Implementation of a method for the generation of representative models of polycrystalline microstructures in LS-PrePost.

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Abstract

The capability of accurately reproducing the microstructural features of polycrystalline materials is of fundamental importance for the correct simulation of the micromechanical behaviour of materials.
This paper describes the development and the implementation of VorTeX algorithm for the generation of numerical models representative of real polycrystalline microstructures, and its integration within LS-PrePost. The method presented offers high control over the grain size distribution of the final structure by adopting the so-called Laguerre-Voronoi tessellation techniques. Additional features implemented allow constraints to be imposed on the structure such as symmetrical boundaries and enables the introduction of interface entities (i.e. contacts and cohesive elements) on the grain boundaries to model inter-granular crack propagation.

Keywords: LS-PrePost, microstructural modelling, Voronoi tessellation

1 Introduction

The capability of accurately modelling the microstructural features of polycrystalline materials is of fundamental importance to increase the understanding of deformation and failure mechanisms of materials. This in turn facilitates the development of new microstructural configurations with increased performance under specific loading conditions.
The numerical modelling methods have been developed to generate accurate models of real microstructures, and can be broadly divided into *specific* and *generic* (or *statistical*). To the first category belong all the methods that aim to reconstruct a specific structure from a single set of direct experimental measurements, either with a destructive (e.g. SEM imaging of serial sections [1]) or non-destructive (e.g. X-ray tomography [2]) approaches. The second category, instead, comprises of all the methods aiming to generate models statistically representative of the target material, focusing on capturing key topological features rather than reproducing a specific microstructure.

Among the several statistical approaches developed, Voronoi-based tessellation techniques have been proven to be able to generate representative models of real microstructural morphology of several polycrystalline materials [3,4], offering a good compromise between simplicity of formulation and representativeness of the generated topologies.
Several modifications of the classic Voronoi tessellation technique have been proposed to provide more control over the final tessellation, thus increasing the representativeness of the generated topologies, either by imposing constraints on the position of the nuclei during the seeding process (e.g. Poisson, Hardcore, extended Hardcore), or by introducing definitions of distances alternative to the Eulerian distance (e.g. Laguerre).
Laguerre-Voronoi technique, in particular, provides extreme control over the size of the single cells composing the tessellation, thus allowing the generation of numerical models representative of a wide range of polycrystalline microstructures.

In this paper, the implementation of a method for the generation of finite elements (FE) models of representative polycrystalline microstructures is presented, alongside its integration into the user interface software LS-PrePost.

2 Generation of numerical microstructures

The good compromise between simplicity of formulation and representativeness of polycrystalline topologies offered by Voronoi tessellations allowed the development of a computationally-efficient and robust algorithm for the generation of microstructural models for the simulation of micromechanical behaviour of polycrystalline materials.
The classic Voronoi tessellation technique, often used to model both metallic and ceramic microstructures, however, exhibits low accuracy in reproducing the variability in grain size observed in real ceramic materials, mainly due to the limited "versatility" of the formulation. A noticeable improvement of the representativeness can be obtained adopting the so-called *Laguerre-Voronoi* formulation that, by introducing additional variables, increases the range of accurately reproducible materials. However, to exploit the increased versatility offered by the Laguerre modification, additional constraints on the seeding of the nuclei are required.

In this section the formulations of the classic and Laguerre Voronoi tessellation techniques are briefly presented, alongside the method for the conditioning of the nuclei seeding developed to avoid the presence of degenerate cells in the tessellation and provide user control over the final cell size distribution.

2.1 Voronoi tessellation techniques

Starting from an arbitrary distribution of *nuclei*, Voronoi tessellation techniques decompose the entire space into convex polyhedral *cells*. A single cell consists of all the points closer to the correspondent nucleus than to any other nuclei. The mathematical definition of the *i-th* cell generated from the seeding of *N* nuclei can be expressed as

$$\left\{R_{P_i}\right\} = \left\{x \in \Re^3 : \left\|P_i - x\right\| \le \left\|P_j - x\right\| \right\} \forall j = 1,2,...,N : j \neq i \tag{1}$$

Where R_P is the set of points associated to the *i-th* nucleus $\boldsymbol{P_i}$, and $\boldsymbol{x}$ represents the position of the any point in the three-dimensional space.
Within the classic formulation the only variables are the coordinates of the nuclei, thus limiting the control on the grain size distribution to the nuclei seeding process, as it is done, for example, for the widely used Hardcore and Poisson formulations. However, the constraints on the nuclei seeding provide a relatively small increase of the achievable grain size distributions, thus hindering the representativeness of the numerical models.

