RESEARCH NOTES

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A METHOD OF LIMITING INTERMEDIATE VALUES OF VOLUME FRACTION IN ITERATIVE TWO-FLUID COMPUTATIONS

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Multidimensional computational analysis of fluid flow is usually done by segmented iterative methods, as the equations sets generated are too large to permit simultaneous solution. Frequently the need arises to compute values for variables which must remain bounded for physical reasons. In two-phase computation, for example, the volume fraction is restricted to values between 0 and 1, but iterative procedures often return intermediate values which violate these bounds. It is fairly straightforward to prevent negative values, however no satisfactory method of imposing the upper limit has been published. A method of smoothly applying the limit in reversible fashion is outlined in this note.

Introduction

Multidimensional computational analysis of fluid flow generates systems of algebraic equations which are too large for simultaneous solution. Segmented schemes have therefore been developed in which each conservation equation is solved in turn to obtain approximate solutions, which are then driven to convergence by a suitable iterative scheme. Most numerical schemes for multidimensional analysis of single fluid flow are of this nature and originate from two sources, the ICE procedures developed at LASL (**1**)‡ and the SIMPLE procedures from Imperial College (**2**). Both use the staggered grid concept in which velocities are assigned at control volume boundaries, and both formulate the conservation equations by using a computation of the pressure field to drive the iteration scheme to convergence. The solution thus consists of a hyperbolic phase in which approximate values of velocity are computed from each momentum equation, and an elliptic phase in which the influence of pressure is extracted from the momentum equations and used to convert the continuity equation into a pressure equation, which is then solved in a manner to promote convergence.

The two schools of thought are quite similar in approach, and differ only in the exact form of the pressure equation derived, the manner in which the equations are integrated over the control volume, the degree of implicitness in the time advancement and in minor details of the solution sequence. Schemes for two-fluid computation, in which individual conservation equations are written and solved for each fluid, have been developed from both bases (**3**) (**4**). This note concentrates, however, on the latter base, and schemes which have evolved from the SIMPLE algorithm (**5**)–(**7**).

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‡ *References are given at the end of this note.*

The SIMPLE algorithm, and a number of generic descendants are described with clarity in Patankar (**8**). Some highlights are given here to establish context.

The SIMPLE iterative scheme

The SIMPLE scheme is based on solving the momentum equations for a first estimate of each velocity component, and also extracting a pressure equation from continuity considerations. In general, each momentum equation is reduced by appropriate discretization, integration, and linearization to an algebraic equation, which can be written

$$\{a_m(\rho U)_m = \sum_n a_n(\rho U)_n + b(P_+ - P_-) + c\}_i \quad i = 1, 3 \qquad (1)$$

This links the mass flux component (ρU) at the point m to neighbouring mass fluxes in all directions, and to the pressure gradient in the i direction. Similarly, the continuity equation can be reduced to a discrete form

$$\sum_i e_i(\rho U_{\text{in}} - \rho U_{\text{out}})_i + f = D \approx 0 \qquad (2)$$

The coefficients a in (1) absorb the nonlinearity of the momentum equations, coefficients a, c, and f may incorporate transient terms, and e is the area available to the fluid at the appropriate control volume face. The precise forms of equations (1) and (2) for a particular case are given below in equations (15)–(18).

First estimates of each velocity component U_i may be obtained by solving equations (1) using an assumed pressure field. When these are inserted in (2), however, the equation will not exactly balance, but instead compute a divergence, D, because of the nonlinearities and inaccuracies in the assumed pressure field. However, a new velocity field which will more closely fulfill continuity may be obtained by computing the pressure changes required to drive D to zero for the next iteration $m + 1$. The Newton–Raphson technique establishes

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these to be

$$dP = P_{m+1} - P_m = \frac{D_{m+1} - D_m}{\mathrm{d}D/\mathrm{d}P} = \frac{-D}{\mathrm{d}D/\mathrm{d}P} \tag{3}$$

or

$$\mathrm{d}D = \frac{\mathrm{d}D}{\mathrm{d}P}\,\mathrm{d}P = -D \tag{4}$$

An expression for $\mathrm{d}D$ is readily determined by differentiating (2)

$$\frac{\mathrm{d}D}{\mathrm{d}P}\,\mathrm{d}P = \sum_i e_i \left\{ \frac{\mathrm{d}(\rho U)_{\text{in}}}{\mathrm{d}P} - \frac{\mathrm{d}(\rho U)_{\text{out}}}{\mathrm{d}P} \right\}_i = -D \tag{5}$$

by differentiating (1) and simplifying

$$\{\mathrm{d}(\rho U)_m\}_i = \{\mathrm{b}(\mathrm{d}P_+ - \mathrm{d}P_-)_m\}_i \tag{6}$$

