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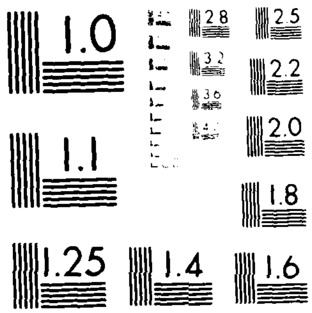

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TWO-DIMENSIONAL FLUX-CORRECTED TRANSPORT

JAYCOR Report Number J206-83-003/6201

FINAL REPORT

by

Raafat H. Guirguis

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TWO-DIMENSIONAL FLUX-CORRECTED TRANSPORT

by

Raafat H. Guirguis

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Alexandria, Virginia

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I. INTRODUCTION AND MOTIVATION

A well-documented module ETBFCT for solving generalized continuity equations was presented in NRL Memorandum Report 3237, dated March 1976. The module PRBFCT was also included to treat the case of periodic boundary conditions. In these modules, the cell centers are specified while the cell boundaries are located midway between the centers. In August 1980, JPBFCT, in which the cell boundaries are tracked, was documented.

The above modules are based on the Flux-Corrected Transport (FCT) technique introduced first by Boris and Book.[1] FCT, instead of adhering to an asymptotic ordering, requires positivity, a physical and mathematical property of continuity equations. To assure positivity, the convective stage includes or is supplemented by a large diffusive flux of zeroth order (in $\varepsilon = \frac{u\delta t}{\delta x}$). Consequently, an antidiffusive or corrective step has to follow. The two stages together are able to tre... steep gradients without generating dispersive ripples. Antidiffusion being a physically (and numerically) unstable process, the corrective flux is limited according to a criterion which may be stated, "The antidiffusion stage should generate no new maxima or minima in the solution, nor should it accentuate already existing extrema."

FCT was shown to be applicable to any finite difference transport scheme and able to improve it.[2] Phoenical FCT, a refinement which minimizes residual diffusive errors, was introduced. Clipping and terracing, two nonlinear processes resulting from the flux limiter were discussed. Finally, splitting techniques were recommended to extend FCT to multi-dimensions.

The most detailed error analysis of FCT algorithms was performed in Ref. 3. Low-residual-diffusion and low-phase-error algorithms were derived. An optimal algorithm, Fourier FCT, was introduced.

The requirements for positivity of a general three-point scheme and the antidiffusion flux for a minimum residual diffusion were derived in Ref. 4.

Zalesak[5] provided a general mathematical interpretation of the antidiffusion flux as the difference between a high-order transport scheme and a low-order one. He also described a generalized fully multidimensional flux limiter guaranteeing that the antidiffusion fluxes on all sides of the control volume, acting in concert, do not create any ripples. It was shown that by proper selection of the flux limiter parameters the clipping and terracing phenomena can be reduced.

The goal of the present work is to extend JPBFCT to a fully two-dimensional algorithm, without time splitting, and incorporate the Zalesak flux limiter while still keeping the implementation of the convective, diffusion and antidiffusion processes as physical fluxes.

II. FOURIER ANALYSIS; DEFINITIONS

A generalized conservation equation can be written in the form:

$$\frac{\partial\rho}{\partial t} + \vec{u}.\nabla\rho = \rho\nabla.\vec{u} + s(\vec{x},t,\rho,\ldots), \tag{1}$$

where $\vec{u}$ is the velocity vector, ρ is the generalized density or the transported quantity whose positivity is to be conserved, and s is a source term including all the remaining terms, i.e., gradients, divergences, body forces, etc.

In the analysis we assume $s = 0$ and $\vec{u}$ = constant. We shall start with the one-dimensional case. Eq. (1) reduces to

$$\frac{\partial\rho}{\partial t} + u_o \frac{\partial\rho}{\partial x} = 0, \tag{2}$$

whose analytic solution is

$$\rho(x,t) = \rho(x - u_o t, 0), \tag{3}$$

a rightward-propagating wave with velocity u_o. Let us Fourier analyze $\rho(x,t)$ in space, assuming periodic boundary conditions. Assuming an initial distribution of density $\rho(x,0) = F(x)$,

$$F(x) = \frac{a_o}{2} + \sum_{k=1}^{\infty} (a_k \cos kx + b_k \sin kx), \tag{4a}$$

where k is assumed to be *normalized*, i.e., k replaces $\frac{2\pi k}{L}$. In complex form

$$F(x) = \sum_{k=-\infty}^{\infty} \hat{\rho}_k e^{ikx} \tag{4b}$$

where $i \equiv \sqrt{-1}$. From the reality of $\rho(x,0)$, the a_k and b_k are real. The quantity $\hat{\rho}_k$ is related to these by

$$\hat{\rho}_k = \begin{cases} \dfrac{a_k - ib_k}{2} & \text{for } k > 0; \\[2ex] \dfrac{a_k + ib_k}{2} & \text{for } k < 0; \\[2ex] \dfrac{a_o}{2} = 0 & \text{for } k = 0. \end{cases} \tag{5}$$

