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Capillary forces: A volume formulation

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ABSTRACT

In this Note we give a simple volume formulation of capillary force. This formulation is not conservative but less singular than that of Lafaurie et al., (1994). Moreover our formulation allows to recover immediately Laplace's law.

1. Introduction

One of the most challenging issue in Computational Fluid Dynamics (CFD) is to capture accurately and robustly multi-fluid flows. Indeed, after spectacular progresses in computational (single) fluid dynamics, both industrial and fundamental issues are demanding for the same state of the art in the case of two (or more) fluid flows. There are mainly two kinds of mathematical models for two non miscible fluid flows. The first one states that the two fluids under consideration are separated by sharp interfaces and the numerical method should capture this interface (or free surface). This is termed as separated flows. The second one acknowledges the fact that interfaces could be too complicated (*e.g.* a bubbly flow) to be computed and introduces averaged equations (Ishii and Hibiki [1]) so that the interfaces are not captured but locally the volume fraction of each fluid is a dependent variable to be computed like the other ones (density, velocities, pressure, ...). These two kinds of models are complementary and sometimes the first one is used to validate the second one according to the usual DNS[1] approach.

In this Note we focus on separated flows. At the interface between two non miscible fluids like air and water or oil and water, to cite a few, a capillary force occurs and enters into the momentum balance:

$$\frac{\partial(\rho\,\boldsymbol{u})}{\partial t} + div(\rho\,\boldsymbol{u}\otimes\boldsymbol{u}) + \nabla p = \rho\,\boldsymbol{g} + 2\,\sigma\,\kappa\,\delta_\Sigma\,\boldsymbol{n}. \tag{1}$$

In this equation, the capillary force is $2\,\sigma\,\kappa\,\delta_\Sigma\,\boldsymbol{n}$ where σ denotes the surface tension coefficient between the two fluids, κ denotes the mean curvature of the interface Σ, $\boldsymbol{n}$ the unit normal on Σ and δ_Σ is the Dirac mass supported by the interface. Observe that in the r.h.s. of (1) the factor 2 appears since in this paper we use the definition of the mean curvature of the interface steaming from differential geometry. In Fluid Mechanics this factor is not present and κ then denotes the sum of the two principal curvatures.

Remark 1. We deal, in this Note, with capillary forces in the simplest context in CFD, namely the Euler equations for perfect fluids. The case of viscous and diffusive fluids (Navier–Stokes equations) is totally parallel.

On the one hand, modern numerical methods in fluid dynamics rely on Finite Volume Methods (FVM) as they allow both to handle real geometries and to ensure exactly local conservations like mass, momentum and energy. On the other hand, the capillary force is highly singular. Indeed surface forces are not adapted to FVM[2] on a fixed mesh (Eulerian methods). In this Note we prove that this force can be expressed in terms of volume forces:

$$2\sigma\,\kappa\,\delta_\Sigma\,\boldsymbol{n} = \nabla(2\sigma\,\kappa\,H_\Sigma) - H_\Sigma\nabla(2\sigma\,\kappa), \tag{2}$$

where H_Σ denotes the Heaviside function.

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[1] Direct Numerical Simulation.

[2] Except for the method proposed by D. Chauveheid [2].

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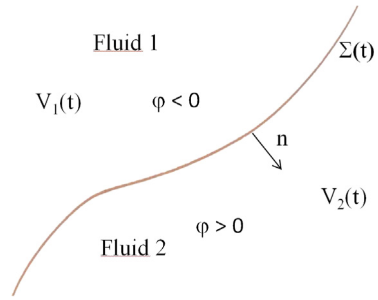

Fig. 1. The interface at time t between the two fluids.

Remark 2. In [3], Lafaurie et al. show that:

$$\kappa\,\delta_\Sigma\,\boldsymbol{n} = div\,((\boldsymbol{I} - \boldsymbol{n}\otimes\boldsymbol{n})\,\delta_\Sigma)\,, \tag{3}$$

which leads also to a volume formulation of the capillary forces. In a certain sense it is more elegant than (2) since it is a conservative expression but, as explained in Section 4.2, it does not allow to recover Laplace's law.

2. Expression of the capillary force

2.1. Geometry

We consider two non miscible fluids (liquids or gases) separated at time t by a smooth interface denoted by:

$$\Sigma(t) \equiv \{\boldsymbol{x} \in \mathbb{R}^d \text{ such that } \varphi(t,\boldsymbol{x}) = 0\}, \tag{4}$$

where $\varphi(t,\boldsymbol{x}) = 0$ is the equation of this hypersurface in $\mathbb{R}\times\mathbb{R}^d$ ($d = 2$ or 3). We assume that this equation satisfies:

$$|\nabla_{\boldsymbol{x}}\varphi| \neq 0 \quad \text{on } \Sigma(t), \tag{5}$$

and that $\varphi < 0$ corresponds to fluid 1 while $\varphi > 0$ corresponds to fluid 2, see Fig. 1. Finally we denote by

$$\boldsymbol{n} = \frac{\nabla_{\boldsymbol{x}}\varphi}{|\nabla_x\varphi|}, \tag{6}$$

the unitary normal on the free surface at time t pointing from fluid 1 towards fluid 2.

