Modelization of partial wetting by macroscopic approach in discrete mechanics

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Abstract

The partial wetting is generally defined by a contact angle between the liquid and the surface in the case of a static equilibrium excluding other types of actions such as gravity, inertia, viscosity, etc. When these last effects are no longer negligible, the modeling of two-phase flows governed by capillary forces cannot be reduced to simple geometrical laws on the surface tensions between the phases. The triple line is subject to accelerations that combine in a complex way to fix in time its motion on the surface. The macroscopic approach adopted is based on the representativity of the discrete equation of motion derived from the fundamental law of dynamics expressed in terms of accelerations. The formalism leads to a wave equation whose form corresponds to the two components of a Helmholtz-Hodge decomposition, the first to the curl-free and the second to the divergence-free. Like all other contributions, the capillary effects are expressed in two terms of the capillary potential, an energy per unit mass. The longitudinal and transverse surface tensions allow for possible anisotropy effects in the tangent plane at the interface. The assignment of the surface tension values on the triple line related to the contact angle allows to take into account the partial wetting effects in a dynamic context. Two examples illustrate the validity of this approach.

Keywords

Discrete Mechanics; Helmholtz-Hodge Decomposition; Conservation of Acceleration; Partial Wetting; Capillary effects

1 Introduction

The physical concepts of partial wetting are now well known at the microscopic and macroscopic scales [1]. If there is an indisputable marker of the wettability of a surface, it is the contact angle θ_c, a reproducible measure for a liquid to wet a solid surface in the presence of a third phase, a gas mixed with the liquid's vapor. This contact angle is defined at mechanical equilibrium in the absence of any disturbance that could distort the interpretation of the measurement; gravity, an electric field, the geometrical structure of the surface on a small scale, the presence of impurities, ... can indeed drastically modify the value of the contact angle. A general analysis by S. Popinet [2] places the problem of partial wetting in the broader context of capillary flows.

Apart from the contact angle measured under ideal conditions, it is difficult to find other indisputable parameters to define the macroscopic connection of the free surface with the solid wall. Let us consider for example the case of a solid surface inclined by an angle α_c on which is deposited a drop of small dimension which reaches a static mechanical equilibrium.

The observation of the latter leads to define two angles, one upstream of the triple line in the downstream direction and the other downstream, the angles of advancing and receding. Under these conditions, the contact angle varies along the triple line defined as the trace of the liquid on the surface. It is then very difficult to exploit this result to model macroscopically and to transpose this result to similar experiments for conditions different from the initial experiment. Similarly, when there is an unsteady motion of the interface due to an external action, the contact

angle θ_c is no longer respected for different reasons, (i) the viscosity of the fluid and in general its rheology, (ii) the inertia which depends in a non-linear way on the velocity of the fluid in the vicinity of the triple line, etc. Consequently, there are no more references allowing to intrinsically model the motion of the triple line as a function of time. The notion of dynamic contact angle sometimes used to account for unsteady phenomena related to the triple line is not acceptable because it ignores the underlying phenomena which have an undeniable reality [3, 1, 4, 5].

Over time, the modeling associated with the contact equilibrium of several phases has been made from global formulas such as the Young-Dupré law that expresses the value of the contact angle as a function of the values of the surface tension of the liquid, vapor and that of the solid. Even if there is a mechanical equilibrium that can be translated into a law of forces or surface tensions, the interpretation of certain quantities, for example here the surface tension between the solid and the vapor, does not lead to an intrinsic quantification of the contact angle. Approaches based on the Cahn and Hilliard's model and a phase field method [6, 7] enable us to consider the problem from a thermodynamic angle and extend the concepts to interfaces close to the critical point. The applications of wetting models are numerous, from the printed droplet microfluidics, paint spreading, and undeniably justify studies of a theoretical nature [8, 9]. The methodologies used are also numerous and are based on techniques used in the more general framework of capillary two-phase flows [10, 11].

The point of view adopted in this framework is different, it postulates that a contact angle θ_c is measured under ideal conditions and adopted in the modeling. It can, like the surface tension itself, depend on the temperature but not on other physical parameters. This angle should naturally be considered as a solution of the problem if the ideal conditions are applied; in all other situations, the real contact angle will be different from θ_c.

The formulation adopted to represent the motion of a fluid in the presence of a triple line is that of discrete mechanics. This physical model postulates that the acceleration of a particle or a material medium is equal to the sum of the accelerations imposed on it by the exterior. The fundamental principle of dynamics becomes an equilibrium of accelerations, the only physical quantity considered as absolute. This model already includes the main contributions related to inertia, viscous effects, compression effects, gravitational acceleration, etc. It can be considered as an alternative to the Navier-Stokes equations for which it allows to find strictly the same solutions, the momentum being replaced by the acceleration. The modeling of capillary effects in general and of the triple line in particular is carried out in a manner consistent with the principles of the derivation of the discrete law of motion. The objective here is to present the general model of this new approach and to analyze the role played by the contact angle in complex flows where the physical phenomena are already described.

2 Framework of discrete mechanics

The concepts of discrete mechanics have already been described in the literature. They can be summarized by the abandonment of some important assumptions of classical mechanics, (i) the notion of continuous medium, (ii) the notion of global reference frame $\mathbb{R}(x, y, z)$ and the change of reference frame, (iii) the derivation at a point, integration and, in general, mathematical analysis, (iv) mass and density, (v) the notion of tensor and axial or polar vectors, (vi) the quantities force and pressure, (vii) the three-dimensional view of volume and (viii) the notion of fictitious force. These fundamental concepts of classical mechanics are replaced by those of a very different approach based on the alliance of differential geometry and electromagnetism. The global frame of reference of classical mechanics is replaced by a local frame of reference on which all effects are modeled. Unlike conventional procedures, the method we use has the particular advantage of producing results that can be used directly in numerical calculations, without the need for additional discretization.

2.1 Local frame of reference

In the absence of an absolute reference frame, Newtonian mechanics took up the concept of velocity relativity enunciated by Galileo; this concept became the principle of Galilean relativity or the principle of inertia or Newton's first law. Any point body having a velocity in a fixed direction maintains its rectilinear motion at constant velocity if it is not subjected to an external force. Its interpretation in discrete mechanics is restricted to two parameters, (i) a length dh called discrete horizon and (ii) the time interval dt between the mechanical equilibria defined at time t^o and $t = t^o + dt$. The mechanical equilibrium corresponds to the exact satisfaction of the discrete law of motion. Length and time allow us to define a velocity or rather a celerity c such that $dh = c\,dt$. An observer located at one end of the line can only distinguish the other for a time greater than dt, hence the notion of horizon. The velocity $\boldsymbol{v}$ on this rectilinear segment cannot exceed the celerity c of the medium.

The local reference frame considered is that of the Figure 1; it is composed of the segment Γ of extremities a and b of length dh oriented by the unit vector $\mathbf{t}$. It is surrounded by a dual contour Δ oriented by the unit vector $\mathbf{n}$ such that the unit vectors are orthogonal, $\mathbf{t} \cdot \mathbf{n} = 0$. The association of several rectilinear segments connected by their extremities forms flat polygonal surfaces $\mathcal{S}$ bounded by a family Γ^* of segments Γ. Similarly, the contour Δ defines the dual surface $\mathcal{D}$. Two quantities are respectively related to the vertices of the segments and to the dual contour, the scalar potential ϕ and the vector potential $\boldsymbol{\psi}$ oriented along $\mathbf{n}$.

Space vectors do not exist in this context. The velocity $\boldsymbol{v}$ will be defined only on Γ, it is one of the components of the space velocity which knowledge is not necessary. Similarly, the acceleration $\boldsymbol{\gamma}$ is limited to its only component on this segment. Discrete mechanics postulates that the acceleration $\boldsymbol{\gamma}$ is the only absolute physical quantity, all the other physical quantities being relative; the velocity is thus defined by the material derivative $\boldsymbol{\gamma} = d\boldsymbol{v}/dt$ such that $\boldsymbol{v} = \boldsymbol{v}^o + \boldsymbol{\gamma}\,dt$ where $\boldsymbol{v}^o$ is the so-called retarded velocity, defined at the instant t^o. Thus, without the knowledge of $\boldsymbol{v}^o$ it is not possible to predict whether the motion is, at time t, at a velocity lower or higher than the celerity of the medium, whatever the physical phenomenon of propagation considered (swell, sound, light).

