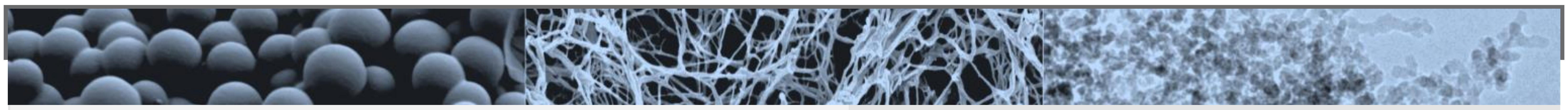
Effect of diffusive and ballistic aggregation on properties of gels



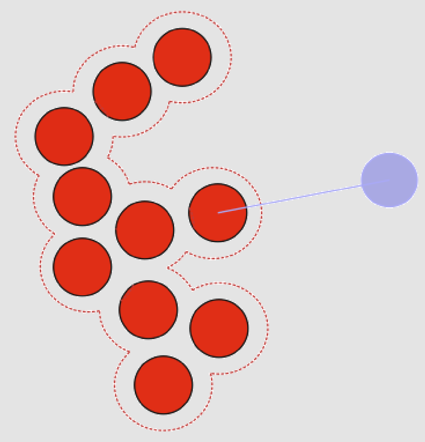
Motivation

Since the formulation of the diffusion equation for the Brownian particles, there has been an increasing interest in the dynamics and mechanism behind the formation of different aggregates. Over the years several aggregation algorithms have been developed, either depending upon the particle movement in the medium, *viz*., diffusion-limited (cluster-cluster) aggregation (DLCA) [1, 2] and ballistic (cluster-cluster) aggregation (BCCA) [3] or their affinity of sticking for forming aggregates, *viz*., reaction- or chemically-limited (cluster-cluster) aggregation (RLCA)[4].

Thus, for theoretically describing the structural properties of colloids and gels that demonstrate such aggregation, it is critical to study these algorithms and their influence on the aggregate's properties.

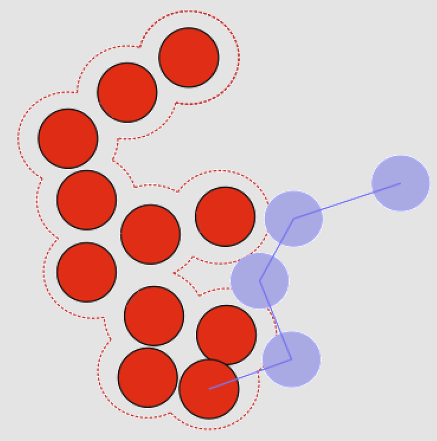
DLCA vs. RLCA – visualisation

Particles stick as soon as encountering another particle



Purely diffusive (stick probability = 1)

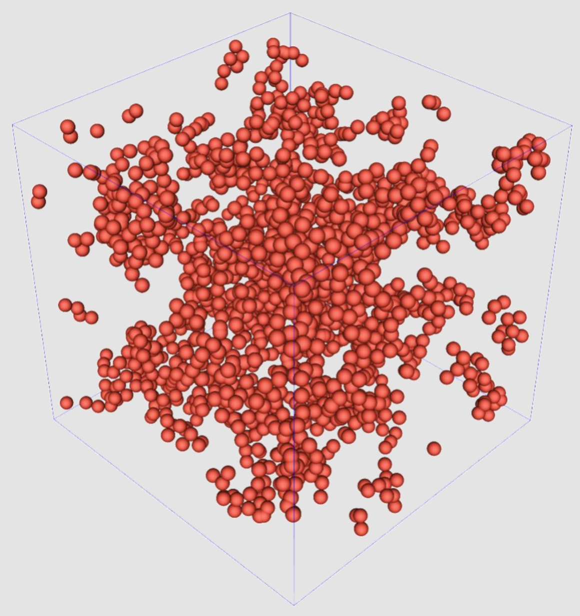
Particles require multiple interactions before finally aggregating



