Microstructure Clustering in Multiphase Materials: Effect of Initial Configuration.

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In disperse multiphase systems, the dispersion/distribution of particles (microstructure) is regarded as a key factor, both affected by processing and in its turn determining performance. Among many miscrostructural features, clustering, that is, the tendency of dispersed particles to agglomerate forming clusters of differnt size, is considered of primary significance. Our purpose in this study is both, to understand the evolution of clustering generated by Monte-Carlo procedure with the change of the initial configuration of the particles. During the MC process, each particle gets displaced, randomly and sequentially, by the small amount relative to its original position. The interaction of each displaced particle is checked against every other particle, and particles are subject to attractive/repulsive forces, while they are also subject to thermal motion, expressed by a dimensionless temperature T. Earlier research has shown that a microstructure generated by the aforementioned procedure would evolve to different equalibrium states, depending on T. However, no formal, quantitative assessment of this was offered (TD Papathanasiou, 2009). In this study, such microstructural clustering is quantified using the Voronoii tessellation approach (Sumbekova, 2017). Three systems containing Random, Uniform and Gaussian dispersions of particles have been supplied as initial conditions, with an area fraction $\phi = 0.2$ and at two system temperatures $T = 0.5, 1.0$. The clustering levels σ of all three initial grids at $T = 1.0$ are in the same range of values from 0.41 ± 0.01, showing relative independence of clustering on initial conditions. The results obtained for $T = 0.5$ however show a substantial difference of clustering levels σ of Gaussian initial particle configuration with respect to the other configurations, which could considered as the result of the breakup of the initial super-cluster (Fig. 23 and 24).

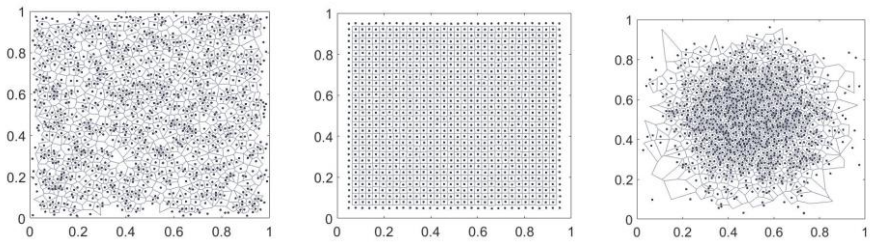

Fig. 23 Random, Uniform and Gaussian initial grids

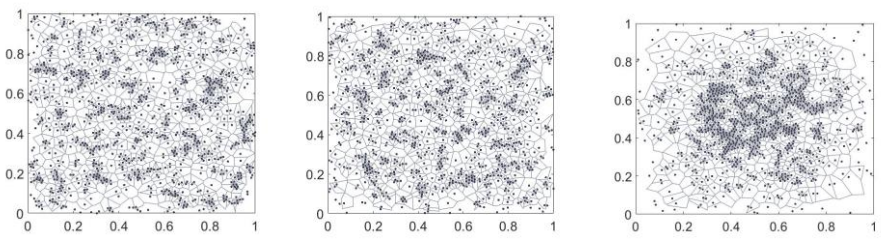

Fig. 24 End step at T = 0.5 and 2.5 million iterations