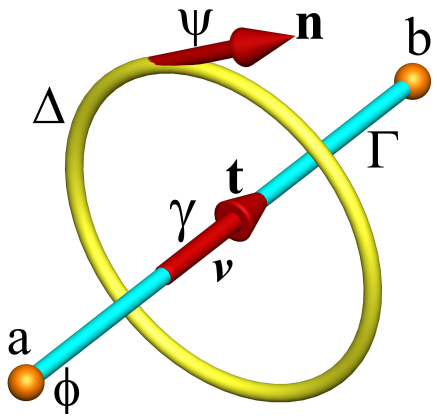

Figure 1. Primal and dual geometric structures of discrete mechanics. The primal structure consists of a segment Γ oriented by the unit vector $\mathbf{t}$ with ends a and b. The dual closed contour Δ is oriented by the unit vector $\mathbf{n}$ orthogonal to $\mathbf{t}$, $\mathbf{t} \cdot \mathbf{n} = 0$. The acceleration $\boldsymbol{\gamma}$ and velocity $\boldsymbol{v}$ vectors are restricted to their components on Γ. The scalar potential ϕ is defined on the vertices and the vector potential $\boldsymbol{\psi}$ is associated to the dual contour. These two structures define a direct local reference frame.

The local frame of reference of Figure 1 represents a discrete form of the existing primal and dual structures whatever the dimension of the space considered; in one, two or three dimensions, this scheme will remain unchanged and the law of motion that follows is strictly independent of the dimension of the space. The dimension dh can take finite values related to the considered problem but it can also be reduced to zero; in this case, it is the whole frame of reference which is reduced in a homothetic way. Thus, just as the volume is reduced to zero in continuum mechanics, this approach leads to a local law. However, unlike classical mechanics, the local reference frame cannot be reduced to a point, the angles and directions are preserved. The two representations, discrete and continuous, are thus preserved.

The structure of the discrete reference frame evokes the remarkable idea of J.C. Maxwell [12] to federate the concepts of magnetism and electrodynamics to define those of electromagnetism. A direct variable current created by an electric potential difference between a and b of the Γ segment induces a variable current in the Δ loop and *vice versa*. In direct current, the interaction disappears and the two phenomena become independent. This scheme is used in discrete mechanics to establish a law of motion in accordance with the fundamental principles of mechanics, notably Newton's second law. Since the laws of electromagnetism are currently dissociated from those of mechanics, how can the two be reconciled? This is only possible by abandoning some of the concepts of classical mechanics mentioned above. As it is not a simple analogy between two phenomena, it is necessary to find a unique law of motion applied to quantities of different nature. This transformation therefore requires the definition of common quantities by drastically reducing the number of physical quantities and the units in which they are expressed. The law of motion thus obtained will be representative of motions in fluids, of stresses and displacements in solids and of wave propagation in all media [13]. The structure of the discrete equation cannot escape the more recent concepts of relativity.

Since the concepts of mathematical analysis are abandoned, they must be replaced by those of differential geometry in the form of operators. Only four operators are needed to transform the information from the primary structure to the dual structure and *vice versa*. The gradient operator of the scalar potential $\nabla\phi$ is the restriction of the classical gradient to its only component on the segment Γ, $\nabla\phi = (\nabla^e\phi \cdot \mathbf{t})\, \nabla^e$ where ∇^e is the gradient vector of space. The primal curl $\nabla \times \boldsymbol{v}$ is defined as the circulation of the vector $\boldsymbol{v}$ on the contour Γ^*, it is carried by the unit vector $\mathbf{n}$. The discrete divergence $\nabla \cdot \boldsymbol{v}$ corresponds to the sum of the fluxes coming from the segments associated to the same vertex a. Finally, the dual curl $\nabla \otimes \boldsymbol{\psi}$ is set by the circulation of the vector $\boldsymbol{\psi}$ on the contour Δ and the result is assigned to the oriented primal contour Γ. The symbol $\otimes$ usually used in mechanics to denote the tensor product of two vectors is adopted because it complements in a harmonious way the concept of rotation of a pseudo-vector in classical mechanics. Since tensors do not exist in discrete mechanics, any confusion is avoided. Remarkable properties mimic those of the continuous medium:

$$\nabla \cdot (\nabla \otimes \boldsymbol{\psi}) = 0; \qquad \nabla \times (\nabla\phi) = 0, \tag{1}$$

since $\nabla \cdot \boldsymbol{v}$ is a scalar and $\nabla \times \boldsymbol{v}$ is a primal curl, the composition of operators provides the following identities:

$$\nabla \cdot (\nabla \otimes (\nabla \times \boldsymbol{v})) = 0; \qquad \nabla \times (\nabla\,(\nabla \cdot \boldsymbol{v})) = 0. \tag{2}$$

These properties are always verified whatever the geometrical structure of the physical domain tessellated by the primary and dual structures; the flat surfaces formed can have any number of sides and the volumes are any polyhedra.

Maxwell's idea leads to a very important result; the direct and induced currents are both carried by the same Γ segment, so they can add up for variable currents or flow without interacting in direct current. The representation of a vector by its three components in a global reference

frame is replaced, in discrete mechanics, by vectors linked to a single direction, that of $\mathbf{t}$. The physical modeling of all direct and induced phenomena is thus to a single direction of space. The consideration of the two-dimensional or three-dimensional space is realized from cause to effect, by the vertices common to two segments. The change of reference frame from $\mathbb{R}$ to a distant reference frame $\mathbb{R}'$ can only be realized under restrictive conditions; in the theory of relativity this condition supposes that the celerity of light c_0 is constant on its whole path. In the present case, the celerity is fixed at the vertices of the primary structures and can be variable from one vertex to another and depend on other quantities, temperature for example.

2.2 Equivalence of conservation of acceleration and energy

The modeling that leads to a unique law of motion for all wave propagation phenomena, including mechanics, requires a return to the Weak Equivalence Principle (WEP) to modify its interpretation. Originally, this principle gives mass a privileged status, the equivalence between inertial and gravitational effects is granted to mass, "inert mass = gravitational mass". However, this principle only reflects the dynamic effects, two bodies of different nature fall with the same velocity and acceleration. Newton's second law confirms Galileo's point of view, $m\,\boldsymbol{\gamma} = \mathbf{F}$ with $\mathbf{F} = m\,\mathbf{g}$. The mass m is the same and yet it is not removed from this relation. Special relativity will take back this notion of momentum $\mathbf{q} = m\,\boldsymbol{v}$. Even more surprisingly, the principle of equivalence between mass and energy will not allow to remove mass from the laws of mechanics. The postulate of discrete mechanics is to discard this notion of mass and to reformulate the fundamental law of dynamics in the form :

$$\boldsymbol{\gamma} = \boldsymbol{h}. \tag{3}$$

The intrinsic acceleration $\boldsymbol{\gamma}$ of a particle or a material medium is equal to the sum $\boldsymbol{h}$ of all the accelerations applied to it. This is a local law and a law of conservation of total energy. Indeed the integration over the length dh of the segment Γ of the acceleration is an energy per unit mass. In general, a vector can always be decomposed as a sum of a gradient of a scalar potential and a dual curl of a vector potential, it is a Helmholtz-Hodge decomposition. This decomposition is not unique *a priori*, it is only defined to within one $\boldsymbol{\mathcal{H}}$ field.

$$\boldsymbol{\gamma} = -\nabla\phi + \nabla \otimes \boldsymbol{\psi} + \boldsymbol{\mathcal{H}}, \tag{4}$$

where $\boldsymbol{\mathcal{H}}$ harmonic term, to divergence-free and curl-free.