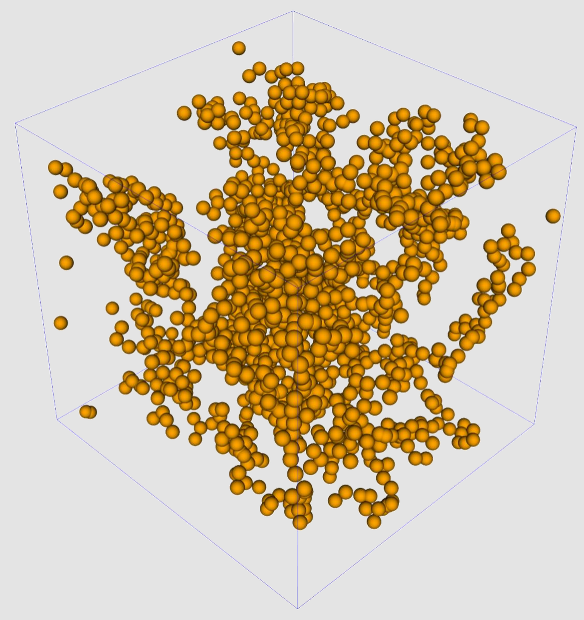
Diffusion with reaction (stick probability < 1)

Diffusive aggregation models

Exemplary **3-d diffusive structures**

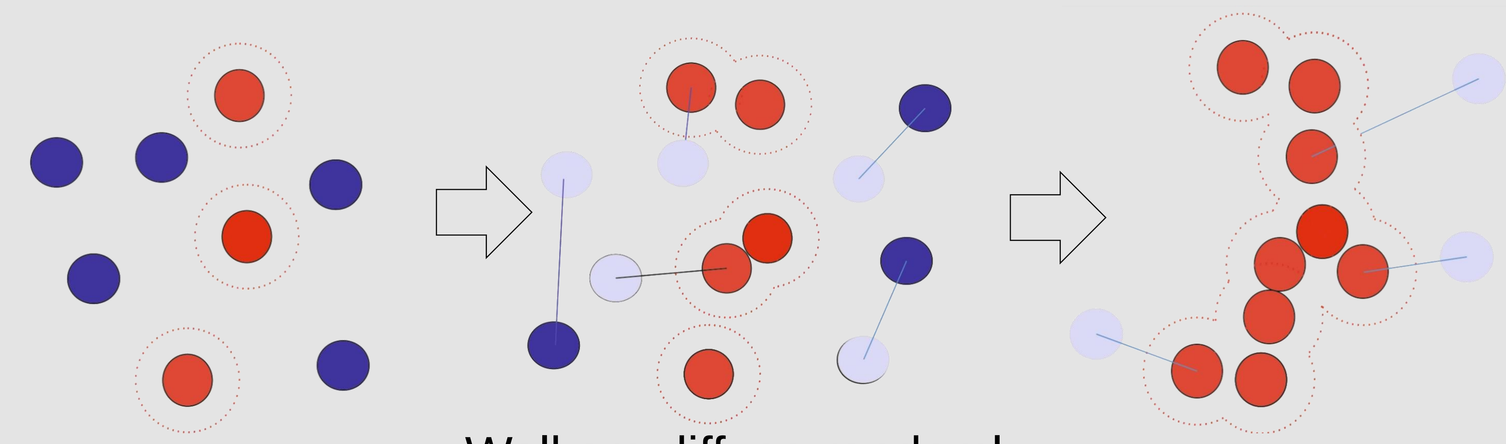


DLCA



RLCA

Illustrative 2-d simulation flow of diffusive aggregation



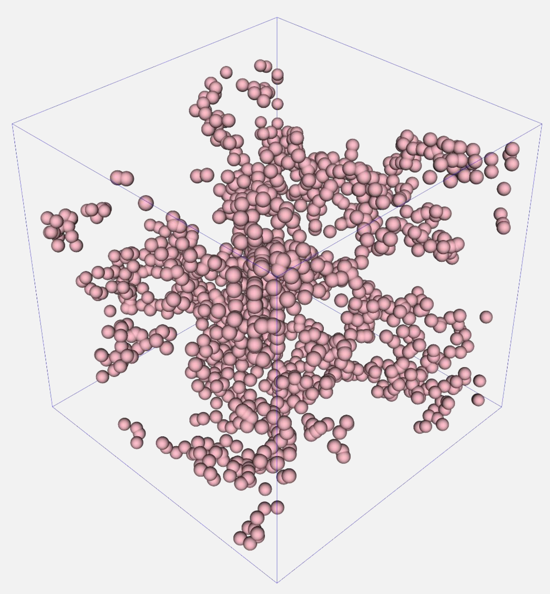
Seeds and walkers initialised

Walkers diffuse randomly towards seeds and aggregate on reaching a critical distance

