Adaptive finite element simulation of three-dimensional surface-tension-dominated free-surface flow problems

M. A. Walkley* P. H. Gaskell† P. K. Jimack*
M. A. Kelmanson‡ J. L. Summers†

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Abstract

An arbitrary Lagrangian-Eulerian (ALE) finite element method is described for the solution of three-dimensional free-surface flow problems. The problems are typified by the motion of the fluid free-surface, hence the geometry evolves as part of the solution, and mesh adaptivity is required to maintain a suitable computational mesh for the physical domain. Continuous mesh adaptivity, in the form of a pseudo-elastic mesh movement scheme, is used to move the interior mesh nodes in response to the motion of the fluid free surface. Periodic, discrete remeshing stages are also used for cases in which the fluid volume has grown, or is significantly distorted, by the free surface motion.

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*School of Computing, University of Leeds, UK. `mailto:markw@comp.leeds.ac.uk`
†School of Mechanical Engineering, University of Leeds.
‡Department of Applied Mathematics, University of Leeds.

1 Introduction

Free-surface-flow problems occur in a wide variety of scientific and engineering applications. Examples include phase-change problems, coating flows, the spreading of viscous fluids and the motion of drops or bubbles. The primary interest of this paper is the development of a numerical technique for the simulation of time-dependent free-surface flows in three dimensions, which represents one of the most important practical computational challenges for this class of problem. The requirement for time dependence is apparent in almost all applications since understanding the evolution and stability of free surfaces provides one of the major incentives for their mathematical and computational study. Furthermore, fully three-dimensional simulations are required in order to capture all of the physically important features of most free-surface flows. For example, the forced spreading of a fluid droplet on a chemically or topologically patterned surface, a problem with significant practical interest in the context of coating flows [3], is necessarily both time-dependent and three-dimensional.

In recent years there has been a significant interest in the computational study of such flows using ALE finite element methods and it is this approach that is pursued here. Baer *et al.* [1] used a linear hexahedral finite element method to solve the incompressible Navier-Stokes equations and also introduced a dynamic contact angle model to describe the evolution of a coating flow. Bänsch [2] developed and analysed a tetrahedral Taylor-Hood finite element method for the Navier-Stokes equations. This model included a static contact angle, allowing fluid slip along solid boundaries, but did not account for dynamic contact angle effects. Zhou and Derby [12] describe a linear tetrahedral finite element model for the Stokes equations and applied this to the sintering of two spherical particles.

The principal aim of this paper is to provide a three-dimensional incompressible free-surface flow solver based upon the use of implicitly stable elements (the so-called Taylor-Hood element); to represent the three-dimensional free surface using piecewise quadratics for optimal accuracy with the chosen elements (this is of particular significance when surface-tension effects are dominant), and; to implement the three-dimensional moving-mesh algorithm in conjunction with a discrete mesh regeneration procedure (to allow for larger geometry changes to occur than is otherwise possible). Previous work was limited in the range of problems that could be handled by restricting the mesh adaptivity to mesh movement techniques. In cases where the fluid volume changes significantly or is distorted due to the flow, for example the formation of a droplet at the end of a tube [11], mesh movement is not sufficient if the simulation is continued for a reasonable time. Particular attention is also paid to the modelling of the contact line, where the fluid free surface meets a solid surface. For steady flows a given static contact angle between these two surfaces can be achieved. This static angle is a physical parameter of the problem and its value is a functuon of the fluid properties and the solid surface characteristics. For time-dependent flows a dynamic contact angle model is implemented which allows motion of the free surface along a solid boundary. Specifying a variation in the distribution of the static contact angle allows simulation of problems where the solid surface has preferential wetting areas and, conversely, areas where wetting is inhibited.

2 Mathematical model

The class of problems to be considered here is generally characterised by three nondimensional parameters: the Reynolds number, Stokes number and capillary number, respectively

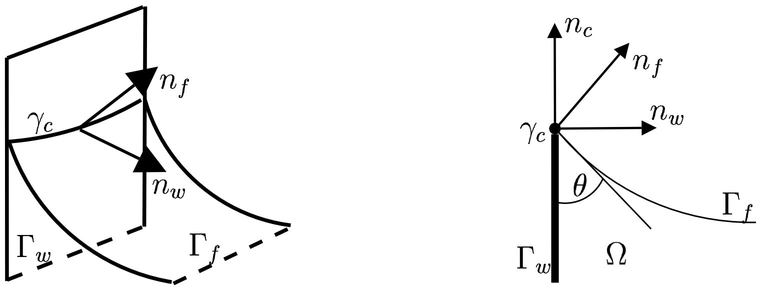
$$Re = \frac{\rho L U}{\mu}, \qquad St = \frac{\rho g L^2}{\mu U}, \qquad Ca = \frac{\mu U}{\sigma}, \tag{1}$$

written in terms of the fluid density ρ, viscosity μ and surface tension parameter σ, a characteristic length L and velocity U, and gravity g. For the purposes of this work flows are considered for which the Reynolds number is small, and the problem to be modelled can be described by the three-dimensional Stokes equations for velocity field $\mathbf{u}$ and pressure p, written in the following non-dimensional form:

$$\mathbf{0} = \nabla \cdot \boldsymbol{\sigma} + St\mathbf{f}, \qquad 0 = \nabla \cdot \mathbf{u}. \tag{2}$$