If the scalar potential can be defined by a divergence of the velocity $\phi = \nabla \cdot \boldsymbol{v}$ and the vector potential by its curl, $\boldsymbol{\psi} = \nabla \times \boldsymbol{v}$, then the harmonic term is eliminated. The demonstration [14] shows indeed that fields with constant divergence or constant curl are discarded from the modeling of the intrinsic acceleration. They are related to uniform expansion and rotation motions with constant velocities. For example, the expansion of the Universe at constant velocity has no effect on the acceleration of a medium on a Γ segment. It follows that the acceleration, an absolute quantity, decomposes in the form $\boldsymbol{\gamma} = -\nabla\phi + \nabla \otimes \boldsymbol{\psi}$. The conservation of the total energy is then written:

$$\int_\Gamma \boldsymbol{\gamma}_\phi \cdot \mathbf{t}\, dl = -\int_\Gamma \nabla\phi \cdot \mathbf{t}\, dl + \int_\Gamma \nabla \otimes \boldsymbol{\psi} \cdot \mathbf{t}\, dl, \tag{5}$$

where the first integral on the right side is the expansion energy and the second the rotation energy. The two accelerations $\nabla\phi$ and $\nabla \otimes \boldsymbol{\psi}$ are the only two mechanical effects to take into account. There are however other effects linked to gravitational, capillary, electromagnetic accelerations, etc.

The law of discrete motion describes the evolution of a system only between the times t^o and $t = t^o + dt$. It is therefore essential to define retarded potentials ϕ^o and $\boldsymbol{\psi}^o$ similar to those of electromagnetism [15]:

$$\phi^o = -\int_0^{t^o} c_l^2 \, \nabla \cdot \boldsymbol{v} \, d\tau, \qquad \boldsymbol{\psi}^o = -\int_0^{t^o} c_t^2 \, \nabla \times \boldsymbol{v} \, d\tau. \tag{6}$$

The law of motion is thus a continuous memory model, only the acceleration is absolute and the other current quantities are defined according to their value at time t^o, the velocity $\boldsymbol{v} = \boldsymbol{v}^o + \boldsymbol{\gamma} \, dt$, the displacement $\boldsymbol{u} = \boldsymbol{u}^o + \boldsymbol{v} \, dt$, the scalar potential $\phi = \phi^o + d\,\phi$, the vector potential $\boldsymbol{\psi} = \boldsymbol{\psi}^o + d\boldsymbol{\psi}$, etc.

2.3 Discrete law of motion

The modeling of the compressive and rotational acceleration increments is done on the basis of simple experiments where the compressive energy is expressed from the divergence of the velocity $d\phi = -dt \, c_l^2 \, \nabla \cdot \boldsymbol{v}$ where c_l is the longitudinal celerity which can also be written from the isentropic compressibility coefficient χ_S. At the same time, the rotational energy is reflected by the primal curl and transverse celerity $d\boldsymbol{\psi} = -dt \, c_t \, \nabla \times \boldsymbol{v}$. The law of discrete motion then becomes:

$$\frac{\partial \boldsymbol{v}}{\partial t} = -\nabla \left(\phi^o + \frac{1}{2} \, |\boldsymbol{v}|^2 - c_l^2 \, dt \, \nabla \cdot \boldsymbol{v} \right) + \nabla \otimes \left(\boldsymbol{\psi}^o + \frac{1}{2} \, |\boldsymbol{v}|^2 \, \mathbf{n} - c_t^2 \, dt \, \nabla \times \boldsymbol{v} \right) + \boldsymbol{h}_s, \tag{7}$$

where the material derivative is written as a Helmholtz-Hodge decomposition [16]:

$$\boldsymbol{\gamma} = \frac{d\boldsymbol{v}}{dt} \equiv \frac{\partial \boldsymbol{v}}{\partial t} + \nabla \phi_i - \nabla^d \times \boldsymbol{\psi}_i = \frac{\partial \boldsymbol{v}}{\partial t} + \boldsymbol{\kappa}_i. \tag{8}$$

The vector κ_i represents the curvature of the inertial potential $\phi_i = |\boldsymbol{v}|^2/2$. The two vector components are also expressed on the segment Γ and can be added or cancelled according to the problem. The law of discrete motion (7) allows to predict the solution of the current velocity $\boldsymbol{v}$ from its value at time t^o. The divergence and primary rotation of the velocity difference, $(\boldsymbol{v} - \boldsymbol{v}^o)$ allows the potentials to be updated from the retarded potentials :

$$\text{updates} \begin{cases} \alpha_l \, \phi^o - c_l^2 \, dt \, \nabla \cdot (\boldsymbol{v} - \boldsymbol{v}^o) \longmapsto \phi^o; \\ \\ \alpha_t \, \boldsymbol{\psi}^o - c_t^2 \, dt \, \nabla \times (\boldsymbol{v} - \boldsymbol{v}^o) \longmapsto \boldsymbol{\psi}^o. \end{cases} \tag{9}$$

The quantities α_l and α_t are respectively the attenuation factors of longitudinal and transverse waves. When $\alpha = 1$ the corresponding energy is fully conserved and when $\alpha = 0$ the waves are fully dissipated; this is the case for a Newtonian fluid where shear leads to the dissipation of energy in the form of heat. The equation of motion being a law of conservation of total energy, the dissipated energy must be compensated in the equation, this is the role of the retarded potentials ϕ^o and $\boldsymbol{\psi}^o$. The symbol $\longmapsto$ corresponds to the actualization of these.

It is possible to group the potentials with the inertia term to obtain the Bernoulli potentials, $\phi_B^o = \phi^o + |\boldsymbol{v}|^2/2$ and $\boldsymbol{\psi}_B^o = \boldsymbol{\psi}^o + |\boldsymbol{v}|^2/2$. The equation of motion then becomes

$$\frac{\partial \boldsymbol{v}}{\partial t} = -\nabla \left(\phi_B^o - c_l^2 \, dt \, \nabla \cdot \boldsymbol{v} \right) + \nabla^d \times \left(\boldsymbol{\psi}_B^o - c_t^2 \, dt \, \nabla \times \boldsymbol{v} \right). \tag{10}$$

The form (10) shows two Lagrangians, the first for the expansion terms and the second for the rotation. Each of them is composed of a potential energy, ϕ_B^o or $\boldsymbol{\psi}_B^o$ and a kinetic energy term expressed as a function of the velocity $\boldsymbol{v}$. This form is the condition for the application of

Noether's theorem [17] which theoretically states that when a law can be written in the form of a Lagrangian or a Hamiltonian, then it has symmetry and invariance properties. Each of them is related to the conservation of a certain physical quantity. In this case, the time invariance ensures the conservation of the total energy, the first term of the second member conserves the compression energy and the last term ensures the conservation of the angular acceleration.

The law of motion (7) has other properties due to its structure. One of them shows that it is relativistic, it integrates the concepts and results of special relativity and general relativity. Consider the displacement $\boldsymbol{u} = \boldsymbol{u}^o + \boldsymbol{v}\, dt$ and suppose that the velocities c_l and c_t are equal, the classical relation of differential calculus :

$$\nabla^2 \boldsymbol{u} = \nabla \left(\nabla \cdot \boldsymbol{u} \right) - \nabla \times \nabla \times \boldsymbol{u}, \tag{11}$$

allows then to transform the discrete equation of motion into a nonlinear wave equation:

$$\frac{1}{c^2} \frac{d^2 \boldsymbol{u}}{dt^2} - \nabla^2 \boldsymbol{u} = -\nabla \phi^o + \nabla \times \boldsymbol{\psi}^o, \tag{12}$$

where the first member can be written as a Dalembertian when inertia is neglected:

$$\Box\, \boldsymbol{u} \equiv \frac{1}{c^2} \frac{\partial^2 \boldsymbol{u}}{\partial t^2} - \nabla^2 \boldsymbol{u}, \tag{13}$$

but here the equation is non-linear and, by grouping the retarded terms, the equation becomes:

$$\frac{1}{c^2} \frac{d^2 \boldsymbol{u}}{dt^2} - \nabla^2 \left(\boldsymbol{u} - \boldsymbol{u}^o \right) = 0. \tag{14}$$

It is then easy to show that a wave equation is relativistic. It is enough to apply the Lorentz transformation of the reference frame $\mathbb{R}$ to show an identical equation corresponding to the reference frame $\mathbb{R}'$. It thus remains invariant with respect to the considered transformation. This invariance is not incompatible with the invariance resulting from the Galilean transformation related to inertia. On the contrary, it is necessary to (i) ensure the filtering of uniform translational and rotational motions and (ii) describe the blocking of the velocity of a particle in its accelerated motion on a linear trajectory at the celerity of the medium.

