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A particle-based model for aggregate formation in biomineralization

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Biosilicification is a process in which meaningful behaviors happen in different temporal and spatial scales. Hence, one might consider different approaches depending which part of the dynamics is under scrutiny. In the kind of simulation that we are currently dealing with, the growth of spicules in sponges has been modeled from the beginning of the intracellular nucleation process. It simulates the interaction of inorganic-organic materials with the view of forming an aggregate of mineral nanoparticles on an organic matrix. It is based on DLA (Diffusion Limited Aggregation) in the first step and then a modification by adding a Poisson equation to describe the interaction of acidic sites of proteins with charged particles. The boundaries of the 3D simulation box have cylindrical symmetry, which has been chosen based on the simplified geometry of the organic matrix. This approach describes the general behavior of silica deposition, but could contain more parameters, both physical and protein-based, in order to produce more realistic results in comparison with growth of real spicules.