

Internal Webinar

Rare events in cluster-cluster aggregation

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Cluster-cluster aggregation (CCA) is a nonequilibrium, irreversible phenomenon where particles, or clusters coalesce on contact to form larger clusters. The most common approach to study CCA is the meanfield Smoluchowski coagulation equation. However, this equation can be exactly solved only when the rate of collision is independent of the colliding masses (constant kernel), is the sum of the masses (sum kernel), or the product of the masses (product kernel). Moreover, the solution of the Smoluchowski equation describes only the typical or average trajectories and moments of the mass distribution, and does not provide any information about atypical or rare trajectories.

In this talk, we establish an analytical path-wise large deviation principle for arbitrary collision kernels, and obtain the explicit large deviation functions, for constant, sum and product kernels, as well as the optimal evolution trajectories for constant and sum kernels, all of which show excellent agreement with Monte Carlo simulations. We use this analytical formalism to obtain the large deviation function of interest and atypical trajectories for *k*-nary coalescence, $kA \rightarrow \ell A$.

I will also briefly describe a biased Monte Carlo algorithm developed to study probabilities of rare events in CCA for arbitrary collision kernels, and the results obtained therein. The algorithm can sample probabilities as low as 10⁻⁴⁰, and obtains atypical and typical trajectories. We establish the efficacy of the algorithm by benchmarking the numerically obtained large deviation function of interest, and the trajectories, with the exact answers for constant, sum and product kernels.

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