A parallel Monte Carlo - Discrete Element Method approach for the shear-induced aggregation of colloidal particles

THEME: Formulation and solution of PB Models

A PARALLEL MONTE CARLO – DISCRETE ELEMENT METHOD APPROACH FOR THE SHEAR-INDUCED AGGREGATION OF COLLOIDAL PARTICLES

Graziano Frungieri [1] *– Marco Vanni*[1]

[1] Department of Applied Science and Technology, Politecnico di Torino, Corso Duca degli Abruzzi 24, 10129 Torino, Italy

The study of colloidal suspensions in which particles undergo simultaneously aggregation and breakage phenomena poses several difficulties.

The use of Population Balance (PB) models, for instance, is hindered by the lack of suitable models to describe aggregation and breakup rates of colloidal clusters with complex geometries. Furthermore, reducing the complexity of particles to a few internal variables, PB models fail to take into account the characteristic disordered structure of the aggregates.

The application of Discrete Element Methods (DEM) to the simulation of the suspension represents a valid alternative; by modelling all the relevant forces acting on the suspended particles, they are able to track the motion of each particles, returning valuable insights into the system dynamics, in terms of both kinetics and morphology of the clusters. However, their use is not free of difficulties; DEM simulations are extremely demanding in terms of computational resources. For this reason, their use has been restricted so far to the simulation of single aggregates or at most of small populations.

In a recent work (Frungieri & Vanni 2017), we have proposed a numerical method to study the dynamics of a population of colloidal particles under the effect of a spatially uniform shear flow; the method is summarised by the flowchart of Fig. 1. It couples the mean-field approach typical of PB models with the accurate predictions obtainable by DEM simulations; the Population Balance governing the suspension dynamics is solved stochastically by an event-driven, rejection-free Monte Carlo (MC) algorithm: the MC, set up on the basis of the Smoluchowsky two-body kinetics, is in charge of sampling a sequence of binary encounter events between the suspended particles. The DEM is instead used to accurately reproduce each event. The DEM is built into the framework of Stokesian Dynamics and coupled with proper models for inter-particle interactions; as such, it is able to model accurately hydrodynamic as well as colloidal interactions. By such a combination, the uncertainty affecting the pure PB models is circumvented and the DEM simulations are performed to track the motion of just two aggregates at a time, thus reducing the computational load compared to a pure DEM simulation of a colloidal system.

For the present work, in order to further speed-up the overall method, a large-scale parallelization strategy of the MC-DEM technique has been developed and implemented

resorting to the Message Passing Interface (MPI) standard. The method is schematically illustrated in Fig. 2. The model of communication is based on a Master/Slave architecture; a Master process is used to sample the encounter events and to assign them to the Slaves; the Slave processes perform the DEM simulation and return the results to the Master.

However, the accuracy of the parallel MC-DEM need to be evaluated; to this purpose, several simulations of a shear-induced aggregation process were performed and the results compared with the one obtained by the serial version of the method. A strategy was developed to match the results both in terms of integral properties of the suspension and particle size distribution, according to the number of Slave processes used. Finally, the method shows a good scalability, and, as such, it is suitable for reproducing a large number of encounter event simultaneously, yielding to a substantial reduction of the run time.

References

Frungieri, G. & Vanni, M., 2017. Shear-induced aggregation of colloidal particles: A comparison between two different approaches to the modelling of colloidal interactions. *The Canadian Journal of Chemical Engineering 95*, pp. 1768-1780.

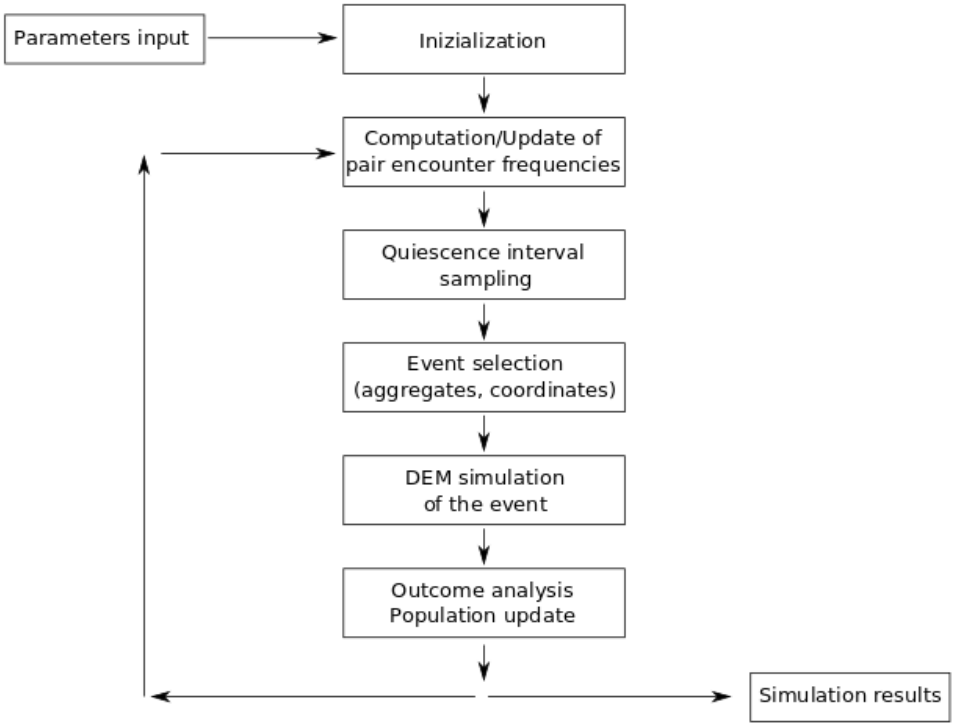

Figure 1: Flowchart of the Monte Carlo – DEM simulation technique.

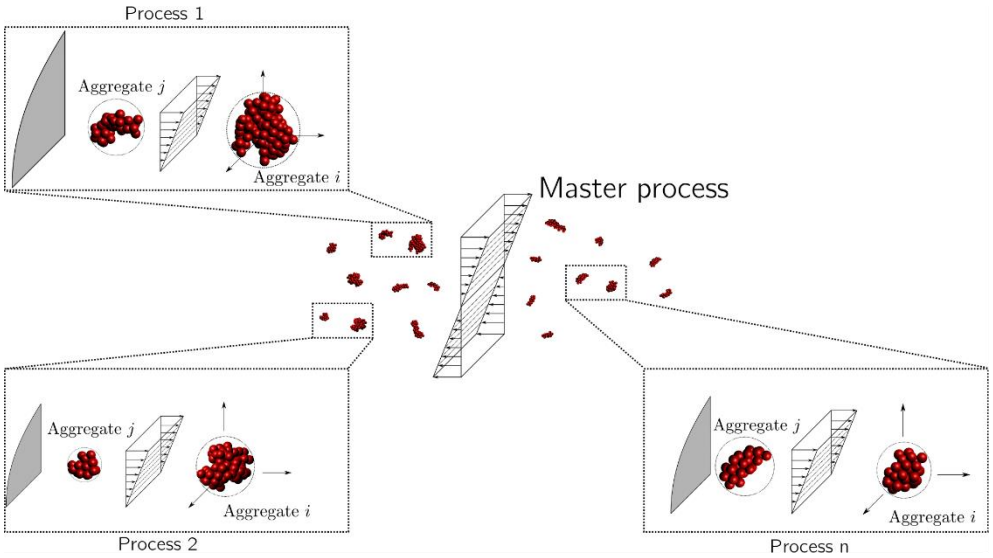

Figure 2: Representation of the parallelized simulation technique.