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Note

Finite-Sized Fluid Particle in a Nonuniform Moving Grid

I. Introduction

The particle-in-cell (PIC) method, which is known as the mixed Eulerian–Lagrangian scheme, has been applied successfully to solve a wide variety of problems where the fluid distortions are large. But the use of the scheme is limited to an idealized situation, because the use of particles produces nonphysical fluctuations of fluid quantities, and makes great demands on computer memory capacity and calculation time. Furthermore, we sometimes need to describe a large density variation, e.g., the variation of several orders from a solid-state region to a rarefied-gas region. Because the minimum density is determined by the density shared with one particle, some automated particle adjusting technique must be introduced.

In this paper, we present a PIC method of a new type, in which an area-weighting technique and a nonuniformly spaced moving grid are employed, respectively, for the suppression of nonphysical fluctuations and for the description of large density variations with few particles. In addition, the reduction of numerical viscosity is discussed.

II. Numerical Algorithm

For a simple description of the basic scheme, the following one-fluid compressible equations are used:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{v} = 0, \tag{1}$$

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \rho \mathbf{v}\mathbf{v} = -\nabla p, \tag{2}$$

and

$$\frac{\partial \rho I}{\partial t} + \nabla \cdot \rho \mathbf{v} I = -p \nabla \cdot \mathbf{v}, \tag{3}$$

where p, ρ, $\mathbf{v}$, and I denote the pressure, density, velocity, and specific internal energy, respectively. The PIC method employs Lagrangian fluid particles to represent mass,

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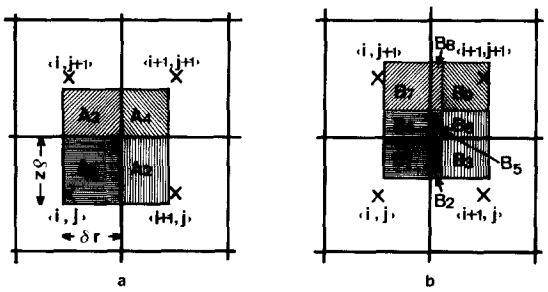

FIG. 1. Schematics of a finite-sized particle's location (●) in cells (×) (a) before, and (b) after the particle moves. In this example, the summation of the areas B_6 and B_3 corresponds to the area A_2.

momentum, and energy convections through Eulerian grids of cells. In Harlow's PIC method [1, 2], the particle has the memory only for its own mass and positions, but momentum and energy are attached to the particle from the cell only when the particle crosses the cell boundary. A nearest-grid-point procedure like this suffers from a large fluctuation with few particles. The area-weighting technique [3] can reduce the effect, but requires some modification before it is applied to the fluid PIC method. The full particle method [4], which means that all quantities are kept in the particle's memory, may use the area-weighting technique without special care, but the multi-streaming problem is still a subject of considerable debate.

Here we present another approach to the PIC method. Let us imagine that a particle center locates at the place denoted by a filled circle in Fig. 1a. In our scheme, the particle has memories for its own mass, positions, and internal energy, but in order to avoid the multi-streaming problem, momentum is attached to the particle only when it moves. The area-weighting procedure places a square of the cell size around each particle, and the fractional area belonging to each neighbor cell determines the fraction of the physical quantities of the particle and cell. The mass and internal energy of a cell are calculated from the fractional areas of particles belonging to the cell. The new internal energy of a particle is corrected by artificial relaxation between the energy of the particle and the area-weighted energy of corresponding cells. Then the numerical thermal diffusion can be successfully reduced without the multi-temperature problem [4, 5]. On the other hand, the momentum is not memorized, and hence the averaging causes a large diffusion. An essential point of our procedure is that the particle preserve the memory of the cell boundary lines in Fig. 1a when it moves. The memorized boundary lines of the particle after it moves are schematically depicted in Fig. 1b. The momentum and kinetic energy of four cells in Fig. 1a are memorized on the particle and are redistributed to new cells in Fig. 1b. In the example depicted in the figure, this procedure can be expressed as

$$
\begin{aligned}
U_{i,j}^{\mathrm{NEW}} &= B_1 U_{i,j}^{\mathrm{OLD}}, \qquad U_{i,j+1}^{\mathrm{NEW}} = B_4 U_{i,j}^{\mathrm{OLD}} + B_7 U_{i,j+1}^{\mathrm{OLD}}, \\
U_{i+1,j}^{\mathrm{NEW}} &= B_2 U_{i,j}^{\mathrm{OLD}} + B_3 U_{i+1,j}^{\mathrm{OLD}}, \\
U_{i+1,j+1}^{\mathrm{NEW}} &= B_5 U_{i,j}^{\mathrm{OLD}} + B_6 U_{i+1,j}^{\mathrm{OLD}} + B_8 U_{i,j+1}^{\mathrm{OLD}} + B_9 U_{i+1,j+1}^{\mathrm{OLD}}.
\end{aligned} \tag{4}
$$

