POSITION, VELOCITY AND PRESSURE CORRECTION ALGORITHM FOR PARTICLE METHOD SOLUTION OF THE PDF TRANSPORT EQUATIONS

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ABSTRACT

In PDF methods (Pope 1985) there is close connection between the normalization (or consistency) condition, the mean mass conservation equation, and the Poisson equation for the mean pressure. In the context of a particle method to solve the PDF transport equations, an algorithm is described which: performs a position correction so that the consistency condition is satisfied; performs a velocity correction so that the mean mass conservation is satisfied; and determines a mean pressure correction. For statistically stationary flows, a steady state is achieved in which these corrections tend to zero (in the mean). This algorithm is incorporated in the code PDF2DV (Pope 1994).

INTRODUCTION

The algorithm is based on the mean mass conservation equation in the form

$$\nabla \cdot \langle \rho \mathbf{U} \rangle = 0. \tag{1}$$

Consequently it is applicable to constant-density flows, or statistically-stationar variable-density flows. It is applicable to three-dimensional flows, but it is described here for plane two-dimensional flows. Figure 1 is a sketch of the rectangular grid considered. The sketch also shows the definition of the *wedge functions* $f^{\pm}_{i\pm\frac{1}{2}}(x)$ and $g^{\pm}_{j\pm\frac{1}{2}}(y)$. As an example, $f^{-}_{i+\frac{1}{2}}$ is defined by

$$\begin{aligned} f^{-}_{i+\frac{1}{2}}(x) &= 0, \quad \text{for } x < x_i \\ &= 1 - (x - x_i)/\Delta x_{i+\frac{1}{2}}, \quad \text{for } x_i \le x < x_{i+1} \\ &= 0, \quad \text{for } x > x_{i+1}. \end{aligned} \tag{2}$$

The bi-linear basis function $b_{ij}(\mathbf{x})$ is defined by

$$b_{ij}(\mathbf{x}) = \left[f^{+}_{i-\frac{1}{2}}(x) + f^{-}_{i+\frac{1}{2}}(x) \right] \left[g^{+}_{j-\frac{1}{2}}(y) + g^{-}_{j+\frac{1}{2}}(y) \right]. \tag{3}$$

The flow is represented by a large ensemble of particles. The general particle has mass m^*, specific volume v^*, position $\mathbf{X}^*$, and velocity $\mathbf{U}^*$. Braces $\{\ \}$ denote the sum over all particles; while $\{\ \}_{i+\frac{1}{2},j+\frac{1}{2}}$ denotes the sum over all particles in the cell centered at $(i + \frac{1}{2}, j + \frac{1}{2})$.

POSITION CORRECTION ALGORITHM

The *consistency condition* is that the volume associated with a sub-ensemble of particles (i.e., the sum of m^*v^*) equals the geometric volume occupied by the particles. A weak form of this condition is obtained by summing over all particles, weighted by the basis function $b_{ij}(\mathbf{x})$

$$\{m^*v^*b_{ij}(\mathbf{X}^*)\} = V_{ij}, \tag{4}$$

where V_{ij} is the geometric volume

$$V_{ij} \equiv \int b_{ij}(\mathbf{x})\, d\mathbf{x}. \tag{5}$$

Notice that Eq. (4) can be written for each grid node.

In the particle method, before the steady state is reached (and because of statistical fluctuations) Eq. (4) is not satisfied. We seek then a *position correction* $\delta\mathbf{X}^*$ for each particle so that the corrected position does satisfy Eq. (4), i.e.,

$$\{m^*v^*b_{ij}(\mathbf{X}^* + \delta\mathbf{X}^*)\} = V_{ij}. \tag{6}$$

For small $|\delta\mathbf{X}^*|$, with high probability $\mathbf{X}^*$ and $\mathbf{X}^* + \delta\mathbf{X}^*$ lie within the same cell. Hence the linear approximation to Eq. (6) is accurate for small $|\delta\mathbf{X}^*|$:

$$\{m^*v^*\left[b_{ij}(\mathbf{X}^*) + \delta\mathbf{X}^* \cdot \nabla b_{ij}\right]\} = V_{ij}. \tag{7}$$

Observe that in the cell $(i+\frac{1}{2}, j+\frac{1}{2})$, we have

$$\frac{\partial b_{ij}}{\partial x} = -\frac{g^-_{j+\frac{1}{2}}}{\Delta x_{i+\frac{1}{2}}}. \tag{8}$$