Notice that we could have started the summation in Eq. (4a) from k = 0 since sin 0 = 0 and cos 0 = 1. The zeroth order term would then be a_o. The form (4a) is preferred, however, since it is compatible with the symmetric formulation of Eqs. (4b) and (5). Then $\hat{\rho}_k$ is given by

$$\hat{\rho}_k = \frac{1}{L}\int_o^L F(x)e^{-ikx}dx. \tag{6}$$

From Eq. (3), the density profile at time t is given by

$$\rho(x,t) = \sum_{k=-\infty}^{\infty} \hat{\rho}_k e^{ik(x - u_o t)} = \sum_{k=-\infty}^{\infty} \hat{\rho}_k(t)e^{ikx}, \tag{7}$$

where

$$\hat{\rho}_k(t) = \hat{\rho}_k e^{-iku_o t}, \tag{8}$$

showing that each harmonic independently advances uniformly in phase without changing its magnitude (see Fig. 1).

Suppose ρ is known at all times only as a set of N + 1 quantities ρ_j; on discrete grid points with separation $\delta x = \frac{L}{N}$; $x_j = j\delta x$ (j = 0,1,..., N-1), since $\rho_o = \rho_N$. We can have only $\frac{N}{2}$ + 1 different harmonics. Namely, wave numbers (0,1,...,N/2) and wave lengths ($\infty = L/0$, $\frac{L}{1}$, $\frac{L}{2}$, ..., $\frac{L}{N/2}$) respectively, where we note that the shortest wave length is $2\delta x$. Let

$$f(x) = \frac{A_o}{2} + \sum_{k=1}^{N/2} (A_k \cos kx + B_k \sin kx), \tag{9a}$$

or

$$f(x) = \sum_{k=-N/2}^{N/2} \hat{\rho}_k e^{ikx} \tag{9b}$$

(see Fig. 2). We notice in Eq. (9a) that at $k = N/2$, $\sin kx_j = \frac{2\pi(N/2)}{L} j\delta x = \sin \pi j = 0$; hence only cos kx is needed at $k = N/2$. There are then N coefficients, A_k ($k = 0,\ldots,N/2$) and B_k ($k = 1,2,\ldots,N/2 - 1$), which can be determined using $f(x_j) = \rho_j^o$ ($j = 0,\ldots,N-1$), where superscript 0 denotes time $t = 0$. Similarly, since for all j, $\exp [i \frac{2\pi}{L}(\frac{-N}{2}) j\delta x] = \exp (i\frac{2\pi}{L}(\frac{N}{2}) j\delta x]$, Eq. (9b) is rewritten as

$$f(x) = \sum_{k=-N/2+1}^{N/2} \hat{\rho}_k e^{ikx} \tag{9c}$$

Again, we get N coefficients $\hat{\rho}_k$($k = -N/2+1,\ldots,0,\ldots,N/2$). The relation between the $\hat{\rho}_k$ and A_k, B_k are given by equations similar to Eq. (5). Formally,

$$\hat{\rho}_k = \frac{1}{N} \sum_{j=o}^{N-1} \rho_j^o e^{ikx_j} \tag{10}$$

Eq. (3) predicts the density at time t as

$$\rho(x,t) = \sum_{k=-N/2+1}^{N/2} \hat{\rho}_k e^{ik(x - u_o t)} = \sum_{k=-N/2+1}^{N/2} \hat{\rho}_k(t) e^{ikx}$$

where $\hat{\rho}_k(t) = \hat{\rho}_k e^{-iku_o t}$. Since we are only concerned with $\rho(x_j,t)$, substituting $x = x_j = j\delta x$, we get

$$\rho(x_j,t) = \sum_{k=-N/2+1}^{N/2} \hat{\rho}_k(t) e^{ikj\delta x} \tag{11}$$

If the time is also discretized, let $t^n \equiv n\delta t$, $\rho_j^n \equiv \rho(x_j, t^n)$, $\hat{\rho}_k^n \equiv \hat{\rho}_k(t^n)$, then