The modified area-weighting procedure removes the zeroth-order diffusion, but the first-order diffusion, called the *numerical viscosity*, still remains. The effect is usually not crucial, except for the case where the fluid velocity relative to the Eulerian grid is greater than the local sound speed, and the velocity gradient is relatively large.

There are several methods to reduce the numerical viscosity. One may, for example, subtract it in the form of a finite difference [1] or assume a velocity distribution within a particle for more correct convection. The former is hard to extend to multi-dimensional simulations, while the latter is more flexible because it tries to remove the origin of the numerical viscosity. The simplest distribution is

$$U(r, z) = \{(U_{i+1,j+1} - U_{i+1,j})(2z - \delta z) + U_{i+1,j}\}(2r - \delta r) - \{(U_{i,j+1} - U_{i,j})(2z - \delta z) + U_{i,j}\}(2r - \delta r - 1), \quad (5)$$

where the particle size is set to unity, and the origin of the (r, z) coordinate system is at the bottom left-hand corner of the particle in Fig. 1a. The momentums of the four parts after convection are easily obtained by integrating $U(r, z)$ over each new area in Fig. 1b. It is easily understood that this procedure also removes the zeroth-order diffusion, and hence does not require the complicated procedure given by Eq. (4). All these procedures are straightforwardly extended to a nonuniformly spaced grid system, where a particle size may be set to the minimum size of the four adjacent cells.

III. Numerical Results

Let us demonstrate the efficiency of our scheme with typical examples. A first example is a one-dimensional adiabatic expansion process. Initially, five particles per cell are loaded in 20 grids which are uniformly spaced, and nonuniformly spaced grids are placed in a vacuum region.

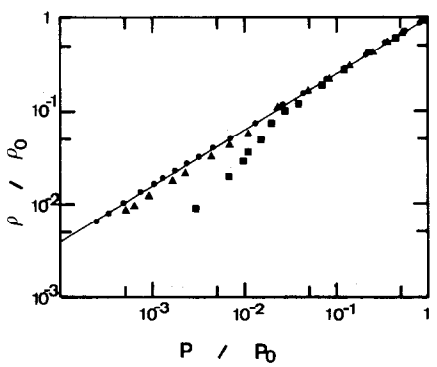

FIG. 2. Comparison between the theoretical adiabatic expansion law (—) and simulation results, where ■, ▲, and ● correspond to the schemes given, respectively, by Eq. (4), by Eq. (5) with fixed grid, and by Eq. (4) with moving grid.

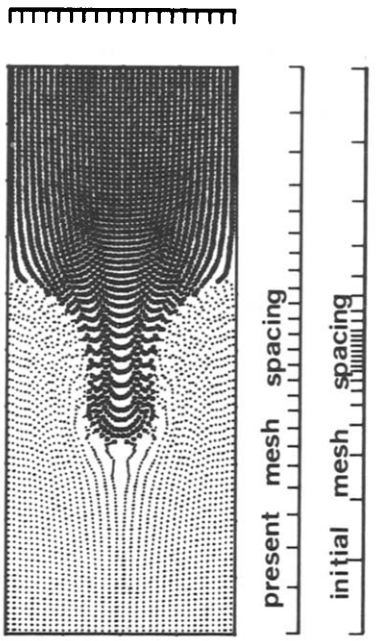

FIG. 3. Sample particle plot at $\gamma t = 5$ and grid arrangements at $\gamma t = 0$ and $\gamma t = 5$. The initial density ratio of the two superposed fluids is 5:1.

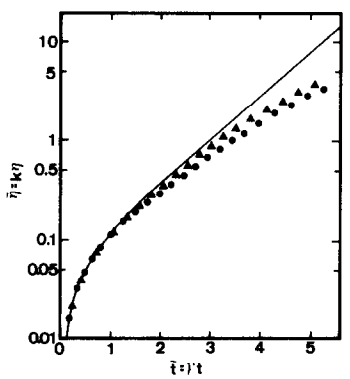

FIG. 4. Comparison between the theoretical linear growth (—) and simulation results. Fine resolution of initial growth is attained by a moving grid. Simulations corresponding to ● and ▲ use the grid of (parallel to, perpendicular to acceleration) equal to (24, 18) and (24, 28). Here the grid is constrained to move only in the direction parallel to acceleration.

