



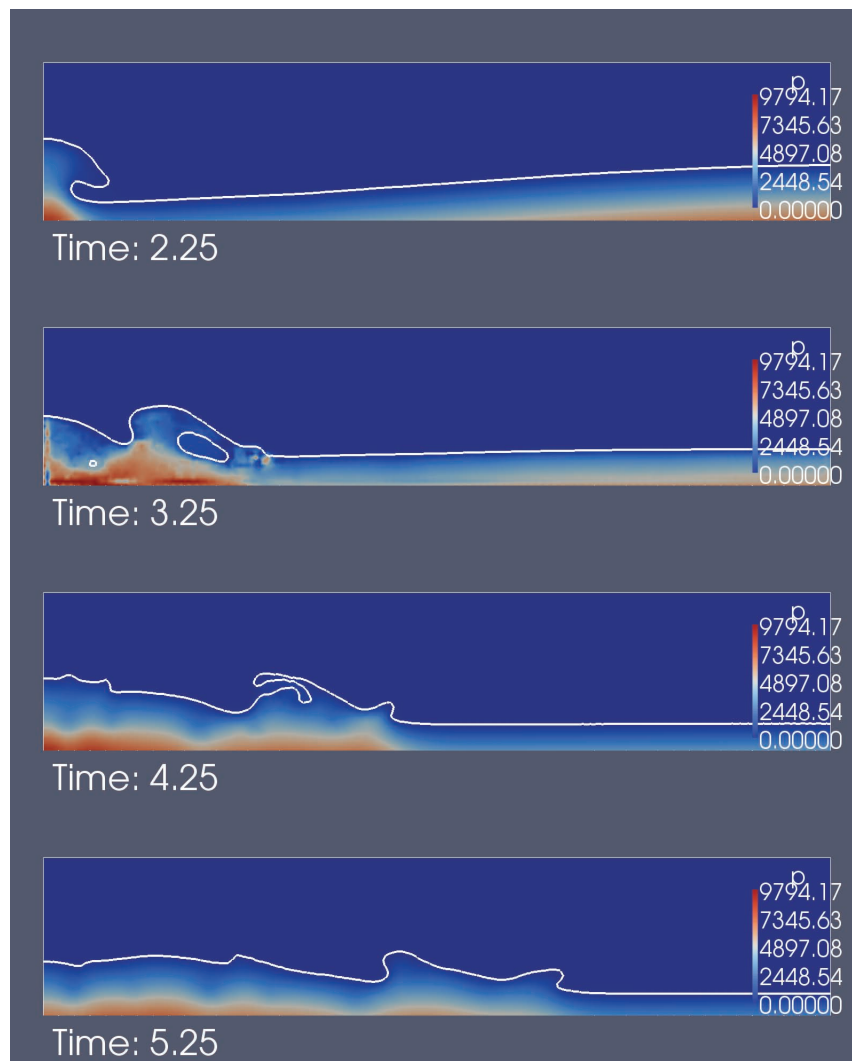
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A Review of Methods for Moving Boundary Problems

C. E. Kees, M. W. Farthing, R. C. Berger and T. C. Lackey

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Abstract: State-of-the-art numerical methods for solving moving boundary problems arising from multiphase flow and fluid-structure interaction modeling are reviewed. The emphasis of the review is on robust methods that do not require the mesh to conform to the moving boundary. The impetus for this review is the Coastal and Hydraulics Laboratory's mission in navigation. Accurately predicting the effect of a vessel on a waterway and the vessel motion are required to support the navigation mission as is accurately predicting wave interaction with coastal and hydraulic structures. A key part of making accurate predictions in these cases is solving moving boundary problems. This report identifies promising directions for research and development of in-house, state-of-the-art computational models.

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Preface

This report is a product of the High Fidelity Vessel Effects Work Unit of the Navigation Systems Research Program being conducted at the U.S. Army Engineer Research and Development Center, Coastal and Hydraulics Laboratory.

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1 Introduction

Consider the problem of simulating a solid (e.g. a vessel) moving in a waterway (Figure 1). Suppose that the primary goal of the simulation is to describe the interaction of the solid's movement on the air and water in some sufficiently large box containing the waterway. The interior of the box is the domain, and the boundaries of the box are the domain boundaries. For simplicity, we assume that the solid is a rigid body. It does not deform, but its motion may depend on surface forces exerted by the fluid and on gravitational forces. The incompressible Navier-Stokes equations will be used to describe both the water and air flow, though in full-scale applications a system of Reynolds Averaged Navier-Stokes equations (RANS) would be required. This problem contains three moving boundaries at the interfaces between the three material types: air-water, air-solid, and water-solid. The movement is relative to the fixed domain boundaries, and the interfaces remain sharp. No significant amounts of material pass through the moving boundaries at the temporal and spatial scales of interest. That is, the moving boundaries are material surfaces. On the other hand, mechanical and thermal energy can and do pass through these moving interfaces. The particular way that mass and momentum fluxes are constrained at the interfaces constitute the boundary conditions for the Navier-Stokes equations along these moving boundaries.