The position correction is specified to be the gradient of a potential ϕ, which is represented at grid nodes. Simple differencing and interpolation in the cell $(i+\frac{1}{2}, j+\frac{1}{2})$ then gives

$$\begin{aligned} \delta X^* &= g^{-*}_{j+\frac{1}{2}}(\phi_{i+1,j} - \phi_{i,j})/\Delta x_{i+\frac{1}{2}} \\ &\quad + g^{+*}_{j+\frac{1}{2}}(\phi_{i+1,j+1} - \phi_{i,j+1})/\Delta x_{i+\frac{1}{2}}. \end{aligned} \tag{9}$$

From Eq. (8) and Eq. (9) we obtain the contribution from δX^* in cell $(i+\frac{1}{2}, j+\frac{1}{2})$ to Eq. (7) to be

$$\left\{ m^* v^* \delta X^* \frac{\partial b_{ij}}{\partial x} \right\}_{i+\frac{1}{2},j+\frac{1}{2}} =$$

$$-\left(\Delta x_{i+\frac{1}{2}}\right)^{-2} \left[\left\{ m^* v^* \left(g^{-*}_{j+\frac{1}{2}} \right)^2 \right\}_{i+\frac{1}{2},j+\frac{1}{2}} (\phi_{i+1,j} - \phi_{i,j}) \right.$$

$$\left. + \left\{ m^* v^* g^{-*}_{j+\frac{1}{2}} g^{+*}_{j+\frac{1}{2}} \right\}_{i+\frac{1}{2},j+\frac{1}{2}} (\phi_{i+1,j+1} - \phi_{i,j+1}) \right]. \tag{10}$$

Adding the contributions from the other three cells and from δY^* yields a nine-point finite-difference equation for $\phi_{i,j}$. This equation is solved (currently using a band-solver) to yield $\phi_{i,j}$.

The simple differencing used in Eq. (9) yields a discontinuous field of $\nabla\phi$. Once $\phi_{i,j}$ has been determined, a continuous, piece-wise linear approximation to $\nabla\phi$ is obtained using staggered grids. This continuous field is used to evaluate $\delta \mathbf{X}^*$.

Because the linearization (Eq. 7) is approximate, and because different finite-difference approximations to $\nabla\phi$ are used, with the corrected particle positions $\mathbf{X}^* + \delta\mathbf{X}^*$, the consistency condition is not exactly satisfied. However, generally 2 or 3 iterations suffice to satisfy the condition to within a few percent. More iterations are required if there are few particles per cell.

There are as many consistency conditions as there are unknowns $\phi_{i,j}$—one at each grid node. Consequently, additional boundary conditions are not needed. However, at an outlet boundary, the consistency condition is not imposed and instead $\phi_{i,j}$ is set to zero. This allows particles to cross the outflow boundary in order to satisfy the global consistency condition, i.e., the total particle volume equals the geometric volume of the solution domain.

VELOCITY CORRECTION

The weak form of the mean mass conservation equation is

$$\int b_{ij}(\mathbf{x}) \nabla \cdot \langle \rho \mathbf{U} \rangle \, d\mathbf{x} = 0. \tag{11}$$

Away from boundaries, integration by parts yields

$$\int \langle \rho \mathbf{U} \rangle \cdot \nabla b_{ij}(\mathbf{x})\, d\mathbf{x} = 0. \tag{12}$$

A velocity correction $\delta \mathbf{U}^*$ is sought such that the corrected velocity satisfies the particle version of Eq. (12), i.e.,

$$\{m^* v^* [\mathbf{U}^* + \delta \mathbf{U}^*] \cdot \nabla b_{ij}\} = 0. \tag{13}$$

The velocity correction is specified to be

$$\delta \mathbf{U} = -\frac{1}{\langle \rho \rangle} \nabla \phi = -\tilde{v} \nabla \phi, \tag{14}$$

where ϕ is a potential (different from that used in the position correction). Then simple differencing and interplotion for $\nabla \phi$, when substituted into Eq. (13) again yields a nine-point finite-difference equation for the potential $\phi_{i,j}$, which is solved using a band-solver.

If the velocity correction $\delta \mathbf{U}^*$ is computed from $\nabla \phi$ in the obvious way, a $2\Delta x$ instability results. To avoid this, the ϕ field is first filtered to remove this mode. Primarily because of this filtering, the residuals in the mass conservation equation are not reduced to zero: but the filtered residuals can be. Even with this filtering, a sub-grid instability occurs in the particle velocities. To control this, fourth-order dissipation is added to the particle velocities.

When the velocity increment is determined via Eq. (14) for a time step Δt, it is equivalent to the effect of a mean pressure correction

$$\delta \langle p \rangle = \phi / \Delta t. \tag{15}$$

Note that Eq. (14) can then be written

$$\delta \mathbf{U} = -\frac{1}{\langle p \rangle} \nabla \delta \langle p \rangle \Delta t. \tag{16}$$

Needless to say, the pressure correction field obtained from Eq. (15) is extremely noisy. A good deal of filtering and damping is applied to yield a stable mean pressure field.