$$\rho_j^n = \sum_{k=-N/2+1}^{N/2} \hat{\rho}_k^n e^{ikj\delta x} \tag{12}$$

where

$$\hat{\rho}_k^n = \hat{\rho}_k e^{-iku_o n\delta t} \tag{13}$$

If we space-discretize only, after we Fourier analyze the initial density profile ρ_j^o, i.e., after getting the $\hat{\rho}_k$ in Eq. (9c), the problem is reduced to that of propagation of the complex harmonics e^{ikx} ($k = 0,\ldots,N/2$). In a nonlinear problem, each harmonic can couple into components of the other harmonics. In the linear problem of Eq. (2), however, each harmonic propagates independently (this is also true if $u = u(t)$). Since the number of spatial points does not change, we can always express the density at any time as a Fourier expansion of the form Eq. (9c). In a nonlinear problem $\hat{\rho}_k(t)$ is a function of $(\hat{\rho}_{-N/2+1},\ldots,\hat{\rho}_o,\ldots,\hat{\rho}_{N/2})$ at time $t = 0$. But in the linear problem $\hat{\rho}_k(t)$ is only a function of $\hat{\rho}_k$ as is obvious from Eq. (13). If the time is also discretized, we can then define a transfer function

$$A(k) \equiv \frac{\hat{\rho}_k^{n+1}}{\hat{\rho}_k^n} \tag{14}$$

which is independent of n if $u = u_o$ as is obvious from Eq. (13) (analytic solution), yielding

$$A(k) = e^{-iku_o\delta t} \tag{15}$$

Eq. (12) may be rewritten then as

$$\rho_j^n = \sum_{k=-N/2+1}^{N/2} \hat{\rho}_k [A(k)]^n e^{ikj\delta x}, \tag{16}$$

Denoting the constant $\frac{u_o \delta t}{\delta x}$ by ε and the dimensionless wave number $k\delta x$ by β, $A(\beta) = e^{-i\beta\varepsilon}$. The amplification is $|A(\beta)| = 1$ and the phase shift is $-\beta\varepsilon$. Notice that the smallest $\beta = 0$ and largest $\beta = \frac{2\pi}{L}\frac{N}{2}\delta x = \pi$. For a finite-difference scheme applied to the linear problem, each harmonic propagates independently. Consequently, a method equivalent to Fourier-analyzing ρ_j^{n+1} and $\rho_j^n (j = 0,\ldots,N-1)$ and evaluating A_k from Eq. (14) is to study the propagation of only one harmonic by assuming $\rho_j^n = \rho^o\, e^{ikj\delta x}$, where ρ^o is constant. Then

$$A(k) = \frac{\rho_j^{n+1}}{\rho_j^n} \tag{17}$$

By writing A(k) as

$$A = |A|e^{i\theta}, \tag{18}$$

we define the amplitude (or diffusion) error and the relative phase error as

$$a = |A| - 1 \tag{19a}$$

and

$$R = \frac{(-\theta) - \beta\varepsilon}{\beta\varepsilon} = \frac{-(\theta/\beta)}{\varepsilon} - 1, \tag{19b}$$

respectively. We define a scheme as stable if $A \leq 1$ (see Fig. 3).

<u>Example</u>:

Assuming $u = \text{const} = u_o$, the original explicit SHASTA Algorithm can be written as

$$\rho_j^{TD} = \rho_j^n - \frac{\varepsilon}{2}(\rho_{j+1}^n - \rho_{j-1}^n) + (\frac{1}{8} + \frac{\varepsilon^2}{2})(\rho_{j+1}^n - 2\rho_j^n + \rho_{j-1}^n)$$

$$\rho_j^{n+1} = \rho_j^{TD} - \frac{1}{8}(\rho_{j+1}^{TD} - 2\rho_j^{TD} + \rho_{j-1}^{TD}) \tag{20}$$

in which we identify $-\frac{\varepsilon}{2}(\rho^n_{j+1} - \rho^n_{j-1})$ as the net transportive flux, denoted by a superscript T, and $(\frac{1}{8} + \frac{\varepsilon^2}{2})(\rho^n_{j+1} - 2\rho^n_j + \rho^n_{j-1})$ as the net diffusive flux, denoted by a superscript D, from which we have the notation ρ^{TD}. Expressing ρ^{TD} as a three-point formula we can write

$$\rho^{TD}_j = [\frac{1}{8} + \frac{\varepsilon^2}{2} - \frac{\varepsilon}{2}]\rho^n_{j+1} + [1 - 2(\frac{1}{8} + \frac{\varepsilon^2}{2})]\rho^n_j + [\frac{1}{8} + \frac{\varepsilon^2}{2} + \frac{\varepsilon}{2}]\rho^n_{j-1}$$

