Discrete Multi-Physics: a particle-based computational method coupling CG-MD, SPH and DEM

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ABSTRACT

The flow of solid-liquid suspensions is a generic problem which poses many challenges to scientists and industrialists across many different areas. Applications range widely from processing of food and pharmaceuticals, through oil and mining industries, to blood and biological applications. Such flows involve a large array of complex phenomena on a wide range of scales, and the reciprocal interaction of liquid and dispersed solids creates a very complex dynamics, which often includes particle deformation, breakage, degradation, melting, swelling, erosion, aggregation etc. The variety of phenomena occurring in these flows can be roughly divided in three main categories mutually linked in a feedback mechanism: fluid phenomena, solid phenomena and contact phenomena. Traditionally, specific modelling techniques have been developed by focusing on certain specific aspects of the flow and simplifying the others. Computational Fluid Dynamics, for instance, accurately describes the fluid dynamics, but the solids phase is simplified by the point-particle assumption. Other techniques, such as the Discrete Element Method, on the other hand, provide a good account of the inter-particle contact forces, but it cannot handle phenomena such as solid-liquid mass transfer or melting. Computational methods dedicated to solid mechanics, on the other hand, describes the elastic and plastic deformations in the solid, but the external stresses coming from the fluid must be known in advance and provided as boundary conditions.

In order to achieve a more sophisticated description of these systems, this study proposes a model based on the combination of Smoothed Particle Hydrodynamics, Coarse Grained Molecular Dynamics and the Discrete Element Method, where these models are linked in a hybrid fashion. This approach can be applied to the simulation of both dispersed solid-liquid flows [1,2] and flow-structure interactions [3,4] and can deal with a large variety of particle types (e.g. non-spherical, elastic, breakable, melting, solidifying, swelling) flow conditions (e.g. confined, free-surface, microscopic) and scales (from meters to microns). Various examples are presented and discussed

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