The introduction of an alternative formulation of the distance, namely the *power distance*, in lieu of the *Eulerian distance* adopted in the classic Voronoi tessellation, hugely increases the control over the cell size distribution by allowing the user to assign the "weight" of each nucleus.
The relative value of the weight ω of two neighbouring nuclei determines the position of the cell boundary by modifying Eq. (1) into:

$$\left\|P_i - x\right\| - \omega_i \le \left\|P_j - x\right\| - \omega_j \tag{2}$$

A graphical representation of the position of a generic cell boundary between two neighbouring nuclei adopting the classic and the Laguerre Voronoi (with $\omega_i < \omega_j$) approaches in presented in Fig.1:.

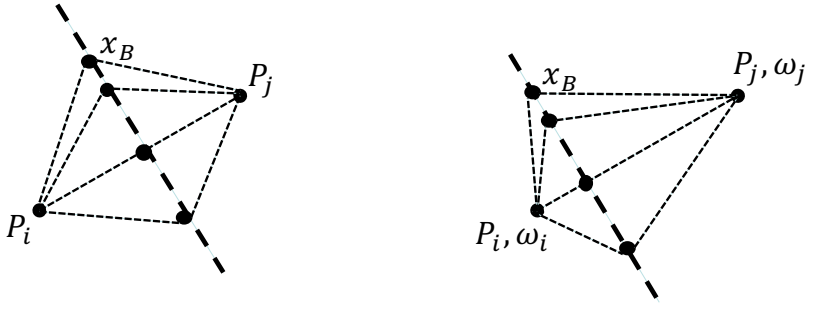

Fig.1: Classic (left) and Laguerre (right) Voronoi definition of cell boundary (dashed line).

The versatility offered by the Laguerre modification, however, comes at the cost of a non-univocal relation between nuclei and cells, which can hinder the quality of the resulting tessellation. To avoid degenerated cases a method for conditioning the nuclei seeding process has been developed and implemented as part of the methodology presented in this paper.

2.2 Conditioning of Laguerre-Voronoi tessellation

The formulation of the Laguerre-Voronoi tessellation presented in Eq. (2) suggests that, under the assumption that all the values of ω are positive, the weights can be interpreted as the square of the radius of a sphere centred in the corresponding nucleus [5].

The so-called *geometrical equivalence* allows to use sphere packing methods as conditioning for the seeding of the nuclei. In particular, the method presented in this paper adopts a geometrical packing approach, presented in [6].
The algorithm implemented is based on the sequential positioning of spheres, with arbitrary size distribution, imposing for each new added sphere the simultaneous tangency with two already positioned spheres, thus creating a spirally growing structure, as presented in Fig.2:.

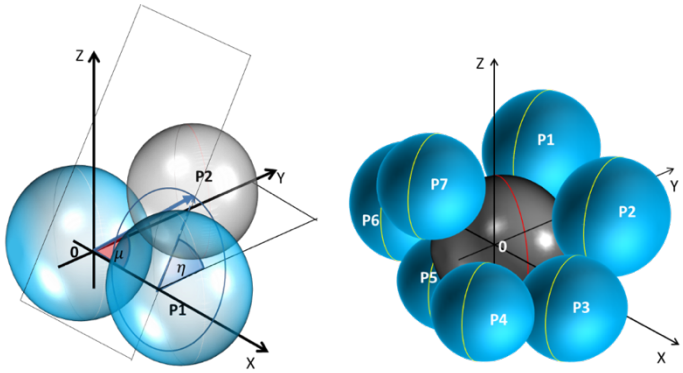

Fig.2: Graphical representation of the tangency condition (left), and the position of the first layer of packed spheres (right).

Of the two angles used to define the position of the newly added sphere (marked as μ and η in Fig.2:), the first is imposed by the tangency condition, whilst the second is assigned arbitrarily, thus guaranteeing the aleatory nature of the final assembly.

The position of the centres and the radii of the spheres are used, respectively, as position and square root of the weight of the nuclei for the discretisation of the entire 3D space using the Laguerre-Voronoi tessellation technique. An example of the application can be found in Fig.3:.

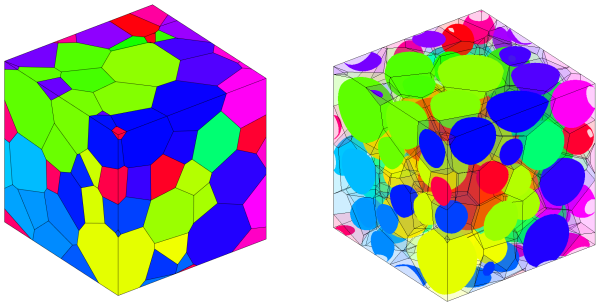

Fig.3: Rendering of the Voronoi cells (left) and underlying conditioning spheres (right).

The approach described in this section has been used to generate three-dimensional tessellations statistically representative, in terms of grain size distribution, of real polycrystalline microstructures, as presented in [7].