Each of the quantities in square brackets is ≥ 0 for $|\varepsilon| \leq \frac{1}{2}$, assuring the positivity of ρ^{TD}_j if $\rho^n_j \geq 0$. The positivity requirement will be discussed later in detail. Assuming $\rho^n_j = \rho^o e^{ikj\delta x}$,

$$\rho^{TD}_j = \rho^o e^{ikj\delta x} - \frac{\varepsilon}{2}(\rho^o e^{ik(j+1)\delta x} - \rho^o e^{ik(j-1)\delta x})$$

$$+ (\frac{1}{8} + \frac{\varepsilon^2}{2})(\rho^o e^{ik(j+1)\delta x} - 2\rho^o e^{ikj\delta x} + \rho^o e^{ik(j-1)\delta x}),$$

giving

$$\rho^{TD}_j/\rho^n_j = 1 - \frac{\varepsilon}{2}(e^{i\beta} - e^{-i\beta}) + (\frac{1}{8} + \frac{\varepsilon^2}{2})(e^{i\beta} - 2 + e^{-i\beta}).$$

Denoting the operator $\frac{e^{i\beta} - e^{-i\beta}}{2} = i \sin \beta$ by t and $e^{i\beta} - 2 + e^{-i\beta}$ $= 2(\cos \beta - 1)$ by d, we have $\rho^{TD}_j = (1 - \varepsilon t + \nu d)\,\rho^n_j$ where $\nu \equiv \frac{1}{8} + \frac{\varepsilon^2}{2}$. Then if $\mu \equiv \frac{1}{8}$, $\rho^{n+1}_j = (1 - \varepsilon t + \nu d)\,\rho^n_j - \mu d(1 - \varepsilon t + \nu d)\rho^n_j$, whence

$$A \equiv \frac{\rho^{n+1}_j}{\rho^n_j} = (1 - \varepsilon t + \nu d)(1 - \mu d). \tag{21}$$

We notice that at $\varepsilon = 0$, $A \neq 1$. In fact, $A = (1 + \frac{1}{8}d)(1 - \frac{1}{8}d)$, a deficiency that led to the introduction of a phoenical algorithm in Ref. 2, in which the antidiffusion operates on a transported density which is free from any zeroth-order diffusion. Phoenical SHASTA is written as

$$\rho_j^T = \rho_j^n - \frac{\varepsilon}{2}(\rho_{j+1}^n - \rho_{j-1}^n) + \frac{\varepsilon^2}{2}(\rho_{j+1}^n - 2\rho_j^n + \rho_{j-1}^n);$$

$$\rho_j^{TD} = \rho_j^T + \frac{1}{8}(\rho_{j+1}^n - 2\rho_j^n + \rho_{j-1}^n);$$

$$\rho_j^{n+1} = \rho_j^{TD} - \frac{1}{8}(\rho_{j+1}^T - 2\rho_j^T + \rho_{j-1}^T). \tag{22}$$

thus yielding

$$A = (1 - \varepsilon t + \lambda\varepsilon^2 d)(1 - \mu d) + \nu d, \tag{23}$$

where $\lambda = \frac{1}{2}$, $\nu = \mu = \frac{1}{8}$, satisfying $A = 1$ at $\varepsilon = 0$.

The importance of phoenicity lies in the fact that the total diffusion through a surface is proportional to the time of diffusion and therefore should vanish as $\delta t \to 0$, i.e., $\varepsilon \to 0$.

Later, in Ref. 6, ETBFCT and JPBFCT, based on the scheme

$$\rho_J^T = \rho_j^n - \frac{\varepsilon}{2}(\rho_{j+1}^n - \rho_{j-1}^n)$$

$$\rho_j^{TD} = \rho_j^T + \nu(\rho_{j+1}^n - 2\rho_j^n + \rho_{j-1}^n)$$

$$\rho_j^{n+1} = \rho_j^{TD} - \mu(\rho_{j+1}^T - 2\rho_j^T + \rho_{j-1}^T), \tag{24}$$

were introduced, yielding

$$A = (1 - \varepsilon t)(1 - \mu d) + \nu d, \tag{25}$$

where $\nu \equiv \frac{1}{6} + \frac{\varepsilon^2}{3}$ and $\mu \equiv \frac{1}{6} - \frac{\varepsilon^2}{6}$. Notice that the zeroth order term is the same in both ν and ν, thus yielding a residual diffusion $O(\varepsilon^2)$, which vanishes as $\delta t \to 0$.