The nonlinear wave equation (14) is naturally deduced from Newton's second law. It is not derived from a Lorentz transformation nor from the use of the factor $\gamma = 1/\sqrt{1 - v^2/c^2}$. The approaches of SRT and discrete mechanics are very different even if the results are identical. The discrete model presented here allows to fully recover the solutions of the Navier-Stokes equation for fluids in a wider context describing waves in general (swell, acoustic waves, light).

The boundary conditions associated with the law of motion (7) are directly integrated in the latter in the form of operators, $-\nabla q + \nabla \otimes \boldsymbol{r}$ where q corresponds to a surface flux and $\boldsymbol{r}$ to a shear stress at the walls. These two potentials allow to simulate any kind of boundary condition in a way consistent with the formulation.

3 Concepts of capillary motion

The abandonment of certain concepts of classical mechanics has an impact on the treatment of capillary flows. First of all, the discarding of mass and density has an effect on the quantities used to simulate two-phase flows in the presence of capillary effects. The surface tension γ used classically becomes $\sigma = \gamma/\rho$, named surface tension per unit mass, this one is expressed in $m^3 s^{-2}$. Its product by the curvature κ is an energy per unit mass, the capillary energy $\sigma\, \kappa$ and, like the others, it will be a scalar or vector potential depending on the term in which it appears. The experimental values assigned to γ will also be those used for σ because the pressure itself becomes

$\phi^o = p/\rho$. The density thus disappears from all the adimensional quantities and parameters that usually characterize capillary effects. Moreover, we find the grouping γ/ρ in most of them.

3.1 Capillary motion law

The capillary potentials noted $\phi_c = \sigma\,\kappa$ and $\boldsymbol{\psi}_c = \sigma\,\kappa\,\mathbf{n}$ are also energies per unit mass and the quantity $c_c = \sqrt{\sigma\,\kappa}$ is the capillary wave celerity which can be interpreted as the capillary velocity $\boldsymbol{v}_c$. The capillary acceleration $\boldsymbol{\gamma}_c$ can also be modeled by stating that it is equal to the sum of the accelerations imposed on it. This leads to an equation of capillary motion:

$$\left\{\begin{array}{l} \boldsymbol{\gamma}_c = \dfrac{d\boldsymbol{v}_c}{dt} = -\nabla\left(\phi_c^o - \sigma_l\,\kappa_l\,dt\,\nabla\cdot\boldsymbol{v}_c\right) + \nabla\otimes\left(\boldsymbol{\psi}_c^o - \sigma_t\,\kappa_t\,dt\,\nabla\times\boldsymbol{v}_c\right), \\ \\ \phi_c^o - \sigma_l\,\kappa_l\,dt\,\nabla\cdot\left(\boldsymbol{v}_c - \boldsymbol{v}^o\right) \longmapsto \phi_c^o, \\ \\ \boldsymbol{\psi}_c^o - \sigma_t\,\kappa_t\,dt\,\nabla\times\left(\boldsymbol{v}_c - \boldsymbol{v}^o\right) \longmapsto \boldsymbol{\psi}_c^o. \end{array}\right. \tag{15}$$

It has exactly the same structure as the equation of motion. It is of course free of the compression and rotation terms of the general law. It applies to the case of a Σ surface, for example a liquid sheet having a surface tension σ and a local curvature κ, these two quantities being defined for the longitudinal and transverse waves. This equation (15) allows to calculate the evolution of the velocity over time of a surface subjected to motions generated by variations of surface tension and curvature. It is possible to represent the stationary solution of a catenoid surface, a minimal surface constrained by two circles, from any initial solution.

Since capillary effects are sometimes modified by gravity, it is desirable to rewrite the equation of fluid dynamics subjected to this acceleration; this should of course lead to the stationary solutions of fluid statics, compressible or not. Its modeling is similar to the general law of motion where the gravitational energy is equal to $g\,r$ where r is a fixed coordinate with respect to a reference frame; it reads:

$$\left\{\begin{array}{l} \boldsymbol{\gamma}_g = \dfrac{d\boldsymbol{v}_g}{dt} = -\nabla\left(\phi_g^o - \mathbf{g}\cdot\mathbf{t}\,r\,dt\,\nabla\cdot\boldsymbol{v}_g\right) + \nabla\otimes\left(\boldsymbol{\psi}_g^o - \mathbf{g}\cdot\mathbf{n}\,r\,dt\,\nabla\times\boldsymbol{v}_g\right), \\ \\ \phi_g^o - \mathbf{g}\cdot\mathbf{t}\,r\,dt\,\nabla\cdot\left(\boldsymbol{v}_g - \boldsymbol{v}^o\right) \longmapsto \phi_g^o, \\ \\ \boldsymbol{\psi}_g^o - \mathbf{g}\cdot\mathbf{n}\,r\,dt\,\nabla\times\left(\boldsymbol{v}_g - \boldsymbol{v}^o\right) \longmapsto \boldsymbol{\psi}_g^o, \end{array}\right. \tag{16}$$

where $\nabla(\mathbf{g}\cdot\mathbf{t}\,r) = (\mathbf{g}\cdot\mathbf{t})\,\mathbf{t}$ corresponds to the projection of the gravity vector onto Γ; the other component projects in the same way onto Δ.

The equation of motion of capillary effects (15) and that of fluid statics (16) can be combined in the general law of motion (7). The new scalar potential is then written $\phi^o + \phi_c + \phi_g \longmapsto \phi^o$ and similarly for $\boldsymbol{\psi}^o$ and for the global velocity $\boldsymbol{v}$. Since all potential source terms are written in the form of a Helmholtz-Hodge decomposition, the form of the general equation remains unchanged:

$$\left\{\begin{array}{l} \dfrac{d\boldsymbol{v}}{dt} = -\nabla\left(\phi^o - \left(c_l^2 + \sigma_l\,\kappa_l + g\,r\right)\,dt\,\nabla\cdot\boldsymbol{v}\right) + \nabla\otimes\left(\boldsymbol{\psi}^o - \left(\dfrac{\nu}{dt} + \sigma_t\,\kappa_t + g\,r\right)dt\,\nabla\times\boldsymbol{v}\right), \\ \\ \phi^o - \left(c_l^2 + \sigma_l\,\kappa_l + g\,r\right)\,dt\,\nabla\cdot\left(\boldsymbol{v} - \boldsymbol{v}^o\right) \longmapsto \phi^o, \\ \\ \boldsymbol{\psi}^o - \left(\nu/dt + \sigma_t\,\kappa_t + g\,r\right)\,dt\,\nabla\times\left(\boldsymbol{v} - \boldsymbol{v}^o\right) \longmapsto \boldsymbol{\psi}^o, \end{array}\right. \tag{17}$$

where ν, the kinematic viscosity replaces the generic term $dt\,c_t^2$ for viscous fluids with large time constants where these effects are always present.

The groupings $dt\,\nabla\cdot\boldsymbol{v}$ and $dt\,\nabla\times\boldsymbol{v}$ are dimensionless; the explicit presence of the time lapse dt between two mechanical equilibria has a very special meaning that does not exist for the Navier-Stokes equations. For small time constants, the exchanges between the potential energy, fixed by ϕ^o or $\boldsymbol{\psi}^o$, and the kinetic energy, associated to $\nabla\cdot\boldsymbol{v}$ or $\nabla\times\boldsymbol{v}$, are important. For large time constants, the products $dt\,\nabla\cdot\boldsymbol{v}$ and $dt\,\nabla\times\boldsymbol{v}$ remain of the same order of magnitude as the other terms in the equation, but $\nabla\cdot\boldsymbol{v}$ and $\nabla\times\boldsymbol{v}$ tend to zero or to constants. The acceleration $\boldsymbol{\gamma}$ becomes zero when the motion is stationary and the two terms $-\nabla\phi+\nabla\otimes\boldsymbol{\psi}$ define the new mechanical balance.

