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A Technique for Including Surface Tension Effects in Hydrodynamic Calculations

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ABSTRACT

A technique is described for including the effects of surface tension in time-dependent, hydrodynamics calculations. The fluid interface is initially marked with a sequence of interface particles, which thereafter move through the computation mesh at the local fluid velocity. At each calculation cycle these particles are joined by sections of cubics in order to determine the orientation of the fluid interface. From this orientation the surface tension contribution to the fluid acceleration is determined.

1. INTRODUCTION

Surface tension plays an important role in a large variety of fluid flows. These range from rather small scale phenomena, such as the breakup or coalescence of raindrops, to large scale flows, like the motion of fuel in a space vehicle under low gravity conditions. Laboratory studies of these phenomena are often complicated, however, by problems encountered in making measurements or in simulating the actual physical situation. For reasons such as these, it is desirable to include the effect of surface tension in numerical fluid flow studies.

In this paper we describe a technique for including the surface tension contribution to time-dependent, multi-material or free surface flow calculations. This technique has been successfully applied to the study of the effects of surface tension on the linear and nonlinear phases of two fluid Rayleigh–Taylor instability [1]. The results of the linear study were found to be in good agreement with the analytic predictions of Chandrasekhar [2], thereby establishing confidence in the accuracy of the method. However, the greatest test of the method came in its application to the highly contorted flow of the nonlinear regime. These tests indicated that the method is well suited to such complicated flow problems.

The description of the technique for computing the surface tension force is presented in detail in this paper. Section 2 explains the basic method for resolving

581/4/1-7

the orientation of the fluid interface and also includes some auxiliary subprograms that have proved to be extremely useful in the calculation of highly contorted flows. Section 3 describes the method used to compute the surface tension force, under normal and unusual circumstances, and for plane as well as cylindrically symmetric coordinate systems. The entire computation is placed in perspective in Sec. 4, indicating the order in which the various subprograms are executed and the situations where they are needed.

2. Resolving the Fluid Interface

A. Interface Particles

The successful calculation of surface tension forces requires a detailed knowledge of the orientation of the fluid interface. In finite difference calculations tied to fixed (or for that matter, moving) calculation meshes, the position of a fluid interface is not sufficiently well resolved to make accurate estimates of surface curvature. In the technique described here, this deficiency is overcome by the use of interface particles. These are marker particles that are initially laid out in order along the fluid interface and thereafter mark the interface as they move at the local fluid velocity. This is their sole function in the numerical computation.

The magnitude and direction of the surface tension force are ordinarily determined from the orientation of a curve that fits the interface particles (Section 2-B), rather than from the orientation of the particles themselves. However, the degree of accuracy, by which this curve actually represents the fluid interface, depends to some extent upon the proper initial placement and spacing of the interface particles. We offer no precise rules in this regard, since the initial particle arrangement should be chosen to fit the problem under consideration. Instead, we present certain guidelines that were found to be useful in the calculations of Ref. [1], which were concerned with the effect of surface tension forces on the growth of Rayleigh–Taylor and Kelvin–Helmholtz instabilities.

In these calculations the interface was subjected to a great deal of stretching along the vertical mesh boundaries. In anticipation of this, the particles were initially packed more closely in the cells adjacent to these boundaries than in the interior of the mesh. The spacing was $0.2s$ in two cells adjacent to the left and to the right boundaries, and $0.4s$ in interior cells, s being the mesh interval. Thus, in the twenty-cell wide mesh the interface was initially represented by about sixty particles, but this could be changed in the course of the calculation through a facility for adding or deleting particles (Section 2-E).

Variations on this spacing were tried and found to be less satisfactory. When the spacing was doubled, so that half as many particles were used, it was found

that short wavelength perturbations of the interface could not properly be resolved. If the perturbation were such that only a few interface particles were displaced from an otherwise smooth sequence, then the curve fitting technique produced an interface that had a jagged appearance, not only in the vicinity of the perturbation, but in the adjacent smooth sections as well. These erroneous curvatures would then produce erroneous surface tension forces. These difficulties disappeared when the resolution was increased, but it was important not to overcorrect. For when the particles were too closely packed, any slight fluctuation of particle position away from a smooth arrangement could give rise to a large curvature of the interface. In this way, an insignificant wiggle in the line of particles could produce a strong surface tension force. A proper balance was achieved when the particles were spaced sufficiently close to resolve the smallest physical disturbance expected in the finite difference calculation, but not significantly closer than this.

In Ref. [1] it was possible to obtain good surface resolution right up to the mesh boundaries. This was accomplished by placing the first and last particles a very small distance, $0.0001s$, away from the boundaries. Since these were lines of symmetry, the particles moved tangent to the boundaries throughout the calculation.

