Application of a finite-element level-set method to wetting and filling problems at low to moderate capillary numbers

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Introduction and Background

Applications that involve time-evolving capillary free surfaces offer significant challenges to any numerical method, especially when surface tension forces play an important role. Arbitrary Lagrangian-Eulerian (ALE) moving mesh methods have advantages when it comes to application of surface tension forces and other interfacial phenomena, but one quickly learns that significant motion of the interfacial surface will result in frequent remeshing and reinterpolation of the variable fields. An alternative is to track the free surface with embedded interface methods such as the volume-of-fluid. However, the discontinuity in the volume-of-fluid function at the interface presents problems when applied within the context of a finite element method. The level-set method, however, is an embedded-interface method that employs a smooth representing function that is much better suited for the finite element method. In addition, it provides a precise location for the interface surface at all times and also provides an easy means for finding surface normals and curvatures.

The level set method, however, is not without its flaws. The need for periodic renormalization provides an additional path for mass balance errors. The location of the interface is always known, yet capillary forces usually must be applied as body forces in a vague "interfacial" region between one and two elements wide. In addition, the motion of the "gas" phase is usually of no interest, yet this motion may serve as the primary limitation on the computation. A chief example is the spurious oscillations that develop in the light phase ahead of the interface curve at low capillary numbers. Their short time scale often presents a barrier to an efficient time marching algorithm.

This paper will describe the approach we took to implementing a finite-element, level set method and addressing some of these issues. We shall describe its application to a problem of filling a millimeter scale feature with liquid, and we will compare the results with a solution obtained from an ALE moving mesh approach. This problem presents several challenging physical features similar to a coating flow, including the application of a dynamic contact line condition and fluid/solid contact. We will also demonstrate the method we have devised for introducing velocities at the contact line , which depend upon the local contact angle, among other things.

The Basic Level Set Formulation

The level set method is based upon a scalar function that is defined as the minimum distance from a point to the interface surface itself. The sign assigned to these distance values will distinguish between the phases. That is, in one phase the level set function values are defined to be all negative while in the other phase they are all positive. The consequence of this is then the zero contour of level-set function should coincide with the interface surface. It is also the case that the gradient of the level set function on this contour is the normal to the interface and the divergence of this vector is proportional to its curvature.

This function is evolved in time by applying a straightforward advection operator; for filling problems, we deploy the global velocity field for this purpose. Variations of the material properties across the interface are accomplished by summing the Heaviside-weighted individual phase properties. Generally, we employ diffused Heaviside functions that transition between zero and one smoothly in the interface zone. Solution of the fluid momentum and incompressibility constraint with these variable material properties yields a global velocity field that is coupled to the level set evolution. In our approach, we solve the completely coupled non-linear system, in which fluid momentum, continuity and level set advection (and mesh motion where applicable) are solved for simultaneously.

Although the level set function is defined originally as a distance function, this evolution scheme is not constrained to retain it as such. Over time the level set function might deviate significantly from a distance function with consequences for model accuracy. The standard solution is to periodically reconstruct the new location of the interface curve and re-distance the scalar function with respect to it. This procedure can introduce mass balance errors that we have sought to minimize by including a global mass balance constraint enforced via a Lagrange multiplier.

Introduction of surface tension forces is done by adding a tensor to the fluid stress tensor in the momentum equation of the form:

$$T = \sigma(I - nn)\delta_\alpha(\phi)/|\nabla\phi|$$

where σ is the surface tension, n is the normal to the interface curve, $\delta_\alpha(\phi)$ is a smoothed Dirac function with length scale α, and ϕ is the level set function. In form it is similar to that proposed by Jacqmin (1995):

Extensions to the Method

One of the first things recognized is that the surface tension tensor term is very non-linear and applied very locally around the interface. The standard finite element numerical integration methods, applicable to low order polynomials, are likely not appropriate for accurate integration of this term. One successful approach is to cluster numerical integration points in the interface region based upon a quad-tree refinement (or oct-tree in the case of three dimensions) of the elements that fall within the interface region. Note this refinement did not involve adding degrees-of-freedom, but simply provided a means of adding more integration points. A second successful method involves dynamic tessellation of the elements through which the interface passed such that the borders of sub-elements created conform to the interface surface. This has the benefit of permitting the interface width to be set at zero. The surface tension terms become line integrals and the other volumetric terms are integrated on the subelement triangles.

