Implementation of mass/heat transfer boundary conditions on a moving boundary

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Introduction

Industrial applications of fluid flows with free surfaces are ubiquitous: applications include casting, container filling, extrusion and fluid jetting devices. The accurate determination of these free surfaces is important especially if the flow itself is determined by the position and curvature of the free surface, as it would be if surface tension were significant. It is also essential that any numerical algorithm can cope with merging, folding or separation of free surfaces.

Over the years a number of computational techniques have been developed for solving free surface flows (see, e.g. Shyy et al. (1996)). These may be broadly divided into two categories: interface tracking methods and front-capturing methods. Front or shock-capturing methods are usually associated with compressible fluids; these methods are now extremely sophisticated, explicitly enforcing monotonicity through a nonlinear step while simultaneously maintaining high order. The reader is referred, for instance, to the books by Leveque (1992) and Hirsch (1998).

The Unilever Study Group problem was however, concerned with incompressible flows and we shall focus on front tracking methods. The purpose of this report is two-fold: firstly it provides an up to date survey of the literature of the many approaches that have been proposed; but, knowing that foodstuff is generally a low(ish) viscosity non-Newtonian shear thinning fluid, it also provides a simple, but we believe a perfectly adequate approach to relatively low Reynolds number multiple free surface flows.

Tracking methods may be subdivided into front-tracking and volume-tracking. If high accuracy is required it is generally accepted that front-tracking is needed, when the interface itself is described by additional computational elements. Although the basic idea goes back to Richtmyer and Morton (1967), its primary implementation has been through the work of Glimm and his co-workers (see, eg Glimm et al. (1988)). They represent the moving front by a connected set of points, which form a moving internal boundary. To calculate the evolution inside the fluid in the vicinity of the interface, an irregular grid is constructed and a special finite difference stencil is used on these irregular grids. Authors who have used this approach to different flow regimes include Chern et al. (1986), Daripa et al. (1988), Moretti (1987) and Peskin (1977) (also Fauci and Peskin (1988), and Fogelson and Peskin (1988)). In Peskin's work the connected set of particles carry forces which are adjusted to achieve a specific velocity at the interface. Within this category one might include the so-called boundary integral or boundary element methods and the vortex-in-cell (VIC) method. Boundary integral methods can be effective when inertia forces are negligible (see, for instance, Baker and Moore (1989) or Tsai and Miksis (1994) who solve successfully the axisymmetric problem of gas bubbles rising in a liquid). The vortex-in-cell method, normally used for homogeneous flows, has been extended to cope with weakly stratified flows (Meng and Thomson (1978)) and arbitrary stratification (Tryggvason (1988)). More recently Unverdi and Tryggvason (1992) described a front-tracking method for incompressible, viscous, multi-fluid flows in which the interface is explicitly tracked but maintains a distinct thickness dependent upon the mesh size. The main advantage of this approach is that interfaces can interact in a rather natural way, since gradients simply add or cancel as the grid distribution is constructed from the information carried by the tracked front.

Another approach which has found favour is the level set approach. This would appear to have been first introduced by Osher and Sethian (1988). The level set function is typically a smooth function which eliminates the sorts of problems, like oscillations, that conventional difference schemes often have. It also gets rid of having to add or subtract points to a moving grid and it automatically takes care of merging and breaking up of an interface. More recently, Sussman et al. (1994) has combined the level set method with projection methods (see, eg Bell and Marcus (1992)) to avoid explicitly tracking the interface. A level set approach has also been applied to three-dimensional two-phase flows by Beux and Banerjee (1996).

Volume-tracking methods can be further subdivided into Marker and Cell (MAC) methods and Volume-of-fluid (VOF) methods. Indeed the original MAC method was one of the first such tracking methods dating back to Harlow and Welsh (1965). Both these classes of methods are still popular and, although they suffer from not being able to accurately provide a surface interface, arguably this is less important today - a 100 x 100 x 100 grid is possible on a good workstation and will certainly be easily feasible on even a modest one in the next few years. With the MAC method virtual marker particles are pushed forward according to the Eulerian fluid calculation (with appropriate bilinear interpolation for the velocity components) and it is these that define the fluid region and hence the interface. Ths Simplified Marker and Cell (SMAC) was introduced by Amsden and Harlow (1970). Over the intervening years research into this method has continued, see for example Viecelli (1971), Hirt and Shannon (1971) who also use the immersed boundary technique to handle its interaction with the underlying grid.

