Using Dynamic Graphs to Quantitatively Visualize Agglomeration in Spatial Simulations

Tihamer Geyer
Center for Bioinformatics, Saarland University, D–66041 Saarbrücken

The usual approaches to analyze many-particle simulations of association processes either focus on time-averaged measures for the degree of binding like radial distribution functions or cluster sizes, or movies are generated which in principle provide all the details but in an only qualitative way.

Here we show how dynamic graphs can be used to visualize quantitatively the time dependent events of complex formation and breaking. For this, a simple distance criterion is used to set up a time dependent graph from the snapshots of the spatial simulation [1]. Some examples highlight how even simple graph measures like the degree distribution or the clustering coefficient can be used to follow the dynamics, to unambigiously identify complexes in a sea of monomers and partially assembled fragments, or to quantify how regular of amorphous an aggregate is [2].

In a further step the spatial simulation ad the dynamic graph will be combined such that the simulation can make use of the connectivity encoded in the graph by, e.g., defining temporary pseudo-particles or assigning different diffusion coefficients based on how many neighbors are actually bound.

References:

[1] Florian Lauck, Volkhard Helms, and Tihamér Geyer. Graph Measures Reveal Fine Structure of Complexes Forming in Multiparticle Simulations. *J. Chem. Theor. Comput.* 2009, **5**:641

[2] Tihamér Geyer. Many-Particle Brownian and Langevin Dynamics Simulations with the Brownmove Package. *BMC Biophys.* 2011, **4**:7