A different issue with embedded interface methods is that frequently discontinuities occur across the interface in either the value of a field variable or its gradient. The pressure jump across a capillary surface is the most obvious example. Introducing local enrichment of the interpolating space was found to improve the method significantly. We chose to employ a new method for this, often referred to as the extended finite element method (XFEM), e.g. Chessa, Smolinski, Belytschko (2002). This method introduces an enriching function of the level set field, for example a step change across the interface, and multiplies it by each of the finite element trial functions in the elements that are influenced by the interface. This generates a set of new trial functions to which additional enriching degrees-of-freedom in, for example, the pressure field, can be associated. The pressure field at a point in the interface region is then a sum of the contribution from the regular pressure unknowns and the enriched unknowns, each weighted by their trial functions

We apply wetting line velocities by first introducing the potential for slip on a wetting boundary by replacing the Dirichlet no-slip requirements with a Navier slip condition. The slip coefficient in the latter is chosen to effectively enforce no slip conditions away from the contact line. At the contact line we assume a wetting velocity model, that is, a relationship between local contact angle, model parameters and wetting line velocity. One example is a model proposed by Blake and De Coninck (2002):

$$V_{wet} = V_0 \sinh(\gamma(\cos\theta - \cos\theta_s))$$

Multiplying this velocity by a surface tangent vector yields a vector condition that supplants the momentum equations in the contact line region and produces fluid motion in response to deviations from the static contact angle parameter, θ_s.

Example Application

We demonstrate our approach in a simple two-dimensional example. It consists of a millimeter-high planar channel and a few millimeters downstream of its entrance a millimeter-high square groove in the upper surface. Fluid is supplied to the channel at a fixed average rate, and the primary modeling goal is to determine under what circumstances the feature will fill. This is a challenging problem not only because of the effect of the capillary free surface, but because the wetting line algorithm must function robustly despite the abrupt changes in geometry of the upper surface. Further, we anticipate fluid/solid contact events in the situations where the feature does not fill.

This problem was originally motivated by a process in which the filling occurred because the upper surface was being squeezed onto the lower surface (like in the filling of a gravure cell). Including this dynamic geometry requires that the mesh node displacements be determined while the lower surface is moved upward over time. These displacements were determined with a pseudo-solid mesh motion approach described by Sackinger et.al (1996). The mesh displacement equations are solved in a fully-coupled fashion with the rest of the unknown field variables. This approach is termed arbitrary Lagrangian-Eulerian (ALE) because the fluid velocity and mesh velocities are in general independent except at bounding surfaces.

The surface tension was fixed, and different values of the effective capillary number were obtained by varying the "fluid" side viscosity value. We shall show results for capillary numbers from 10.0 to 0.01. The Blake-De Coninck wetting velocity model was employed as described above and we demonstrate the effect of changing the static contact angle parameter of this model. Finally, we show the effect that dynamic squeezing has on the progress of the fluid front. Our modeled results show that the groove will fill *completely* provided only that the upper wetting line reaches the deepest part of the groove prior to the free surface contacting the downstream reentrant corner. This result is consistent with a much longer and more computationally intensive ALE moving mesh simulation.

In addition to this filling problem, we also shall show the application of the method to startup of a two-dimensional slot coater. In some aspects, this situation is simpler to model than the previous case. However, the contact problem is made more difficult by the tendency of the moving substrate to entrain the "gas" phase and inhibit the contact event. We shall describe an *ad hoc* means for initiating contact in these situations based upon a very simple probabilistic model.

References

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