Proposal for a Master's thesis

Spatial modeling of formation of gel

1 Background

Understanding and controlling the dynamics of colloidal aggregation is important in our everyday life with applications ranging from food processing and gel batteries to medicine. For instance, in biological fluids such as blood and milk, it is crucial to maintain the stability of the system. In this project, we are interested in modeling the aggregation dynamics of silica nanoparticles in three dimensions (3D).

In an earlier work, Norden et al. (2014) studied 2D micrographs of silica gels obtained by scanning transmission electron microscopy (STEM) in order to estimate the number of silica particles at each pixel to draw conclusions on the original 3D structure. Then, Häbel et al. (2016) studied silica gels by using diffusion limited cluster aggregation (DLCA) and reaction limited cluster aggregation (RLCA) processes. The main challenge was to be able to draw conclusions on a 3D dynamic process based on static 2D images. Finally, Häbel et al. (2019) studied the silica particle aggregation in 3D by comparing an experimentally obtained aggregate of silica nanoparticles to simulated structures obtained by DLCA and RLCA. In addition, they fitted static Gibbs point process models for the silica data. To investigate goodness-of-fit of the models, experimentally obtained and simulated structures were compared by means of spatial summary functions.

In the DLCA and RLCA simulations above, the diameter of the silica particles was fixed to 20nm but in the 3D data we have available the diameter varies. In her Master's thesis (2020), Lovisa Köllerström allowed the diameter to vary in the DLCA and RLCA simulations and compared the data and these new simulations. Even though the goodness-of-fit of the models with varying diameter was slightly better than the goodness-of-fit of the models with fixed diameter, the models should be further improved. There are at least two possible approaches to continue: 1) Combine DLCA and RLCA models by e.g. using one of them early during the gel formation process and then, switch to the other, or 2) combine DLCA and RLCA models by letting the aggregation probability to depend on the number of neighbouring particles. The data we have available are stacks of 2D gray-scale STEM images.

2 Project plan

The project will be divided into several subproblems:

1. Get familiar with the DLCA and RLCA processes and the simulation program as well as with spatial point process theory.
2. Choose approach 1) or 2) and (re)write the simulation code accordingly.
3. Fit the models to the 3D STEM data and check the goodness-of-fit of the models by using summary functions from spatial point process theory.

References

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