Possibly the first Volume-in-fluid type code was the Simple Line Interface Calculation (SLIC) of Noh and Woodward (1976). This was employed by Chorin (1980) to model flame propagation, and later by Ghoniem et al. (1982) and Sethian (1984) to model turbulent combustion. However, one usually associates Hirt and Nichols (1981) with the VOF method, whereby a volume fraction is convected forward with the fluid. This then led to many variants and descendants, namely, SOLA-VOF (Nichols et al. (1980)), NASA-VOF 2D (Torrey et al. (1985)), NASA-VOF3D (Torrey et al. (1987)), RIPPLE (Kothe and Mjolsness (1992), Koth et al. (1991)) and Flow 3D (Hirt (1988)). These have been widely used in industrial applications. Most recently, an interesting idea of a second order VOF tracking method, employing an approximate projection operator, has been put forward by Puckett et al. (1997)).

Recently, Tomé and McKee (1996) (see also Tomé et al. (1997)), motivated by industrial filling processes, returned to the SMAC methodology and developed the GENSMAC code. GENSMAC simulates incompressible time dependent fluid flows in

Cartesian coordinates within arbitrary, user specified two-dimensional domains. In addition, it can handle free-slip and no-slip boundary conditions, there can be a number of inflows and outflows, and a number of arbitrary shaped obstacles can be contained within the general flow domain. GENSMAC has been modified to cope with axisymmetric flow (Tomé et al.); and the techniques of solid modelling have been applied to permit, through a graphic interface, enhanced flow visualization (Castelo et al.). A full three dimensional code in an arbitrary domain is under development.

A methodology

We shall briefly describe the MAC and VOF Eulerian codes. Briefly the technique involves the following steps:

1. Use the Euler method to compute $\tilde{\mathbf{u}}$ from $\dfrac{\partial \tilde{\mathbf{u}}}{\partial t} + (\tilde{\mathbf{u}} \cdot \nabla)\tilde{\mathbf{u}} = -\nabla p + \dfrac{1}{\mathrm{Re}}\nabla^2 \tilde{\mathbf{u}} + \mathbf{f}$.
2. Solve $\nabla^2 \psi = -\nabla \cdot \tilde{\mathbf{u}}$ where $\mathbf{u} = \tilde{\mathbf{u}} + \nabla \psi$ (NB: $\nabla \cdot \mathbf{u} = 0$).
3. Compute new particle positions using $\dfrac{d\mathbf{x}}{dt} = \mathbf{u}$. (MAC approach).

or

4. Compute volume of fluid via a convection equation (VOF approach).

To illustrate how to construct a simple (but in our view for our purposes, adequate) free surface, we shall consider the sessile drop.

meth

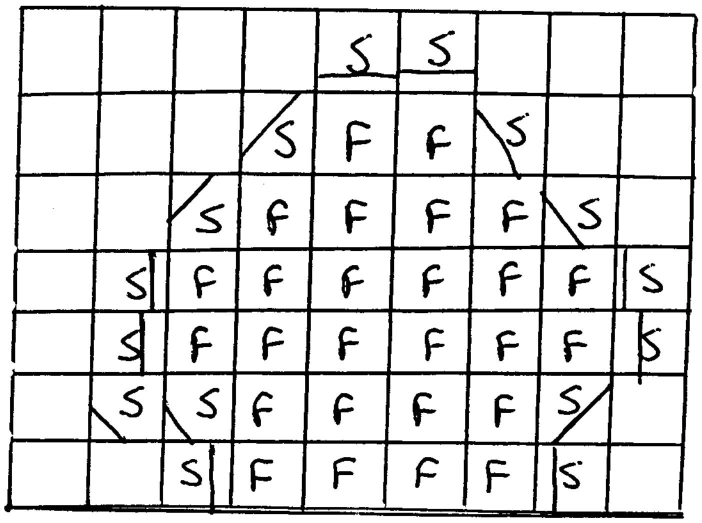

Diagram 1 – Sessile Drop

VOF approach

Surface cells have $F_i (0 \leq F_i \leq 1), i = 1, 2, \ldots, n$.