$\boldsymbol{\sigma} = -p\mathbf{I} + \nabla\mathbf{u} + \nabla\mathbf{u}^T$ is the stress tensor and $\mathbf{f}$ is the exterior force. The fluid domain Ω is assumed to be simply-connected and is bounded by either a fluid free surface Γ_f or a solid wall Γ_w. The contour defined by the interface of these two surfaces is termed the contact line γ_c. On the solid boundary Γ_w a no-slip condition is applied and, at the free surface Γ_f the following kinematic condition and stress condition are applied:

$$\mathbf{n}_f \cdot (\mathbf{u} - \dot{\mathbf{x}}_f) = 0, \qquad \mathbf{n}_f \cdot \boldsymbol{\sigma} = -\mathbf{n}_f p_{\text{ext}} + \frac{1}{Ca}\left(\nabla_S \cdot \mathbf{n}_f\right)\mathbf{n}_f \, . \tag{3}$$



(a) 3d model

(b) 2d section in the plane of $\mathbf{n}_w$ and $\mathbf{n}_f$

Figure 1: Geometrical description of the contact line

In (3) $\mathbf{n}_f$ represents the outward normal to the free surface whose location is given by $\mathbf{x}_f$, the dot above a variable denotes its time derivative, $\mathbf{u}$ represents the fluid velocity at a point on the free surface, p_{ext} is the external pressure, which may be taken as zero for simplicity, and $\nabla_S = (\mathbf{I} - \mathbf{n}_f\mathbf{n}_f) \cdot \nabla$ is the surface gradient operator.

For some applications [10] it can be assumed that the contact line γ_c is fixed and a no-slip condition applies. In these cases there is, in effect, no restriction on the angle formed between the fluid free surface and the solid boundary. However in general it more appropriate to allow the position of the contact line to evolve as part of the flow. It is desirable in these cases to specify a static contact angle, θ_s, on this boundary, the value of which is determined *a priori* by properties of both the fluid and the solid surface and can be given as a physical parameter of the problem. For transient flow the contact line is allowed to move forming a dynamic contact angle, θ, between the fluid and solid surfaces. Experimental observations have been reported [4] that show that while not at equilibrium the fluid can support contact angles that differ from the static value.

Fig. 1 depicts the geometry of the contact line on which the model is based. In practice $\mathbf{n}_f$ and $\mathbf{n}_w$ (the outward normal to the solid boundary) are computed from the current geometry whilst $\mathbf{n}_c$, the tangent to the solid surface in the plane of $\mathbf{n}_f$ and $\mathbf{n}_w$, defines locally the direction in which the free surface is allowed to move. Strictly, this problem cannot be uniquely defined within the Stokes flow framework since the contact line is both part of the solid boundary, which is subject to the no-slip condition, and the fluid boundary, which is subject to the kinematic condition. Detailed mathematical analyses of this problem and alternative mathematical models appear in the literature, *e.g.* [7, 9]. In general these models may be expressed in the form

$$\mathbf{n}_w \cdot \mathbf{n}_f \;=\; cos(\theta) \;=\; f(\theta_s, \dot{x}_c), \tag{4}$$

with the precise definition of $f(\theta_s, \dot{x}_c)$ determined by the selected model. Equation (4) may be used to compute the local speed of the contact line $\dot{x}_c$ in the direction $\mathbf{n}_c$. The specific model used in this paper is taken from [4] and has previously been applied in three dimensions by Baer *et al.* [1]:

$$f(\theta_s, \dot{x}_c) \;=\; cos(\theta_s) - c_T\, Ca\, \dot{x}_c. \tag{5}$$

The constant c_T in this model is arbitrary and an appropriate value should be determined empirically to scale the contact line speed relative to the dynamic contact angle. It is straightforward to include this general model of the contact line in the current algorithm, as is described in the following section.