The velocity at which the interface particles are moved through the finite difference mesh is determined from an area-weighted average of the local cellular velocities. The procedure is illustrated in Fig. 1 for the case of cell centered

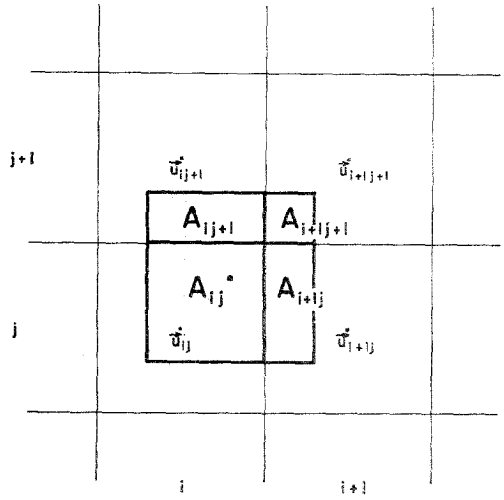

FIG. 1. The procedure for determining the area weighted average of local cellular velocities for the purpose of moving interface particles. A cell-size box is centered about the particle and the percentage of area overlap in adjacent cells gives the weighting to be applied to those cell velocities.

velocities. A rectangle the size of a calculation cell is placed over and centered at the particle. This rectangle overlays parts of four neighboring cells. In the figure these are cells ij, $i+1j$, $ij+1$, and $i+1j+1$. The velocity with which particle k is moved is given by

$$\mathbf{u}_k = \frac{1}{A}\left(A_{ij}\mathbf{u}_{ij} + A_{i+1j}\mathbf{u}_{i+1j} + A_{ij+1}\mathbf{u}_{ij+1} + A_{i+1j+1}\mathbf{u}_{i+1j+1}\right).$$

where A is the mesh area and the subscripted A's give the overlapped areas of adjacent cells. Detailed area weighting formulas may be obtained from Ref. [3] for cell centered velocities or from Ref. [4] for boundary centered velocities.

B. *Interface Line*

For the purpose of determining slopes and curvatures along the fluid interface, the interface particles are connected at each cycle of calculation to form an interface line. The particles are joined by sections of cubics through the application of a spline fit interpolation scheme [5]. (This reference describes the excellent approximation properties of the spline fit technique.) Consider an interface that is represented by an ordered sequence of interface points:

$$(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n),$$

that is single valued in x. Following Walsh *et al.* [5], we represent the interface line by an approximating function, $y(x)$, that has second derivatives, M_k, $k = 1, 2, \ldots, n$, at the interface points. Between the points, the second derivative varies linearly,

$$y''(x) = M_{k-1}\frac{x_k - x}{l_k} + M_k\frac{x - x_{k-1}}{l_k} \qquad x_{k-1} \leqslant x \leqslant x_k \tag{1}$$

where $l_k = x_k - x_{k-1}$. Integrating twice and requiring that $y(x_k) = y_k$ gives

$$y'(x) = -M_{k-1}\frac{(x_k - x)^2}{2l_k} + M_k\frac{(x - x_{k-1})^2}{2l_k} + \frac{y_k - y_{k-1}}{l_k} - \frac{(M_k - M_{k-1})\,l_k}{6}, \tag{2}$$

$$y(x) = M_{k-1}\frac{(x_k - x)^3}{6l_k} + M_k\frac{(x - x_{k-1})^3}{6l_k} + \left(\frac{y_k}{l_k} - \frac{M_k l_k}{6}\right)(x - x_{k-1}) + \left(\frac{y_{k-1}}{l_k} - \frac{M_{k-1}l_k}{6}\right)(x_k - x), \tag{3}$$

over the same range in x. The M's are then determined by requiring that the slopes vary continuously at the interface points, i.e., that $y'(x_k -) \equiv y'(x_k +)$. This yields a system of n simultaneous equations,

$$\frac{l_k}{6} M_{k-1} + \frac{l_k + l_{k+1}}{3} M_k + \frac{l_{k+1}}{6} M_{k+1} = \frac{y_{k+1} - y_k}{l_{k+1}} - \frac{y_k - y_{k-1}}{l_k}, \tag{4}$$

which, together with the two end conditions, can be solved for the M's.

In the calculations that have been performed to date, the interface line has been constrained to begin at the left boundary of the mesh and to terminate at the right boundary. Since these boundaries are lines of symmetry, we require that the interface line intersect them normally. This is equivalent to placing an imaginary particle outside each boundary in symmetry with the first particle inside the boundary and making the second derivative the same at the two points. Thus, when the left boundary coincides with $x = 0$ and the right boundary with $x = L$, we construct two imaginary points:

$$\begin{aligned} x_0 &= -x_1 & \qquad x_{n+1} &= 2L - x_n \\ y_0 &= y_1 \qquad \text{and} & y_{n+1} &= y_n \\ M_0 &= M_1 & M_{n+1} &= M_n . \end{aligned} \tag{5}$$

With these substitutions, the system of equations (4) becomes

$$\begin{aligned} \left(x_1 + \frac{l_2}{3}\right) M_1 + \frac{l_2}{6} M_2 &= \frac{y_2 - y_1}{l_2} \\ \frac{l_2}{6} M_1 + \frac{l_2 + l_3}{3} M_2 + \frac{l_3}{6} M_3 &= \frac{y_3 - y_2}{l_3} - \frac{y_2 - y_1}{l_2} \\ \frac{l_3}{6} M_2 + \frac{l_3 + l_4}{3} M_3 + \frac{l_4}{6} M_4 &= \frac{y_4 - y_3}{l_4} - \frac{y_3 - y_2}{l_3} \\ &\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ \frac{l_n}{6} M_{n-1} + \left(\frac{l_n}{3} + L - x_n\right) M_n &= -\frac{y_n - y_{n-1}}{l_n} \end{aligned} \tag{6}$$

The coefficients of the M's form a tri-diagonal matrix for which Peaceman and Rachford [6] give a convenient explicit inversion technique. When the M's are determined using that technique, one has sufficient information to solve Eqs. (1)–(3) for any abscissa in the range, $0 \leqslant x \leqslant L$. This provides the information needed to determine the magnitude and direction of the surface tension force (Section 3) at any point along the interface line.