2.2. Proof of formula (2) in the 2D case

According to (5) one can build on Σ a curvilinear abscissa s and the Dirac mass supported by Σ is the distribution on the plane defined by:

$$\langle\delta_\Sigma, \Psi\rangle \equiv \int_\Sigma \Psi(s)\,ds, \quad \forall\Psi, \tag{7}$$

where Ψ is a smooth function on $\mathbb{R}^2$ whose compact support is a neighborhood of Σ.

Again thanks to (5), locally on Σ, after rotation on the (x, y) coordinates if necessary, it is possible to assume that:

$$\varphi(t, x, y) = y - \Phi(x, t), \tag{8}$$

so that (7) implies:

$$\delta_\Sigma(x, y) = \sqrt{1 + \Phi_x^2(x,t)}\,\delta(y - \Phi(x,t)), \tag{9}$$

where this time δ denotes the classical Dirac mass on $\mathbb{R}$:

$$\langle\delta, \psi\rangle \equiv \psi(0), \quad \forall\psi \text{ smooth and compactly supported on } \mathbb{R}. \tag{10}$$

On the other hand we have:

$$\kappa = \frac{\Phi_{xx}}{(1+\Phi_x^2)^{3/2}} \quad \text{and} \quad \boldsymbol{n} = \frac{1}{\sqrt{1+\Phi_x^2(x,t)}}(-\Phi_x, 1). \tag{11}$$

Hence in this case the second term in the r.h.s. of (1) is:

$$2\,\sigma\,\kappa\,\delta_\Sigma\,\boldsymbol{n} = 2\,\sigma\,\frac{\Phi_{xx}}{(1+\Phi_x^2)^{3/2}}\,\delta(y - \Phi(x,t))(-\Phi_x, 1). \tag{12}$$

Introducing the usual Heaviside function H on $\mathbb{R}$ and observing that:

$$\frac{\partial}{\partial x}H(y - \Phi(x,t)) = -\Phi_x\,\delta(y - \Phi(x,t)), \tag{13}$$

and

$$\frac{\partial}{\partial y}H(y - \Phi(x,t)) = \delta(y - \Phi(x,t)), \tag{14}$$

we deduce that:

$$2\,\sigma\,\kappa\,\delta_\Sigma\,\boldsymbol{n} = \nabla_{x,y}\mathcal{H}(x,y,t) + \mathcal{S}(x,y,t), \tag{15}$$

where:

$$\mathcal{H}(x,y,t) \equiv 2\,\sigma\,\frac{\Phi_{xx}(x,t)}{(1+\Phi_x^2(x,t))^{3/2}}\,H(y - \Phi(x,t)), \tag{16}$$

$$\mathcal{S}(x,y,t) \equiv \left(-2\,\sigma\left(\frac{\Phi_{xx}(x,t)}{(1+\Phi_x^2(x,t))^{3/2}}\right)_x, 0\right) H(y - \Phi(x,t)). \tag{17}$$

Returning to the intrinsic formulation, we can write:

$$2\,\sigma\,\kappa\,\delta_\Sigma\,\boldsymbol{n} = \nabla_{x,y}(2\,\sigma\,\kappa\,H_\Sigma) - H_\Sigma\,\nabla_{x,y}(2\,\sigma\,\kappa), \tag{18}$$

where H_Σ is the distribution on the plane defined by:

$$\langle H_\Sigma, \Psi\rangle \equiv \int_{V_2(t)} \Psi(x,y)\,dx\,dy, \quad \forall\Psi, \tag{19}$$

where Ψ is a smooth function on $\mathbb{R}^2$ with compact support. That is H_Σ is the characteristic function of the volume occupied by Fluid 2 ($\varphi(x, y, t) > 0$). We have shown (2) in the 2D case.

2.3. Proof of formula (2) in the 3D case

The proof is totally similar to the previous one. Here thanks to (5), one can build on Σ a normal parametrization s_1 and s_2 and the Dirac mass supported by Σ is the distribution on the space defined by:

$$\langle\delta_\Sigma, \Psi\rangle \equiv \int_\Sigma \Psi(s_1, s_2)\,ds_1\,ds_2, \quad \forall\Psi, \tag{20}$$

where Ψ is a smooth function on $\mathbb{R}^3$ whose compact support is a neighborhood of Σ.

Again thanks to (5), locally on Σ, after rotation on the (x, y, z) coordinates if necessary, it is possible to assume that:

$$\varphi(t, x, y, z) = z - \Phi(x, y, t), \tag{21}$$

so that

$$\delta_\Sigma(x, y) = \sqrt{1 + \Phi_x^2 + \Phi_y^2}\,\delta(z - \Phi(x,y,t)). \tag{22}$$

On the other hand we have:

$$\kappa = \frac{(1+\Phi_x^2)\Phi_{yy} + (1+\Phi_y^2)\Phi_{xx} - 2\,\Phi_x\,\Phi_y\,\Phi_{xy}}{(1+\Phi_x^2+\Phi_y^2)^{3/2}}, \tag{23}$$