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Numerical simulation of wetting phenomena by a meshfree particle method

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HIGHLIGHTS

- Accurate interface between two phases.
- Meshfree particle methods are appropriate candidates for flows with changing interface in time.
- Wetting phenomena can be naturally handled by Lagrangian particle methods.

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ABSTRACT

Simulations of wetting phenomena by a meshfree particle method are presented. The incompressible Navier–Stokes equations are used to model the two-phase flow. The continuous surface force model is used to incorporate the surface tension force. Chorin's projection method is applied to discretize the Navier–Stokes equations. The different fluid phases are identified by assigning different colors and different material properties (density, viscosity) to the particles that remain unchanged throughout a simulation. Two-phase flow is captured by a one-fluid model via using weighted averages of the density and viscosity in a region around the fluid–fluid interface. The differential operators at each particle are computed from the surrounding cloud of particles with the help of the least-squares method. The numerical results are compared with specific analytical solutions, but also with previously considered test cases involving wetting of a container and sessile drops. A good overall agreement is found.

1. Introduction

Surface-tension driven flows occur when the surface-tension forces acting on a liquid are of equal or even larger magnitude than the inertial, viscous or gravitational forces. There exist numerous applications in which such flows are important, for example in the areas of microfluidics [1,2], coating technology [3], two-phase heat transfer [4] or oil recovery [5,6]. Correspondingly, there is a high demand for efficient numerical models and schemes to compute surface-tension driven flows.

In the past decades, a large number of CFD approaches have been presented that explicitly resolve the interface between two immiscible fluids. Often these are classified either as interface-tracking or interface-capturing schemes. In the former, the time evolution of the interface is represented by the time evolution of the numerical grid whose structure contains information about the interface shape. In the latter, the evolution of the interface is decoupled from the grid. Instead, the

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interface is reconstructed from field quantities represented on the grid. The most popular examples of interface capturing schemes are probably the volume-of-fluid [7] and the level-set method [8]. While interface-tracking schemes tend to be very accurate, they are not well suited to study flows with topological changes occurring when, for example, drops or liquid sheets break up or merge. For the latter, interface capturing schemes are suitable candidates.

In the past decades, fast progress has been made in the development of particle-based or meshfree methods to compute various types of flows. In such schemes Lagrangian particles, serving as the basic building blocks for discretization of the fluid dynamic equations, are advected with the flow. This has the advantage of a certain degree of inherent adaptivity, i.e. the numerical resolution is provided only where it is needed. Classical examples for the application of meshfree methods are astrophysical flows [9] in which the set of Lagrangian particles co-evolves with an astrophysical structure, e.g. a plasma cloud. Often, in gas–liquid flows a similar division in an important and an unimportant subdomain occurs. Compared to the liquid, the stresses in the gas phase are often negligible, which means that it is sufficient to compute the flow in the liquid phase alone. Meshfree methods lend themselves for this purpose. Furthermore, in contrast to interface-tracking schemes, meshfree methods easily allow studying free-surface flows with topological changes. In total, meshfree methods appear to be ideal candidates for the simulation of complex gas–liquid flows. Among these, surface-tension driven flows form an important subclass.

The first meshfree Lagrangian method that has been formulated to solve fluid dynamics equations is denoted Smoothed Particle Hydrodynamics (SPH) [10]. Another meshfree Lagrangian CFD approach is the moving particle semi-implicit method [11]. In this article we use a meshfree particle method, called Finite Pointset Method (FPM), to solve the incompressible Navier–Stokes equations. FPM is a fully Lagrangian particle method and has a similar character as the SPH method except for the approximation of spatial derivatives and the treatment of boundary conditions. In SPH the spatial derivatives at an arbitrary particle position are approximated by an interpolation approach from the surrounding particles. However, in FPM the spatial derivatives are approximated using the finite-difference approach [12], where the spatial differential operators at an arbitrary particle position are approximated by the moving least squares approach [13]. The Poisson equation for the pressure field is also solved in the sense of constrained least squares. The domain boundaries are represented by boundary particles, and boundary conditions are directly prescribed on those particles.

Meshfree particle methods are appropriate tools to simulate surface-tension driven flows. Each phase is indicated by the color of the respective particles. When particles move, they carry all the information about the flow with them such as their color, density, velocity, etc. The colors, densities and viscosity values of all particles remain constant during the time evolution. The fluid–fluid interface is easily determined with the help of the color function. To the best of the author's knowledge, the first implementation of the continuous surface force (CSF) model to account for surface-tension forces was presented in [14]. In [15] an implementation of the CSF model within the FPM was presented to simulate surface-tension driven flows. The present article is an extension of [15], devoted to studying wetting phenomena.

The paper is organized as follows. In Section 2 we present the mathematical model and the numerical scheme. In Section 3 some specific aspects of the FPM are presented. The numerical test cases are presented in Section 4. In some cases analytical solutions can be calculated, and the numerical solutions are compared with the analytical ones. In those cases where analytical solutions are not known, the results are compared to numerical results published earlier. Moreover, some convergence studies are presented in Section 4. The paper finishes with concluding remarks and suggestions for future work.

2. Mathematical model and numerical scheme

2.1. Mathematical model

We consider two immiscible fluids, for example, liquid and gas, where both of them are incompressible. We use the one fluid formulation of two-phase flows from [16]. We model the two-phase flows by the incompressible Navier–Stokes equations. The equations are expressed in the Lagrangian form

$$\frac{d\vec{x}}{dt} = \vec{v} \tag{1}$$

$$\nabla \cdot \vec{v} = 0 \tag{2}$$

$$\frac{D\vec{v}}{Dt} = -\frac{1}{\rho}\nabla p + \frac{1}{\rho}\nabla \cdot (2\mu D) + \vec{g} + \frac{1}{\rho}\vec{F}_S, \tag{3}$$

where $\vec{v}$ is the fluid velocity vector, ρ is the density, μ is the dynamic viscosity, D is the viscous stress tensor $D = \frac{1}{2}(\nabla\vec{v} + \nabla^T\vec{v})$, $\vec{g}$ is the gravitational acceleration and $\vec{F}_S$ is the surface tension force. In general, ρ and μ are discontinuous across the interface and remain constant in each phase. The surface tension force $\vec{F}_S$ is computed using the classical continuum surface force (CSF) model [16]. It acts on the vicinity of the interface between the fluids. In the CSF model the surface tension force $\vec{F}_S$ is defined by

$$\vec{F}_S = \sigma\kappa\vec{n}_I\delta_S, \tag{4}$$