Note

A Method of Time-Centering the Lagrangian Marker Particle Computation

The method of computing the Marker particle positions in the Marker and Cell method which is presented in detail in Ref. [1] may be applied to the prediction of, for example, either the streamlines of simulated steady flows or the pathlines of simulated unsteady flows. Where the streamlines or pathlines of such flows are curved, there is a strong tendency for the Marker particles to drift in such a way that the true streamlines or pathlines and those indicated by the Marker particles are not coincident. By substantially reducing the time step which is used in this standard particle trajectory calculation, such particle trajectory errors can be significantly reduced. Unfortunately, the computational costs involved in this method of reducing the trajectory errors are considerable. In this paper, attention will be directed to the examination of the source of such errors and their reduction by more efficient means.

For simplicity, the ideas presented in this paper are illustrated in plane Cartesian coordinates, in which case the particle trajectory equations are

$$dx/dt = u(x, y), \tag{1a}$$

$$dy/dt = v(x, y). \tag{1b}$$

The standard numerical analog of these equations is

$$x^{n+1} = x^n + \delta t(u^n), \tag{2a}$$

$$y^{n+1} = y^n + \delta t(v^n), \tag{2b}$$

where (x^n, y^n) and (x^{n+1}, y^{n+1}) are the coordinates of the particle position at the present (n) and the predicted $(n + \delta t)$ respective locations. Typically, u^n and v^n are obtained from the discrete velocity field data with bilinear interpolation at the coordinate location (x^n, y^n).

The proposed discrete analog of Eqs. (1) is

$$x^{n+1} = x^n + (\delta t)\,(u^n + u^{n+1})/2, \tag{3a}$$

$$y^{n+1} = y^n + (\delta t)\,(v^n + v^{n+1})/2, \tag{3b}$$

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where u^{n+1} and v^{n+1} are the interpolated velocity components evaluated at $(x, y)^{n+1}$. Equations (3) are implicit and as such require some special means for solution. A proposed means of solution is to rewrite Eqs. (3) in iterative form as

$$x^{n+k/km} = x^n + \delta t \, (u^n + u^{n+(k-1)/km})/2, \tag{4a}$$

$$y^{n+k/km} = y^n + \delta t \, (v^n + v^{n+(k-1)/km})/2, \tag{4b}$$

where k is a count integer whose minimum value is one and whose maximum value is k_m. k_m is the total number of estimates which are used to approximate the predicted particle location. It has been found that this iterative scheme is convergent provided that δt is restrained to less than or equal to the value which permits a particle to move a cell width or height in one time step. For δt chosen in this region, this procedure may be used to approximate Eqs. (3) to any degree desired simply by a suitable choice of k_m.

In computing practice, Eqs. (4) and the equations for the bilinear particle velocity interpolation for u and v may be incorporated in that sequential order in a common Fortran DO loop which ranges from $k = 1$ to k_m where k_m is chosen among the numbers, two thru six. The choice for k_m depends upon the trade-off between minimizing the computational time which is expended and maximizing the accuracy which the user desires.

One method of analyzing the inherent errors associated with discrete approximations of continuous equations is to determine the size of the neglected terms of a Taylor expansion relative to the retained terms. The errors inherent in the approximations expressed by Eqs. (2) and (3) will be examined in this fashion, and a test problem is included to show the relative magnitude of various of the neglected terms and the manner in which these influence the discrete solution.

Equation (1a) may be expressed with a truncated Taylor expansion to fourth order as

$$x^{n+1} = x^n + (\delta t) \, u^m + (\delta t)^2/2 \left(\frac{d(u)}{dt}\right)^m + (\delta t)^3/6 \left(\frac{d^2(u)}{dt^2}\right)^m$$

$$+ (\delta t)^4/24 \left(\frac{d^3(u)}{dt^3}\right)^m, \qquad \text{where} \qquad m = n, \tag{5}$$

or

$$x^{n+1} = x^n + \delta t \, u^m + (\delta t/2)^3/3 \left(\frac{d^2(u)}{dt^2}\right)^m, \qquad \text{where} \qquad m = n + \tfrac{1}{2} \tag{6}$$

and where the operator is

$$\left(\frac{d(\ )}{dt}\right)^m = u^m \frac{\partial(\ )^m}{\partial x} + v^m \frac{\partial(\ )^m}{\partial y}.$$