Various other boundary conditions could be employed in this interface treatment. Of particular interest for engineering applications is the static meniscus end condition. This is illustrated in Fig. 2 for the case of a wall located at $x = 0$. The interface makes a constant contact angle, φ, with this wall at all times. To incorporate this condition, one might proceed in a manner similar to that used

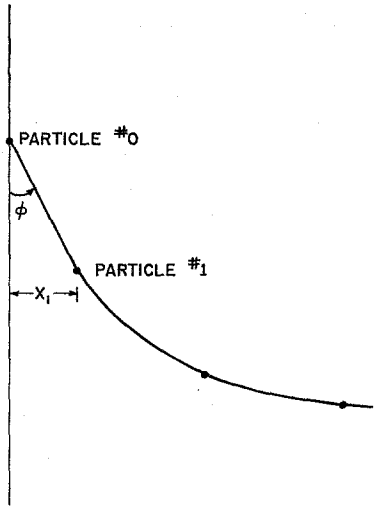

FIG. 2. The figure illustrates a procedure for incorporating a static meniscus boundary condition in spline fit calculations.

above for a line of symmetry. The first real interface particle, #1, would be placed a distance x_1 from the wall, where x_1 measures the width of the (approximately) linear part of the meniscus. An additional particle, #0, can then be imagined to lie on the wall at such a position that the interface line connecting it with the first real particle has slope $-\cot\varphi$. By evaluating Eq. (2) at $x = 0$, $k = 1$, one may verify that this requires that $M_0 = -\frac{1}{2}M_1$. Particle #0 is then defined by

$$\begin{aligned} x_0 &= 0, \\ y_0 &= y_1 + x_1 \cot\varphi, \\ M_0 &= -\tfrac{1}{2}M_1 . \end{aligned} \tag{7}$$

Using this end condition, the first equation in (6) becomes

$$\left(\frac{x_1}{4} + \frac{l_2}{3}\right) M_1 + \frac{l_2}{6} M_2 = \frac{y_2 - y_1}{l_2} + \cot\varphi.$$

This method of including static meniscus end conditions has not yet been applied in numerical calculations. Before use is made of it, it should be carefully tested for accuracy and completeness. One possible shortcoming would be the change in the width of the meniscus due to the motion of particle #1 relative to the wall. This could be corrected by relocating this particle to the point on the interface line that lies the initial distance, x_1, from the wall after each cycle of calculation.

C. *Subdividing the Interface Line*

In the treatment above, it is assumed that the interface line is fitted to a sequence of interface particles that is monotonic in x. In fact, however, it is quite likely that in highly contorted flows the line of particles could become folded back upon itself and be double valued in x. In that case infinite slopes would be obtained and the spline fit technique could not be applied.

In order to be able to calculate such complicated fluid flows, a technique for subdividing the interface particles into monotonic subsequences has been included in the surface tension treatment. The entire line of particles is tested and subdivisions are determined before the spline fitting begins. The criterion for changing from one abscissa to another is that the slope of straight line segments connecting the particles exceed 1.5 in magnitude for five contiguous particles. Thus one would change from a subsequence of particles in which x is the abscissa to one in which y is the abscissa at particle k if

$$\left| \frac{y_{i+1} - y_i}{x_{i+1} - x_i} \right| > 1.5, \qquad i = k, k+1, k+2, k+3, k+4,$$

and

$$\left| \frac{y_k - y_{k-1}}{x_k - x_{k-1}} \right| < 1.5.$$

This criterion was arrived at as the result of experimentation in calculations of the effect of surface tension on Rayleigh–Taylor instability [1]. The test was found to be sufficiently severe to avoid unnecessary changes in abscissa in that calculation. For other calculations it may be less appropriate. In particular, if the particles are widely spaced, the requirement of five successive slopes exceeding 1.5 in magnitude may be excessive.

In the calculation of Ref. [1], it is quite common to have three or five (the number is always odd since the interface is constrained to begin and end with a subsequence monotonic in x) separate sequences when the fluid interface becomes extended and contorted with time. The roles of abscissa and ordinate are interchanged in alternate sequences, but each sequence can be either monotone increasing or

decreasing in the abscissa. Each is designated as a separate array in storage, with its increasing or decreasing character indicated by a simple logic test. When a sequence contains fewer than five interface particles, the spline fit technique should not be used. In those cases, the surface tension force is calculated through the use of an alternative method (Sections 3-B and D).

A separate spline fit is computed for each subsequence of the interface line, and it is desirable that these sections of the curve fit together as smoothly as possible. Experience has shown that an important consideration for smooth joining of segments is that the break in the interface line be made well away from a region of large or infinite slope for either abscissa. Thus, in the example cited above, it would be necessary to insure that the increasing (or decreasing, as the case may be) trend in x extend to particles $k + 1$ and $k + 2$, and that the trend in y extend to $k - 1$ and $k - 2$. If this were not done, one might introduce serious error in the application of the boundary condition at the juncture.

Two different types of boundary conditions have been tested at break points. In both, the spline fit determination is made as though the curve passed through the first particle beyond the break (particle $k + 1$ for the x subsequence above), but they differ in the manner in which the second derivative (M_{k+1}) is defined at that point. In the first approach, M_{k+1} is determined by taking finite differences of the coordinates of k, $k + 1$ and $k + 2$, i.e.,

$$M_{k+1} = \frac{2}{x_{k+2} - x_k}\left(\frac{y_{k+2} - y_{k+1}}{x_{k+2} - x_{k+1}} - \frac{y_{k+1} - y_k}{x_{k+1} - x_k}\right), \tag{8}$$

whereas, in the second approach,

$$M_{k+1} = M_k\,. \tag{9}$$

The first proved to be unacceptable because of the very large slopes encountered at break points, but the second method has worked quite well and is recommended.