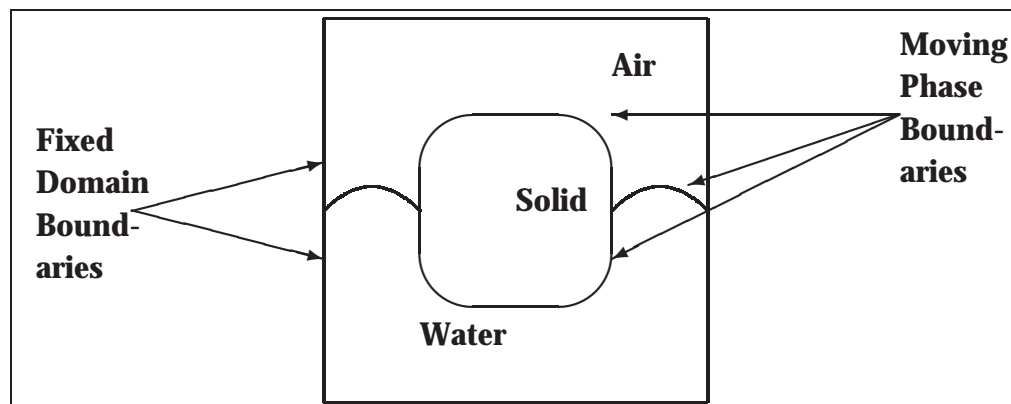


Figure 1. Domain with three mobile phases.

A classic method for describing this moving boundary problem is to shift from the fixed frame of reference associated with the box to a material or Lagrangian frame that moves with the fluids or solid. Due to the as-

sumption that interfaces are material boundaries, the moving boundaries in the fixed frame become fixed boundaries in the moving frame and vice versa. This approach may complicate the application of boundary conditions at the domain boundary, and in the present case it is further complicated by the fact that the moving boundaries are moving relative to one another. The transformation from fixed to moving frame becomes a part of the solution to the problem—it is based on integration of the flow velocity. Instead of a purely Lagrangian perspective, so-called Arbitrary Lagrangian-Eulerian (ALE) space-time formulations that blend the Lagrangian perspective near the moving boundaries with the fixed “Eulerian” frame away from moving boundaries are often preferred (e.g. (Donea, 1982; Hughes and Hulbert, 1998)). The ALE formulation requires additional decisions about the blending of Eulerian and Lagrangian frames that do not follow from the physics alone. These decisions form part of the solution method.

In many cases, the resulting flow dynamics may cause the material domains to undergo changes in topology. For instance, breaking waves or flow over the top of the vessel may change the connectedness of the water and air domains. The time-dependent space transformation in the ALE formulations becomes degenerate during such topological changes. Furthermore, even when no topological changes occur, the numerical ALE formulation must be carefully designed to prevent numerical instabilities from polluting the results.

This review focuses instead on the fixed or Eulerian perspective because of the difficulties associated with ALE formulations of the moving boundary problem. We also exclude various other particle-based numerical methods that can be used to approximate multiphase flow models (e.g. the Lattice-Boltzmann method (Frisch et al., 1986) and the particle finite element method (Idelsohn et al., 2006)). For Eulerian approaches, the primary difficulty becomes accurately locating the moving boundary and applying boundary conditions there. In the next section we provide some mathematical background on free boundary problems. Then we review and discuss the current trends in numerical methods. We conclude with a list of recommendations for further numerical modeling work.

2 Background

We begin by reviewing the basic mathematical framework of moving boundary problems for two-phase flow. First, we describe the Eulerian flow model and then popular techniques for modeling the moving boundary.

2.1 Navier-Stokes equations for incompressible, Newtonian fluids

We partition the spatial domain, Ω , into two subdomains Ω_w (water) and Ω_a (air). In each subdomain we write the incompressible Navier-Stokes equations as:

$$\nabla \cdot \mathbf{v} = 0 \quad (1)$$

$$\frac{\partial \mathbf{v}}{\partial t} + \nabla \cdot (\mathbf{v} \otimes \mathbf{v} - \bar{\boldsymbol{\sigma}}) - \mathbf{g} = 0 \quad (2)$$

where $\mathbf{v} = \mathbf{v}_w, \mathbf{v}_a$ and $\bar{\boldsymbol{\sigma}}$ is the stress tensor, given by

$$\bar{\sigma}_{ij} = -p\bar{\delta}_{ij} + \mu \left(\frac{v_i}{x_j} + \frac{v_j}{x_i} \right) \quad (3)$$

We let $\Gamma(t) = \Omega_w \cap \Omega_a$. Note that both the subdomains and $\Gamma(t)$ are actually time dependent. As a simple example, the boundary conditions on $\Gamma(t)$ could be

$$\mathbf{v}_a - \mathbf{v}_w = 0 \quad (4)$$

$$p_a - p_w = 0 \quad (5)$$

The first condition reflects continuity of the normal and tangential components of the velocity and the second continuity of the pressure. Or, equivalently, these jump conditions in the unknowns follow from an assumption of continuity of the mass and momentum flux. While it typically makes sense to assume that the interface has no mass and therefore that the mass flux is continuous at points on Γ , the well-known phenomena of surface tension implies that the interface can absorb or impart momentum. Hence, a more general set of jump conditions is

$$(\mathbf{v}_a - \mathbf{v}_w) \cdot \mathbf{n} = 0 \quad (6)$$

$$(\bar{\boldsymbol{\sigma}}_a - \bar{\boldsymbol{\sigma}}_w) \cdot \mathbf{n} = \mathbf{f} \quad (7)$$

where \mathbf{f} is the force due to the interface and \mathbf{n} is the outward unit normal vector on Γ_w . Surface tension results in a force on the fluid directed entirely in the normal direction and typically given by

$$\mathbf{f} = \sigma_{w,a} \mathbf{n} \quad (8)$$

where κ is the mean curvature of $\Gamma(t)$ defined as

$$\kappa = -\nabla \cdot \mathbf{n} \quad (9)$$

and $\sigma_{w,a}$ is the surface tension coefficient for the air/water interface. For related formulations see (Harlow and Welch, 1965; Popinet and Zaleski, 1999; Tornberg and Enquist, 2000).