Simulation continues till single cluster in system

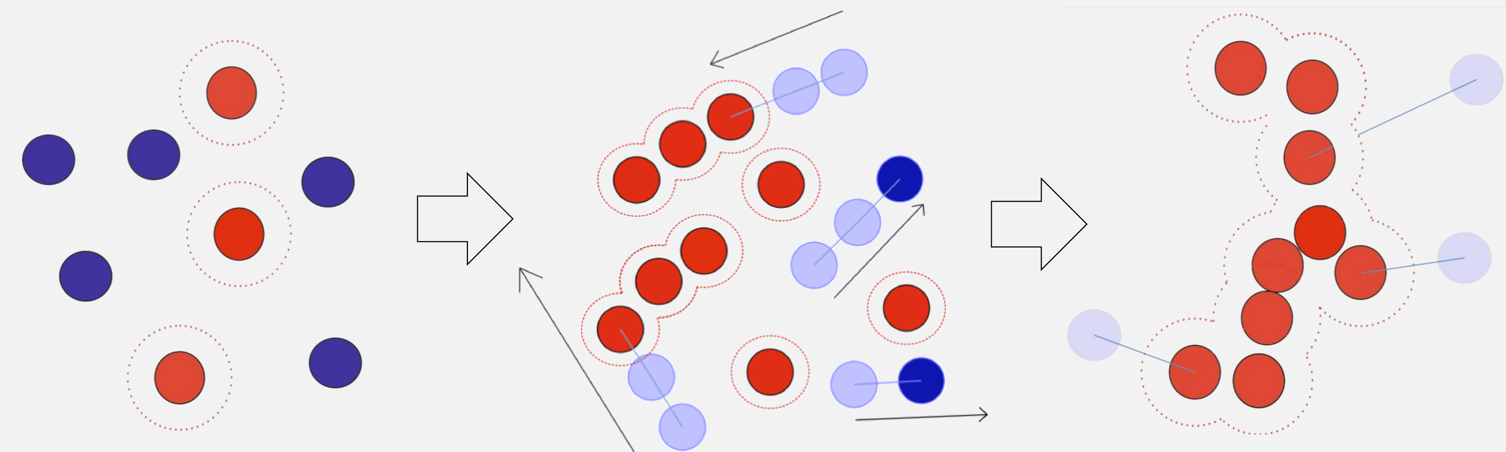
Ballistic aggregation models

Exemplary **3-d ballistic structure**



BCCA

Illustrative 2-d simulation flow of ballistic aggregation



Seeds and walkers initialised

Walkers move in a ballistic motion along a single axis chosen at random and aggregate on reaching critical distance.