D. *Smoothing*

In the original formulation of this surface tension technique, it was anticipated that the interface particles would require smoothing prior to each spline fit. Such has not proved to be the case. In fact, particle smoothing has been needed only very occasionally, even when calculating highly contorted flows. It has been used to smooth out flexures in the interface line that are of such short wavelength that they would not likely be resolved in the surface tension computation. In Ref. [1], these flexures were usually associated with very short wavelength Rayleigh–Taylor instabilities or with nearly right angle interface curves in the neighborhood of Kelvin–Helmholtz instabilities.

The most difficult aspect of smoothing short wavelength interface flexures is sensing their existence. This is done by comparing the value of the second derivative of the interface curve, as calculated by the spline fit technique, with a suitable criterion. To determine this criterion, note that the contribution of the surface tension force to the magnitude of the fluid acceleration is like

$$\left| \frac{d\mathbf{u}}{dt} \right| \rightarrow \frac{T}{\rho_{\text{av}}} \, | \kappa(\mathbf{r}) | \, \delta(\mathbf{r} - \mathbf{r}_i), \tag{10}$$

where T is the surface tension coefficient associated with the two fluids, ρ_{av} is the average density, $\kappa(\mathbf{r})$ is the curvature of the interface at $\mathbf{r}$, and $\delta(\mathbf{r} - \mathbf{r}_i)$ is the Dirac function that limits the surface tension effect to the locality of the interface, $\mathbf{r}_i$. In finite difference formulation this becomes

$$\left| \frac{\delta u}{\delta t} \right| \rightarrow \frac{T \, | \, \kappa \, |}{\rho_{\text{av}} s}, \tag{11}$$

where s is the mesh interval. For accuracy, we require that

$$\frac{| \, \delta u \, | \, \delta t}{s} < 1.$$

In plane coordinates this implies that

$$\frac{| \, y'' \, |}{[1 + (y')^2]^{3/2}} = | \, \kappa \, | < \frac{\rho_{\text{av}}}{T} \frac{s^2}{\delta t^2}.$$

The worst case is when $y' = 0$. Therefore, smoothing is applied at particle k when

$$| \, M_k \, | > \frac{\rho_{\text{av}}}{T} \frac{s^2}{\delta t^2}. \tag{12}$$

The magnitude of each second derivative, M_k, determined from the spline fit computation, is compared with this parameter. If, for any particle in the sequence, the second derivative exceeds this criterion, smoothing is applied only to the particular particle (or particles) at which the criterion is exceeded. Its ordinate is changed by an amount determined from a five point least square fit to a parabola; the five points being the interface particle in question and the two nearest interface particles in either direction. The method used is a straightforward extension of that described by Scarborough [7] to the case of unevenly spaced abscissas.

When smoothing has been applied to all of the particles that require it, the spline fit computation is repeated. Again, the second derivatives are tested against the criterion (12) and smoothing is repeated if necessary. If, after four

cycles of smoothing and spline recomputation, there are further violations of the criteria, they are ignored. Generally, this situation would indicate that some additional treatment, such as improved particle spacing (Section 2-E) or improved boundary conditions at subsequence break points (Section 2-C), is required.

E. *Deleting or Adding Particles*

The interface particles, which were evenly spaced along the fluid interface initially, do not always retain that even spacing. After long periods of calculation, parts of the interface may be sparsely populated with particles, while in another section of the interface the particles may be very closely packed. Either extreme is bad. When the particle separations are too large, the interface is not well resolved. When they are too small, minor fluctuations in particle position can give rise to strong surface tension forces.

The check on particle spacing is the first step in the surface tension calculation. If a pair of particles is separated by more than three times the initial spacing, a new particle is inserted between them. If the spacing between successive particles is less than one third the initial particle spacing, one of the particles is deleted. This can be accomplished simply by determining which of the two particles is closest to its other neighbor, removing it from the storage array, and adjusting the array to account for its absence. The coordinates of the remaining interface particles are unchanged.

Inserting a new particle in an interface line is slightly more difficult. Tentatively, its coordinates are taken to be the average coordinates of its neighbors. If the interface is curved, however, the new particle may not fit the arc, so its position is adjusted by smoothing. The smoothing technique described in Section 2-D is used for this purpose, and both the x and y coordinates of the particle are moved. When this has been accomplished, the storage array is adjusted to accommodate the new particle.

The facility for adding and deleting interface particles has proved to be of immense value in calculating long-running, highly-contorted flows.

3. Calculating the Surface Tension Force

A. *Plane-Coordinates, Spline Fit*

The surface tension force is directed toward minimizing the surface area of a fluid interface. In plane coordinates the magnitude of this force per unit surface area at a point $\mathbf{r}$ in space is

$$T\kappa(\mathbf{r}),$$

where, as indicated earlier, T is the surface tension coefficient of the fluid pair and $\kappa(\mathbf{r})$ is the curvature of the interface at $\mathbf{r}$. The force is directed normal to the interface, on the concave side.

In numerical calculations, the surface tension effect can be included in two equivalent ways: Either as a boundary condition at the fluid interface or as an accelerative force that is applied only in those portions of the mesh that lie on the fluid interface. The first approach is most appropriate if, in the finite difference technique, boundary conditions are otherwise explicitly applied at the interface. If not, then it is more convenient to include the surface tension as an accelerative force in the Navier–Stokes equation, but with the stipulation that it be applied only in those cells which lie along the fluid interface. This is the approach that was used in Ref. [1] and it is the basis for the description that is presented here.