Weak formulation

In order to formulate numerical methods and incorporate the jump conditions, we will use a weak formulation of the Navier-Stokes equation. For now we consider a domain Ω and assume that Γ cuts through Ω and divides it into two domains Ω_w and Ω_a . Multiplying the continuity equation by a smooth test function w with compact support in Ω , integrating by parts, and applying the jump condition on the normal component of the velocity yields

$$-\int_{\Omega_w} \mathbf{v}_w \cdot \nabla w dV + \int_{\Gamma} \mathbf{v}_w \mathbf{w} \cdot \mathbf{n}_w dS - \int_{\Omega_a} \mathbf{v}_a \cdot \nabla w dV + \int_{\Gamma} \mathbf{v}_w \mathbf{w} \cdot \mathbf{n}_a dS = 0 \quad (10)$$

$$-\int_{\Omega} \mathbf{v} \cdot \nabla w dV - \int_{\Gamma} (\mathbf{v}_a - \mathbf{v}_w) \mathbf{w} \cdot \mathbf{n} dS = 0 \quad (11)$$

$$-\int_{\Omega} \mathbf{v} \cdot \nabla w dV = 0 \quad (12)$$

where we have defined a global fluid velocity

$$\mathbf{v} = \begin{cases} \mathbf{v}_w & \mathbf{x} \in \Omega_w \\ \mathbf{v}_a & \mathbf{x} \in \Omega_a \end{cases} \quad (13)$$

Treating the momentum equation in the same manner yields

$$\int_{\Omega} \left[\frac{(\rho \mathbf{v})}{t} - \boldsymbol{\sigma} \right] \mathbf{w} dV - \int_{\Omega} (\rho \mathbf{v} \otimes \mathbf{v} - \boldsymbol{\sigma}) \cdot \nabla \mathbf{w} = \int_{\Gamma} \mathbf{f} \mathbf{w} dS \quad (14)$$

where

$$\mathbf{p} = \begin{cases} \mathbf{p}_w & \mathbf{x} \in \Omega_w \\ \mathbf{p}_a & \mathbf{x} \in \Omega_a \end{cases} \quad (15)$$

$$= \begin{cases} \mu_w & \mathbf{x} \in \Omega_w \\ \mu_a & \mathbf{x} \in \Omega_a \end{cases} \quad (16)$$

$$\bar{\boldsymbol{\sigma}} = \begin{cases} \bar{\boldsymbol{\sigma}}_w & \mathbf{x} \in \Omega_w \\ \bar{\boldsymbol{\sigma}}_a & \mathbf{x} \in \Omega_a \end{cases} \quad (17)$$

Note that in general we only know that $\mathbf{v} \cdot \mathbf{n}$ is continuous at points on Γ while \mathbf{v} , \mathbf{p} , μ , and $\boldsymbol{\sigma}$ may be discontinuous. Since the viscosity is always positive and \mathbf{f} acts normal to the interface, however, \mathbf{v} may be continuous.

2.2 Moving boundary models

We require a representation for the moving boundary, $\Gamma(t)$, and an equation for its evolution. As noted in (Sethian, 2001), there are three classic mathematical perspectives on representing the boundary. First, $\Gamma(t)$ can be given in parametric form,

$$[\mathbf{x}(\xi, \eta, t), y(\xi, \eta, t), z(\xi, \eta, t)] = \mathbf{x}(\xi, \eta, t) \quad (18)$$

where $(\xi, \eta) \in \mathbb{R}^2$ are surface coordinates. For example, the surface depicted in figure 2 can be parameterized as

$$\mathbf{x}(\bar{\mathbf{x}}) = (\xi, \eta, \sqrt{2 - \xi^2 - \eta^2}) \quad (19)$$

where $(\xi, \eta) \in [-1, 1] \times [-1, 1]$. Second, $\Gamma(t)$ can be given in implicit form,

$$\mathbf{u}(\mathbf{x}, y, z, t) = \mathbf{u}(\mathbf{x}, t) = 0 \quad (20)$$

In the example above we could use

$$\mathbf{u}(\mathbf{x}, y, z) = 2 - \mathbf{x}^2 - \mathbf{y}^2 - \mathbf{z}^2 \quad (21)$$

We will call \mathbf{u} a level set (LS) function for the surface since the surface is given by the zero LS of the function \mathbf{u} . Third, instead of representing $\Gamma(t)$, the subdomains Ω_w and Ω_a can be represented in set-theoretic form via their characteristic functions $\chi_w(t)$ and $\chi_a(t)$ defined by

$$\chi_w(\mathbf{x}) = \begin{cases} 1 & \text{for } \mathbf{x} \in \Omega_w \\ 0 & \text{for } \mathbf{x} \in \Omega_a \end{cases} \quad (22)$$