As an example, Fig.4: reports the comparison of the cell size distribution of classic and Laguerre-Voronoi tessellation technique against experimental measurements of the grain size of polycrystalline alumina.

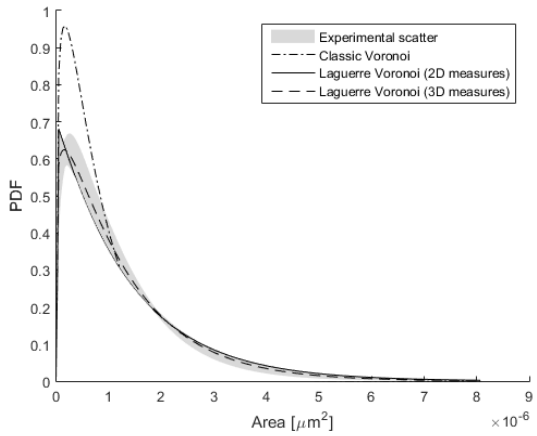

Fig.4: Validation of numerical tessellations generated with different Voronoi-based techniques against experimental measurements.

The Laguerre-Voronoi tessellation provides a noticeable improvement in representativeness, even when using values of weights inferred from 2D measurements of the cross-sectional area of the grains. Further improvement can be obtained by optimising the input values to match the actual (three-dimensional) size of the grains.

Further constraints can be added to the seeding process, to impose the symmetry boundary condition in the desired directions. Specifically, the assembly of conditioning spheres is replicated along the specified directions, thus assuring the compatibility of the cells on two opposite faces.

3 FE models of the microstructure

The so-generated tessellations can be discretised with either tetrahedral or hexahedral elements to build Finite Elements (FE) models representative of real polycrystalline microstructures.

The discretisation with – linear or quadratic – tetrahedral elements is performed singularly on each cell, imposing the same characteristic length, thus ensuring the compatibility of meshes on coincident faces, and allowing for the insertion of interface entities (e.g. cohesive elements, contacts) along the grain boundaries, as presented in Fig.5:. The use of tetrahedral elements allows the planarity of cell faces, and of any interface entities inserted to model the grain boundaries, to be preserved, at the cost of the possible presence of highly distorted elements in the model.

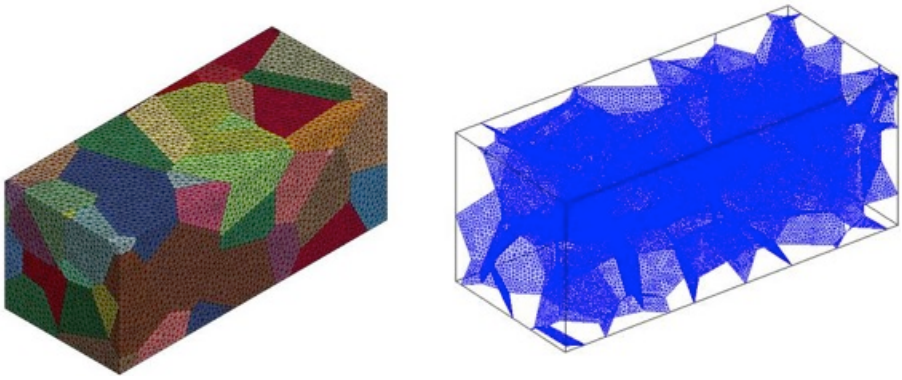

Fig.5: Tetrahedral meshing of a tessellation (left), and corresponding interface entities on the grain boundaries (right)

The *rasterization* of the structure into hexahedral elements, instead, allows for a highly regular structured mesh which provides more accurate results with a higher computational efficiency. This, however, comes at the cost of non-planar surfaces that require more complex interface models for accurate prediction of crack initiation and propagation.
To guarantee high computational efficiency of the algorithm, the rasterization is implemented as a two-step method. First a fast-screening of the position of the Gaussian point with respect to the *minimum bounding box* of each grain is performed to evaluate a subset of potentially intersecting cells, followed by a more accurate comparison of the position of the Gaussian point against the actual grain boundaries of the subset of cells. Finally, also for rasterised models, interface entities can be inserted between grains, as presented in Fig.6:.