The calculations of Ref. [1] make use of the two-fluid Marker and Cell [4] numerical technique for incompressible flow studies, which employs the velocity components and the pressure as dependent variables. In that method, the horizontal and vertical components of the velocity are centered on the vertical and horizontal mesh cell edges, respectively. The difference equations are centered about these same points, and therefore these are the places where the components

The arrows on the cell edges mark the locations where the components of the surface tension force are applied. The length of the arrow indicates qualitatively the magnitude of the force component, while the arrowhead shows its direction.

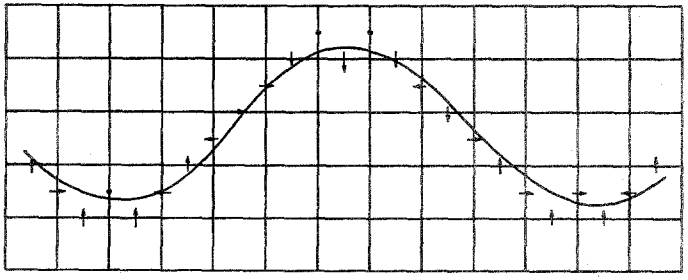

FIG. 3. A fluid interface within a calculation mesh. The arrows on the cell edges mark the locations where the surface tension force is applied.

The surface tension force is actually calculated at points where the interface line intersects lines through cell centers. For example, the y component is computed at each place where the interface line crosses a vertical line through a cell center. The procedure for calculating this component along a sequence of interface

particles monotonic in x is as follows: After the spline fit to the particle positions has been made, one checks the abscissas of the interface particles until two are found that bracket the first cell center, i.e.,

$$x_{k-1} \leqslant \frac{s}{2} \leqslant x_k .$$

The values of $y''(s/2)$, $y'(s/2)$ and $y(s/2)$ are determined from Eqs. (1)–(3), and the magnitude of the surface tension force per unit volume is computed from

$$T\kappa/s = Ty''/s[1 + (y')^2]^{3/2}. \tag{13}$$

The y component can be obtained through multiplication by $[1 + (y')^2]^{-1/2}$. For subsequences monotonic in x, the sign of the y component is the sign of y''. (I.e., where the curve is concave up, the vertical component of surface tension is upward.) Therefore, the y component of the surface tension force at $x = s/2$, $y = y(s/2)$, is

$$ST_y = Ty''/s[1 + (y')^2]^2, \tag{14}$$

where y' and y'' are evaluated at $s/2$. This term is added to the accelerative terms of the y component of the Navier–Stokes equation at the mesh point X, Y, where

$$X = \frac{s}{2}$$

$$Y = \text{the horizontal cell edge such that } \left| Y - y\left(\frac{s}{2}\right)\right| < \frac{s}{2}.$$

The same procedure is applied to determine the vertical component of surface tension in other cells through which the interface line passes. Each time, the abscissa is incremented by s, the bracketing interface particles are determined, and the values of y, y' and y'' are found. These are used to evaluate ST_y and that force component is added to the Navier–Stokes equation at the nearest horizontal cell boundary.

The horizontal component of the surface tension force is determined in a similar way. Beginning with the first particle in the sequence, the ordinates of the interface particles are checked until two are found that bracket a horizontal line through cell centers. The abscissa of the point of intersection is determined by linear interpolation, and the first and second derivatives are evaluated from Eqs. (1) and (2). With these, the x-component of the surface tension force is computed from

$$ST_x = -Ty'y''/s[1 + (y')^2]^2, \tag{15}$$

and applied in the Navier-Stokes equation at the vertical cell boundary closest

to the point of intersection. Succeeding interface particles are tested until two are found whose ordinates again bracket a line through cell centers, and the procedure above is repeated.

If the sequence of interface particles has been subdivided into several subsequences, then the surface tension determinations above are repeated for each subsequence in turn. Only after all of the surface tension contributions from the first subsequence have been computed is the spline fit to the second subsequence made, and similarly for other subsequences. The calculations for monotone decreasing x segments is the same as for monotone increasing x segments, except that particles are incremented in the reverse order (from last to first). For subsequences monotonic in y, the procedure is again similar except that formulas (14) and (15) become

$$ST_y = -Tx'x''/s[1 + (x')^2]^2, \tag{16}$$

$$ST_x = Tx''/s[1 + (x')^2]^2, \tag{17}$$

where $x' = dx/dy$, $x'' = d^2x/dy^2$ at the appropriate point on the curve.

B. *Plane-Coordinates, Non-Spline Fit*

When a subsequence of the interface line contains fewer than five interface particles, one should not use the spline fit method for calculating slopes and curvatures of the interface. An alternative method that can be used under those circumstances involves fitting three consecutive interface points with a circular arc, and using the radius of the circle as the radius of curvature of the interface line.

