TECHNISCHE UNIVERSITÄT DARMSTADT

Thesis (B.Sc. / M.Sc.)
Self-Replication of Colloidal Particles

Fachbereich 18
Elektrotechnik und Informationstechnik
Selbstorganisierende Systeme

Department 18
Electrical Engineering and Information Technology
Self-Organizing Systems

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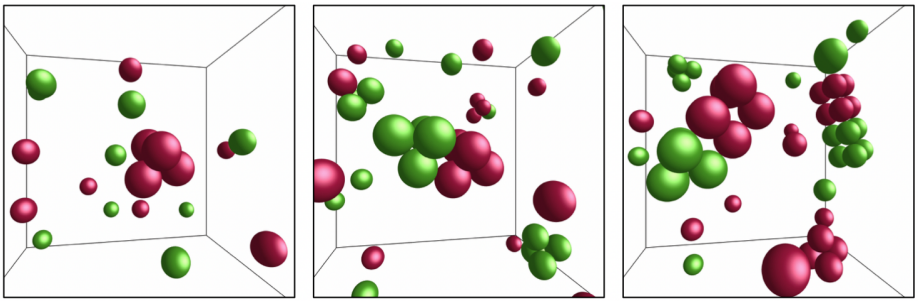

Figure 1: Examples of self-replication process involving colloidal clusters that consist of varying number of colloids.

There is a growing interest in the construction of self-replicating materials. Whereas modern materials science primarily concentrates on synthesis, there has been much less success at building artificial self-replicating materials. Its potential applications might include protein complexes with designed interactions [1] and photonic crystals [2]. One framework to achieve self-replication was proposed in [3, 4] for systems of colloidal particles (see Fig. 1). According to that framework, once considers a system of generic particles. Each particle is represented as a sphere with stickers uniformly distributed over its surface via which it can bind to other spheres. An initial condition consists of a target colloidal cluster, e.g., an octahedron, and a catalyst, e.g., a dimer. Each constituent sphere of colloidal clusters and catalysts has a type and can bind to other spheres of a specific type. When a colloidal cluster is immersed into a monomer bath, it serves as a template and starts to collect other spheres around itself. However, it cannot assemble a new replicated cluster due to geometrical constraints of colloidal interactions. Instead, this can be achieved in the presence of a catalyst that drives some required newly attached particles to one side of the existing colloidal cluster. Afterwards, disassociation occurs that results in one new colloidal cluster and one new catalyst. The resulting self-replication scheme is a hypercycle, along the run of which one observes the exponential growth of replicas of both colloidal clusters and catalysts. The computational side of this approach involves numerical integration of dissipative particle dynamics [5, 6] and the main task of this project is to implement a self-replicating scenario using the aforementioned modelling technique. As an alternative, one is welcome to try other particle dynamics modelling methods for colloidal suspensions, such as fast lubrication dynamics and multiparticle collision dynamics [7].

A potential candidate should be familiar with some of the following:

- Materials science and self-assembly
- Numerical analysis of ordinary / stochastic differential equations
- C++ / MATLAB / Python

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References

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[7] Dan S. Bolintineanu, Gary S. Grest, Jeremy B. Lechman, Flint Pierce, Steven J. Plimpton, and P. Randall Schunk. Particle dynamics modelling methods for colloid suspensions. *Computational Particle Mechanics*, 1, 2014.