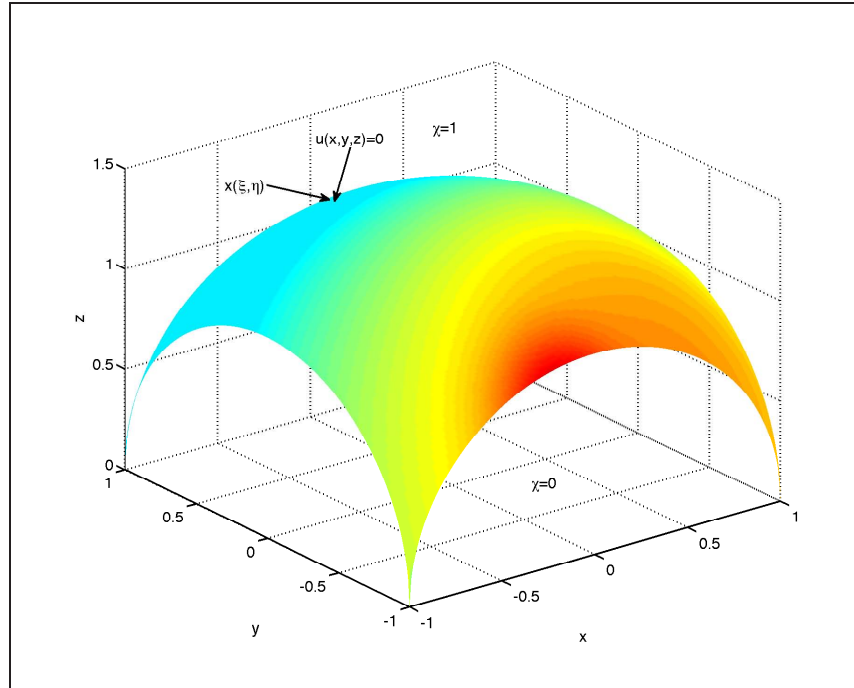


Figure 2. Parametric, implicit, and characteristic representations of a surface in \mathbb{R}^3 .

and $a = 1 - w$. For the example above, assuming that water lies below air, we could use

$$a(\mathbf{x}) = \begin{cases} 0 & \text{if } 2 - \mathbf{x}^2 - \mathbf{y}^2 - \mathbf{z}^2 \geq 0 \\ 1 & \text{if } 2 - \mathbf{x}^2 - \mathbf{y}^2 - \mathbf{z}^2 < 0 \end{cases} \quad (23)$$

It is convenient to consider the basic numerical methods as proceeding from one of these three perspectives

Level set methods

First, note that if the initial surface is described as $u(\mathbf{x}) = 0$ then there is no reason why this $u(\mathbf{x})$ cannot be defined for all $\mathbf{x} \in \mathbb{R}^3$. This is apparent in the 3D example above. Given an initial condition for u on \mathbb{R}^3 , we now wish to define equations for its evolution on all of \mathbb{R}^3 as well. Let $\mathbf{x}(t)$ be a fluid particle path such that $\mathbf{x}(0)$ is on $u = 0$. It can be shown that $\mathbf{x}(t)$ remains on $u = 0$ for all time. Therefore $u(\mathbf{x}(t), t) = 0$. Differentiating with respect to t yields

$$\frac{d\mathbf{x}}{dt} + \nabla u \cdot \frac{d\mathbf{x}}{dt} = 0 \quad (24)$$

Again by definition, the velocity of water particles at the boundary is $\mathbf{v}_w = \frac{d\mathbf{x}_w}{dt}$. Furthermore by continuity of the normal component of the ve-

locities, we know that on Γ , $\nabla \mathbf{u} \cdot \mathbf{v}_w = \nabla \mathbf{u} \cdot \mathbf{v}_a$ so we can use either velocity and henceforth drop the subscript. Hence \mathbf{u} is related to \mathbf{v} through

$$-\frac{\mathbf{u}}{t} + \nabla \mathbf{u} \cdot \mathbf{v} = 0 \quad (25)$$

We denote this the non-conservative interface (NCI) equation. Note that it is known as the kinematic boundary condition for the free surface Γ . We know from calculus that $\mathbf{n} = \nabla \mathbf{u} / \|\nabla \mathbf{u}\|$ where $\|\cdot\|$ is the Euclidean norm. The normal speed is then

$$\mathbf{s}_n = \mathbf{v}_w \cdot \frac{\nabla \mathbf{u}}{\|\nabla \mathbf{u}\|} = \frac{-\frac{\mathbf{u}}{t}}{\|\nabla \mathbf{u}\|} \quad (26)$$

We can thus rewrite the NCI equation in terms of the normal speed as a Hamilton-Jacobi interface (HJI) equation

$$-\frac{\mathbf{u}}{t} + \|\nabla \mathbf{u}\| \mathbf{s}_n = 0 \quad (27)$$

For the special case of $\nabla \cdot \mathbf{v} = 0$ we can also rewrite the NCI equation as a conservative interface (CI) equation

$$-\frac{\mathbf{u}}{t} + \nabla \cdot (\mathbf{u}\mathbf{v}) = 0 \quad (28)$$

Note that \mathbf{v} need only agree with the physical velocity along Γ , and in fact many implicit representations of Γ are possible that agree only on Γ . For example, suppose Γ is $[-1, 1] \times [-1, 1]$ and Γ is simply the circle of radius $1/2$. A signed Euclidean distance to this circle makes sense for all (x, y) . The zero LS of this signed distance function is an implicit representation of the boundary. In this simple case the LS function is given by $u(x, y) = 1/2 - \sqrt{x^2 + y^2}$. The level sets are shown in Figure 3. Note that $u^2 = 0$ is a different LS function that still has the same zero LS as u . The signed Euclidean distance from \mathbf{x} to the set Γ is generally a good choice for the LS because it provides additional geometric information: its value gives both the distance to the interface from a point and which side of the interface the point lies on. It can be shown that the signed distance function is the unique vanishing viscosity solution of the boundary value problem for the eikonal equation:

