

MTEX2Gmsh: a tool for generating 2D meshes from EBSD data

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Software

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Summary

Micromechanics of polycrystalline aggregates consists in evaluating the thermo-mechanical behaviour of the aggregates at their grain scale. It is of great interest for investigating the influence of grain morphology (size and shape) and crystallographic texture on the macroscopic behaviour. If the investigated material is subjected to macroscopic deformation, the local strain can be obtained either experimentally, thanks to full-field measurement methods such as microgrid technique (Allais, Bornert, Bretheau, & Caldemaison, 1994) or Digital Image Correlation (DIC) (Hild, Raka, Baudequin, Roux, & Cantelaube, 2002), or thanks to numerical simulation of the microstructure. The latter needs to take into account the mechanical heterogeneities (due to the different constituents) and the anisotropy of each phase, depending on its crystalline orientation.

Orientation Imaging Microscopy (OIM), usually made from Electron Backscatter Diffraction (EBSD) data, is now widely used in the literature for investigating the grain morphology and local crystal orientations in crystalline materials. Raw EBSD data can be considered as matrices of measurements of crystallographic data: each dot contains information about the phase and its orientation at the corresponding position.

In order to perform Finite Element Analysis (FEA) on a polycrystal, one needs to first generate a mesh based on either EBSD or reconstructed grains. In this mesh, the Grain Boundaries (GBs) must be accurately described since they play an important role in the overall behaviour of aggregates. Indeed, it is known that GBs increase the energy of the materials. The interfacial energy between two adjacent grains due to their boundary depends, among other parameters, on their misorientation and on the surface normal of the boundary (Priester, 2012). In addition, Zhong, Rowenhorst, Beladi, & Rohrer (2017) mentioned that the GB curvature is one of the most important properties of a microstructure. For instance, the driving force for grain growth depends on the local curvature of the GBs.

Latypov, Shin, De Cooman, & Kim (2016) proposed a program to generate regular pseudo-3D mesh, consisting in brick elements with only one element in thickness. Nevertheless, because of the regular structure, the GBs can not be smoothly described. In addition, the element size must be constant, possibly resulting in a huge number of elements, depending on the size and the spatial resolution of the orientation map. Dancette, Browet, Martin, Willemet, & Delannay (2016) proposed the following method to generate a conforming mesh with smooth GBs:

- computation of the GBs based on a proper criterion;
- grain reconstruction using a graph theory -based method;
- spline interpolation of the GBs;
- meshing.

The criterion used by the previous authors for defining the GBs, called weight in the context of graph theory, was specially designed for cubic phases. The geometry was meshed using the Gmsh software (Geuzaine & Remacle, 2009).

The proposed software, named [MTEX2Gmsh](#), provides a customisable and robust method for generating a 2D mesh based on EBSD with smooth and accurate definition of the GBs. It is based on the MTEX toolbox for Matlab (Bachmann, Hielscher, & Schaeben, 2011) and the Gmsh software. Figure 1 schematically illustrates the proposed algorithm. [MTEX2Gmsh](#) allows to mesh the volume with a couple of options, such as:

- increasing element size with increasing distance from the grains boundaries;
- element type (tetrahedron, wedge or brick elements);
- nesting the Region of Interest (ROI) into a larger medium.

This software comes with an Abaqus plugin for importing the mesh and allocating the phase and Euler Angles of each grain.

