8th. World Congress on Computational Mechanics (WCCM8)
5th. European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2008)
June 30 – July 5, 2008
Venice, Italy

Numerical modeling of nanostructures

***A. Benabbou [1], H. Borouchaki [2], P. Laug [3] and J. Lu [4]**

[1] INRIA Paris - Rocquencourt
BP 105, 78153 Le Chesnay Cedex, France
azeddine.benabbou@inria.fr
http://www.inria.fr

[2] University of Technology of Troyes
BP 2060, 10010 Troyes Cedex, France
houman.borouchaki@utt.fr
http://www.utt.fr

[3] INRIA Paris - Rocquencourt
BP 105, 78153 Le Chesnay Cedex, France
patrick.laug@inria.fr
http://www.inria.fr

[4] Hong Kong Polytechnic University
Kowloon, Hong Kong
jian.lu@inet.polyu.edu.hk
http://www.polyu.edu.hk

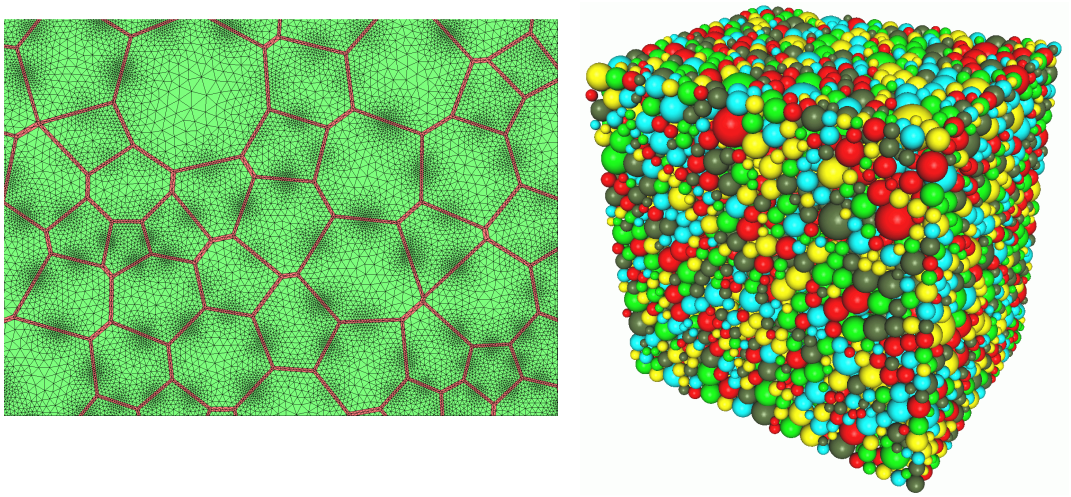
Key Words: *nanostructures, sphere packing, granular structures, power diagram, Laguerre diagram.*

ABSTRACT

During the past three decades, many researchers have been interested in tools and techniques to synthesize nanomaterials and understand their exceptional properties. Experiences and researches have proved that nanostructures properties are very different than those of bulk structures, and that the nanocrystallisation globally enhances the behavior of materials. Owing to the scientific and industrial interests in nanomaterials, investigations and studies of the grain refinement mechanisms in metals and alloys represent one of the most advanced directions in physical metallurgy. In this paper, we focus on the geometrical modeling of nanostructures issued from the SMAT (Surface Mechanical Attrition Treatment) process, in order to simulate their behavior by the finite element method. The principle of the SMAT process is to result in a grain refinement by introducing a maximum of plastic deformation on the surface of the material [1]. In fact, in most cases, material failures occur on surfaces (fatigue fracture, wear and corrosion, etc.). These phenomena are very sensitive to the structure and the properties of the material surface. Hence, the overall properties, performance and lifetime of materials can be improved by a grain refinement on the surface.

The geometrical modeling of nanostructures is similar to the packing sphere problem which consists in filling a domain by disks in two dimensions (spherical balls in three dimensions) whose radii follow a size distribution. In this geometrical modeling, grains (usually polygonal or polyhedral cells) are approximated by disks in 2D and spherical balls in 3D, the grain size distribution experimentally obtained must be verified, the disks (spherical balls) must neither overlap each other nor intersect the domain boundary, and they must be separated by grain boundaries with a specific thickness. A new filling constructive algorithm based on an advancing-front approach, usually used in the context of mesh generation, is proposed [5]. This filling algorithm is compared to some existing constructive and dynamic methods in 2D [2,3]. The gains in computation time and in density show the efficiency of our new method. The aggregates generated by the advancing-front approach contain empty areas (considered as grain boundaries)

near front collisions. This geometrical anisotropy can lead to physical errors in the simulation (indeed grain boundaries are mainly responsible for the nanomaterial behavior). A point relocation algorithm using the weighted Delaunay triangulation is then introduced to balance the grain boundaries thicknesses on the whole structure. Furthermore, using Laguerre (or power) diagrams, we can transform the disks (spherical balls) into polygonal (polyhedral) cells which are very similar to the grain shapes observed in many material structures.
Numerical 2D and 3D examples are provided to illustrate the capability and the efficiency of our approach. The algorithms and techniques presented here can find applications to generate aggregates in all fields concerned by the granular structures such as metallurgy, ceramics, soil science, biology, cements, etc.



Models of nanostructures in 2D (left) and in 3D (right).

REFERENCES

[1] K. Lu and J. Lu. Nanostructured surface layer on metallic materials induced by surface mechanical attrition treatment. Materials Science and Engineering A, Vol. 375-377, p. 38-45, 2004.

[2] K. Bagi. An algorithm to generate random dense arrangements for discrete element simulations of granular assemblies. Granular Matter (2005) 7: 31-43.

[3] B.D. Lubachevsky and F.H. Stillinger. Geometric properties of random disk packings. Journal of Statistical Physics, Vol. 60, Num. 5-6, p. 561-583, September 1990.

[4] A. Benabbou, H. Borouchaki, P. Laug and J. Lu. Geometrical modeling and meshing of granular domains. 6th Symposium on Trends in Unstructured Mesh Generation. 9th US National Congress on Computational Mechanics. San Francisco, California, July 22-27, 2007.

[5] A. Benabbou, H. Borouchaki, P. Laug and J. Lu. Geometrical modeling, mesh and simulation of granular structures, application to nanostructures. Part I. Theoretical and algorithmic aspects of the modeling in 2D. INRIA Research report N°6414, January, 2008.