An equation analogous to Eq. (5) for the y direction may be derived. The terms involving the operator derivatives are evaluated with centered difference expressions. The use of these discrete equations will be referred to as an explicit procedure for predicting the particle trajectory with accuracies which are referred to as first, second, third, and fourth order for the approximations including the terms through δt, δt^2, δt^3, and δt^4, respectively. Similarly, an equation analogous to Eq. (6) may be derived for the y direction (Eq. (1b)). The use of this equation in conjunction with Eq. (6) as approximated with the iterative scheme represented by Eqs. (4) and with centered approximations for the operator derivatives will be referred to as an implicit procedure for predicting the particle trajectory with accuracies which are referred to as second and fourth order for the approximation including the terms thru δt and δt^3, respectively.

In order to illustrate the magnitude of the truncation errors in explicit and implicit procedures of various orders of accuracy, consider the following thought problem. A cluster of four adjoining square ($\delta x = \delta y$) computational cells have a prescribed steady clockwise incompressible circulation. The exterior faces of the cells are impervious to flow and have the free slip boundary condition for the particle prediction calculations. The bottom left corner of the four-cell cluster is taken as the origin of the coordinate system in which x and y increase rightward and upward, respectively. The test particle location is defined initially at $(\delta x, \delta y/2)$ and the time step (δt) is defined as $\delta x/|\,u\,| = \delta y/|\,v\,|$. Equations (4) predict particle locations of $(0, \delta y/2)$, $(\delta x/2, 3/4\ \delta y)$, $(3/8\ \delta x, 7/8\ \delta y)$, $(29/64\ \delta x, 15/16\ \delta y)$ etc., for $k_m = 1, 2, 3, 4$, respectively. The predicted coordinate location approaches the location of $(\frac{1}{2}\delta x, \delta y)$ as k_m is increased and the convergence rate toward this value is great. The predicted location with the first order, second order, and third order explicit approximations are, respectively, $(0, \frac{1}{2}\delta y)$, $(0, \delta y)$, and $(\frac{1}{4}\delta x, \delta y)$, and are approaching the vicinity of the location $(\frac{1}{2}\delta x, \delta y)$ with the increasing order of the approximation. In order to aid in comparison, these data and those of the proposed second order implicit scheme are presented in Figure 1. Implied from these data is that the order of the explicit approximations must be high if the pitch error of simulated flow with a curved path is to be held small. Thus, the test particle path in the four cell cluster generated with explicit approximations of any practical finite order of accuracy would show a helical pathline which eventually must intersect one of the four bounding walls of the four cell cluster. However, this difficulty does not result with the second order implicit procedure if k_m is taken at an appropriate value. As a result, Eqs. (4) are adequate for the illustration of steady flows. For the prediction of the particle trajectories of simulated unsteady flows, there are two principle sources of errors with this method. The first is associated with the time step while the second is related to the time plane chosen for the estimation of the interpolated velocity components. In the first instance, the fourth and higher order implicit approxi-
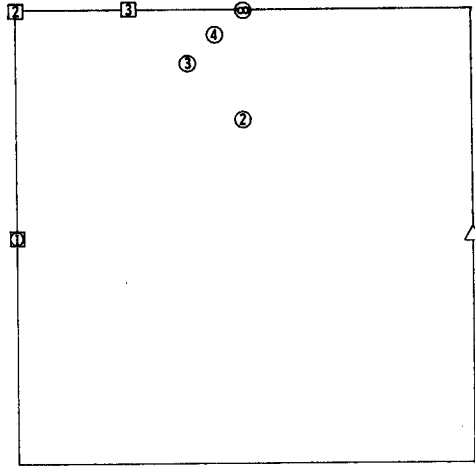
FIG. 1.   Comparison of Explicit and Implicit Procedures for the predicted test particle location in one computational cell with flow out the top and in at the right side $\delta t = \delta x / |u| = \delta y / |v|$. Δ = Initial test particle location; $\bigcirc$ = position of estimated particle location for km = 1, 2, 3, 4 and ∞ with the second order implicit scheme; $\square$ position of particle location for explicit procedure of order 1, 2 and 3.

mations can improve this aspect of the computation for $\delta t \approx (\delta x / |u|, \delta y / |v|)_{min}$, but since δt is usually restrained to one half or less this value for unsteady flow simulations, these terms are typically more than two orders of magnitude smaller than the leading terms. Thus, these higher order analogs of Eqs. (4) are not significantly more accurate than that expressed by Eqs. (4) for practical applications.