III. AMPLITUDE AND PHASE ANALYSIS

If in Eq. (18) A is expressed as $A = A_R + iA_I$, where R stands for real and I for imaginary, then

$$|A|^2 = A_R^2 + A_I^2, \tag{31a}$$

$$\theta = \tan^{-1}(A_I/A_R). \tag{31b}$$

Equations (31) yield numerical values of $|A|$ and θ for a given β. These should be expanded, however, in a power series in β and plugged into Eqs. (19) to get an estimate of the order of a given scheme. Expanding Eqs. (31) in power series is a huge task. Instead, we use a scheme based on successive differentiation, as follows:

PHASE ERRORS

As seen from Eqs. (21), (23), and (25), three-point schemes can be expressed in terms of a transport operator $t \equiv i \sin \beta$ and a diffusion operator $d \equiv 2(\cos \beta - 1)$. In other words, $A = A(t,d)$ where $t = t(\beta)$ and $d = d(\beta)$. Taking the logarithm of Eq. (18), we obtain $\log A = \log |A| + i\theta$, yielding

$$\theta = \mathrm{Im}[\log A]. \tag{33}$$

Expanding θ in a power series of β, near $\beta = 0$, we have

$$\theta = \theta_o + \theta_o' \frac{\beta}{1!} + \theta_o'' \frac{\beta^2}{2!} + \ldots$$

where $(\ )' \equiv \frac{d(\ )}{d\beta}$ and the subscript 0 denotes the value at $\beta = 0$. Since, from Eq. (33),

$$\frac{d^n \partial}{d\beta^n}\Big|_{\beta=0} = \mathrm{Im}\,\{\frac{d^n}{d\beta^n}(\log A)\Big|_{\beta=0}\},$$

all we need are the derivatives of (log A) with respect to β, at $\beta = 0$.

First, by direct differentiation we get $(\log A)' = A'/A$, $(\log A)'' = A''/A - (A'/A)^2$ and so on. Noticing that the "consistency" of any scheme requires $A(\beta = 0) = 1$, we can write

$$(\log A)'_o = A'_o; \tag{35a}$$

$$(\log A)'_o = A''_o - A'^2_o; \tag{35b}$$

$$(\log A)'''_o = A'''_o - 3A'_o A''_o + 2A'^3_o; \tag{35c}$$

$$(\log A)^{iv}_o = A^{iv}_o - 4A'_o A'''_o - 3A''^2_o + 12A'^2_o A''_o - 6A'^4_o; \tag{35d}$$

$$(\log A)^{v}_o = A^{v}_o - 5A'_o A^{iv}_o - 10A''_o A'''_o + 20A'^2_o A'''_o + 30A''^2_o A'_o$$
$$- 60A'^3_o A''_o + 24A'^5_o. \tag{35e}$$

Next denoting $\frac{\partial(\cdot)}{\partial t}$ by $(\ )^t$ and $\frac{\partial}{\partial d}(\ )$ by $(\ )^d$, we get by direct differentiation $A' = t'A^t + d'A^d$, $A'' = t''A^t + d''A^d + t'^2A^{tt} + 2t'd'A^{td} + d'^2A^{dd}$, and so on. Confining our scope to schemes of first degree in t (composite transport excluded) and of second degree in d, we have

$$A^{tt} = 0,\ A^{tdd} = \text{constant, and } A^{ddd} = 0. \tag{36}$$

We obtain then

$$A_o = 1;$$

$$A'_o = t'A^t_o + d'A^d_o; \tag{37a}$$

$$A''_o = t''_o A^t_o + d''_o A^d_o + 2t'_o d'_o A^{td}_o + d'^2_o A^{dd}_o; \tag{37b}$$

$$A_o''' = t_o''' A_o^t + d_o''' A_o^d + 3(t_o'' d_o' + t_o' d_o'') A_o^{td} + 3 d_o' d_o'' A_o^{dd} + 3 t_o' d_o'^2 A_o^{tdd}; \qquad (37c)$$

$$A_o^{iv} = t_o^{iv} A_o^t + d_o^{iv} A^d + (4t_o''' d_o' + 6t_o'' d_o'' + 4t_o' d_o''') A_o^{td}$$

$$+ (4d_o' d_o''' + 3d_o''^2) A_o^{dd} + (12t_o' d_o' d_o'' + 6t_o'' d_o'^2) A_o^{tdd}; \qquad (37d)$$

$$A^v = t_o^v A_o^t + d_o^v A_o^d + (5t_o^{iv} d_o' + 10t_o''' d_o'' + 10t_o'' d_o'''$$

$$+ 5t_o' d_o^{iv}) A_o^{td} + (5d_o' d_o^{iv} + 10d_o'' d_o''') A_o^{dd} + (30t_o'' d_o' d_o''$$

$$+ 5t_o' d_o''^2 + 20t_o' d_o' d_o''' + 10t_o''' d_o'^2) A_o^{tdd}. \qquad (37e)$$

Going back to the definition of t and d

$$t_o = 0,\ t_o' = i,\ t_o'' = 0,\ t_o''' = -i,\ t_o^{iv} = 0,\ \text{and}\ t^v = i, \qquad (38a)$$

$$d_o = 0,\ d_o' = 0,\ d_o'' = -2,\ d_o''' = 0,\ d_o^{iv} = 2,\ \text{and}\ d_o^v = 0. \qquad (38b)$$

