Numerical simulations of buoyancy-driven droplets in non-Newtonian media using a variance-reduced, micro-macro, particle-level set method

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ABSTRACT

In this presentation we introduce the main features and explore the capabilities of a recently developed multi-scale, particle level-set method for the simulation of non-Newtonian fluids, termed SLEIPPNNIR [Comput. Methods. Appl. Mech. Eng, 307 (2016),164-192]. We show simulations of buoyancy-driven droplets rising in non-Newtonian media, featuring different viscoelastic effects.

INTRODUCTION

The origin of numerical methods for interface flows can be dated back to 1931 and the seminal paper by Rosenhead[1], where the method of "small oscillations" was used to predict vortex-shedding in a counterflow configuration.In 1957, Harlow[2] proposed the Particle in Cell (PIC) method for surface deformation, using mass particles carrying information about the species. From then on, most schemes have employed either of these latter approaches: namely, the description of the interface in a Lagrangian fashion by placing markers which follow and define the surface, usually adjusting the mesh to account for these changes; or the definition of the interface by means of a certain auxiliary implicit function dependent on the flow, producing an Eulerian scheme over a fixed mesh. The methods are commonly classified as *interface-tracking* or *interface-capturing m*ethods, according to the Lagrangian or Eulerian representation of the free surface.

Half a century later, the field of non-Newtonian Fluid Mechanics has taken advantage of the rich methodology developed for multiphase flows. However, Brownian Dynamics simulations of free-surface flows are still somewhat scarce in the literature: the CONNFFESSIT approach[3] was used e.g. by Grande et al.[4] and by Prieto[5]; the Brownian Configuration Fields (BCF) method[6] was applied by Bajaj et al.[7]; and recently, a Particle Level Set method with a variance-reduced technique was presented by Prieto[8]: the purpose of the next lines is to sketch the main features of this so-called SLEIPNNIR method.

MATHEMATICAL DESCRIPTION

The SLEIPNNIR technique uses a second-order accurate, Finite-Element discretization, along with a semi-Lagrangian approach ("method of the characteristic curves") to deal with the convective terms and to evolve the *level set* function defining each of the fluids in the domain, Eq.1:

$$\begin{cases} \dfrac{\partial \phi}{\partial t} + \boldsymbol{u} \cdot \nabla \phi = 0, & \text{in } D \times (0, T]; \\ \phi(\boldsymbol{x}, 0) = \phi_0(\boldsymbol{x}), & \forall \boldsymbol{x} \in D. \end{cases} \qquad (1)$$

As the simulation goes on, the level set function loses its initial signed-distance property, so that a *reinitialization* step has to be carried out; in SLEIPNNIR, a second-order accurate redistancing scheme based on the eikonal equation[10] is used for that purpose. Surface tension effects are considered through the Laplace-Beltrami[11] operator to circumvent the need for curvature computations, and thus avoid excessive oscillations due to high-frequencies when the mesh grows refined.

Non-Newtonian fluids are modeled by means of a *variance-reduced*, micro-macro approach, in which a collection of ensembles of polymer particles are scattered over the domain. The internal degrees of freedom of these *polymer particles* are advanced according to Eq. 2 (for details on the notation, see[8]):

$$d\mathbf{Q} = \left[\boldsymbol{\kappa}\cdot\mathbf{Q} - \frac{2}{\zeta}\mathbf{F}\left(\mathbf{Q}\right)\right]dt + \sqrt{\frac{4k_B\Theta}{\zeta}}d\mathbf{W},$$

(2)

with a suitable kinetic model such as “Hookean” or the “Finitely Extensible Non-linear Elastic” (FENE) model providing the form of the elastic spring force in Eq. 2. The resulting polymer (extra-stress) tensor is then computed via a Compactly-Supported Radial Basis Function (CSRBF) approach providing a high-degree of mesh independency.

RESULTS

In this talk, we show numerical simulations of buoyancy-driven droplets rising in both Newtonian and non-Newtonian media, for a range of inertial, surface tension and viscoelastic effects. As an example, we next collect the isolines of the rise velocity in a series of droplets rising in a viscoelastic (FENE, b=20) fluid, using a mesh of size h=1/160 with the SLEIPNNIR method and FENE (b=20) model, for values of the Reynolds, Froude and Weber number of Re=35, We=35, Fr=1; the density and viscosity ratios between the fluids are 10; 50000 ensembles are scattered over the domain, each of them collecting 2500 dumbbells carrying the internal configurations of the polymer. As we see in Figs. 1 and 2, downward velocities (*negative wake effect*) arise at a certain point of the simulation when the concentration parameter and the Deborah number are high enough.