As in the spline fit calculation, the y and x components of the surface tension force are computed at each point where the interface line crosses a vertical or a horizontal line through a cell center, respectively. The y components are calculated by testing the abscissas of this sequence of interface particles until two are found that bracket the abscissa of a cell center. A test is made to see which of the two particles, say $k - 1$ and k, has an abscissa closest to that of the cell center. Assume that this is particle k. Then we wish to determine the radius of a circle that passes through the coordinates of particles $k - 1$, k and $k + 1$. This is given [8] by

$$R_1 = abc/4[d(d - a)(d - b)(d - c)]^{1/2} \tag{18}$$

where

$$a = [(x_k - x_{k-1})^2 + (y_k - y_{k-1})^2]^{1/2},$$
$$b = [(x_{k+1} - x_k)^2 + (y_{k+1} - y_k)^2]^{1/2},$$
$$c = [(x_{k+1} - x_{k-1})^2 + (y_{k+1} - y_{k-1})^2]^{1/2},$$
$$d = \tfrac{1}{2}(a + b + c).$$

Then y component of the surface tension force per unit volume is then

$$ST_y = (\text{sgn } \zeta)\ T/sR_1(1 + m^2)^{1/2}, \tag{19}$$

where m is the slope of the straight line joining particles $k - 1$ and $k + 1$ and

$$\zeta = m(x_k - x_{k-1}) - (y_k - y_{k-1}).$$

ζ is positive if the circular arc is concave up and negative if it is concave down. The expression (19) contributes to the accelerative terms of the y component of the Navier–Stokes equation at the horizontal mesh boundary closest to particle k.

This procedure is repeated for all of the particles in the subsequence, testing the abscissas of each pair of particles to determine whether they bracket the abscissa of a cell center. If so, the computation leading to expression (19) is repeated for those particles. When all such contributions to vertically directed surface tension forces have been calculated, the determination of x-directed forces is made. This time the ordinates of each pair of adjoining interface particles are tested to determine whether they bracket the ordinate of a cell center. When two such particles are found, the radius of curvature, R_1 is determined as shown above and then the x-component of the surface tension force per unit volume is calculated from

$$ST_x = -m(\text{sgn } \zeta)\ T/sR_1(1 + m^2)^2. \tag{20}$$

The sign of ST_x is positive if the concave side is on the right and negative if it is on the left. Expression (20) contributes to the x-component of the acceleration in the Navier–Stokes equation centered at the nearest vertical mesh boundary to particle k.

C. *Cylindrical-Coordinates, Spline Fit*

In three dimensions the curvature at a point $\mathbf{r}$ on a surface is

$$\kappa(\mathbf{r}) = \frac{1}{R_1} + \frac{1}{R_2}, \tag{21}$$

where R_1 and R_2 are the principal radii of curvature at $\mathbf{r}$. When the surface is cylindrically symmetric, with the axis of symmetry coinciding with the z axis, then one of the R's is the radius of curvature at $\mathbf{r}$ of a curve formed by the intersection of the surface and a plane through the z-axis. This corresponds to the radius of curvature in two dimensions. The other R is the radius of curvature of a curve formed by the intersection of the surface with a cone which is tangent to the surface at $\mathbf{r}$ and has symmetry about the z axis. In this paper, we call the first radius R_1 and the second R_2, and we refer to the corresponding surface tension effects as the transverse and circumferential forces, respectively.

Figure 4 demonstrates the contribution of these two tension effects to the total surface tension force. The figure shows a trace of the fluid interface in a constant θ plane in the r, θ, z coordinate system. Due to angular symmetry about the z axis, one could observe the same trace at all values of θ. At three points, a, b and c, along the curve, a portion of the trace of the tangential cone is shown and the direction of the transverse surface tension force (solid line arrow) and the circumferential force (dashed line arrow) are indicated. Also included are the radial distances to the three points and the normal distances to the axis of symmetry from the points of tangency.

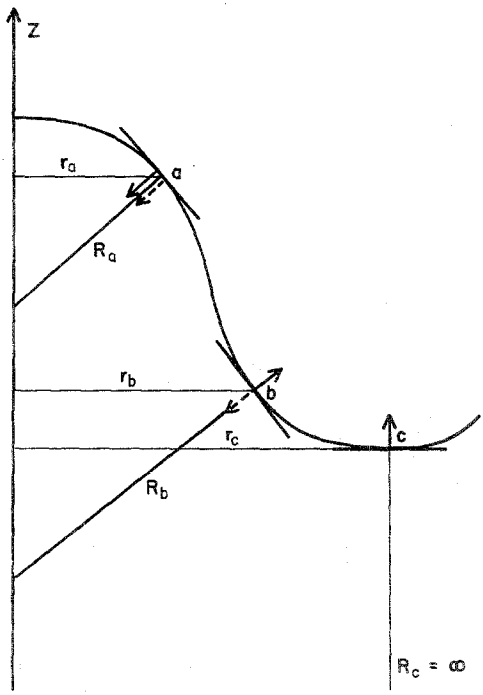

FIG. 4. A trace of the fluid interface in a constant θ plane. The solid line arrows show the direction of the transverse surface tension force at points a, b and c. The dashed line arrows show the direction of the circumferential force.

The nature of the transverse surface tension contribution is clear, since it is identical to the plane coordinate case, but the circumferential force requires some additional discussion. It can be thought of as a tension pull along a ring (formed

by the intersection of the surface with the tangent cone) about the cylindrical axis, tending to reduce the radius of the ring to zero. The direction of this force is therefore normal to the interface in the negative r direction. The magnitude of the radius of curvature associated with this force, R_2, is the normal distance to the axis of symmetry as indicated by the R's in the figure.

The direction of the transverse force is always toward the concave side of the curve. Thus, when the concave side of the curve in a constant θ trace is on the direction of decreasing r, the two forces act together; when it is on the increasing r side, the forces oppose one another. In Fig. 4, point a represents a case where the two forces act in the same direction, while b is a case where they oppose one another. At point c the curve has zero slope, so that the normal distance to the axis of symmetry is infinite and there is no circumferential contribution to the surface tension force.