Substituting in Eqs. (37), we get

$$A_o = 1;$$

$$A_o' = iA_o^t; \qquad (39a)$$

$$A_o'' = -2A_o^d; \qquad (39b)$$

$$A_o''' = -i(A_o^t + 6A_o^{td}); \qquad (39c)$$

$$A_o^{iv} = 2(A_o^d + 6A_c^{dd}); \qquad (39d)$$

$$A_o^v = i(A_o^t + 30A_o^{td} + 60A_o^{tdd}). \qquad (39e)$$

Finally, with Eqs. (30), Eqs. (35) yield

$$(\log A)_o = 0;$$

$$(\log A)'_o = iA^t_o; \tag{40a}$$

$$(\log A)''_o = -2A^d_o + (A^t_o)^2; \tag{40b}$$

$$(\log A)'''_o = -iA^t_o(1 - 6A^d_o) - i[6A^{td}_o + 2(A^t_o)^3]; \tag{40c}$$

$$(\log A)^{iv}_o = 12A^{dd}_o + 2(1 - 6A^d_o)[A^d_o - 2(A^t_o)^2] - 6A^t_o[4A^{td}_o + (A^t_o)^3]; \tag{40d}$$

$$(\log A)^v_o = 60iA^{tdd}_o + iA^t_o[1-30A^d_o - 60A^{dd}_o + 120(A^d_o)^2] + 20i(A^t_o)^3[1 - 6A^d_o] + 30iA^{td}_o[1 - 4A^d_o + 4(A^t_o)^2] + 24i(A^t_o)^5. \tag{40e}$$

Eqs. (40) invoke the fact that only the odd derivatives of log A are imaginary. Therefore, with the use of Eqs. (33) and (34), we get

$$\theta = \frac{(\log A)'_o}{i}\beta + \frac{(\log A)'''_o}{i}\frac{\beta^3}{3!} + \ldots \tag{41}$$

<u>Example</u>:

Let us phase-analyze the scheme described by Eqs. (22), i.e., the transfer function of Eq. (23)

$$A = (1 - \varepsilon t + \lambda\varepsilon^2 d)(1 - \mu d) + \nu d$$

where $\nu = \mu = \frac{1}{8}$ and $\lambda = \frac{1}{2}$.

First we notice that it is phoenical: $A = 1$ at $\varepsilon = 0$. By direct differentiation, $A^t = -\varepsilon(1 - \mu d)$ and $A^d = \lambda\varepsilon^2(1 - \mu d) - \mu(1 - \varepsilon t + \lambda\varepsilon^2 d) + \nu$; $A^{td} = \varepsilon\mu$, $A^{dd} = -2\lambda\varepsilon^2\mu$, and $A^{tdd} = 0$.

At $\beta = 0$, $t = 0$ and $d = 0$, yielding $A_o^t = -\varepsilon$, and $A_o^d = \lambda\varepsilon^2 + (\nu - \mu) = \frac{\varepsilon^2}{2}$; $A_o^{td} = \varepsilon\mu = \frac{\varepsilon}{8}$, $A_o^{dd} = -2\lambda\varepsilon^2\mu = -\frac{\varepsilon^2}{8}$, and $A_o^{tdd} = 0$. Substituting in Eqs. (40), (41), we get

$$\theta = -\varepsilon\beta + \frac{1}{6}(\frac{1}{4}\varepsilon - \varepsilon^3)\beta^3 + \ldots$$

Using Eq. (19b), the relative phase error is found to be

$$R = \frac{1}{6}(\frac{1}{4} - \varepsilon^2)\beta^2 + O(\beta^4),$$

showing that the scheme is second order in phase.

Alternatively, let us derive an expression for ν which renders the scheme of Eqs. (24) fourth-order in phase. Upon differentiating the transfer function $A = (1 - \varepsilon t)(1 - \mu d) + \nu d$ we get, when we substitute $\beta = 0$,

$$A_o^t = -\varepsilon; \text{ and } A_o^d = \nu - \mu;$$

$$A_o^{td} = \varepsilon\mu,\ A_o^{dd} = 0, \text{ and } A_o^{tdd} = 0, \tag{42}$$

which with Eqs. (39a) through (39c) gives

$$A_o' = -i\varepsilon$$

$$A_o'' = -2(\nu - \mu)$$

$$A_o''' = -i(-\varepsilon + 6\varepsilon\mu). \tag{43}$$

Substituting in Eq. (35c), we obtain

$$\text{Im } (\log A)_o''' = \varepsilon(1 - 6\mu) - 6\varepsilon(\nu - \mu) + 2\varepsilon^3 = \varepsilon(1 - 6\nu + 2\varepsilon^2).$$