$$\|\nabla u\| = 1 \text{ for } \mathbf{x} \in \Omega \quad (29)$$

$$u = 0 \text{ for } \mathbf{x} \in \Gamma \quad (30)$$

where $\|\cdot\|$ is the Euclidean norm. Solutions of the eikonal equation can in turn be characterized as steady state solutions of the initial value problem

$$\mathbf{u}_t + \text{sgn}(\mathbf{u}_0)(\|\nabla \mathbf{u}\| - 1) = 0 \quad (31)$$

$$\mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x}) \quad (32)$$

where \mathbf{u}_0 is any LS function describing and sgn is the signum function given by

$$\text{sgn}(\mathbf{u}) = \begin{cases} -1 & \mathbf{u} < 0 \\ 0 & \mathbf{u} = 0 \\ 1 & \mathbf{u} > 0 \end{cases} \quad (33)$$

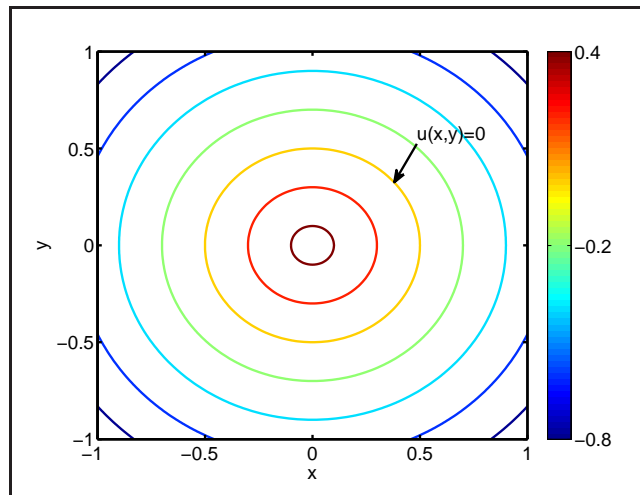


Figure 3. Signed distance level sets for moving boundary at $z = 1/2$.

One additional element is needed to make this description complete: the extension of s_n or \mathbf{v} to all of Ω . This extension is not unique because it need only match the normal of the fluid velocities on Γ . Two natural choices are the fluid velocities themselves and a speed s_n that preserves the signed distance structure of u .

The modern LS method based on the HJI equation was first formulated in (Osher and Sethian, 1988). The LS method can lead to loss of mass because no discrete mass conservation properties can be derived from the fluid and LS equations alone (even the CI formulation). This is a significant drawback of the basic LS method, which we discuss briefly below.

To complete the method for modeling two-phase flow we combine the LS representation with the two-phase Navier-Stokes formulation. As an example we choose to preserve a signed distance representation of the LS using the eikonal equation and use the NCI equation for the LS dynamics. The complete system of equations in weak form is

$$\int (\|\nabla \mathbf{u}\| - 1) \mathbf{w} dV = 0 \quad (34)$$

$$-\int \mathbf{v} \cdot \nabla \mathbf{w} dV = \int_{N_s} \mathbf{q} dS \quad (35)$$

$$\int \left[\frac{(\mathbf{v})}{t} - \mathbf{g} \right] \mathbf{w} dV - \int (\mathbf{v} \otimes \mathbf{v} - \bar{\boldsymbol{\sigma}}) \cdot \nabla \mathbf{w} = \int \mathbf{f} dS + \int_{N_{s,v}} \mathbf{q}_v dS \quad (36)$$

$$\int \left(\frac{\hat{\mathbf{u}}}{t} + \nabla \hat{\mathbf{u}} \cdot \mathbf{v} \right) \mathbf{w} = 0 \quad (37)$$

where

$$= \mu_a \mathbf{H}(\mathbf{u}) + \mu_w [1 - \mathbf{H}(\mathbf{u})] \quad (38)$$

$$\boldsymbol{\mu} = \boldsymbol{\mu}_a \mathbf{H}(\mathbf{u}) + \boldsymbol{\mu}_w [1 - \mathbf{H}(\mathbf{u})] \quad (39)$$

$$\mathbf{H}(\mathbf{u}) = \begin{cases} 0 & \mathbf{u} < 0 \\ \frac{1}{2} & \mathbf{u} = 0 \\ 1 & \mathbf{u} > 0 \end{cases} \quad (40)$$

and the boundary and initial conditions are

$$\mathbf{u} = \hat{\mathbf{u}} \text{ for } \mathbf{x} \in \quad (41)$$

$$\mathbf{p} = \mathbf{p}_d \text{ for } \mathbf{x} \in D_p \quad (42)$$

$$\mathbf{v} = \mathbf{v}_d \text{ for } \mathbf{x} \in D_v \quad (43)$$

$$\mathbf{v} \cdot \mathbf{n} = \mathbf{q}(\mathbf{x}, t) \text{ for } \mathbf{x} \in N_s \quad (44)$$

$$(\mathbf{v} \otimes \mathbf{v} - \bar{\boldsymbol{\sigma}}) \cdot \mathbf{n} = \mathbf{q}_v \text{ for } \mathbf{x} \in N_{s,v} \quad (45)$$

$$\mathbf{p} = \mathbf{p}_0 \text{ for } \mathbf{x} \in \quad , t = 0 \quad (46)$$

$$\mathbf{v} = \mathbf{v}_0 \text{ for } \mathbf{x} \in \quad , t = 0 \quad (47)$$

$$\hat{\mathbf{u}} = \hat{\mathbf{u}}_0 \text{ for } \mathbf{x} \in \quad , t = 0 \quad (48)$$