Let us now consider the respective roles of each of the expansion c_l^2, capillary $\sigma\,\kappa_l$ and gravitational $g\,r$ and those of the vector potentials. Let us fix for that orders of magnitude compatible with the capillary movements in a viscous liquid subjected to gravity, $\sigma_l=10^{-4}\,m^3s^{-2}$, $\kappa=1/R=10^3\,m$, $c_l=10^3\,ms^{-1}$, $g=10\,ms^{-2}$ and $\nu=10^{-6}\,m^2s^{-1}$. Let us summarize the different potential groupings by considering that is of the same order of magnitude as the ratio of a dimension by a celerity $dt=1/(\kappa\,\sqrt{\sigma\,\kappa})\approx 10^{-2}\,s$:

$$\frac{\sigma_l\,\kappa_l}{c_l^2}=10^{-7};\quad \frac{g}{\kappa_l\,c_l^2}=10^{-8};\quad \frac{\nu}{dt\,\sigma_t\,\kappa_t}=10^{-3};\quad \frac{\nu\,\kappa_t}{dt\,g}=10^{-2};\quad \frac{g}{\sigma_l\,\kappa_l^2}=10^{-1};\quad \frac{g}{\sigma_t\,\kappa_t^2}=10^{-1}. \tag{18}$$

The groupings $(g/\kappa_l)/c_l^2$ and $(g/\kappa_l)/c_l^2$ show that the effects due to capillarity or gravity are respectively seven and eight orders of magnitude smaller than those related to the compressibility of the liquid and can therefore be neglected. The same is not true for rotation where the quantities related to viscosity, capillarity and gravity form sets closer to unity. Of course, this exercise must be reproduced according to the problem at hand, but it shows the interest of such a global approach to define adimensional parameters whose quantities are all expressed exclusively by a length and a time. Contrary to the classical adimensional analysis, the adimensional parameters are not defined by orders of magnitude of the velocity, the density or a characteristic length whose choices can be discussed.

There are many dimensionless parameters related to capillary effects, for example the Weber number $We=\rho\,v^2\,L/\gamma$, the capillary number, $Ca=v\,\mu/\gamma$, the Froude number, $Fr=v/\sqrt{g\,L}$, the Laplace number, $La=\gamma\,L\,\rho/\mu^2$, the Ohnessorge number, $Oh=\mu/\sqrt{\rho\,\gamma\,L}$ or the Bond number, $Bo=\rho\,g\,L^2/\gamma$, to name a few. They are not all independent and can be combined to form others. There are of course a few in the list (18) including the Bond number, $Bo=g/(\sigma\,\kappa^2)$ as the ratio of gravitational energy to capillary energy.

The most notable difference is the presence of the ratio ν/dt, representing the energy per unit mass of viscous friction. The true notion of viscosity is complex. The fact that it is measured by steady-state experiments does not give it the desired general character. Moreover, Newton's shear law $\tau=\mu\,dv/dy$ induces a paradox in the Navier-Stokes equation at small time constants when a sudden shear is imposed on a fluid at a given time. The perturbation is theoretically instantaneously felt at infinity and the initial stress is itself infinite. The hyperbolic character of the discrete equation (7) overcomes this drawback.

3.2 Modelization of partial wetting

This section presents how this formulation (17) is likely to take into account the notion of partial wetting between a surface and a liquid. Many models are based on the static contact angle which is sometimes extended in dynamics. In fact these approaches are set aside in the framework of the presented formulation. Indeed, it is very difficult to predict what happens to the contact angle when capillary effects are intermingled with those due to viscosity, inertia, gravity, etc. The principle adopted here is different, the modeling of all the effects is carried out in a coherent way and, if the equation of motion is representative of the phenomena, it is then used without trying to analyze each phenomenon separately. Indeed, the instantaneous

local angle is a complex function of the terms of the equation of motion. Young-Dupré's law, $\cos\theta = (\gamma_{SV} - \gamma_{SL})/\gamma_{LV}$ where γ_{SV} is the surface tension between the solid and the vapor, γ_{SL}, the surface tension between solid and liquid, and γ_{LV}, the surface tension between liquid and vapor, provides an equilibrium relation but does not allow to describe the dynamics of the interface formation; moreover, the tension γ_{SV} is difficult to quantify.

In the case of capillary flows without connection to a triple line, the equation (17) allows to find the classical results [18]. For example the solution of the Laplace problem of a drop of average curvature $\kappa_l + \kappa_t = 2/R$, $p/\rho = \phi_c = 2\sigma\kappa$ is obtained exactly (to machine precision). The dynamic case of an ellipse oscillating around a mean position is solved precisely (to second order) from an Arbitrary Lagrangian Eulerian method to obtain the theoretical oscillation frequency equal to $f = m\,(m^2-1)\,\sigma\,R^3$ [19]. Many other cases of two-phase flows show the validity of the proposed approach. In all cases, the static or dynamic solution of the problem does not depend on the density, which is integrated both in the capillary potential $\phi = p/\rho$ and in the surface tension per unit mass, $\sigma = \gamma/\rho$. Moreover, the notion of average curvature is replaced by the two curvatures κ_l and κ_t which form an orthogonal reference of the tangent plane of the interface.

Let us now introduce the concept of partial wetting in the discrete model associated with the equation of motion (17). In fact this equation remains unchanged, it is only necessary to introduce an information on the desired contact angle at the capillary equilibrium. Indeed this notion of contact angle defined as a property of a surface-liquid couple is only realized in one case, the one where all the other effects, inertial, viscous, gravitational, compressible are negligible before the surface tension. In this situation, the shape of the surface of the liquid in contact with the solid is a portion of a sphere and this is also true for more complex situations, for example a lens of a liquid in equilibrium between two other liquids. In other cases, the contact angle is not respected either in static or in dynamic. Simplistic laws or reasoning neglecting other effects cannot represent the reality of such complex phenomena. The point of view adopted is based on an equation of motion which already describes correctly all physical phenomena. Only a global model allows to assemble the contributions linked to each of them in an essentially macroscopic vision; the effects at very small scale will not be taken into account.

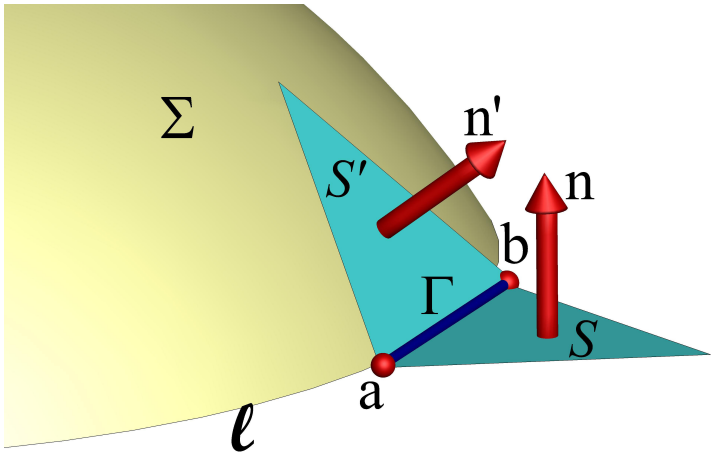

Figure 2. Drop of surface Σ placed on a solid plane; two facets $\mathcal{S}$ and $\mathcal{S}'$, associated to the common segment Γ of the triple line $\boldsymbol{\ell}$, respectively of normals $\mathbf{n}$ and $\mathbf{n}'$ define the dihedral angle additional to the contact angle θ_c.

Let us consider the Σ interface of the Figure 2, for example that of a drop of liquid on a solid surface partially wetted by it. The liquid is in contact with the solid on a surface delimited by the triple line $\boldsymbol{\ell}$. This line is formed by the line segments Γ whose ends a and b are oriented

by the unit vector t. The interface Σ and the solid surface are tessellated by surfaces such as $\mathcal{S}$ and $\mathcal{S}'$ which have, in this case, the triple line segment $\boldsymbol{\ell}$ in common. The normals to these two facets are called $\mathbf{n}$ and $\mathbf{n}'$. As in the general case of capillary flows, the capillary accelerations are written as a Helmholtz-Hodge decomposition:

$$-\nabla\left(\sigma_l\,\kappa_l\right)+\nabla\otimes\left(\sigma_t\,\kappa_t\,\mathbf{n}\right). \tag{19}$$

The first term is evaluated from the quantity $\sigma_l\kappa_l$ defined at the vertices of the segment Γ and the second term is the dual curl related to the circumferences of the two primary facets. The center of $\mathcal{S}$ located at c is the intersection of the perpendicular bisectors of the triangle sides. In general, the curvature is related to the divergence of the normals on the interface. The use of the dihedral angle is particularly well suited in this context because the normals $\mathbf{n}$ and $\mathbf{n}'$ are defined exactly from the coordinates of the vertices of each triangle. The dihedral angle θ_d is defined by the two normals $\mathbf{n}$ and $\mathbf{n}'$ such that $\cos\theta_d=\mathbf{n}\cdot\mathbf{n}'$, it is the supplementary angle of the contact angle $\theta_c=\pi-\theta_d$. It is possible to define a contact curvature named $\boldsymbol{\kappa_\ell}$ by the outer product of the normals $\mathbf{n}$ and $\mathbf{n}'$ attributed to the segment Γ oriented by $\mathbf{t}$ is obtained by considering a distance, the one joining the circumferences of the two triangles:

$$\boldsymbol{\kappa_\ell}=\frac{\mathbf{n}\wedge\mathbf{n}'}{\|c\,c'\|}, \tag{20}$$

where $\|c\,c'\|$ is the norm of the distance between the circumcenters of the two facets $\mathcal{S}$ and $\mathcal{S}'$. The symbol $\wedge$ defines the exterior product which corresponds to the component normal to the considered surface, of the vector product noted with the symbol $\times$. In the absence of a global reference frame, the outer product is particularly adapted to the writing of the laws of discrete mechanics. Unlike the vector product which is defined for a three dimensional space, the outer product is defined for any n dimensional vector space.