For $i = 1(1)n$ do

Determine the orientation

(a) One neighbour a full cell

$$N, S \Rightarrow \text{line } \| E, W$$

$$E, W \Rightarrow \text{line} \| N, S$$

(b) Two neighbours a full cell

$$NE, NW, SE, SW @ 45^\circ$$

(c) Otherwise mesh to coarse – refine.

diag1

The application of the heat/mass transfer boundary condition may be achieved as follows: As an example consider diagram 2 and the boundary condition

$$K\nabla T \cdot \mathbf{n} = h(T - T_g)$$

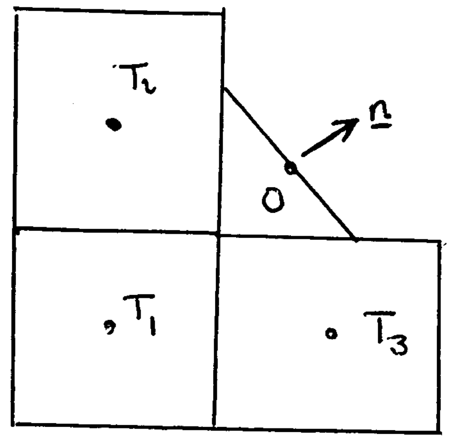

Diagram 2

For the example given in diagram 2 the boundary condition is

$$K\left(\frac{1}{\sqrt{2}}\frac{\partial T}{\partial x} + \frac{1}{\sqrt{2}}\frac{\partial T}{\partial y}\right) = h(T - T_g) \tag{1}$$

and an acceptable discretisation is

$$\frac{K}{\sqrt{2}}\left(\frac{T_3 - T_1}{\Delta x} + \frac{T_2 - T_1}{\Delta y}\right) = h(T_1 - T_g). \tag{2}$$

We may consider (2) applied at node 0 as a consistent approximation to (1) – straightforward Taylor series expansion verifies this.

heatmass

MAC Method

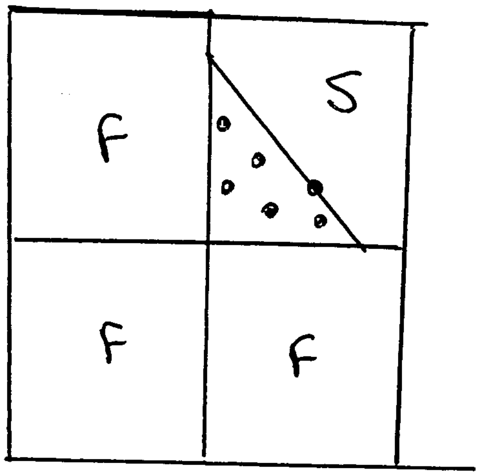

Diagram 3

With the orientation illustrated in diagram 3, choose a straight line with gradient $-\frac{1}{\sqrt{2}}$ and passing through any particle. Iterate on all particles in S to obtain the best one–sided linear fit.

A similar approach of using a straight line with gradient $-\frac{1}{\sqrt{2}}$ may be used for the VOF method.

mac

The same ideas may be extended to surface tension where we require a C^2 curve (at least locally).

For the MAC method consider diagram 4.

