FLUID PARTICLES IN MESOSCOPIC MODELLING OF COLLOIDALS AND SUSPENSIONS

Witold Dzwinel¹,
David A. Yuen²,
Krzysztof Boryczko¹,²,
1 Institute of Computer Science, AGH University of Technology, Mickiewicza 30, 30-059 Kraków, Poland, 2 Minnesota Supercomputing Institute, University of Minnesota, MN 55455, Minneapolis, USA
dzwinel@uci.agh.edu.pl, boryczko@uci.agh.edu.pl, davey@msi.umn.edu

Abstract

When mesoscopic features embedded within macroscopic phenomena in polymers are coupled together with micro-structure dynamics and boundary stoichiometries, the complex multi-resolution behavior observed in polymer dynamics are difficult to capture with the continuum models [1]. Therefore, the approaches based on the Navier-Stokes and the Cahn-Hillard equations, which use partial differential equations, become useless when employed in microscopic and mesoscopic scales. They must be augmented with discretized atomistic microscale models, such as molecular dynamics (MD) to provide an effective solver across the diverse scales with different physics. The two-level fluid particle model [2] is a discrete-particle method, which is a mesoscopic version of molecular dynamics (MD) technique combined with fluid particle method (FPM). Unlike in MD, where the particles represent atoms and molecules, in our model they represent both colloidal beds and fluid particles. The fluid particles mimic the "lumps of fluid", which interact with each other, not only via the central conservative forces as in MD, but with non-central, dissipative and stochastic forces as well.

We show that by using discrete particles we can model realistic behavior of such the mesoscopic phenomena such as the thin-film evaporation in mesoscale [3], mixing instabilities in suspensions [4,5], phase separation [6,7], creation of colloidal arrays [7] and colloidal aggregates [8]. The modeled multi-resolution patterns and qualitative behavior of mesoscopic features are amazingly similar to the results found in laboratory experiments and predicted by theory. The combination of two different types of interactions: postulated by the DLVO theory - representing realistic interactions between colloidal beds - and arbitrary defined dissipative and random interactions acting between fluid particles result in spontaneous creation of many multi-resolutional structures. They represent a single micelle, colloidal crystallate, large-scale colloidal aggregates up to scales of hydrodynamic instability [9,10] and the macroscopic phenomena involving the clustering of red blood cells in capillaries. We can summarize the computationally homogenous discrete particle model in the following hierarchical scheme [11]: non-equilibrium molecular dynamics (NEMD), dissipative particle dynamics (DPD), fluid particle model (FPM), smoothed particle hydrodynamics (SPH), and thermodynamically consistent DPD. The large scale-simulations involving up to 10 million fluid particles in 3-D were carried out on a broad range of parallel systems from IBM SP multi-computer, SGI Origin coMURA multiprocessor to the shared memory clusters such as IBM Regatta and SGI Altix machines resulting in an efficient and universal discrete-particle algorithms and codes [11-13]. A powerful toolkit over the GRID can be formed from these discrete particle schemes to model successfully multi-scale phenomena such as biological vascular and mesoscopic porous-media systems.

References


Multiresolution Structures – Colloidal Aggregates and Agglomerates

FUTURE DIRECTIONS

The discrete particle methods can be used as the components of the problem solving environment (PSE) based on the concept of multi-resolution workflow. As show below the whole cycle of simulations can be performed over three different spatial-temporal scales simultaneously due to the "wavelets" nature of the models. The spatial and temporal resolutions expected in each level of the three-level modeling concept will be compared. The main advantage of this approach is the possibility of the short range interaction can be treated as some sort of "wavelets". The interactions are short range with compact support and well localized in space. The total force acting on each particle is a linear combination of “wavelets” of various locations. However, unlike wavelets we cannot get "details" for the whole macroscopic spatial domain but rather for some part of it. This does not matter for homogeneous system but gets clumsily for more interesting - anisotropic system. Thus the global simulation localized in space. The final total forces acting on each particle are linear combinations of "wavelets" of various locations.

It does not matter for homogeneous system but gets clumsily for more interesting - anisotropic system. Thus the global simulation localized in space. The final total forces acting on each particle are linear combinations of "wavelets" of various locations. The interactions are short ranged with compact support and well localized in space. The total force acting on each particle is a linear combination of “wavelets” of various locations.