Note that equation 34 “redistances” or “re-initializes” $\hat{\mathbf{u}}$ so that the flow equations are always able to depend on a LS description that provides the signed distance to the interface. This system is typically solved using operator splitting. For example, the solution at time t can be approximated by first solving equation 34 (redistance), then solving equations 35 and 36 (Navier-Stokes) using $\mathbf{u}(0)$, then finally equation 37 (LS) at

$\mathbf{t} = \mathbf{t}$ using $v(\mathbf{t})$. A common variant of this approach is to use smooth (regularized) approximations of the Heaviside function, H , and the Dirac delta function to evaluate the discontinuous coefficients and surface force integral:

$$\mu_a \mathbf{H}_\epsilon(\mathbf{u}) + \mu_w [1 - \mathbf{H}_\epsilon(\mathbf{u})] \quad (49)$$

$$\mu \quad \mu_a \mathbf{H}_\epsilon(\mathbf{u}) + \mu_w [1 - \mathbf{H}_\epsilon(\mathbf{u})] \quad (50)$$

$$\int \mathbf{f} d\mathbf{S} \quad \int \epsilon(\mathbf{u}) \mathbf{f} \|\nabla \mathbf{u}\| d\mathbf{V} \quad (51)$$

$$\mathbf{H}_\epsilon(\mathbf{u}) = \begin{cases} 0 & \mathbf{u} < -\epsilon \\ \frac{1}{2} \left(1 + \frac{\mathbf{u}}{\epsilon} + \frac{\sin(\frac{\mathbf{u}}{\epsilon})}{\epsilon} \right) & \mathbf{u} = 0 \\ 1 & \mathbf{u} > \epsilon \end{cases} \quad (52)$$

$$\epsilon(\mathbf{u}) = \begin{cases} 0 & \mathbf{u} < -\epsilon \\ \frac{1}{2} \left(\frac{1}{\epsilon} + \frac{\cos(\frac{\mathbf{u}}{\epsilon})}{\epsilon} \right) & \mathbf{u} = 0 \\ 0 & \mathbf{u} > \epsilon \end{cases} \quad (53)$$

where ϵ is a mesh-dependent parameter (e.g. $\epsilon = 1.5 \mathbf{x}$ is recommended in (Osher and Fedkiw, 2003)). It was pointed out in (Tornberg and Enquist, 2003) that these simple regularizations of the Heaviside and Dirac functions are inaccurate and that significantly better alternatives exist. Furthermore, direct evaluation of the surface force term is also feasible as are related immersed boundary methods described in (Li and Ito, 2006). It is also common in surface tension calculations to introduce a filtering step to remove high frequency oscillations from the surface normal $\|\nabla \mathbf{u}\|$ or (Tornberg and Enquist, 2000).

We note that the primary advantage of the LS formulation is that accurate and efficient finite element and finite volume methods exist for solving equations 34–37. Such methods automatically compute the viscosity solutions for the LS functions, which are the correct solutions for cases in which the connectivity of the fluid regions change (i.e. during breaking or merging of the fluid regions).

Before continuing we consider the conservation properties of the basic LS method. The mass of water in the domain is given by

$$\int_w \mathbf{w} d\mathbf{V} = \int \mathbf{w} \mathbf{H}(\mathbf{u}) d\mathbf{V} \quad (54)$$

The integral form of mass conservation can likewise be extended to the entire domain or any subdomain as

$$-\frac{d}{dt} \int_{\Omega} \rho_w H(\mathbf{u}) dV + \int_{\partial\Omega} \rho_w H(\mathbf{u}) \mathbf{v}_w \cdot \mathbf{n}_w dS \quad (55)$$

Of course, for incompressible fluids this implies volume conservation as well so that we could cancel out ρ_w . Neither a global nor a local statement of mass or volume conservation can be obtained from any of the LS equations derived above.

Front tracking (parametric) methods

Next we consider the parametric representation of the surface, $\mathbf{x}(\boldsymbol{\xi}, t)$. It is easy to show from the implicit representation of $\phi(\mathbf{x}, t)$ that $\frac{d\mathbf{x}}{dt} \cdot \mathbf{n} = s_n$, hence the front tracking (FT) formulation can be written as

$$\frac{d\mathbf{x}}{dt} = \mathbf{v}_{FT} \quad (56)$$

where \mathbf{v}_{FT} is any velocity such that $\mathbf{v}_{FT} \cdot \mathbf{n} = s_n$. Given a discrete representation of the $\mathbf{x}(\boldsymbol{\xi}, t)$ the FT equation is set of (uncoupled) ordinary differential equations. Early examples of FT for two-phase flow include (Glimm et al., 1987; Tryggvason and Unverdi, 1990; Unverdi and Tryggvason, 1992). The primary drawback of FT is that for many realistic velocities, the trajectories defined by \mathbf{v}_{FT} intersect, leading to degeneracy in the parametric representation. These problems can be dealt with using additional, rather complex, “untangling” algorithms based on additional physical and geometric information (Glimm et al., 1988). We consider these methods Eulerian methods because the underlying mesh for resolving physics is fixed, even though the Lagrangian particle tracking is a key part of the method. Given an implementation of a complete algorithm, the two-phase model is similar in overall design to the LS model above, with the exception that the LS advection step is replaced by the FT step and the coefficients are evaluated using the parametric form of the surface.