Combining (5) and (6) gives a matrix equation for the pressure change field, which can be written in general form

$$q_m\,\mathrm{d}P_m = \sum q_n\,\mathrm{d}P_n - D \tag{7}$$

Equation (6) can be used to solve for the required pressure change field, which in turn is applied to correct the velocities according to equation (7). The entire process must be iterated to converge through the nonlinearities.

It is useful to note that equations (1) and (7), and in fact most other relevant transport equations, can be written in a general form

$$a_m \phi_m - \sum_n a_n \phi_n = S \tag{8}$$

This is a general matrix equation which relates a variable ϕ at the point m to its neighbours at points n. All other variables are collected in the source term, S. Thus, the same matrix algorithm may be used to solve all such equations. Equation (8) can be one-, two-, or three-dimensional. Exact solutions are expensive, so inner iteration may be used to solve (8). Iteration is all the more economical, as (8) itself need not be iterated to convergence as the whole process (1)–(7) is repeated.

Equations (1)–(8) are the foundations of the SIMPLE scheme; a number of variations have been developed from the same basic scheme (**8**). Two-fluid schemes based on these principles are required to solve twice as many equations and incorporate linkage between the two fluids, but all of these again reduce to the common form of equation (8), which may be solved by the same methods (**5**)–(**7**).

The volume fraction equation in two-fluid analyses

In two-fluid analyses, the momentum equations can be written in a form similar to equation (1) for each fluid in each direction. The individual continuity equations are then used to derive a pressure correction equation and an equation for volume fraction, α. It is advantageous to use linear combinations of the continuity equations. A suitable equation for pressure correction can be obtained by adding the continuity equations (2) subscripted for each fluid, k (**5**).

$$\sum_{k=1}^{2} \left\{ \sum_i e_i[(\alpha\rho U)_{\text{in}} - (\alpha\rho U)_{\text{out}}]_i + f \right\}_k = D_1 + D_2 \tag{9}$$

A more suitable equation is obtained by normalizing each continuity equation with respect to a reference density of each phase ρ_{Ok}

$$\sum_{k=1}^{2} \left(\left\{ \sum_{i=1}^{3} e_i[(\alpha\rho U)_{\text{in}} - (\alpha\rho U)_{\text{out}}]_i + f \right\} \Big/ \rho_O \right)_k = \frac{D_1}{\rho_{O1}} + \frac{D_2}{\rho_{O2}} \tag{10}$$

This equation is then differentiated together with equations (1) to derive the pressure equation (7) which now contains D_1 and D_2. Similarly, a suitable volume fraction equation can be derived by subtracting the normalized continuity equations, with $D_1 = D_2 = 0$, $\alpha_1 = (1 - \alpha_2)$, $r_k = [\rho U e/\rho_O]_k$, and $i = 1, 3$.

$$\alpha_1 \left\{ \sum_i (r_1 + r_2) \right\}_{\text{out}} = \left\{ \sum_i \alpha_1 (r_1 + r_2) \right\}_{\text{in}} + \left\{ \sum_i r_2 \right\}_{\text{out}} - \left\{ \sum_i r_2 \right\}_{\text{in}} + \frac{f_1}{\rho_{O1}} - \frac{f_2}{\rho_{O2}} \tag{11}$$

Note that equations (9)–(11) may also be written in the general form of equation (8). However, equation (10) is subject to the additional constraint that $\alpha \in (0, 1)$. If the solution of equation (11) returns any values of α outside this range, the iterative process will no longer maintain the continuity of each individual fluid. Also, as equation (11) is itself an expression of continuity, it is not sufficient merely to solve (11), and then correct stray values back into range. This again detracts from continuity, as the remaining variables cannot be rationally readjusted to reflect the correction. Instead, a method of maintaining the bounds within the calculation is sought.