To reduce the coefficient of β^2 in the R expansion to zero we require $(\log A)_o''' = 0$, yielding

$$\nu = \frac{1}{6} + \frac{\varepsilon^2}{3} \tag{44}$$

AMPLITUDE ANALYSIS

Denote the complex conjugate by a bar on top:

$$|A|^2 = A\,\bar{A}. \tag{45}$$

Since $\frac{d^n}{d\beta^n}\overline{(\;)} = \overline{\frac{d^n(\;)}{d\beta^n}}$, we get by successive differentiation of Eq. (45)

$$(|A|^2)_o = 1;$$

$$(|A|^2)_o' = A_o'\bar{A}_o + A_o\overline{A_o'}; \tag{46a}$$

$$(|A|^2)_o'' = A_o''\bar{A}_o + 2A_o'\overline{A_o'} + A_o\overline{A_o''}; \tag{46b}$$

$$(|A|^2)_o''' = A_o'''\bar{A}_o + 3A_o''\overline{A_o'} + 3A_o'\overline{A_o''} + A_o\overline{A_o'''}; \tag{46c}$$

$$(|A|^2)_o^{iv} = A_o^{iv}\bar{A}_o + 4A_o'''\overline{A_o'} + 6A_o''\overline{A_o''} + 4A_o'\overline{A_o'''} + A_o\overline{A_o^{iv}}. \tag{46d}$$

Noticing from Eqs. (39) that the odd derivatives of A are pure imaginary while the even ones are pure real.

$$A_o = +\bar{A}_o = 1;$$

$$A_o' = -\overline{A_o'};$$

$$A_o'' = +\overline{A_o''};$$

$$A_o''' = -\overline{A_o'''}; \tag{47}$$

and

$$A_o^{iv} = +\overline{A_o^{iv}}.$$

Substituting in Eqs. (46), we get

$$(|A|^2)_o = 1; \tag{48a}$$

$$(|A|^2)_o' = 0; \tag{48b}$$

$$(|A|^2)_o'' = 2[A_o'' + (\frac{A_o'}{i})^2]; \tag{48c}$$

$$(|A|^2)_o''' = 0; \tag{48d}$$

$$(|A|^2)_o^{iv} = 2[A_o^{iv} + 4(\frac{A_o'}{i})(\frac{A_o'''}{i}) + 3(A_o'')^2], \tag{48e}$$

where we notice that the odd derivatives vanish. Accordingly, $|A|^2$ can be expanded as

$$|A|^2 = 1 + (|A|^2)_o'' \frac{\beta^2}{2!} + (|A|^2)_o^{iv} \frac{\beta^4}{4!} + \ldots \tag{49}$$

Example:

Let us derive an expression for μ to render the diffusion error of ETBFCT fourth order. Substituting Eqs. (42) into Eq. (39d), we find

$$A_o^{iv} = 2(\nu - \mu), \tag{50}$$

Using Eqs. (43) with (48), we obtain $(|A|^2)_o'' = 2[-2(\nu - \mu) + \varepsilon^2]$, which has to vanish for a fourth-order diffusion, yielding

$$\nu - \mu = \frac{\varepsilon^2}{2}. \tag{51}$$

Solving Eqs. (44) and (51), we have $\mu = \frac{1-\varepsilon^2}{6}$, whence $\frac{A_o'}{i} = -\varepsilon$, $A_o'' = -\varepsilon^2$, $\frac{A_o'''}{i} = \varepsilon(1 - 6\mu) = \varepsilon^3$, and $A_o^{iv} = \varepsilon^2$. We can then write

$$(|A|^2)_o^{iv} = 2[\varepsilon^2 + 4(-\varepsilon)(\varepsilon^3) + 3\varepsilon^4] = 2\varepsilon^2(1 - \varepsilon^2),$$

which when substituted into Eq. (49) gives

$$|A|^2 = 1 \frac{\varepsilon^2}{12} (1 - \varepsilon^2)\beta^4 + O(\beta^6), \tag{52}$$

showing a slight instability near $\beta = 0$ (the coefficient of β^4 is positive).

A warning is in order at this point. Although a positive coefficient of the leading term in the expansion implies unstable behavior, a negative one does not guarantee a stable scheme, since the expansion is valid only near $\beta = 0$.

Figure 4 shows the amplification $|A|$ versus β. We notice a maximum value of $|A| = 1.0018$ at $\beta = 53.668° \pm 0.001$ for $\varepsilon = \frac{1}{2}$. We can get rid of the potential instability by using a slightly different expression for μ,

$$\mu = \frac{1}{6} - \alpha \frac{\varepsilon^2}{6}. \tag{53}$$

By trial and error, α was found to be ≥ 1.056. The dashed line in Fig. 4 shows the resulting amplification for $\alpha = 1.056$. The maximum value of $|A|$ becomes 0.999998 at $\beta = 45.775° \pm 0.001$. Since the phase error depends on ν only, the resulting scheme is still fourth-order in phase error. The zeroth-order antidiffusion being kept at $\frac{1}{6}$, phoenicity is preserved, i.e., the residual diffusion is $O(\varepsilon^2)$. Later, a modified algorithm which is stable and has sixth-order diffusion and fourth-order phase error is described.

