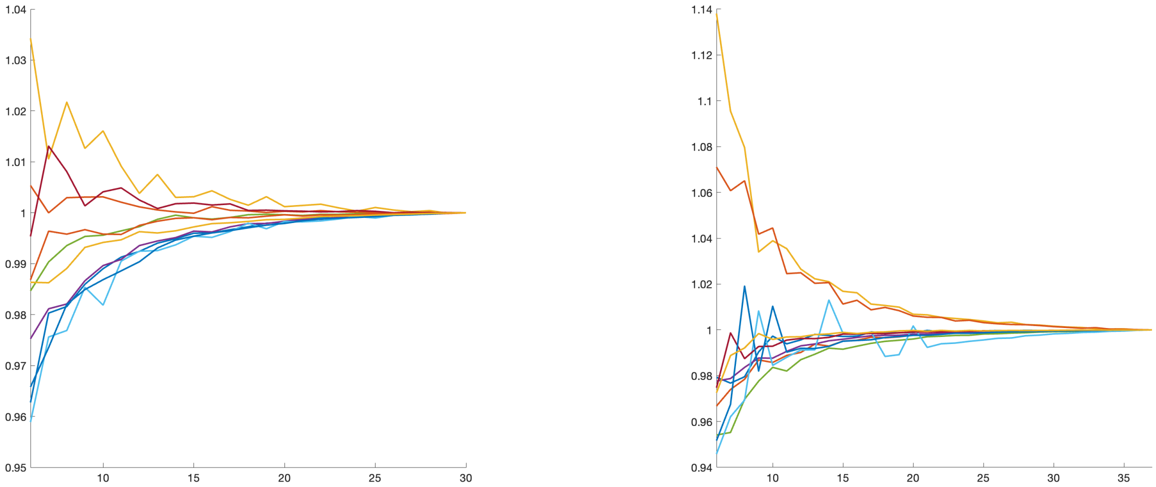
The computation of analytic boundaries with a high number of particles is a challenging process. For this reason, we attempt to take advantage of the higher computing power that is available today and try to simplify the process. We use the idea of generating points on the particle boundary. In this case, the boundaries are represented by a large number of straight lines (Schaller et al., 2013). The composition of these lines results in a semilinear cell boundary. This boundary resembles an analytically exact curve given a sufficient number of points. This has the advantage of being easily algorithmizable, and using today's hardware power, the process is noticeably faster. It also gives us the ability to create particles of arbitrary shapes that will even more closely match the real structure of the material. Once the particles have been created, the equilibrium equations will then be generated in the same way as for classical LDPM model structure generation.

We used the Matlab software (MATLAB, 2021) for the calculation. Our algorithm first creates the particles according to the given parameters. This is followed by the generation of points at the boundary of each particle. Then, a dense network of Voronoi cells between the points is computed. This is followed by the composition of the complex Voronoi cells according to the initial particle to generate the resulting tessellation of the material structure.



(a) 12 points per edge *(b) 25 points per edge* *(c) 44 points per edge*

Fig. 3: Voronoi tessellation formed from elliptical particles.



(a) Circular particles *(b) Elliptical particles*

Fig. 4: Convergence of the relative volume for a set of ten particles as a function of the number of points representing the particle boundary.

Fig. 2a shows a tessellation of circular particles where the edge is represented by 6 points. At first glance, it is clear that the shape of the boundary involves large inaccuracies that affect the content and length of the cell boundary. Fig. 2b shows the same set of particles, which are represented by 16 points in the calculation. In this case, the boundaries between cells are without significant fragments. Small fragments are visible for close particles or when there is a significant difference in radii. In Fig. 2c, particles represented by 50 points are visible. In this case, the boundaries are fragment-free, and as the amount of points on the particle edge is increased, the variation in boundary length and cell volume is negligible.

Voronoi 3a shows a set of elliptical particles with an edge represented by 12 points. Compared to the circular particles, the fragments are much more distinct despite the higher number of points due to the greater curvature of the cell boundary. Voronoi 3b shows ellipses represented by 25 points. In this example, the boundary is absent of distinct fragments, but minor noise is still evident near the particles. Voronoi 3c with ellipses represented by 44 points shows that at higher counts the boundary is clear of significant fragments.

Voronoi 4 shows the rate of convergence of the cell volume as a function of the number of points representing the edge of the particle. In the case of convergence of the circular particles 4a, a volume deviation of max 1% is reached at approximately 16 points per particle. For elliptic particles, Fig. 4b, which have boundaries with more curvature, a 1% deviation occurs at up to 25 points per particle. As the number of points increases, the volumetric variation only decreases.

4. Conclusion

In this paper, we discussed the use of Voronoi cells for non-circular particle shapes used in the LDPM. The planar structures composed of circular particles and elliptical particles are shown. Preliminary results show that Voronoi particles could represent grains in polymer particles or concrete, represented by rotating ellipsoids or arbitrary asymmetric particles. The convergence rate, which represents the accuracy of the Voronoi cells with respect to their exact boundary, was briefly discussed. Future work will need to validate the use of Voronoi particles with the LDPM model and quantify the differences between these approaches.

Acknowledgments

The financial support provided by the GAČR grant No. 21-28525S and by the Czech Technical University in Prague within SGS project with the application registered under the No. SGS20/155/OHK1/3T/11 is gratefully acknowledged.

References

Abali, B. E., Vorel, J., and Wan-Wendner, R. (2020) Thermo-mechano-chemical modeling and computation of thermosetting polymers used in post-installed fastening systems in concrete structures. *Continuum Mechanics and Thermodynamics*, pp. 1–19.

Cusatis, G., Mencarelli, A., Pelessone, D., and Baylot, J. T. (2011a) Lattice Discrete Particle Model (LDPM) for failure behavior of concrete. II: Calibration and validation. *Cement & Concrete Composites*, 33, 9, pp. 891–905.

Cusatis, G., Pelessone, D., and Mencarelli, A. (2011b) Lattice Discrete Particle Model (LDPM) for failure behavior of concrete. I: Theory. *Cement & Concrete Composites*, 33, 9, pp. 881–890.

Du, Q., Faber, V., and Gunzburger, M. (1999) Centroidal Voronoi Tessellations: Applications and Algorithms. *Siam Review*, 41, 4, pp. 637–676.

Ghobarah, A. (2001) Performance-based design in earthquake engineering: State of development. *Engineering Structures*, 23, 8, pp. 878–884.

MATLAB (2021) *9.11.0.1837725 (R2021b) Update 2*. The MathWorks Inc.

Schaller, F. M., Sebastian C. Kapfer, Kapfer, S. C., Evans, M. E., Hoffmann, M., Aste, T., Saadatfar, M., Mecke, K., Gary W. Delaney, Delaney, G. W., Delaney, G. P., and Schröder-Turk, G. E. (2013) Set Voronoi diagrams of 3D assemblies of aspherical particles. *Philosophical Magazine*, 93, pp. 3993–4017.

Wen, Y. (2001) Reliability and performance-based design 73. *Structural Safety*, 23, 4, pp. 407–428.

Yan, Z., Ge, H., Guo, S., Xiaoyong, W., and Zhao, G. (2021) Flexural strength test and meso-mechanical evolution behavior of cement concrete based on discrete element method. *Computational particle mechanics*, pp. 1–15.