Imposing the lower bound

The positivity constraint is relatively easily imposed by following Patankar (**8**). Equation (8) is rewritten as follows

$$(a_m + S_m)\phi_m = \sum_n a_n \phi_n + S_C \tag{12}$$

The constraint for positivity of ϕ is now that both S_m and S_C remain positive. Thus, if the source term S in equation (8) has a positive component S_1 and a negative component S_2, equation (12) is used with $S_C = S_1$ and $S_m = S_2/\phi_m^\circ$, where ϕ_m° is the current value of ϕ_m. ($S = S_1 - S_2$, $S_1 \geqslant 0$, $S_2 > 0$). This ensures that the computed ϕ_m will always retain a positive sign, providing the initial value of ϕ_m° is also positive.

Imposing the upper bound

Patankar also suggests a means of ensuring $\phi \leqslant 1$. Unfortunately, this applies only to equations in which the source term is dominant.

His procedure is to monitor current values ϕ_m°, and if the source term S is positive when a particular ϕ_m° approaches 1, to write the associated source terms $S_C = S_m = S/(1 - \phi_m^\circ)$, which will return $\phi_m = 1$, providing the source dominates the equations. Unfortunately, in the two-fluid volume fraction equation above, this does not appear to be the case. A method based on under-relaxation was therefore developed and this proved to be satisfactory.

The standard under-relaxation procedure is as follows. In order to promote stability, a certain proportion of the original variable is retained in the solution. Instead of solving (8) directly for ϕ_m, which would yield ϕ_m^c, one prefers to return a value $\phi = \beta\phi_m^c + (1 - \beta)\phi_m^\circ$ where $\beta \in (0, 1)$. Relaxation may be imposed after the solution but this may detract from the integrity of the solution. It is preferred to pre-relax, making the relaxation implied in the solution. Equation (8) is thus rewritten in terms of ϕ and ϕ° by substituting for ϕ_m^c

$$a'_m \phi_m = \sum a_n \phi_n + S' \tag{13}$$

where $a'_m = a_m/\beta, S' = S - (1 - \beta)a'_m \phi_m^\circ$.

The new procedure suggested here to improve the upper constraint is to again monitor current values of ϕ_m°, but to approach unity by means of under-relaxation. Equation (8) is first rewritten in point Jacobi form

$$\phi'_m = (\sum a_n \phi_n + S)/a_m \tag{14}$$

Although (8) is to be solved in the matrix sense, equation (14) will give a good indication of the likelihood that a particular ϕ in (8) will return greater than unity. Thus if $\phi'_m > (1 - \varepsilon)$, individual point relation is applied in the form $\beta = \max(1 - \phi_m^\circ, \gamma)$. The parameters ε and γ are small, values of 0·05 and 10^{-10} have proved satisfactory. Equation (8) is then solved in the matrix form of equation (13) with individually assigned relaxation parameters.

The method permits the calculation to proceed smoothly to unity, and also subsequently depart from unity if required to do so, meanwhile ensuring that continuity is maintained throughout. It also merges readily with the lower constraint, as positivity is assured first in an automatic manner, and the arguments concerning the upper bound are merely applied to the resulting coefficients of equation (12). The imposition of the upper limit does not require the source terms to be dominant or even significant.

At first sight one might postulate some advantage in reformulating equation (8) to solve for a correction $\delta\phi$, such that $\phi = \phi^\circ + \delta\phi$ satisfies (8). The resulting equation for $\delta\phi$ is analogous to (8) but is doubly constrained such that $\delta\phi \in (0, 1)$ and $(\phi^\circ + \delta\phi) \in (0, 1)$. Although these constraints may also be imposed through under-relaxation, the increased overhead destroys any advantage inherent in the correction formulation.

Application

The new method of constraints has been incorporated in a two-fluid code which is documented in (**9**). The particular application considered for illustration of the method is a comparison with the experiments of Gardner and Nelles (**10**). In these experiments, air and water flow through a duct consisting of a vertical riser followed by a 90 degree elbow and finally a horizontal section. Volume fraction profiles were measured at various stations.