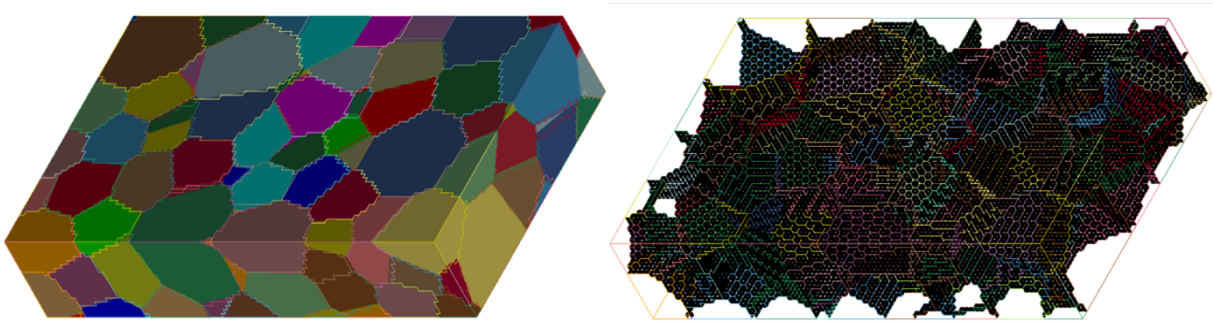

Fig.6: Visualisation of actual and rasterised cells (left), and underlying interface elements along the grain boundaries (right).

4 Integration with LS-PrePost

VorTeX algorithm has then been integrated into LS-PrePost, thus providing the capability to generate and visualise the microstructural model from the graphic interface of the software.
The tessellation properties can be inserted in the ad-hoc implemented user-interface, and the models are generated following three sequential processes: packing of arbitrarily defined spheres to condition the nuclei seeding process, tessellation of the 3D space with the Laguerre-Voronoi technique, and spatial discretisation of the structure into a structured hexahedral mesh.
Additionally, the tessellation can be cropped along arbitrarily oriented planes into any desired user-defined shape, following the methodology presented in [8].

The capability of visualising each of the three steps of the process presented – namely the spheres representing the conditioning of the nuclei seeding procedure (Fig.7:a), the unconfined tessellation (Fig.7:b), and the cropped geometry (Fig.7:c) – offers the user increased control over the whole process to build a finite element model of a representative polycrystalline microstructure.

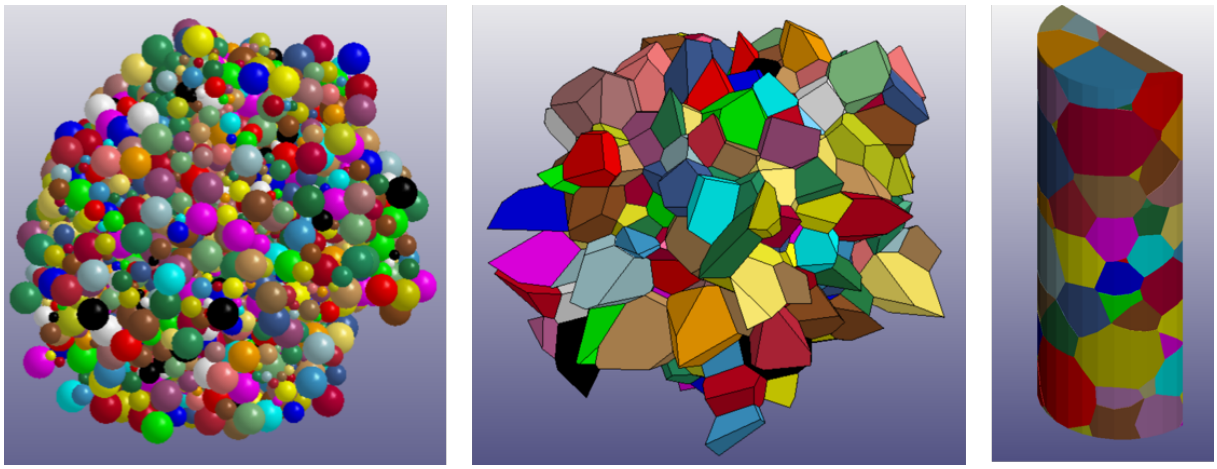

Fig.7: LS-PrePost visualisation of the conditioning spheres (left), the unconfined tessellation (centre), and the arbitrarily shaped structure(right).

In the FE model generated, each grain is implemented as a unique part, thus allowing the user to assign any available constitutive material compatible with solid elements to each grain separately. Furthermore, the interface entities on the grain boundaries can be modelled with any segment-based contact or cohesive element formulation available in LS-Dyna.

5 Summary

The work presented illustrates the integration of VorTeX algorithm, for the generation of representative models of polycrystalline microstructures, with the user interface software LS-PrePost.
First the method implemented to build FE models representative of real polycrystalline microstructures is described, focusing particularly on the high flexibility offered by the specific approach adopted, i.e. preconditioned Laguerre-Voronoi tessellation technique.
The spatial discretisation approaches implemented, either with tetrahedral or hexahedral elements, are described, highlighting the capability of inserting interface entities on the grain boundaries within both structured and unstructured meshes.
Finally, the integration into the software LS-PrePost provides a user interface for the algorithm, both for the input of the tessellation parameters and for the visualisation of each step of the process to generate the representative models.

Acknowledgement

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