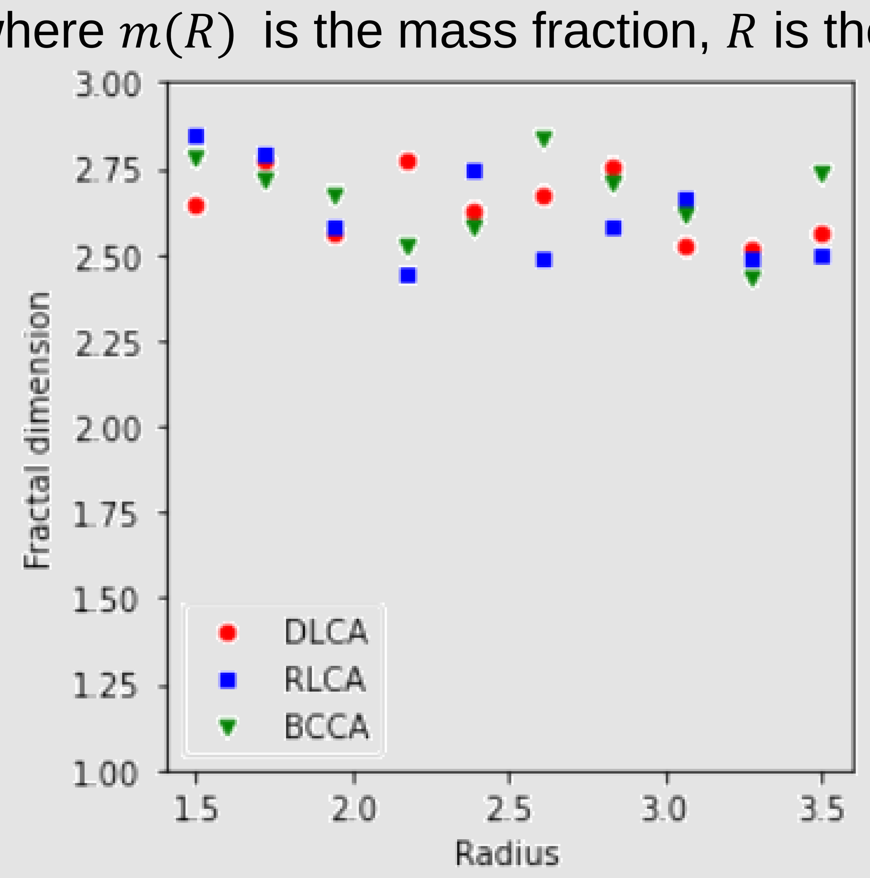
Simulation continues till single cluster in system

Fractal dimension *vs.* radius, density and reactivity for different aggregate types

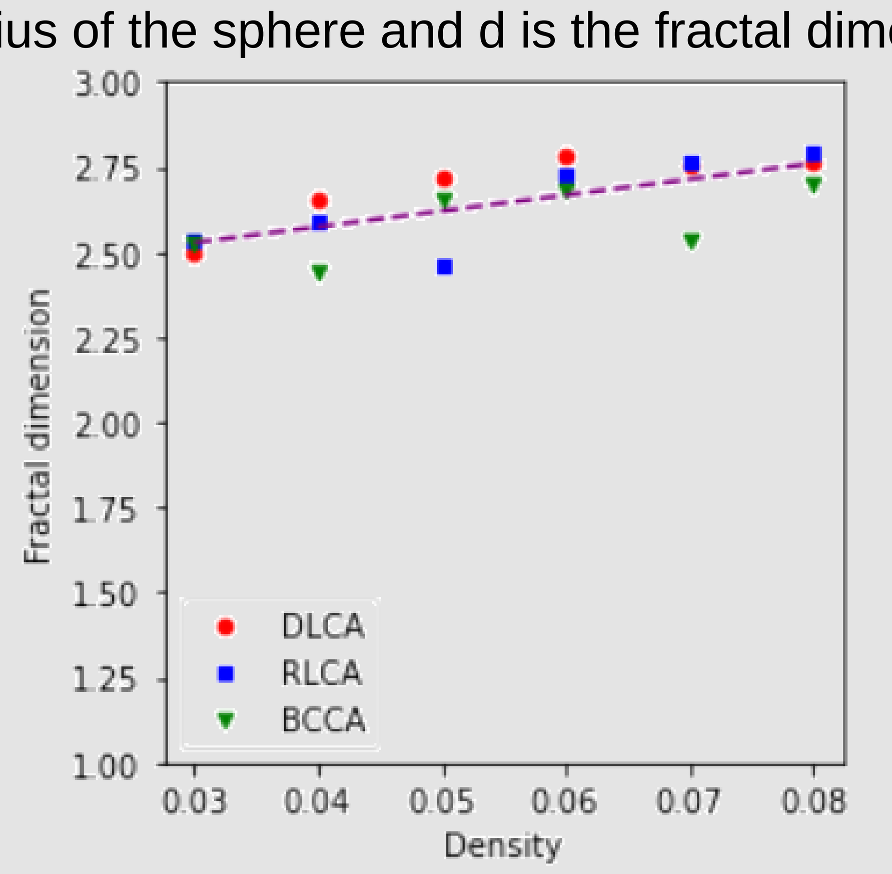
Fractal dimension: The fractal dimension is a factor to define the complexity of a feature as a ratio of the change in detail to the change in scale. For the scope of this research, the mass fractal method is used to calculate the fractal dimension. This is done by calculating the number of particles in a spherical region within the simulation box of increasing radii. The fractal dimension is then calculated by taking the slope of the log-log plot of the equation given as