For an ideal fluid, the pressure and density should obey the adiabatic law as shown by the solid line in Fig. 2. The result of the scheme given by Eq. (4) is shown by squares. Although the large density variation is successfully described with few particles, the pressure is appreciably detached from the adiabatic law at lower density. The velocity distribution method given by Eq. (5) presents a favourable result, as shown by triangles. The full particle method and finite difference subtraction method reproduce the same result. We may use a more complicated profile than that given by Eq. (5), if improved accuracy is required.

On the other hand, there exists a more interesting method which employs a moving grid. The effect of numerical viscosity becomes relatively smaller than the pressure effect when fluid velocity relative to the grid is less than the local sound speed. This effect is demonstrated and its result shown by circles in Fig. 2, where each grid is forced to move at 80% of the local fluid velocity. The prominent feature of our scheme is that the grid can move with almost arbitrary speed without any complicated technique, because each particle preserves the memories of physical quantities and the grid only plays a temporary role.

The second example is the Rayleigh–Taylor instability [6]. Because a fine grid is required for the description of initial linear growth, partially nonuniformly spaced grids (24×18), as shown in Fig. 3, are preferred. The grids are forced to move in the direction parallel to acceleration, so as to be uniformly spaced at the end of calculation, that is, at the time when the perturbed region expands over a whole system. It is found that the effects of nonuniformly spaced moving grids are small, because the similar simulation with uniformly spaced 90×18 grids shows the same growth. The linear growth rate of the simulation γ_s is 87% of the theoretical prediction γ_T; both are shown in Fig. 4. The discrepancy between them comes primarily from the coarseness of horizontal grid spacing. Another simulation with a 24×28 grid justifies this expectation, and $\gamma_s \simeq 0.94\gamma_T$ is obtained, as shown in the figure.

IV. Summary

A PIC method of a new type is developed and shown to be useful for the description of large density variation with few particles. Nonphysical noise, numerical thermal diffusion, and viscosity are successfully reduced. A nonuniformly spaced moving grid system can be used for locally fine resolution of processes.

The detailed description of the scheme and its application to real situations will appear in a forthcoming paper, where the extension to a polar coordinate system will also be discussed.

Appendix

Here we briefly describe the PIC method. Each cycle of calculation is divided into two phases, the Eulerian phase and the Lagrangian phase. In the first phase, Eulerian

field variables are calculated, neglecting the transport due to fluid motion, that is, the second terms of the left-hand sides of Eqs. (1)–(3). In order to conserve the total energy even in nonuniform grids, the following finite difference representations in two-dimensional plane coordinates are employed:

$$\tilde{u}_{i,j} = u^n_{i,j} - (\Delta t/\rho^n_{i,j}\,\Delta r_i)(p_{i+1/2,j} - p_{i-1/2,j}),$$

$$\tilde{v}_{i,j} = v^n_{i,j} - (\Delta t/\rho^n_{i,j}\,\Delta z_j)(p_{i,j+1/2} - p_{i,j-1/2}),$$

$$\tilde{I}_{i,j} = I^n_{i,j} - (\Delta t/\rho^n_{i,j}\,\Delta r_i)\{(p\bar{u})_{i+1/2,j} - (p\bar{u})_{i-1/2,j}\} - (\Delta t/\rho^n_{i,j}\,\Delta z_j) \times \{(p\bar{v})_{i,j+1/2} - (p\bar{v})_{i,j-1/2}\} - \bar{u}_{i,j}(\tilde{u}_{i,j} - u^n_{i,j}) - \bar{v}_{i,j}(\tilde{v}_{i,j} - v^n_{i,j}),$$

where Δr_i and Δz_j represent the cell size of r direction and z direction, respectively, and Δt is the time step. The half integer indicates the value on the cell boundary, which is calculated by linear interpolation using the value defined on the grid points. Here, $\bar{u} = (\tilde{u} + u^n)/2$ and $\bar{v} = (\tilde{v} + v^n)/2$ are used for pressure work calculation. In the second phase, the fluid convections are accomplished with finite-sized particles. This part is described in the body of this paper.

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