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Stochastic Rotation Dynamics simulations of wetting multi-phase flows

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ABSTRACT

Multi-color Stochastic Rotation Dynamics (SRD^{mc}) has been introduced by Inoue et al. [1,2] as a particle based simulation method to study the flow of emulsion droplets in non-wetting microchannels. In this work, we extend the multi-color method to also account for different wetting conditions. This is achieved by assigning the color information not only to fluid particles but also to virtual wall particles that are required to enforce proper no-slip boundary conditions. To extend the scope of the original SRD^{mc} algorithm to e.g. immiscible two-phase flow with viscosity contrast we implement an angular momentum conserving scheme (SRD^{mc}_{+}). We perform extensive benchmark simulations to show that a mono-phase SRD^{mc} fluid exhibits bulk properties identical to a standard SRD fluid and that SRD^{mc} fluids are applicable to a wide range of immiscible two-phase flows. To quantify the adhesion of a SRD^{mc}_{+} fluid in contact to the walls we measure the apparent contact angle from sessile droplets in mechanical equilibrium. For a further verification of our wettability implementation we compare the dewetting of a liquid film from a wetting stripe to experimental and numerical studies of interfacial morphologies on chemically structured surfaces.

1. Introduction

Capillarity dominated flows of immiscible fluids on the micro-scale are of central importance in many coating processes [3,4], secondary oil recovery [5,6] or the advancing field of microfluidics [7,8]. Motion of fluid interfaces and their topological changes such as droplet pinch-off or coalescence are difficult to capture by finite element methods and become even more complex in the presence of rigid walls [9]. Capillary flows with wall contact depend crucially on wettability [7,8] but the disproportionately high computational costs to capture the specific wall interactions in e.g. level-set or phase field models make it virtually impossible to study large scale systems.

Over the last decades several particle based methods including dissipative particle dynamics (DPD) [10,11], Lattice Boltzmann (LB) [12–14] or multi-particle collision dynamics (MPC) [15–18] have been developed to study a wide range of soft condensed matter systems on the meso-scale. Particle based methods share the idea of a coarse graining procedure that lumps together the microscopic degrees of freedom of the fluid particles into larger macroscopic entities that, after suitable

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spatial and temporal averaging, display the fluid mechanical properties. The DPD method, closely related to Molecular dynamics (MD) [19] is still too detailed to provide an efficient Navier–Stokes solver and the integration of Newton's equation of motion comes with high numerical costs. Although widely used in computational sciences LB models have some limitations especially when enforcing certain boundary conditions. Because LB models consider particle populations with discrete velocities residing on a regular spatial lattice, embedded objects that are of irregular shape or off-lattice lead to further treatment of the fluid-solid interface by e.g. immersed boundary methods [20,21].

More recently the MPC method introduced by Malevanets and Kapral [15] has gained attraction in the field of computational fluid dynamics. It provides a robust method to obtain the correct transport of mass, momentum, and energy on the macro-scale. In their pioneering work on polymer solutions in meso-scale systems [16] the authors coupled MPC to simulate the solvent and MD to study the solute dynamics. This hybrid approach has since been used to study equilibrium colloidal suspensions [17,18,22–25] and polymer [17,18,26,27] solutions. An even more eminent relevance to real applications is the use of MPC to study systems out of equilibrium that are driven by flow including colloids [28–32], polymers [26,33–35], liquid crystals [36] and fluid vesicles or blood cells [37–39]. Furthermore, MPC was also successfully applied to study bacteria [40], sperm cells [41] and swimmers and squirmers in general [42–45].

The method employed in this work belongs to a subset of MPC methods termed stochastic rotation dynamics (SRD). The name originates from the specific realization of momentum exchange between fluid particles during collisions. In all SRD variants the diffusive transport of momentum is achieved through a stochastic rotation of the relative velocities of the particles in a collision cell [15,46–48]. In the course of this work we will use the term SRD rather than MPC even though some general statements may refer to both types of methods.

In recent years, different SRD variants have been used to model phase separating binary and ternary fluid mixtures [49–51]. A modified SRD algorithm that accounts for an arbitrary number of fluid phases has been proposed by Inoue et al. [1,2,52]. Inoue's multi-color algorithm (SRD^{mc}) employs a collision operator that actively maintains a segregation of particles with different colors. Whilst the multi-color model accounts for phase immiscibility, the interaction of the fluids with the walls, or embedded objects with different wall affinities was not yet addressed. To this end, we implemented an extension to the SRD^{mc} scheme in order to account also for surface wettability. Especially for capillary dominated flows where the fluid-surface interaction is of central importance [7,8] this extension can be employed to study colloidal suspensions in immiscible fluid phases, porous media, micro- or nanofluidics or other fields of soft condensed matter.

The standard SRD method is a well established tool to study mono-phase fluids on the meso-scale and its properties have been thoroughly investigated by several authors over the last years [24,46–48,53–65]. In their introductory work Inoue et al. [1] only measured the surface tension qualitatively for a 2D droplet and showed that the Brownian motion of the center of mass of a droplet follows a Maxwell–Boltzmann distribution. What the SRD^{mc} method has been lacking so far is the characterization of bulk fluid properties as well as the interaction of two immiscible phases, especially in three dimensions. To this end, and before introducing our wettability implementation, we perform a series of benchmark simulations to determine the relevant hydrodynamic properties of a SRD^{mc} fluid. To the best of our knowledge this is the first time that such an extensive study is carried out for SRD^{mc} fluids to verify the reliability of the method. To present a coherent description this work is outlined as follows. Section 2 introduces the theoretical foundations of the methods employed in this work. In Sec. 3 we determine the dynamic viscosity of a SRD^{mc} fluid from local measurements of the shear rate and stress tensor in a linear shear flow. In Sec. 4 we determine the interfacial tension between two immiscible fluid phases with three independent methods and verify the beforehand determined values with predictions for the deformation of a droplet in a linear shear flow. In Sec. 5 we present our extension to the SRD^{mc} scheme that accounts for varying surface wettability. We test our wetting implementation on homogeneously and heterogeneously wettable surfaces and compare the resulting interfacial configurations with previous experiments and numerical studies.

2. Model and methods

In the following we briefly present the standard SRD algorithm (Sec. 2.1) and an extension that respects angular momentum conservation (Sec. 2.2). After introducing the SRD^{mc} algorithm of Inoue et al. [1] in Sec. 2.3 we present our implementation of stress measurements based on area-weighted averages (Sec. 2.4). This allows us to localize very precisely the momentum transport inside a collision cell. The necessity of this approach is shown later in the course of this work (see Sec. 4.1).

2.1. Stochastic Rotation Dynamics

Particle based simulation methods obtain the collective dynamics of the fluid phases from the motion of a large number N of point particles i of mass m that can adopt continuous positions, $\mathbf{x}_i$, and velocities, $\mathbf{v}_i$, in three dimensional Euclidean space. The dynamics of the particles consist of a sequence of streaming and collision steps. During free streaming, particles move deterministically between time t and $t + \Delta t$. New positions $\mathbf{x}_i(t + \Delta t)$ and velocities $\mathbf{v}_i'(t + \Delta t)$ at the end of the streaming step are consequently given by

$$\mathbf{x}_i(t + \Delta t) = \mathbf{x}_i(t) + \mathbf{v}_i(t)\Delta t + \frac{\mathbf{f}_{\text{ex}}}{2m_i}\Delta t^2, \tag{1}$$