In a sense, the mean pressure is irrelevant and does not need to be determined. For, any error in the mean pressure field is compensated by the pressure correction. That is, the potential ϕ is such that the total pressure effect, i.e.,

$$\delta \mathbf{U}' = -\frac{1}{\langle \rho \rangle} \nabla (\langle p \rangle + \delta \langle p \rangle) \, \Delta t, \tag{17}$$

is the same, whatever the value of $\langle p \rangle$. But numerically, the errors are less if $\langle p \rangle$ determined accurately. Splitting errors are avoided, and variance reduction techniques can be applied to generate mean momentum conservation.

References

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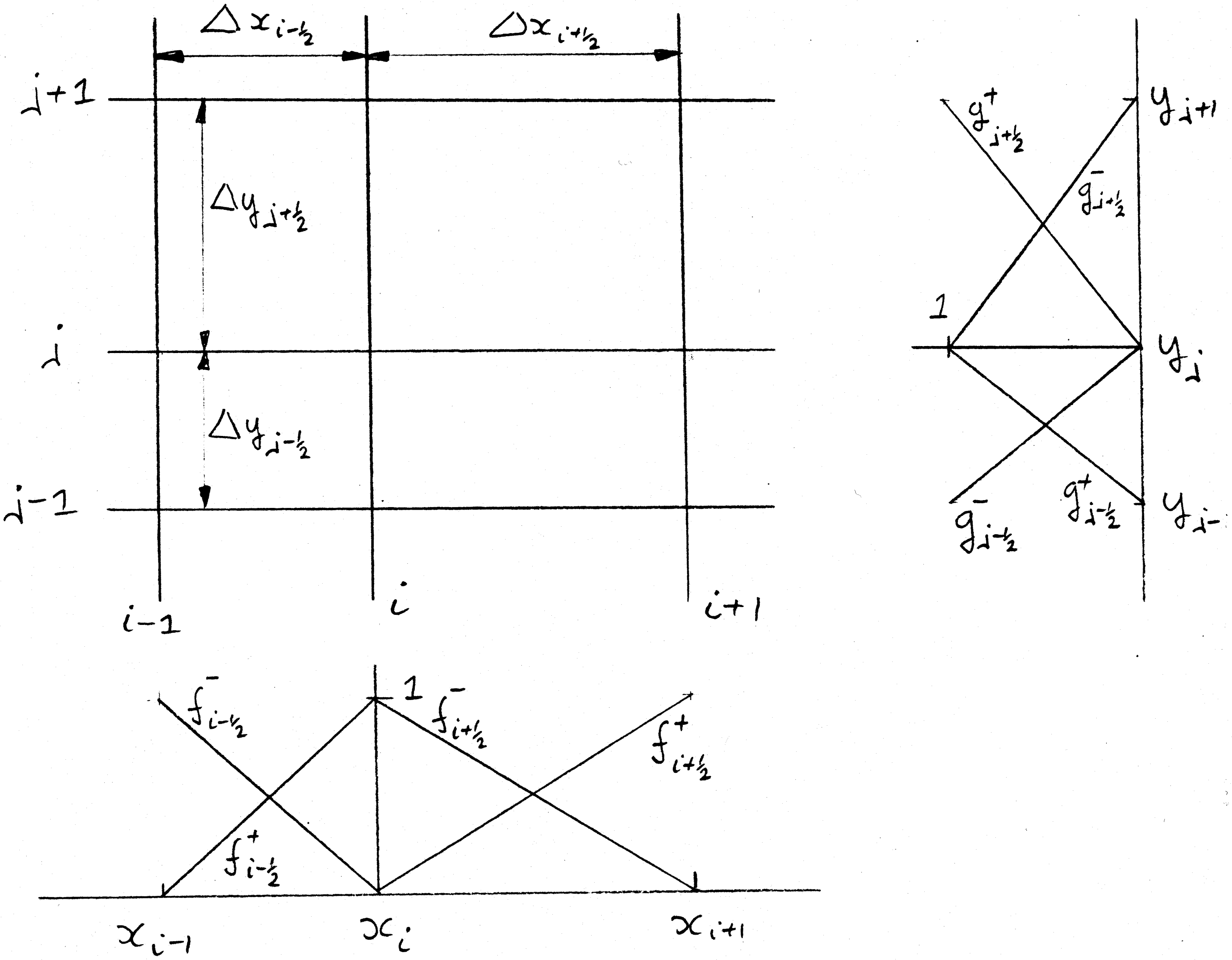

Fig.1: Sketch of grid and the linear wedge functions.