In the second instance, the accuracy may be improved in some circumstances by evaluating the interpolated velocity components for predicted location $(x, y)^{n+1}$ from the $(n + \delta t)$ time plane. Such a procedure can be implemented in a straight-forward fashion in situations in which the Marker particle display does not enter in the velocity predictions. However, in methods like the MAC method when the Marker particles are an intricate part of the velocity predictions, the particle position predictions and the velocity predictions would have to be iterated. (It would be interesting to know, in this case, what impact the foregoing consid-erations have for accuracy of MAC calculations involving free surface.)

To summarize the comparison of the explicit and implicit procedures, the primary advantage of the second order implicit procedure, which is approximated by Eqs. (4), is that for the same accuracy it is substantially more economical to compute and practical to implement than the explicit procedures besides more nearly eliminating the pitch errors of curved flow paths. Such results can also be shown for the prediction of particle paths in polar coordinates.

Finally, a sample test problem is included to show the improvement in the fidelity of the Marker particle movement with the proposed implicit iterative procedure compared with the first order explicit procedure. The test problem involves the bouyantly driven flow of incompressible fluid in a square two dimensional cavity for a Raleigh number of 10^4 and a Prandtl number of one. The left and right wall temperatures are set for all time at equal plus and minus temperature differences from the uniform initial bulk temperature, respectively. The fluid state is initially quiesent. The top and bottom walls are perfectly insulated and the no-slip condition is applied at all surfaces. The simulated flow proceeds through a starting transient and after a time a steady clockwise circulation is established. Figure 2 shows the results of using the computational method which is presented
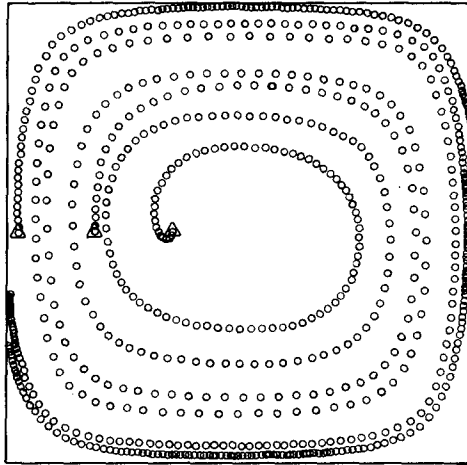

FIG. 2   Three marker partical paths in a square cavity predicted by the Standard Method; Δ = starting point.

in Ref. [1]. The principle feature of this picture is that the three Marker particles move helically outward through the prevailing circulation and collide with the wall where they stick. Figure 3 shows the path of the same three Marker particles which have been moved with the previously proposed iterative method for the same time step. Note that the pitch of the helix of each particle path is now essentially zero. Figure 3 is generated with two estimates of the proposed procedure ($k_m = 2$) with the time step at one half the smallest value which moves the fluid a cell width. Figure 3 was also generated with six estimates ($k_m = 6$) and no distinguishable difference between these results was noted. The plots were generated with an SC 4020 plotting machine.
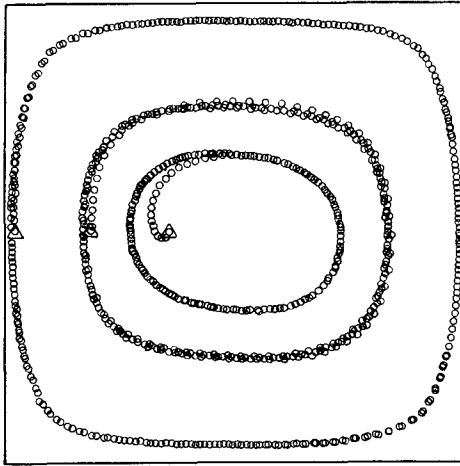
FIG. 3. Three marker particle paths in a square cavity predicted by the Proposed Method; $\varDelta$ = starting point.

Based upon the foregoing discussion, it is recommended that the proposed scheme for the prediction of the particle trajectory be considered in applications where the use of the Lagrangian marker particle calculations are desired.

REFERENCES

1. J. E. WELCH, F. H. HARLOW, J. P. SHANNON, AND B. J. DALY, The MAC Method, Los Alamos Scientific Lab, Report No. LA-3425, 1965.

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