Grain and pore shape analysis and generation of digital twins from digital images

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Abstract

The properties of granular or sintered manufactured materials or natural materials depend on their microstructure. Obtaining meaningful insights on the microstructure of these materials often relies on the correct identification of individual grains and pores. Their direct identification on 3D digital images is challenging but opens the possibility to detailed simulations and accurate prediction of material behavior, such as mechanical simulations that depend on the grain orientation. Such simulations give vital information to figure out the most promising designs of manufactured materials such as electrodes or to reach decisions based on reservoir rock properties and determined by Digital Rock Physics.

With this motivation, several new algorithms have been integrated into the GeoDict® [1] software. GeoDict’s capabilities to segment 3D scans, e.g. CT or FIB-SEM scans have been expanded to identify also individual grains and pores through the new modules GrainFind and PoreFind that are presented here, together with the option to use the results of GrainFind for the creation of digital twins of granular materials.

Keywords: pore identification, grain identification, digital rock physics, porous media, ceramics

1 Pore Identification

PoreFind is the GeoDict module dedicated to the analysis of the shape of individual pores. First, pores are identified from the segmented image by watershed and region-growing algorithms. Next, PoreFind extracts an equivalent ellipsoid for each individual pore. Finally, the statistics of pore positions, pore orientations, and size distributions are determined from the equivalent ellipsoids. Another pore shape property is the sphericity of the pore. Taken together, these statistics provide useful parameters to engineer material models that are needed [2], for example, to predict properties of sintered ceramic materials.

Figure 1: Model created after segmentation of a µCT-scan of a rock (left), the result of the pore identification (middle) and illustration of the visualization and animation of the results where green identified pores are represented as red ellipsoids with orientation, position in the whole domain and some statistical information about the individual pores

2 Grain Identification

GrainFind is the GeoDict module dedicated to the analysis and identification of grains. Again, grains are identified from the segmented image by watershed and region-growing algorithms. Next, GrainFind extracts an equivalent ellipsoid for each individual grain. The statistics of grain positions, grain orientations, and size distributions are found from the equivalent ellipsoids. The sphericity of the grain is also analyzed. From these statistics, one can create a digital twin of the scan, i.e. one has a computer model that allows the creation of voxelized 3D grain models with the same statistics. Furthermore, with GeoDict, this virtual twin can be used as a starting point such that it may better fit to those physical properties you want to optimize. One such property, for example, is the tortuosity of electrode materials as considered in [3].
Figure 2: Comparison of a CT scan of a rock and the result of the grain identification

3 Digital Twin Model Generation

By using the results of GrainFind as input to the GrainGeo module, a digital twin of a granular material can now easily be created with GeoDict. Here, we use an electrode material from [4] for illustration purposes. In GrainGeo, one can now simply opt to load the results of GrainFind as the generator settings as illustrated in Figure 3.

After a few additional settings, for example enforcing periodicity, adjusting the overlap between grains, and adding some amount of binder (which is not automatically detected by GrainFind, yet), a digital twin can be generated in minutes as illustrated in Figure 4. Now, any metrics that we deem useful can be applied to the original data and the digital twin. The following figures illustrate this by comparing simply the GrainFind results for the two, but of course many other metrics could be used here as well.
Figure 4: Visualization of (left) the structure model created from the imported original data set of 1400 x 1400 x 200 voxels and (right) the digital twin generated with GrainGeo by loading the grain identification results obtained with GrainFind on the imported original data set, with slight overlap (1.5%) and addition of binder (5%, with contact angle of 10°).

Figure 5: Main results of GrainFind illustrating that the number of Grains (1931 vs 1922) agrees very well

Figure 6: Comparison of Grain shapes for the original data and the digital twin
4 Conclusion

The identification of individual pores and grains was shown and demonstrated to have several benefits in the literature. The newest and maybe biggest benefit that is elaborated on here is the capability to create parameterized statistically correct geometric models that agree with the original scan in several metrics.

References

[1] www.geodict.com