Volume of fluid methods

This approach could be described as “pseudo-mixture theory” because the set characteristic functions ϕ_w and ϕ_a are derived from the volume

fraction of each discrete cell or element, as if it were filled with a mixture of the two fluids. Instead of solving the free boundary problem explicitly, the entire fluid domain is described by a single set of equations for the two-fluid mixture with a particular choice of “constitutive laws” for the mixture properties. Let $\phi_e(x, t)$ be the ratio of water volume to total fluid volume in a computational element e . If initially all elements contain either water or air then $\phi_e = \phi_w$. We then define the density and viscosity of the two-fluid mixture as

$$\rho = \phi_w \rho_w + (1 - \phi_w) \rho_a \quad (57)$$

$$\mu = \phi_w \mu_w + (1 - \phi_w) \mu_a \quad (58)$$

In a sense these are “constitutive laws” of the mixture, though they are introduced as a numerical convenience as are the smoothed Heaviside functions in the LS methods. The flow equations for the mixture are simply the Navier-Stokes equations for the fluid mixture, which necessarily has variable density and viscosity (though it is still incompressible). An additional transport equation for ϕ_w represents conservation of volume for either phase:

$$\frac{\partial \phi_w}{\partial t} + \nabla \cdot (\phi_w \mathbf{v}) = 0 \quad (59)$$

where \mathbf{v} is the velocity of the fluid mixture. Since mass conservation is explicitly enforced one need only discretize carefully in order to conserve mass in the fully discrete model. On the other hand, Eulerian methods for the volume of fluid (VOF) equation tend to smear the jumps in ϕ_w , which results in a loss of information about the precise location of the interface. Interface reconstruction and sharpening techniques must be used to counteract this problem and to obtain precise information on the interface geometry. Early work on VOF methods includes (Noh and Woodward, 1976; Hirt and Nichols, 1981)

Relationships among interface representations

We now relate the FT and VOF interface representations to the LS representation. The simplest relationship is among solutions. Given a parametric representation $\mathbf{x}_{mp}(\xi, \eta, t)$ then the signed distance LS function is given by $u(\mathbf{x}, t) = \min_{(\xi, \eta)} \|\mathbf{x} - \mathbf{x}_{mp}(\xi, \eta, t)\|$. Given a signed distance LS function $u(\mathbf{x}, t)$ ($u < 0$ being the water phase) the characteristic function is $\phi_w = 1 - H(u(\mathbf{x}, t))$ where H is the Heaviside function defined in equation 40

The methods for obtaining solutions are also related. We can rewrite the HJI equation as

$$\mathbf{u}_t + \nabla \mathbf{u} \cdot (\mathbf{s}_n \mathbf{n}) = 0 \quad (60)$$

This equation is the directional derivative along the curve determined by the characteristic equations

$$\frac{d\mathbf{x}_s}{dt} = \mathbf{s}_n \mathbf{n} \quad (61)$$

$$\mathbf{x}_s(0) = \mathbf{x}(\mathbf{s}, 0) \quad (62)$$

which are equations for a FT representation. Thus, if the FT equations can be solved then the HJI equation can be as well via $\mathbf{u}(\mathbf{x}_s(t), t) = \mathbf{u}(\mathbf{x}_s(0), 0)$ and whatever method is used to extend \mathbf{u} to all of space. It is well known that the method of characteristics does not yield the solution of the HJI equations for large time because the characteristics trajectories, $\mathbf{x}_s(t)$, will cross in many settings as mentioned above. On the other hand, the theory of viscosity solutions yields a method for extending solutions of the HJI equation past the point when characteristics cross. For example, far enough from a curved boundary the signed distance LS function will form corners, see Figure 4

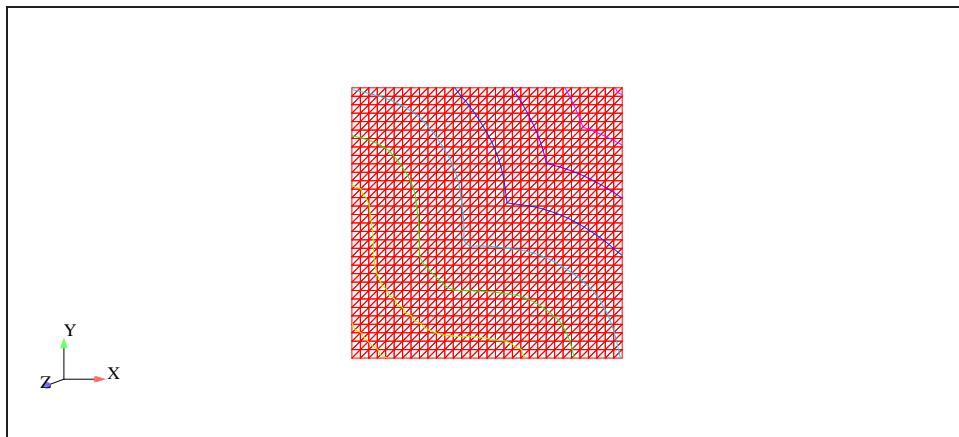


Figure 4. Level sets with corners.

As we have seen, the volume fractions can be derived directly from the LS function via the Heaviside function. Since the VOF model is a conservation law, it can also be interpreted in terms of a method-of-characteristics solution which may break down but can be continued via the viscosity solution, similarly to the HJI equation. The volume fraction drops some of the information provided in the LS function, however, using only its sign.