The relevant equations are the continuity equation and two momentum equations for each fluid k. The equations for fluid 1 are

$$\frac{1}{r}\left\{\frac{\partial}{\partial r}(r\rho\alpha V) + \frac{\partial}{\partial\theta}(\rho\alpha U)\right\}_1 = 0 \tag{15}$$

$$\frac{1}{r}\left\{\frac{\partial}{\partial r}(r\rho\alpha UV) + \frac{\partial}{\partial\theta}(\rho\alpha V^2)\right\}_1 = -\frac{\alpha}{r}\frac{\partial P}{\partial\theta} + \rho_1\alpha_1\left(g_\theta + \frac{UV}{r}\right) + k_{12}(U_2 - U_1) + \Gamma_{\theta 1} \tag{16}$$

$$\frac{1}{r}\left\{\frac{\partial}{\partial r}(r\rho\alpha U^2) + \frac{\partial}{\partial\theta}(\rho\alpha UV)\right\}_1 = -\alpha_1\frac{\partial P}{\partial r} + \rho_1\alpha_1\left(g_r + \frac{U^2}{r}\right) + \Gamma_{r1} \tag{17}$$

Γ denotes friction and viscous source terms.

These are transformed to cartesian form by substituting $r = 1$, $\partial/\partial r = \partial/\partial X$ and $\partial/\partial\theta = \partial/\partial y$ and omitting the coriolis and centrifugal terms. The equations are readily transformed into the simplified form of equations (1) and (2) by integrating over a finite control volume dimension $r\,\mathrm{d}r\,\mathrm{d}\theta$. Thus equation (15), for example, becomes

$$\int \frac{1}{r}\left\{\frac{\partial}{\partial r}(r\rho\alpha V) + \frac{\partial}{\partial\theta}(\rho\alpha U)\right\}_1 r\,\mathrm{d}r\,\mathrm{d}\theta = 0 \tag{18}$$

This reduces to

$$\{(r\rho\alpha V)_{\text{in}} - (r\rho\alpha V)_{\text{out}}\}\,\mathrm{d}\theta + \{(\rho\alpha U)_{\text{in}} - (\rho\alpha U)_{\text{out}}\}\,\mathrm{d}r = 0 \tag{19}$$

which is equivalent to equation (2).

In equations (16) and (17) the gravitational and centrifugal forces tend to separate the fluids, the interphase drag terms counteract this tendency.

Computed results for the Gardner and Nelles conditions are shown in Fig. 1 in the form of bar graphs depicting radial air volume fraction profiles at various axial stations. Initially in the elbow, the centrifugal force drives the heavier water toward the outer radius and the

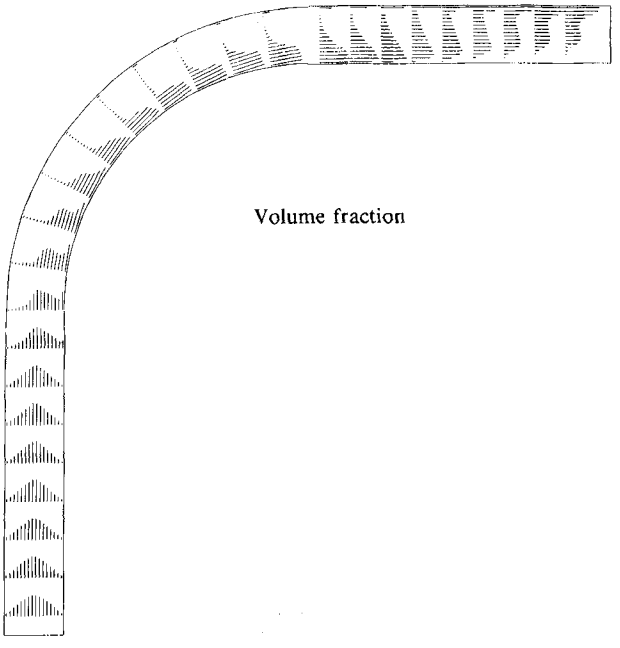

Fig. 1. Bar graph showing computed air volume fraction at various axial stations from two-fluid simulation of Gardner and Nelles experiment

air inward. Eventually, however, the gravity term dominates and the fluids return to the opposite walls. This switchover makes the simulation numerically difficult, particularly as zero or unit local volume fractions are generated at various points in the profiles. However, continuity is maintained throughout. Quantitative experimental comparisons are given in (**9**).

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