3 Numerical model

The system of equations described in the previous section represent a time-dependent, nonlinear flow in which the spatial domain evolves with the problem. The computational algorithm used here has been described in detail in [10]. In previous work, *e.g.* [1], this problem has been solved in a fully coupled fashion, however here the flow solution is decoupled from the boundary motion at each time step in the following manner. First, solve the steady Stokes equations to compute the pressure and velocity field. Equation (2) is approximated with an isoparametric tetrahedral Taylor-Hood finite element method. This admits a piecewise quadratic approximation of the fluid geometry allowing an accurate model of the surface curvature and hence the free-surface stress boundary condition. The discretised finite element problem is solved with a preconditioned GMRES iteration using the solution from the previous time step as the initial guess. Second, update the free surface position Γ_f using the computed velocity. This involves an explicit time discretisation of the kinematic condition (3) and is subject to a CFL-like time step restriction. The contact line model (4), which prescribes the motion of the mesh nodes on γ_c, is incorporated at this stage. Finally, adapt the interior mesh through a pseudo-elastic solid motion of the mesh points, subject to displacements enforced by the motion of the free-surface due to the kinematic condition. This linear elastic problem is discretised using a linear finite element method and solved with a Gauss-Seidel iterative technique [10]. In general two iterations are sufficient to produce a satisfactory evolution of the interior mesh. However, mesh movement is only effective if the fluid volume does not change significantly, the domain does not distort significantly and the free surface mesh quality is maintained. In cases where these conditions do not apply it is also necessary to discretely remesh the whole domain. The quality of the existing mesh is monitored through the integral of the curvature on the mesh edges: $I_\kappa = \int_s |\kappa| \, ds$, where κ is the curvature [8], which can be computed directly as a piecewise constant on the locally quadratic edge. This measure indicates regions in which surface curvature is large relative to the local mesh resolution.

4 Computational examples

The range of capillary number and Stokes number applicable to this model can be derived from the fluid data presented by Martinez [5]. If the length scale L is of the order of L_c, termed the capillary length, where $L_c^2 = \frac{\sigma}{\rho g}$, fluid data for pure glycerin results in $Re \ll 1$ with Ca and St of order 1, which is within the Stokes flow regime.

The problem comprises a hemispherical droplet of nondimensional radius 1 initially located at the origin with $Ca = 1$ and $St = 4$. The static contact angle is defined as $2\pi/3$ for $x < -1$ or $y < -1$ (depicted as the shaded area) and to be $\pi/2$ elsewhere. The initial domain is discretised with 2141 nodes and 1159 elements using the NETGEN software [6]. A constant timestep of 10^{-3} is used. Figures 2(a)-(c) show the droplet at 3 instants during the simulation. The droplet spreads under the action of gravity but is inhibited from moving into the shaded area by the larger static contact angle. The problem is remeshed twice during the simulation and the final mesh has 1164 nodes and 564 elements.

5 Conclusions

An adaptive ALE finite element method for the solution of three-dimensional moving-boundary problems in the presence of dynamic contact lines has been described. In particular, when considering the implementation at the contact line, the piecewise quadratic model can accurately represent the required contact angles and surface curvature at the solid boundary. The mathematical model of the contact line is quite general and alternative models [7, 9] are possible within the framework of equation (4) which should be investigated and contrasted. At present the model is limited to Stokes flow and further work is required to extend the model to the Navier-Stokes regime, which would allow a wider range of practical applications to be addressed.

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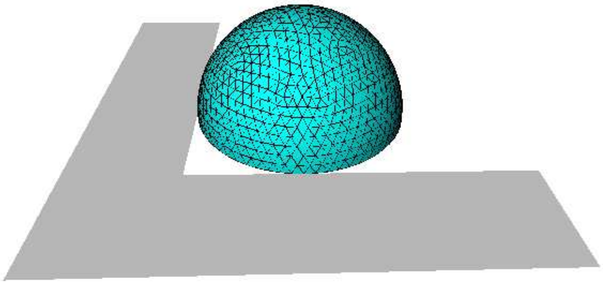
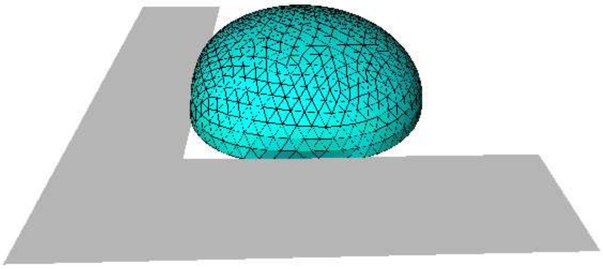
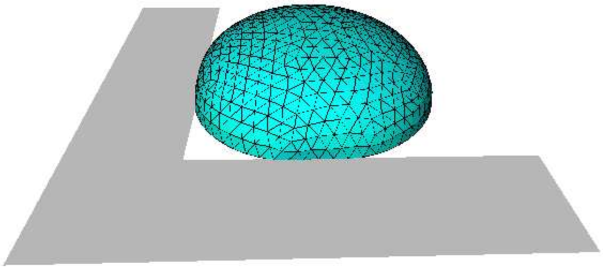


(a) t=0.0



(b) t=4.0



(c) t=20.0

Figure 2: Droplet spreading on a patterned surface