Very little modification of the surface tension force computation is required in going from plane to cylindrical coordinates. The spline fit computation follows exactly as before. All that is required is the addition of the circumferential contribution to Eqs. (14)–(17), and this necessitates the determination of R_2. For a subsequence of interface points monotonic in r, one can see from Fig. 4 that

$$R_2 = r/\sin \alpha,$$

where $\tan \alpha$ is the slope, z'. Thus

$$R_2 = r[1 + (z')^2]^{1/2}/z'. \tag{22}$$

As the radius of the fluid interface approaches zero, the circumferential surface tension force becomes very large if the slope remains nonzero. This shows, for example, why the final stage of breakup of a Rayleigh jet [9] occurs very rapidly.

Thus, with R_2 given by Eq. (22), we can write the component forms of the surface tension force per unit volume for the case of cylindrical symmetry. Along a sequence of interface points monotonic in r, these are

$$ST_z = \frac{T}{s}\left\{\frac{z''}{[1 + (z')^2]^2} + \frac{z'}{r[1 + (z')^2]}\right\}, \tag{23}$$

$$ST_r = -\frac{T}{s}\left\{\frac{z'z''}{[1 + (z')^2]^2} + \frac{(z')^2}{r[1 + (z')^2]}\right\}. \tag{24}$$

The sign of the z-component of the circumferential surface tension force is the same as the sign of z', while the r-component is negative definite. The signs of the components of the transverse force follow the pattern indicated for Eqs. (14) and (15).

Along a sequence monotonic in z, these components of the surface tension force per unit volume are

$$ST_z = \frac{T}{s}\left\{\frac{-r'r''}{[1 + (r')^2]^2} + \frac{r'}{r[1 + (r')^2]}\right\} \tag{25}$$

$$ST_r = \frac{T}{s}\left\{\frac{r''}{[1 + (r')^2]^2} - \frac{1}{r[1 + (r')^2]}\right\}. \tag{26}$$

D. *Cylindrical Coordinates, Non-Spline Fit*

In Section 3-B a technique was described for calculating the surface tension force along subsequences of the interface line that are too short to accurately apply the spline fit method. That technique applies equally well in cylindrical-coordinates, except that it must be extended to include the circumferential surface tension force. As shown in the previous section, this requires a determination for R_2, the radius of curvature associated with the circumferential force.

This technique makes use of triplets of interface particles for calculating the surface tension forces. As in Section 3-B, we demonstrate the method with three interface particles, which have coordinates (r_{k-1}, z_{k-1}), (r_k, z_k) and (r_{k+1}, z_{k+1}). For this case, Eq. (22) for R_2 becomes

$$R_2 = r_k(1 + m^2)^{1/2}/m, \tag{27}$$

where the slope, $m = (z_{k+1} - z_{k-1})/(r_{k+1} - r_{k-1})$. With the transverse radius of curvature given by Eq. (18), the components of the surface tension force per unit volume are written,

$$ST_z = \frac{T}{(1 + m^2)^{1/2}}\left[\frac{(\text{sgn } \zeta)}{R_1} + \frac{1}{R_2}\right], \tag{28}$$

$$ST_r = -\frac{mT}{s(1 + m^2)^{1/2}}\left[\frac{(\text{sgn } \zeta)}{R_1} + \frac{1}{R_2}\right], \tag{29}$$

where

$$\zeta = m(r_k - r_{k-1}) - (z_k - z_{k-1}).$$

In Eqs. (27)–(29) we always take the positive square root for the term $(1 + m^2)^{1/2}$. Thus R_2 has the same sign as the slope, m. From Eq. (28) we see that the z-component of the circumferential surface tension force also has the same sign as m. The r-component in Eq. (29) is negative definite, however.

4. The Calculation in Perspective

Sections 2 and 3 present a technique for including surface tension effects in numerical calculations. That presentation includes descriptions of several sub-programs, which have proved to be extremely useful in calculations of highly

distorted interface motions but which would not necessarily be needed in studies of less complicated flows. In this section we attempt to put the entire computation in perspective, indicating the order in which the various subprograms are executed and giving some idea of the situations where they would be needed.

In this discussion we assume that the interface particles have initially been placed along the fluid interface at a spacing that is appropriate to the particular problem and that a technique exists for moving these particles through the mesh at each subsequent calculation cycle (see Section 2-A). We concern ourselves here with the procedure for determining at each calculation cycle the components of the surface tension force from the known position of the interface particles. Figure 5 shows a flow diagram that outlines the major steps in such a program.