$$m(R) \propto R^d$$

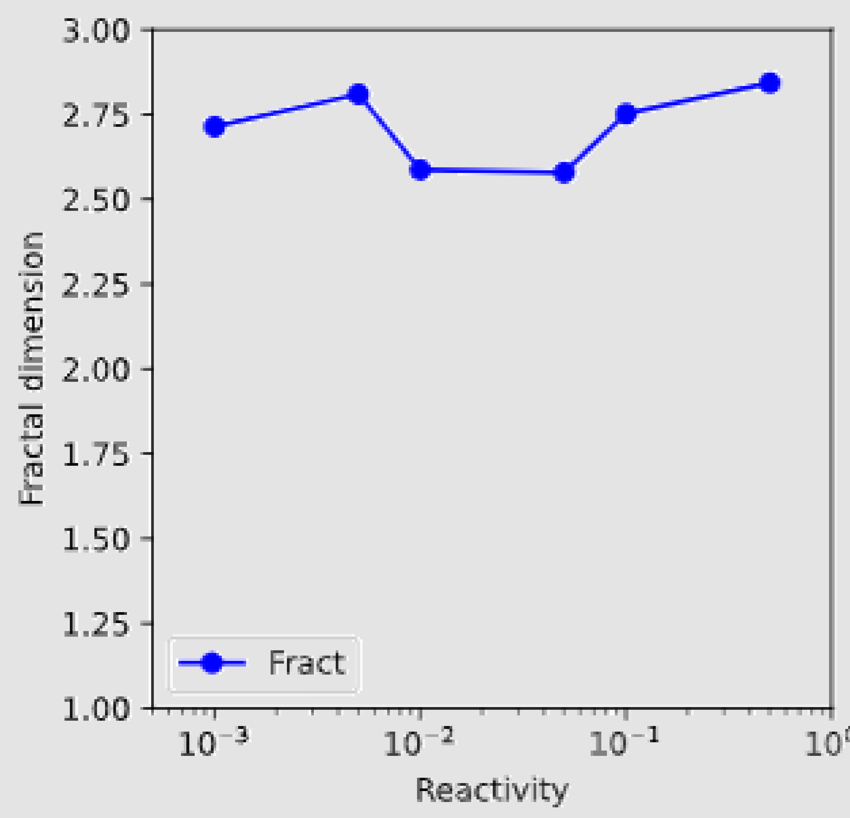
where $m(R)$ is the mass fraction, R is the radius of the sphere and d is the fractal dimension.



Radius



Density



Reactivity

[1] P. Meakin, *Physical Review Letters*, **51**, 1119–1122 (1983).
[2] P. Meakin, *Journal of Colloid and Interface Science*, **102**, 491–504 (1984).
[3] M. J. Vold, *Journal of Colloid Science*, **18**, 684–695 (1963).
[4] M. Kolb and R. Jullien, *Journal de Physique Lettres*, **45**, L977 (1984).

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