The quantity $\boldsymbol{\kappa_\ell}$ can also be named curvature of the triple line, it characterizes indeed, with the surface tension $\sigma_{\boldsymbol{\ell}}$, the acceleration due to the partial wetting. Thus the transverse curvature κ_t applied to all the facets of the interface Σ will take, on the triple line, the value $\boldsymbol{\kappa_\ell}$. The global formulation then remains unchanged, only the transverse curvatures will be kept equal to $\boldsymbol{\kappa_\ell}$ during a simulation. The link between the experimentally evaluated contact angle θ_c and the curvature of the triple line is direct. In the case of a drop of radius R, the contact curvature, at capillary equilibrium, is equal to $\boldsymbol{\kappa_\ell}=2/R$. From a practical point of view, the calculation of the curvature of a tessellated interface by triangles computed from the formula (20) provides a good approximation of the theoretical value.

Let us consider the case of an evolution in time of the shape of an interface Σ subjected to various accelerations due to the effects of gravity, viscosity, inertia, etc. The value of the contact curvature $\boldsymbol{\kappa_\ell}$, once defined as a function of the contact angle θ_c, is maintained over time on the triple line of the equation (17) but not, for all that, the value of the normals $\mathbf{n}$ and $\mathbf{n}'$, and, in general, the shape of the interface is not fixed. It appears only as a constraint to be satisfied, in the absence of these actions, to reach the capillary equilibrium. For example, let us consider a drop that spreads on a partially wetting surface characterized by a contact angle θ_c in the presence of a gravitational field. In this case, the contact angle at capillary equilibrium is not θ_c, it results from an equilibrium including the gravitational acceleration. The velocity at equilibrium is strictly zero.

Thus, mechanical equilibrium, whether static or dynamic, cannot be defined by a single parameter such as the contact angle (static or dynamic). The physics of these phenomena

is complex but it is inscribed in the law of motion (17). Its resolution is essentially computational because it is non-linear and the interactions between the different phenomena it models are particularly intertwined. From an initial condition fixed by the shape of the interface Σ and the source terms at time t^o, the solution of the equation allows to predict the solution on the velocity $\boldsymbol{v}$ at the current time $t^o + dt$; the potentials ϕ^o and $\boldsymbol{\psi}^o$ are updated and the new shape of the interface is computed using this velocity. If a static equilibrium is possible, the velocity tends to zero, but all terms that no longer depend on it must still strictly satisfy the equation. A conservation equation must always be satisfied, even when the velocity tends to zero; no residual velocities must remain, e.g. the unphysical stray currents frequently reported in the literature.

4 Analyses of some capillary flows

4.1 Spreading and equilibrium of a drop

The dihedral angle and the contact curvature $\boldsymbol{\kappa_\ell}$ are implemented in the case of the spreading of a drop of liquid partially wetting the substrate on which it is placed under the assumption that the initial equilibrium is not assured. In this situation, the liquid spreads or retracts in order to finally satisfy the theoretical contact angle θ_c between the liquid and the solid surface.

A drop having the shape of a semicircle of radius $R = 0.625\,10^{-3}\,m$ is placed on a plane whose wettability can be modified over time from the contact curvature $\boldsymbol{\kappa_\ell}$. The density of the fluid is equal to $\rho = 1000$ and its viscosity equal to $\mu = 10^{-2}\ kg\ m^{-1}\ s^{-1}$ and the external medium is air. The curvature of the initial semicircle is equal to $\boldsymbol{\kappa_\ell} = 1600$. From the initial time we impose a contact curvature $\boldsymbol{\kappa_\ell} = 750$ to simulate a wetting surface and, from a time equal to $t = 0.2\ s$ we modify this value which is brought to $\boldsymbol{\kappa_\ell} = 2230$ to represent a non wetting surface. The table (1) gives the characteristics of the drop for each step of the simulation.

Curvature	Radius of meniscus	Contact angle	Capillary pressure
$1600\ m^{-1}$	$0.625\ 10^{-3}\ m$	$90°$	$112\ Pa$
$750\ m^{-1}$	$1.333\ 10^{-3}\ m$	$48.2°$	$52.5\ Pa$
$2230\ m^{-1}$	$0.415\ 10^{-3}\ m$	$150°$	$155.04\ Pa$

Table 1. Evolution of a drop on a plane; characteristics of the meniscus for each step of the simulation.

The simulation is performed using equation (17) and maintaining on the contact line the $\boldsymbol{\kappa_\ell}$ curvature in two space dimensions. The computational methodology used is that described previously [18]; the unstructured primal mesh, composed of regular triangles, tessellates the two domains, the initially hemispherical drop and the complement of the rectangular cavity shown in Figure 3. The interface tracking method is similar to Front-Tracking [19], the triple line corresponds to a line of the mesh and this and all vertices of the primal mesh are advected by the velocity field $\boldsymbol{v}$. The boundary condition on the horizontal plane corresponds to a non-slip except on the segment where the junction point of the Σ interface and the plane is located, i.e. on the triple line. Indeed the condition

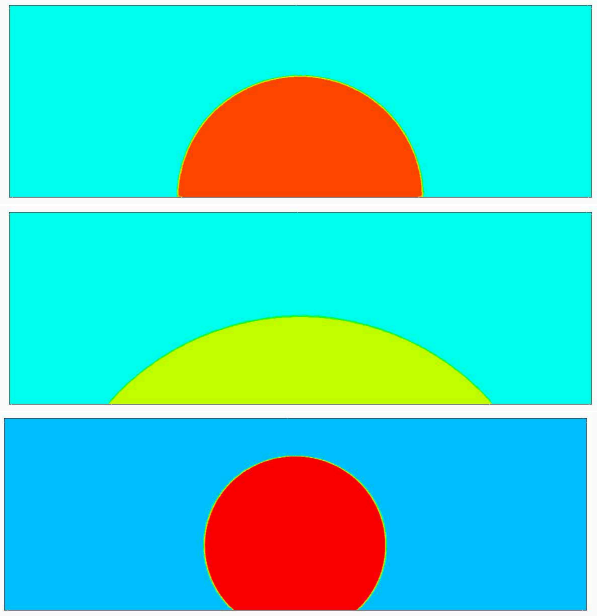

Figure 3. Simulation of the evolution of a drop on a flat surface as a function of the curvature applied to the wall. On top a drop in equilibrium where the curvature $\boldsymbol{\kappa_\ell} = 1600$ and the contact angle $\theta_c = 90°$ are given as initial condition, in the center the curvature $\boldsymbol{\kappa_\ell} = 750$ ($\theta_c = 48.2°$) is imposed on the triple line and at a time of $t = 0.2\ s$ we impose $\boldsymbol{\kappa_\ell} = 2230$ ($\theta_c = 150°$).

of adhesion would lead to a zero velocity of the triple line on the plane which is false. In fact this problem of inadequacy of the boundary condition of the triple line results from the globalization of the velocity field $\boldsymbol{v}$ which contains in fact two components, one at the absence of divergence and the other at the absence of curvature. The triple line must be free to move on a solid surface, which corresponds only to the condition $\boldsymbol{v} \cdot \mathbf{n} = 0$. In the present case, the Γ segment of the plane containing the vertex of the triple line is thus kept sliding, the other segments of the plane ensuring the condition of no sliding.