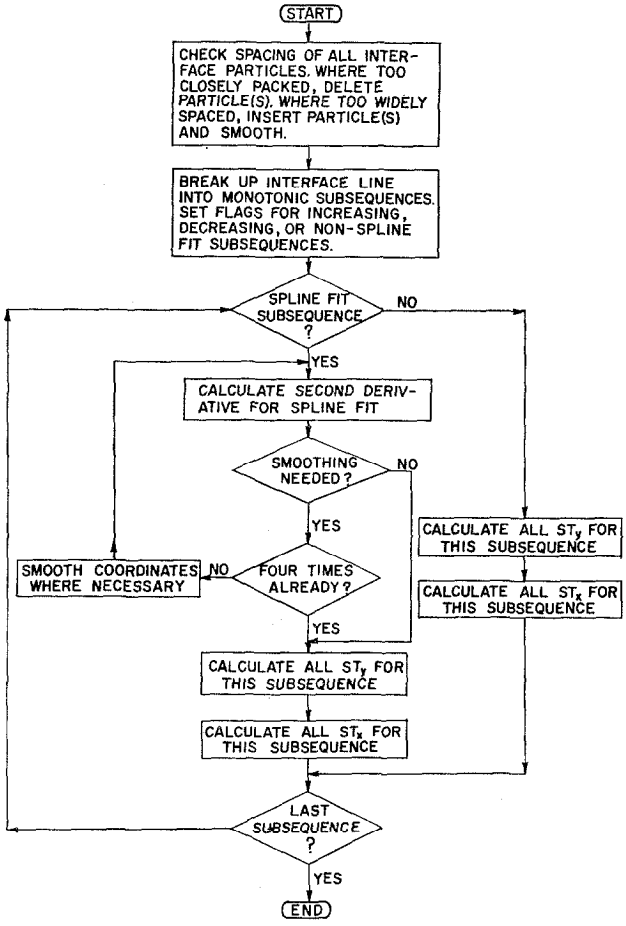

FIG. 5. A flow diagram of a program for surface tension calculation.

The first step in the surface tension computation is a test to determine whether an excess or a scarcity of particles exists anywhere along the interface line

the stretching of the interface and the concentration of particles in certain parts of the interface, particularly near the center of a vortex. The concentrations result from the area weighting technique for determining the particle velocity and are most pronounced in regions where one fluid has a greater velocity tangential to the interface than the other fluid. For this reason, the provision for adding and deleting particles is perhaps essential for the successful long term calculation of highly contorted flows. But in less complicated, uniform shear flows, this portion of the surface tension calculation can be bypassed.

The next major part of the calculation is the subdivision of the ordered sequence of interface particles into subsequences that are monotonic in the x and y (r and z) coordinates. This procedure is necessary in highly contorted flows, since the spline fit technique requires a monotonically varying abscissa and a finite slope. If one could be sure that the interface would not be subjected to strong folding in the problems to which the method would be applied, then this section could be omitted and at least fifty percent of the later programming of the surface tension calculation could be avoided. However, if a provision for subdivision of the full sequence of interface particles is necessary, then this phase of the calculation should be completed before any curve fitting is begun.

Generally one has some *a priori* knowledge of the interface orientation that can be put to good use in the logical process of subdividing the interface into monotonic segments. For example, if it is known that the interface begins and ends at vertical boundaries of the mesh, then one can require that the first and last segments of the interface line have x as the abscissa. In the intermediate section of the line, a considerable amount of testing is required. The determination of the proper abscissa for each section requires tests to see if monotonic trends are reversed or if slopes exceed the criterion outlined in Section 2-C. When a change in abscissa is called for, further tests are needed to insure that the break occurs well away from regions of infinite slope. We also have to make provision for short sequences of particles to which the spline fit technique cannot be applied. Then, for each subsequence of interface particles, an index must be formed to indicate the first particle and the number of particles in the subsequence, and a technique for flagging must be developed to mark the subsequence as increasing, decreasing or non-spline fit.

When the monotonic subdivisions of the interface particles have been identified, then each subdivision is treated independently for the calculation of the surface tension force components. The first step in this treatment is to determine whether a non-spline fit technique should be applied to this sequence. This should be a fairly rare occurrence if the interface is sufficiently well resolved and the numerical

calculation is stable. In fact, a non-spline fit method for calculating surface tension forces would probably not be required in most programs unless short wavelength interface fluctuations (on the order of a few particle spacings) or severe interface folding were anticipated. However, if these are required, the necessary procedure is specified in Sections 3-B or D.

In the more likely event of a subsequence to which the spline-fit technique will be applied, the next stage of the calculation is the evaluation of the second derivatives of the approximating function at the interface points, following the outline presented in 2-B. This involves the explicit inversion of a tri-diagonal matrix. The second derivatives are then tested against the criterion described in Section 2-D to determine whether any particle coordinate require smoothing.

In the calculations of Ref. [1], criterion violations were quite rare and usually were associated with short wavelength Rayleigh–Taylor instabilities or with the use of boundary condition (8) at subsequence junction points. In problems for which the fluid configuration is physically and numerically stable and not highly contorted, and in which condition (9) is used, there should be little need for smoothing, except when new points are added to the interface line (see Section 2-E). When smoothing is applied, at least some particles experience a change of coordinates and this requires a recomputation of the spline fit data. Since this is time-consuming for large subsequences, only four smoothing operations per subsequence, per cycle of calculation are permitted.

The final step of this process, the computation of the components of the surface tension force, is next. The two components are calculated separately, according to the description given in Sections 3-A and C, and the order of calculation is immaterial. As they are calculated, these force components per unit volume are added to the accelerative forces at the appropriate mesh points. In the calculations of Ref. [1], it was found to be convenient to make the surface tension computation the first step in the calculation cycle, since temporary computer storage needed in the spline fit calculation was available at that time.

When the calculations for this subsequence are complete, a test is made to determine whether there are any additional subsequences for which the procedure needs to be repeated. If not, then the surface tension computation is complete, except for the printing of results if this is desired.

The computer time required for the entire surface tension computation is not large compared to the time used in a two-dimensional, incompressible flow calculation. In the highly contorted flows of Ref. [1], the computer time was increased by about ten percent per cycle when the surface tension capability was added to the calculation. The reason that increase is relatively modest is that the determination of the surface tension force involves only a one-dimensional array of particles.

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