3 Current Trends

Each basic method or viewpoint has strengths and weaknesses:

- **FT methods give very accurate representations of smooth interfaces. They require complex untangling algorithms to deal with topological changes and are not strictly mass or volume conserving.**
- **LS methods that deal with topological changes are easy to implement. They are not strictly mass or volume conserving and tend to be less accurate than FT methods.**
- **VOF methods are strictly mass conserving. They can deal with topological changes, but they tend to be the least accurate of the three methods.**

The following advice from (Sethian, 2001)

Good numerics is ultimately about getting things to work; the slavish and blind devotion to one approach above all others is usually a sign of unfamiliarity with the range of troubles and challenges presented by real applications.

Much of the recent work on Eulerian methods reflects attempts at combining aspects of all three methods in order to obtain the best properties of all the methods.

3.1 Recent work on free boundary modeling

One approach to improve the mass conservation properties of LS methods is the conservative LS/VOF (CLSVOF) method (Sussman and Puckett, 2000). In this approach both the VOF and LS representations are computed and the VOF function is used to obtain the correct mass. The CLSVOF method is currently being modified and extended to problems with surface tension (Sussman, 2003; Sussman et al., 2007). A related approach simply uses a LS function that mimics a smoothed Heaviside

function rather than a signed distance function in order to mimic the shape of the set characteristic function (Olsson and Kreiss, 2005).

A different approach to maintaining mass conservation and improving the resolution of LS methods is the particle-LS method presented in (Enright et al., 2002). This approach seeds both sides of the interface with “fluid” particles that are then used to correct the interface. This method improves the mass conservation properties of the method. Lagrangian tracking ideas are also being explored to improve the accuracy of low order methods for the LS advection (Enright et al., 2005).

Much of the research on VOF methods has focused on obtaining higher accuracy and better representations of the interface geometry. The original piecewise linear interface reconstruction technique (PLIC) (Youngs, 1982) has been improved upon using parabolic (PROST) (Renardy and Renardy, 2002) and least squares (Puckett et al., 1997) techniques. A nice set of comparisons presented in (Gerlach et al., 2006) indicated that the CLSVOF was generally superior than most state-of-the-art reconstruction techniques based purely on VOF. Other notable comparisons of reconstruction algorithms include (Rider and Kothe, 1995; Pilliod and Puckett, 1997; Rider and Kothe, 1998; Scardovelli and Zaleski, 2003)

The FT research has also continued to mature so that three-dimensional simulations of problems with complex topological changes are now possible. A recent set of comparisons and a freely available library of FT tools are described in (Du et al., 2006).

Other recent directions in LS research includes the use of various methods for enriching the finite element space locally (Coppola-Owen and Cordina, 2005; Chessa and Belytschko, 2003). The particle finite element methods of (Idelsohn et al., 2006) is a promising new Lagrangian technique that may challenge Eulerian methods even with respect to robustness.

3.2 Recent work on multiphase flow modeling

Recently, (Kadioglu et al., 2005) used LS methods for modeling underwater explosions requiring both compressible and incompressible flow over a wide range of Mach number. Of particular interest to inland navigation is (Price and Chen, 2006), which considers a standard LS formulation of two-phase flow for free surface waves. Reynolds-averaged Navier-Stokes equations are used to model the fluid flow while a smoothed

Heaviside function is used for material properties (surface tension is neglected). The signed distance property is preserved by time marching the eikonal equation to equilibrium. Problems considered include oscillating flow in a tank (sloshing), a dam break problem, and a ship hull moving in calm water. Another interesting application is the physics-based simulations described in (Irving et al., 2006), which combines some aspects of shallow-water modeling with three-phase Navier-Stokes/solid body modeling.

3.3 Modeling with unstructured tetrahedral meshes

Most of the the methods above are compatible with unstructured meshes, but much of the work has been carried out on Cartesian meshes. The LS method was extended to triangular and tetrahedral meshes in (Barth and Sethian, 1998). That method was extended to air/water flow in porous media in (Holm and Langtangen, 1999). Recently (Nagrath et al., 2005) use stabilized finite element for two-phase flow using LSs with a smoothed Heaviside function for material properties. A discontinuous Galerkin method appropriate for unstructured meshes is given in (Marchandise et al., 2006). VOF methods have also been extended to triangular and tetrahedral meshes (Aliabadi et al., 2003; Tezduyar et al., 1998).

4 Conclusions

We have reviewed a range of methods for accurately and efficiently solving two- and three-phase boundary problems. There is as yet no consensus on a best method. Instead, there is still much activity in the area of computational physics and engineering directed at deriving improved algorithms by combining mass/volume conservation, particle tracking, and LS methods. Given that state of affairs we conclude that

1. A mass conservative hybrid method organized around a core LS implementation is the most practical choice for initial development, having a good mix of robustness, accuracy, and efficiency. Additionally, the tools will have a wide range of applicability outside of two- and three-phase flow.
2. Including Lagrangian (particle path) information has consistently been a route toward higher accuracy results so that some form of particle tracking will likely also be involved in an effective algorithm. We should begin experimenting with both hybrid particle-LS methods and the more complex open source FT implementations.
3. Completion of a two-phase test set (e.g. (Rider and Kothe, 1995; Du et al., 2006)) should be the highest priority for the next phase of the project. A test set will allow quantitative studies of accuracy and efficiency on problems of concern to inland navigation as well as guide laboratory and field data collection for model validation.

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