The Figure 4 shows the shape of the drop in each quasi-stationary state where the velocities are negligible. The pressure inside the drop is then almost constant. As soon as the $\boldsymbol{\kappa_\ell}$ is changed, the forces exerted on the triple line act to bring the drop back to an equilibrium state where the $\boldsymbol{\kappa_\ell}$ contact curvature is satisfied. Over time, the velocities evolve in the domain first to spread the drop to a contact angle of 48.2° and then to contract the interface to a contact angle of 150°.

Figure 4 shows the evolution of the scalar potential difference ϕ^o between the interior and exterior of the drop as a function of time; in each of the two domains, liquid and gas, the potential is uniform and the velocity and inertia become very low very quickly after a phase of rapid evolution of the interface. The results obtained from the computationally simulated data are consistent with the theoretical predictions. In this example, the interfaces correspond exactly to a constant curvature, for example of spheres (or cylinders in two spatial dimensions). This is of course no longer the case when gravity is taken into account, the interfaces between air and liquid are no longer spheres and the contact angle θ_c is no longer respected; the real angle of static equilibrium is a complex function of the capillary potentials ϕ_c and that of gravity ϕ_g.

This first characteristic example of capillary flows translates the principle of the use of the law of discrete motion (17), only the physical parameters are adjusted according

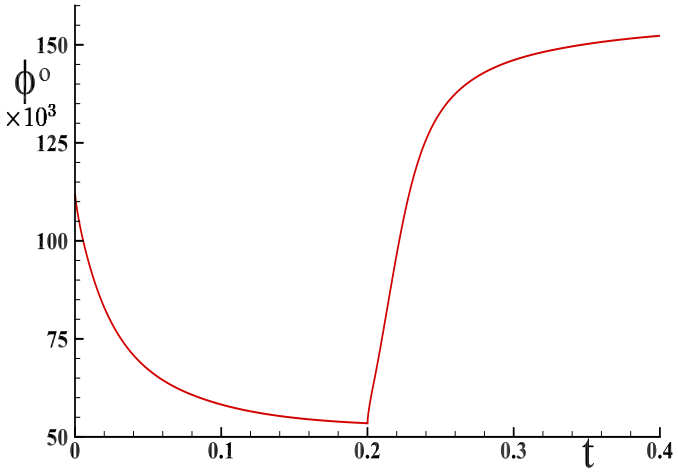

Figure 4. Evolution of the average energy difference per unit mass (in $m^2\ s^{-2}$) between the drop and the exterior on a flat surface as a function of time with respect to curvature variations at the wall. The asymptotes of the capillary potential lie at $\phi^o = 52.5\,10^{-3}$ and $\phi^o = 155\,10^{-3}$.

to the considered problem but the form of the equation itself remains unchanged. For example, when the incompressibility of the flow is required, it is not the divergence term of the velocity $\nabla \cdot \boldsymbol{v} = 0$ that is removed from the equation but the value of the celerity is increased. Similarly, when a contact angle θ_c between a liquid and a solid is desired, it is not maintained explicitly and will not be assured if there are other constraints.

4.2 Capillary rise between two vertical planes

The problem of the capillary rise of a liquid in a pipe is particularly emblematic of capillary flows. The phenomenon is simple to describe, the liquid rises in the pipe of radius r and partially wets the walls of the pipe, eventually stabilizing at a height h fixed by Jurin's law. This law is established on the basis of an equilibrium taking into account the weight of the liquid column of density ρ, $F_p = \pi\, r^2\, h\, \rho\, g$ and that of the capillary force given by $F_c = 2\,\pi r\,\gamma\,\cos\theta_c$ où θ_c where θ_c is the contact angle and γ is the surface tension; an energy balance per unit mass instead of a force balance leads to the same conclusion:

$$h = \frac{2\,\gamma\,\cos\theta_c}{\rho\, g\, r} = \frac{2\,\gamma}{\rho\, g\, R} = \frac{\sigma\,\kappa}{g}, \tag{21}$$

where $\sigma = \gamma/\rho$; as for the other laws related to capillary effects it is the surface tension that appears naturally.

The case proposed here is that of a liquid of density $\rho_2 = 1000$ and viscosity μ_2 in capillary ascent between two planes whose contact angle θ_c with the vertical walls corresponds to $\cos\theta_c = 0.9$; the average curvature of the interface is thus equal to $\boldsymbol{\kappa_\ell} = 1800$. The medium above the liquid has density $\rho_1 = 1$ and viscosity μ_1. The surface tension $\gamma = 0.055555$ is constant. The domain is planar, rectangular, of dimensions $[-0.0005, 0.0005] \times [0, 0.01]$ and the base of the interface between the two fluids in static equilibrium is placed at $y = 0.005$. The value of gravity in the downward vertical direction is chosen to obtain an upward or downward shift of the interface or static equilibrium. The primal topology corresponds to a mesh based on regular triangles bounding the two

media by a mesh line. The boundary conditions are associated with vertical solid walls ($\boldsymbol{v} = 0$) and horizontal free walls where the pressure is constant and equal to $p = 0$. The pressure difference on both sides of the interface resulting from the simulations must be equal to $\Delta p = \gamma\,\kappa$ or $\phi = \sigma\,\kappa$ at static equilibrium.

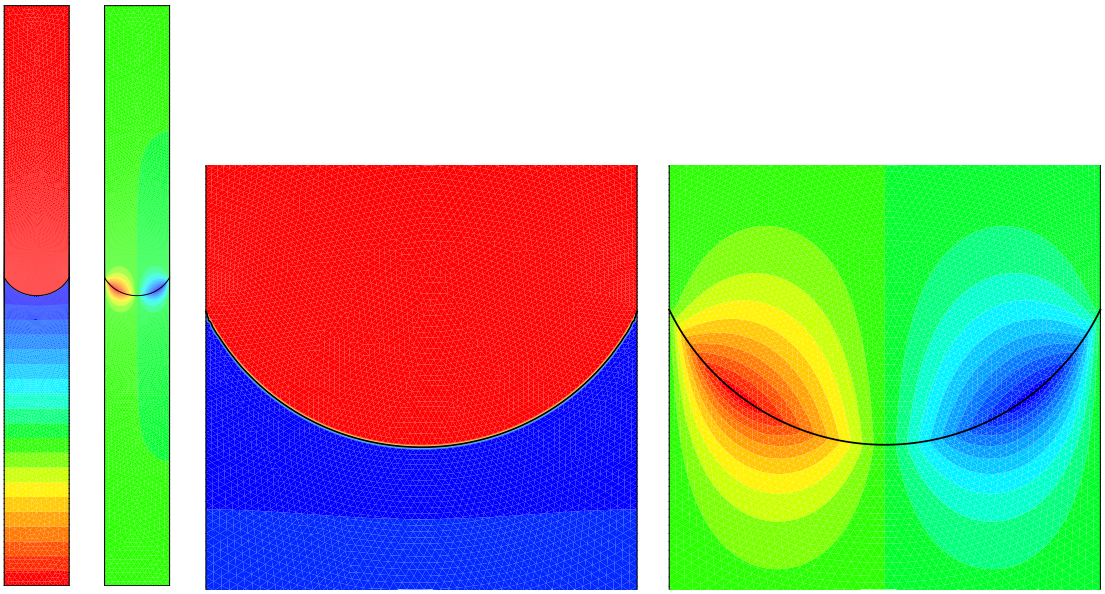

Figure 5. Static mechanical equilibrium defined by the two scalar ϕ^o (left) and vector $\boldsymbol{\psi}^o$ (right) potentials; the two images on the right show the details of these two potentials near the interface.

When gravity is less than the value corresponding to static equilibrium, capillary forces are dominant and the heavier fluid is pulled upward near the walls. These same forces then act to restore a shape close to the circle and a curvature equal to $\boldsymbol{\kappa_\ell} = 1/R$ where R is the radius of curvature. The unsteady vortex motions are induced by all the physical phenomena present in the problem. On the contrary, when gravity is more important, the associated forces pull the interface down until static equilibrium is reached in more or less important times which depend on the exchanges between inertia and viscosity forces. We observe that the boundary conditions of the problem are well satisfied, in particular that the top and bottom of the cavity are at the same pressure and that the pressure jump at the interface corresponds to the exact value $\Delta p = 100$. The value of gravity used for the static situation is equal to $g = 19.636112$. We notice that the height of the meniscus h to be considered to find Jurin's law is not the minimum height of the meniscus on the axis but the average value which is $h = 5.092657\,10^{-3}m$.