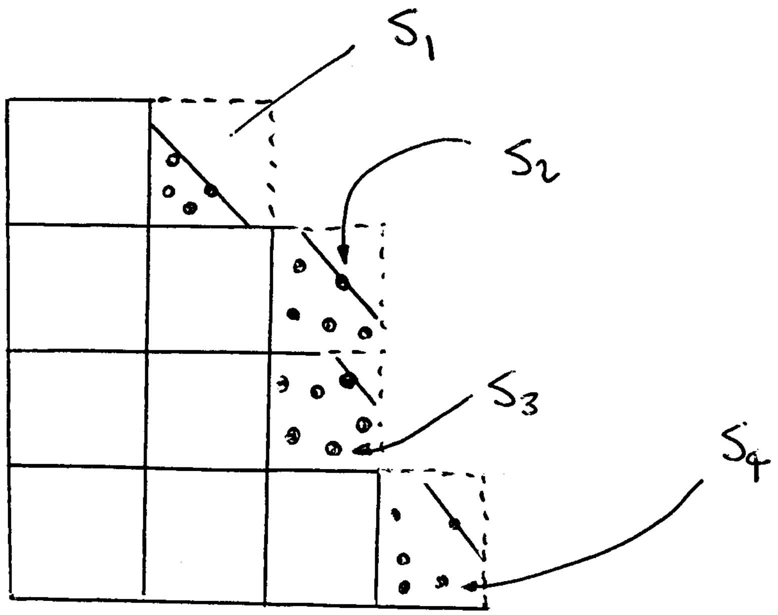

Diagram 4

Consider the union of all particles (points) in S_1, S_2 and S_3.
Determine the best (say L_2) one–sided approximation

$$\text{ie.} \min_{a,b,c} \sum_{i=1}^{N} [y_i - (ax_i^2 + bx_i + c)]^2$$

s.t.

$$y_i - (ax_i^2 + bx_i + c) \geq 0$$

(sign depends on orientation)

mac2

Evaluate the curvature at the mid–point of the arc passing through S_2. Now consider S_2, S_3, and S_4 and continue.

Note: L_1 approximation gives rise to a linear programming problem. Consider

$$\min_{\mathbf{a}} \sum_{j=1}^{N} |y_j - \sum_{i=0}^{m} a_i x_j^i|$$

subject to $y_j - \sum_{i=0}^{m} a_i x_j^i \geq 0, j = 1, 2, \ldots, N$.

Clearly the objective function may be rewritten as

$$\sum_{j=1}^{N} y_j - N a_0 - \sum_{i=0}^{m} a_i \sum_{j=1}^{N} x_j^i.$$

Thus the problem may be stated as

$$\max_{\mathbf{a}} [N a_0 + \sum_{i=1}^{m} a_i (\sum_{j=1}^{N} x_j^i)]$$

subject to $A\mathbf{a}^T \leq (y_1, y_2, \ldots, y_N)^T$ where

$$A = \begin{pmatrix} 1 & x_1 & \ldots & x_1^m \\ 1 & x_2 & \ldots & x_2^m \\ \vdots & \vdots & & \vdots \\ 1 & x_N & \ldots & x_N^m \end{pmatrix}$$

N$\times m$

Application of Surface Tension on VOF

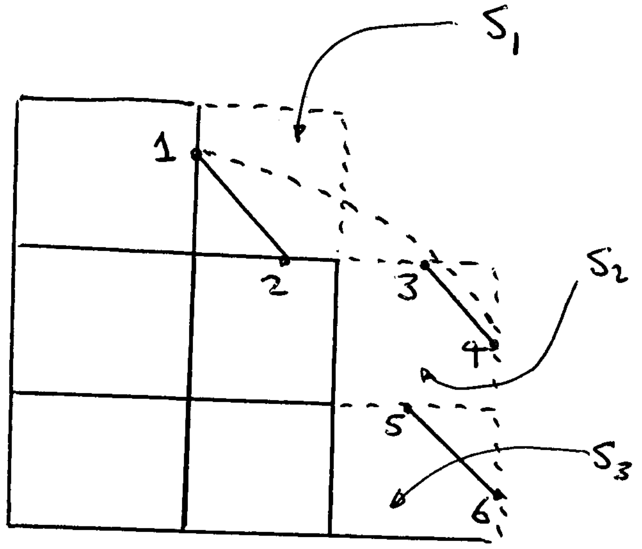

Diagram 5

Determine the points $1, 2, \ldots, 6$. Form a quadratic through points 1 and 6 and specify it exactly by making it pass through all points in turn, checking at each time to see if it is one–sided.

Evaluate the curvature @ S_2 (mid-point of arc), parametrically or otherwise, and apply the boundary condition on the free surface

$$-\sigma_{ij} n_i n_j = p_a + 2\gamma\kappa$$

or

$$-p\delta_{ij} + \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) = p_a + 2\gamma\kappa$$

To evaluate the curvature at S_3 consider S_2, S_3 and S_4.

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