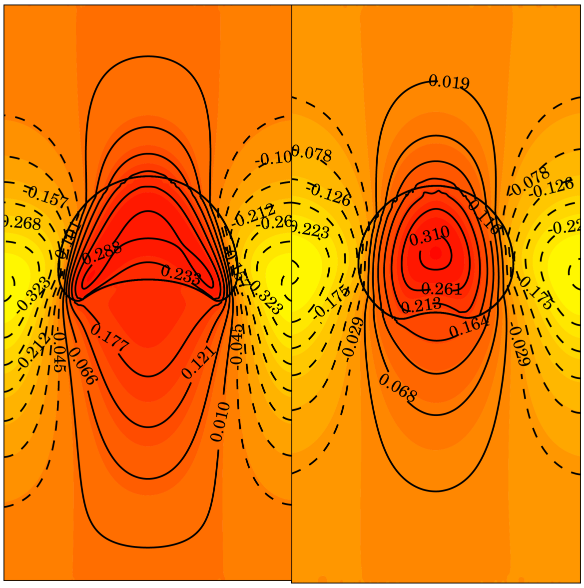

Figure 1. Isolines of rise velocity at time t=3.5. Left panel: c=1,De=1;. Right panel: c=3,De=1.

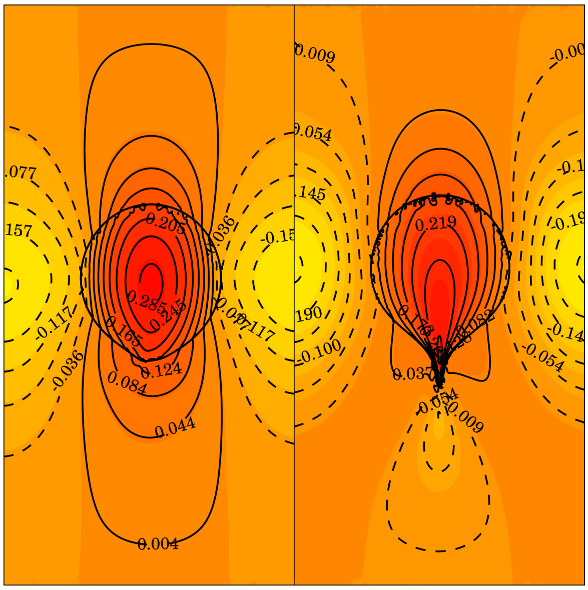

Figure 2. Isolines of rise velocity at time t=3.5. Left panel: c=5,De=1;. Right panel: c=7,De=5.

CONCLUSIONS

Within its limitations, the SLEIPNNIR technique has good capabilities for the computation of accurate and efficient simulations of multiphase, non-Newtonian flows, using a “micro-macro” stochastic approach.

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REFERENCES

1. Rosenhead, L. (1931), "The Formation of Vortices from a Surface of Discontinuity", *Proc. R. Soc. Lond. A,* **134**(823), 170-192.

2. Harlow, F.H. (1957), "Hydrodynamic Problems Involving Large Fluid Distortions", *J. Assoc. Comp. Mach.*, **4**(2), 137-142.

3. Laso, M. and Öttiger, H.C. (1993), "Calculation of viscoelastic flow using molecular models: the CONNFFESSIT approach", *J. Non-Newtonian Fluid Mech.*, **47,** 1-20.

4. Grande, E., Laso, M. and Picasso, M. (2003), "Calculation of Variable-Topology Free Surface Flows Using CONNFFESSIT", *J. Non-Newtonian Fluid Mech.*, **113,** 127-145.

5. Prieto, J.L. (2015), "Stochastic particle level set simulations of buoyancy-driven droplets in non-Newtonian fluids", *J. Non-Newtonian Fluid Mech.*, **226,** 16-31.

6. Hulsen, M.A., van Heel, A.P.G. and van den Brule, B.H.A.A. (1997), "Simulation of viscoelastic flows using Brownian Configuration Fields", *J. Non-Newtonian Fluid Mech.*, **70,** 79-101.

7. Bajaj, M., Bhat, P.P., Prakash, J.R. and Pasquali, M (2006), "Multiscale simulation of viscoelastic free surface flows", *J. Non-Newtonian Fluid Mech.*, **140,** 87-107.

8. Prieto, J.L. (2016), "SLEIPNNIR: A multiscale, particle level set method for Newtonian and non-Newtonian interface flows", *Comput. Methods Appl. Mech. Engrg.*, **307,** 164-192.

9. Bermejo, R. and Prieto, J.L. (2013), "A Semi-Lagrangian Particle Level Set Finite Element Method for Interface Problems", *SIAM J. Sci. Comput.*, **35**(4)**,** A1815-A1846.

10. Cheng, L.T. and Tsai, Y.H. (2008), "Redistancing by flow of time dependent eikonal equation", *J. Comput. Phys.*, **227,** 4002-4017.

11. Gross, S. and Reusken, A. (2007), "Finite element discretization error analysis of a surface tension force in two-phase incompressible flows", *SIAM J. Numer. Anal.*, **45,** 1679-1700.