Figure 5 shows the result obtained for the static equilibrium; the velocity is zero in the whole domain at the accuracy of the machine and the two potential fields of compression ϕ^o and rotation $\boldsymbol{\psi}^o$ alone define this mechanical equilibrium:

$$-\nabla\phi^o + \nabla \otimes \boldsymbol{\psi}^o = 0. \tag{22}$$

The two scalar and vector potentials integrate, respectively for compression and rotation, the energies accumulated over time by the terms of viscosity, inertia, gravity and capillary effects. The law (22) represents what remains of the equation of motion (17) when the velocity is equal to $\boldsymbol{v} = 0$. Thus the dynamics of the capillary rise leads to a static state which respects Jurin's law; this is what is observed experimentally, the

velocity becomes strictly zero. This result is remarkable from the point of view of mechanical equilibrium in a system where the phenomena are complex and intertwined. From a mathematical point of view, the relation (22) translates the equality of two orthogonal components which are both projected on the same segment Γ and which can thus add up. This simulation carried out from the Navier-Stokes equation, with strictly the same parameters, does not lead at all to the same conclusions; when the velocity is equal to zero in the latter one obtains $\nabla p^o = 0$ or $p^o = 0$, a wrong solution. Since static equilibrium cannot be reached, the velocities predicted by the simulation can never be attenuated and large spurious currents remain near the triple line. This result is one of the paradoxes of the Navier-Stokes equation, which does have the equivalent of the scalar potential, the pressure, but does not have the vector potential that accumulates the shear stress.

Static equilibrium (22) represents a general law satisfied in particular by an elastic solid subjected to compressive and shear stresses but also in the case of a fluid whose velocity physically tends towards zero as in the example treated in this section. Moreover, it is valid in the case of a stationary flow where the velocity field $\boldsymbol{v}$ does not depend on time but remains defined by all effects, viscous, gravitational, inertial, capillary, etc. There are two possibilities, (i) to use only one of the potentials, ϕ^o or $\boldsymbol{\psi}^o$, and obtain a non-zero velocity field $\boldsymbol{v}$, and (ii) to keep both potentials which leads to a zero velocity field. In the first case, the solution is written $(\phi^o, \boldsymbol{v})$ or $(\boldsymbol{\psi}^o, \boldsymbol{v})$ and in the second case, it takes the form $(\phi^o, \boldsymbol{\psi}^o)$; the velocity field is not part of the solution anymore. We show that the knowledge of one of the potentials introduced in the discrete equation of motion leads instantaneously to the velocity field $\boldsymbol{v}$ retained previously. In the case of persistent unsteady solutions, for example for a periodic, chaotic or turbulent flow, the acceleration is non-zero and all the terms of the discrete equation are nested.

5 Conclusions

The modeling of two-phase flows dominated by capillary phenomena requires to retain multiple other physical phenomena related to viscosity, gravity, inertia, etc. It is difficult, if not impossible, to predict the evolution of these flows over time or even the static solutions except in a few canonical examples. The principle adopted in discrete mechanics is to derive an equation of motion as general as possible, likely to represent at least the flows of fluids, the stresses and displacements of solids or the propagations of waves. The law of motion thus established requires a thorough validation that will give it sufficient legitimacy to apprehend other complex situations.

The law of motion, which can already account for two-phase flows in general, is confronted with capillary phenomena related to the triple line. The contact angle is most often the parameter most used to translate the phenomenon of partial wetting between a liquid and a solid in the presence of a gas. This parameter is well measured by different techniques in the case of a static equilibrium. As the spatial scales chosen in the presence of the Earth's gravity are necessarily small, the time constants are small and the static equilibrium is reached very quickly. The application of an essentially static parameter to dynamic flows must be done with some precautions, it is not possible, for example, to impose a contact angle, static or dynamic, explicitly. The notion of contact curvature is more flexible because it does not have to be satisfied formally, it allows to obtain the correct contact angle at static equilibrium without explicitly imposing its value in dynamics. The two examples provided highlight some aspects of its use.

Declaration of competing interest

There are no conflict of interest in this work.

References

[1] P. G. de Gennes, Wetting: statics and dynamics, Rev. Mod. Phys. 57 (1985) 827–863. doi:10.1103/RevModPhys.57.827.

[2] S. Popinet, Numerical models of surface tension, Annual Review of Fluid Mechanics 50 (1) (2018) 49–75. doi:10.1146/annurev-fluid-122316-045034.

[3] R. E. Johnson, R. H. Dettre, D. A. Brandreth, Dynamic contact angles and contact angle hysteresis, Journal of Colloid and Interface Science 62 (2) (1977) 205–212. doi:https://doi.org/10.1016/0021-9797(77)90114-X.

[4] J. Göhl, A. Mark, S. Sasic, F. Edelvik, An immersed boundary based dynamic contact angle framework for handling complex surfaces of mixed wettabilities, International Journal of Multiphase Flow 109 (2018) 164–177. doi:https://doi.org/10.1016/j.ijmultiphaseflow.2018.08.001.

[5] Z. Zhang, X. Xu, Effective boundary conditions for dynamic contact angle hysteresis on chemically inhomogeneous surfaces, Journal of Fluid Mechanics 935 (2022). doi:10.1017/jfm.2022.33.

[6] R. Prud'homme, Écoulements et réactions chimiques, 1. Équations générales, Vol. 24, Hermès-Lavoisier, Cachan, 2012.

[7] H. Gouin, P. Seppecher, Temperature profile in a liquid-vapor interface near the critical point, Proceedings of the Royal Society of London. Series A 473 (2017) 20170229. doi:10.1098/rspa.2017.0229.

[8] P. Haley, M. Miksis, The effect of the contact line on droplet spreading, Journal Fluid Mechanics 223 (1991) 57–81. doi:10.1017/S0022112091001337.

[9] Y. Guo, Y. Lian, M. Sussman, Investigation of drop impact on dry and wet surfaces with consideration of surrounding air, Physics of Fluids 28 (2016). doi:10.1063/1.4958694.

[10] D. Legendre, M. Maglio, Comparison between numerical models for the simulation of moving contact lines, Computers & Fluids 113 (2015) 2–13. doi:10.1016/j.compfluid.2014.09.018.

[11] R. Guillaument, S. Vincent, J.-P. Caltagirone, An original algorithm for vof based method to handle wetting effect in multiphase flow simulation, Mechanics Research Communications 63 (2015) 26–32. doi:10.1016/j.mechrescom.2014.11.002.

[12] J. Maxwell, A dynamical theory of the electromagnetic field, Philosophical Transactions of the Royal Society of London 155 (1865) 459–512.

[13] R. Prud'homme, Quadri interfaces, Thermodynamique des interfaces et mécanique des fluides 5 (1) (2021). doi:10.21494/ISTE.OP.2021.0665.

[14] J.-P. Caltagirone, Extension of galilean invariance to uniform motions for a relativistic equation of fluid flows, Phys. Fluids 35 (2023). doi:10.1063/5.0128422.

[15] A. Liénard, Champ électrique et magnétique produit par une charge électrique concentrée en un point et animée d'un mouvement quelconque, L'Éclairage électrique XVI (27) (1898) 5–112.

[16] J.-P. Caltagirone, On Helmholtz-Hodge decomposition of inertia on a discrete local frame of reference, Physics of Fluids 32 (2020) 083604. doi:10.1063/5.0015837.

[17] Y. Kosmann-Schwarzbach, Noether Theorems. Invariance and Conservations Laws, Springer-Verlag, New York, 2011. doi:10.1007/978-0-387-87868-3.

[18] J.-P. Caltagirone, Application of discrete mechanics model to jump conditions in two-phase flows, Journal of Computational Physics 432 (2021) 110151. doi:10.1016/j.jcp.2021.110151.

[19] A. Prosperetti, G. Tryggvason, Computational Methods for Multiphase Flows, Cambridge University Press, Cambridge UK, 2007.