Journal of Computational Physics 256 (2014) 367–387

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

A fictitious domain approach for the simulation of dense suspensions

Stany Gallier [a,b,*], Elisabeth Lemaire [b], Laurent Lobry [b], François Peters [b]

[a] SAFRAN-Herakles, Le Bouchet Research Center, 91710 Vert le Petit, France
[b] CNRS, University of Nice LPMC, UMR, 6622, Parc Valrose, 06108 Nice, France

ARTICLE INFO

Article history:
Received 25 May 2013
Received in revised form 2 September 2013
Accepted 5 September 2013
Available online 16 September 2013

Keywords:
Suspensions
Fictitious domain
Lubrication
Discrete element method

ABSTRACT

Low Reynolds number concentrated suspensions do exhibit an intricate physics which can be partly unraveled by the use of numerical simulation. To this end, a Lagrange multiplier-free fictitious domain approach is described in this work. Unlike some methods recently proposed, the present approach is fully Eulerian and therefore does not need any transfer between the Eulerian background grid and some Lagrangian nodes attached to particles. Lubrication forces between particles play an important role in the suspension rheology and have been properly accounted for in the model. A robust and effective lubrication scheme is outlined which consists in transposing the classical approach used in Stokesian Dynamics to our present direct numerical simulation. This lubrication model has also been adapted to account for solid boundaries such as walls. Contact forces between particles are modeled using a classical Discrete Element Method (DEM), a widely used method in granular matter physics. Comprehensive validations are presented on various one-particle, two-particle or three-particle configurations in a linear shear flow as well as some $\mathcal{O}(10^3)$ and $\mathcal{O}(10^4)$ particle simulations.

1. Introduction

Suspensions of solid particles embedded in a liquid are a class of two-phase flows that are ubiquitous in industry as well as in biological or natural flows. Fresh concrete or uncured solid rocket fuel are two examples of industrial concentrated suspensions for which the highest particle volume fraction is desired while keeping correct rheological properties and flowing behavior. Such dense suspensions do exhibit an intricate physics which is hitherto far beyond complete understanding. This complexity mainly stems from the wide variety of fluid–particle or particle–particle interactions [1] so that even the idealized case of hydrodynamically-interacting smooth monodisperse spherical particles in a Newtonian fluid can involve strong non-Newtonian effects such as yield stress, shear-thickening, particle migration or anisotropic microstructures (see [2,3] for a review).

The development of numerical simulation can help shed light on the complex physics of suspensions. However, due to the importance of flow–particle interactions, only microscale methods – wherein the flow is fully resolved around each particle – are relevant. In contrast, macroscale methods are less computationally demanding but require a local averaging – because computational cells are much larger than particles – which loses the essential details of the flow. For low Reynolds number suspensions, well-suited techniques include Stokesian Dynamics (SD) [4–7] and Force-Coupling Method (FCM) [8–10]. Although different, both methods rely on a truncated multipole expansion solution of the Stokes equations. They undoubtedly have numerous upsides and appear to be instrumental in providing among the most influential results

* Corresponding author at: SAFRAN-Herakles, Le Bouchet Research Center, 91710 Vert le Petit, France. Tel.: +33 1 64991193; fax: +33 1 64991118.
E-mail address: stany.gallier@herakles.com (S. Gallier).

0021-9991/$ – see front matter
http://dx.doi.org/10.1016/j.jcp.2013.09.015

in the field of suspension physics. Nevertheless, they are highly specialized and may not tackle any kind of flows. Because they rest on special solutions of the Stokes equations (multipole expansion), they are inherently restricted to non- or weakly-inertial flows. By and large, multipole expansions are mostly available for spheres, thereby preventing from simulating arbitrary-shaped particles. Furthermore, it is not possible to consider non-Newtonian fluids with these techniques. Therefore, direct numerical simulation (DNS) has emerged as an attractive alternative. In this approach, governing equations (Navier–Stokes or Stokes equations) are solved without any further assumptions other than numerical approximations. This makes possible to solve particulate flows with arbitrary particle shape, flow Reynolds number or fluid rheological constitutive equation. The very first class of DNS methods dedicated to particulate flows followed a boundary-fitted approach wherein only the domain occupied by the fluid is meshed [11,12]. As particles move, the constantly evolving fluid domain poses complex remeshing issues. For sheared concentrated suspensions, in which particle separation can be vanishingly small, remeshing becomes extremely involved and makes this approach impractical for more than a few particles. As an exception, let us mention the works of [13] who performed impressive 3D simulations with up to 100 particles with such body-fitted techniques. In contrast, non-boundary-fitted methods are much more suited for the simulation of suspensions with a large number of particles. The whole domain is mapped onto an Eulerian fixed grid and particles are embedded in this regular non-moving grid. Non-boundary-fitted methods for particulate flows include different techniques, such as immersed boundary methods [14–16], fictitious domain methods [17–19] or lattice Boltzmann methods [20–22]. Fictitious domain methods have met considerable interest and have been widely used so far [23–27]. They have been successfully applied to non-Newtonian flows [28–31], heat transfer in suspensions [32] or non-spherical particles such as ellipsoids [25], cubes [24], polygons [33], plates [23] or fibers [34]. Fictitious domain methods are generally body-force-based methods since solid particles are modeled via a body-force (or momentum forcing) introduced in the momentum equation to enforce a rigid body motion. There exist various methods to handle this body-force and a review is provided in [25]. In the original fictitious domain approach by Glowinski et al. [17,18,35], the body-force is introduced as a Lagrange multiplier in a weak formulation and solved in an iterative way. However, the method is computationally expansive as a saddle-point problem must be solved. Patankar's works [23,36] were the first to develop a non-Lagrange multiplier version of fictitious domain in order to improve computational performance. More recent studies [24–26] have still continued in this way of non-Lagrange multiplier methods by working out an explicit equation on the body-force. These previously cited studies share many similarities and only slightly differ.

