

# Improving Monte Carlo simulations for an accurate modeling of nanoparticles coagulation

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## Introduction

The growth of suspended nanoparticles by coagulation (aggregation and/or coalescence) is found in many industrial, combustion and environmental processes (Friedlander, 2000). In this context particles naturally evolve into polydisperse sizes. These particles experience a movement characterized by very different momentum relaxation times. Thus, accurate numerical methods, such as Langevin Dynamics, become computationally expensive to simulate the coagulation of a large population of particles (Buesser *et al.*, 2009). On the other hand, the Monte Carlo (MC) method (simply consisting in selecting a particle at time and moving it in a random orientation), is a very computationally efficient alternative to overcome this issue. However, it is usually regarded as a technique that relies on an artificial description of time making it difficult to study coagulation (Lazzari *et al.*, 2016). Despite this, some efforts have been made to obtain a more physical description of time (Hasmy & Jullien, 1995; Lazzari & Lattuada, 2017). Unfortunately, as we will show, they usually lead to incoherent time progress for the ensemble of polydisperse particles and/or they are restricted to specific flow regimes (diffusion limited or ballistic). Also, in different studies based on the MC method, the probability of moving a particle is adapted to the flow regime with some rules whose expressions are lack of justification (Kim *et al.*, 2010). Moreover, in such studies, particles are usually displaced along a constant distance in the order of monomers' diameter, regardless of their sizes. A few studies have considered size-dependent displacement (Hayashi *et al.*, 1999). In this study, we propose a new MC method with justified probabilities of particles' movement, considering size-dependent displacement and able to bring a validated and consistent physical time evolution for individual as well as for the ensemble of polydisperse particles.

## Results

The method is firstly presented and compared with previous methods found in the literature to finally validate it by a comparison with Langevin Dynamics simulations. The evolution of calculated mean squared displacements for different-sized particles is compared with theoretical values in

Figure 1, observing a good agreement between the numerical simulations and Einstein's theory (Friedlander, 2000).

## Conclusions

The method is able to efficiently simulate the dynamics of coagulation. For the first time, consistent and coherent residence times of particles are obtained. The proposed MC method could be used to study more complex dynamic processes such as surface growth, sintering or breakage of aggregates.

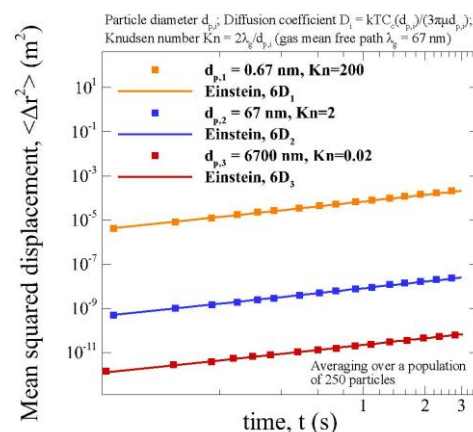


Figure 1. The  $\langle r^2 \rangle$  of a system of 3 off-lattice particles (suspended in air at standard conditions).

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