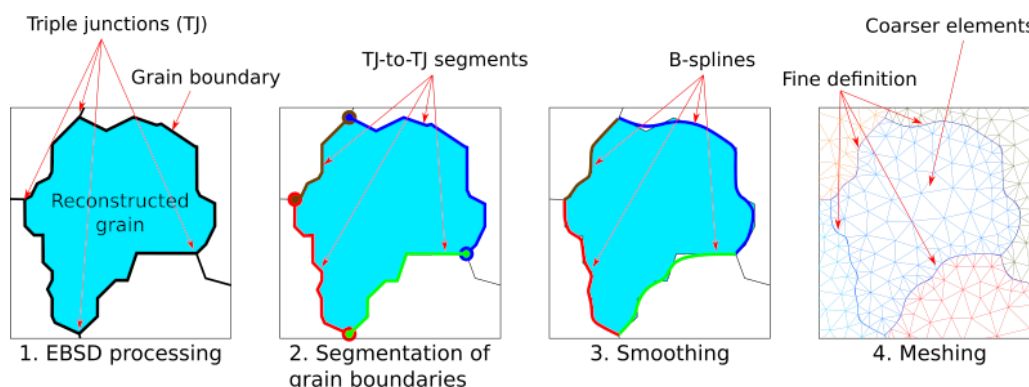


Figure 1: Schematic representation of the algorithm used in MTEX2Gmsh: 1) once the grains are reconstructed using to MTEX (Bachmann et al., 2011), the algorithm fetches all triple junctions (TJ) in the whole map; 2) each grain boundary is divided into TJ-to-TJ segments; 3) all those segments are smoothed using Bspline approximation; 3) this descriptions of the grains can be converted into Gmsh-readable files, allowing to mesh the whole region efficiently. The Bspline approximation results in very accurate definitions of the GBs, with limited serration (usually introduced by the EBSD resolution) and limited number of elements.

References

- Allais, L., Bornert, M., Bretheau, T., & Caldemaison, D. (1994). Experimental characterization of the local strain field in a heterogeneous elastoplastic material. *Acta Metallurgica et materialia*, 42(11), 3865–3880. doi:[10.1016/0956-7151\(94\)90452-9](https://doi.org/10.1016/0956-7151(94)90452-9)
- Bachmann, F., Hielscher, R., & Schaeben, H. (2011). Grain detection from 2d and 3d ebsd data—specification of the mtex algorithm. *Ultramicroscopy*, 111(12), 1720–1733. doi:[10.1016/j.ultramic.2011.08.002](https://doi.org/10.1016/j.ultramic.2011.08.002)
- Dancette, S., Browet, A., Martin, G., Willemet, M., & Delannay, L. (2016). Automatic processing of an orientation map into a finite element mesh that conforms to grain boundaries. *Modelling and Simulation in Materials Science and Engineering*, 24(5), 055014. doi:[10.1088/0965-0393/24/5/055014](https://doi.org/10.1088/0965-0393/24/5/055014)
- Geuzaine, C., & Remacle, J.-F. (2009). Gmsh: A 3-D finite element mesh generator with built-in pre-and post-processing facilities. *International journal for numerical methods in engineering*, 79(11), 1309–1331. doi:[10.1002/nme.2579](https://doi.org/10.1002/nme.2579)

Hild, F., Raka, B., Baudequin, M., Roux, S., & Cantelaube, F. (2002). Multiscale displacement field measurements of compressed mineral-wool samples by digital image correlation. *Appl. Opt.*, 41(32), 6815–6828. doi:[10.1364/AO.41.006815](https://doi.org/10.1364/AO.41.006815)

Latypov, M. I., Shin, S., De Cooman, B. C., & Kim, H. S. (2016). Micromechanical finite element analysis of strain partitioning in multiphase medium manganese TWIP+TRIP steel. *Acta Materialia*, 108, 219–228. doi:[10.1016/j.actamat.2016.02.001](https://doi.org/10.1016/j.actamat.2016.02.001)

Priester, L. (2012). *Grain boundaries: From theory to engineering* (Vol. 172). Springer Science & Business Media.

Zhong, X., Rowenhorst, D. J., Beladi, H., & Rohrer, G. S. (2017). The five-parameter grain boundary curvature distribution in an austenitic and ferritic steel. *Acta Materialia*, 123, 136–145. doi:[10.1016/j.actamat.2016.10.030](https://doi.org/10.1016/j.actamat.2016.10.030)