Surprisingly, despite the availability of these DNS methods, quantitative simulations of dense suspensions are heretofore a privilege of SD or FCM methods. Only scarce studies address the DNS of suspension rheology [25,28,29,37] but they remain mostly qualitative and far from actual configurations as they consider 2D particles (cylinders) with low volume fractions. As far as the authors know, there have been no attempts at simulating the rheological behavior of dense suspensions using DNS in the way it is done by SD or FCM. With an eye to demonstrating that DNS is well-adapted for detailed simulations of concentrated suspensions, this study intends to develop a non-Lagrange multiplier version [24,25] of the fictitious domain approach since it alleviates the computational burden of the original version. However, those methods define body-force values at some Lagrangian nodes attached to the particles moving in the Eulerian background grid. This consequently involves several interpolation steps between Eulerian and Lagrangian nodes, which are known to induce numerical instabilities [25] and impose a careful choice of the interpolation kernel [14,38]. It is also attested that the arrangement itself of the Lagrangian particle nodes may alter results. For spheres, the best results are obtained with nodes adequately arranged in concentric shells and with the nodes closest to the particle surface slightly retracted from it [25,39]. A generalization to arbitrary-shaped particles is believed to be tedious. Therefore, our approach intends to keep the simplicity of a fully Eulerian method. Body-force quantities are defined at the Eulerian grid points, like the other fluid variables, and an Eulerian advection step is inserted in the method, so that the body-force remains attached to the particle as it moves along.

A peculiar feature of concentrated suspensions is that the average separation distance $a\xi$ between particles, where a denotes the particle radius, becomes extremely small. The so-called lubrication forces arise between particles in near-contact because of the draining of interstitial fluid in the gap. The magnitude of these forces rises dramatically as particles approach each other and is singular in the limit of touching particles as the normal and tangential forces diverge as ξ^{-1} and $\ln\xi$, respectively. Consequently, the rheology of suspensions is markedly modified by lubrication forces and qualitatively important effects occur at small separations, typically down to $\xi \sim 10^{-2}$. For accurate simulations of low Reynolds suspensions, a numerical method should be able to capture those short-range lubrication forces. The required grid spacing should however be smaller than at least $10^{-3}a$–$10^{-4}a$ to resolve lubrication, making long-term simulations of many-particle systems unfeasible. Typical grid spacings are about $10^{-1}a$ which means that – albeit implicitly accounted for by DNS – lubrication forces are less and less accurately described as particles come to near contact. A first simple approach consists in adding the theoretical lubrication force $F^{th}_{lub}(\xi)$, known for two spheres in near-contact [40], to the computed hydrodynamic force. To put it more precisely, this rather takes the form $F^{th}_{lub}(\xi) - F^{th}_{lub}(\xi_{cut})$ where ξ_{cut} is a cut-off separation below which this lubrication correction is activated. This approach is widely employed whatever the numerical technique chosen: fictitious domain [32], dissipative particle dynamics [41], lattice Boltzmann method [42] or boundary element method [43]. Yet, such simple approach is not rigorous because – as previously stressed – a part of the lubrication is already partially included in the numerical solution. Just adding the theoretical force consequently results in double-counting the resolved part of the lubrication force. A more rigorous method is proposed in SD [6,44]. The analytical two-sphere resistance interactions are added to the long-range hydrodynamic resistance matrix. However, in order not to count twice the far-field part of the exact two-sphere resistance interactions, the authors subtract off this contribution, which is found by inverting a two-sphere