IV. POSITIVITY AND ANTIDIFFUSION

The concept underlying FCT is "positivity." This means that the sign of the dependent variable must be preserved under the influence of convection alone. Source terms can alter the sign. Positivity is particularly important near steep gradients where the convective fluxes tend to make the transported quantity undershoot or overshoot. Positivity is ensured by supplementing the convective step with a large diffusive flux of zeroth order in δt. For example, in the scheme of Eq. (24), consider the transport step alone,

$$\rho_j^T = \rho_j^n - \frac{\varepsilon}{2}(\rho_{j+1}^n - \rho_{j-1}^n),$$

applied to the discontinuities of Fig. 5(a) and (b), where $\varepsilon = + 1/2$. The negative density in Fig. 5(a) and overshoot in Fig. 5(b) are obviously major errors. By supplying enough diffusion,

$$\rho_j^{TD} = \rho_j^T + (\frac{1}{6} + \frac{\varepsilon^2}{3})(\rho_{j+1}^n - 2\rho_j^n + \rho_{j-1}^n),$$

we see the negative density in Fig. 5(a) disappear, as does the overshoot in Fig. 5(b). Formally, in the expression

$$\rho_j^{TD} = [1 - 2(\frac{1}{6} + \frac{\varepsilon^2}{3})]\ \rho_j^n + [(\frac{1}{6} + \frac{\varepsilon^2}{3}) - \frac{\varepsilon}{2}]\rho_{j+1}^n + [(\frac{1}{6} + \frac{\varepsilon^2}{3}) + \frac{\varepsilon}{2}]\rho_{j-1}^n,$$

the quantities in square brackets are all ≥ 0 for $|\varepsilon| \leq 1/2$, therefore ensuring positivity of ρ_j^{TD} as long as $\rho_j^n \geq 0$.

A side benefit of the zeroth-order term is more accurate propagation i.e., high-order phase preservation. As seen from Eq. (44), selecting $\nu = \frac{1}{6} + \frac{\varepsilon^2}{3}$ assures a fourth-order phase error.

A byproduct of this large added diffusion is antidiffusion, which is needed to extract at least the zeroth order part. This leaves a residual diffusion $O(\varepsilon^2)$ near almost uniform distributions. Near steep gradients, antidiffusion fluxes have to be reduced enough to maintain the positivity of ρ^{TD}. This process is called correction of fluxes, and gives rise to the name "flux-corrected transport." In the case of a discontinuity, the local antidiffusion flux is cancelled completely. This trimming means that the amplitude no longer has the order of accuracy derived above. But near steep gradients the concept of order is meaningless anyway. On the other hand, Eq. (44) is independent of μ. The fourth order phase error is therefore assured regardless of the antidiffusion fluxes. Specifically, "the antidiffusion stage should generate no new maxima or minima in the solution, nor should it accentuate already existing extrema" (Ref. 1).

The first mathematical formulation of the above statement was given in connection with explicit SHASTA,[1]

$$\rho_j^{TD} = \rho_j^n - \frac{\varepsilon}{2}(\rho_{j+1}^n - \rho_{j-1}^n) + (\frac{1}{8} + \frac{\varepsilon^2}{2})(\rho_{j+1}^n - 2\rho_j^n + \rho_{j-1}^n) \tag{61a}$$

$$\rho_j^{n+1} = \rho_j^{TD} - (f_{j+\frac{1}{2}}^c - f_{j-\frac{1}{2}}^c) \tag{61b}$$

The corrected antidiffusion flux,

$$f_{j+\frac{1}{2}}^c = \text{sign}\ \Delta_{j+\frac{1}{2}} \cdot \max\{0, \min[\Delta_{j-\frac{1}{2}} \cdot \text{sign}\ \Delta_{j+\frac{1}{2}}, \frac{\text{"}1\text{"}}{8}|\Delta_{j+\frac{1}{2}}|, \Delta_{j+3/2} \cdot \text{sign}\ \Delta_{j+\frac{1}{2}}]\} \tag{62}$$

is the corrected form of the raw flux

$$f_{j+\frac{1}{2}} \equiv \frac{1}{8}\Delta_{j+\frac{1}{2}} \equiv \frac{1}{8}(\rho_{j+1}^{TD} - \rho_j^{TD}), \tag{63}$$

which in this scheme is always in the same direction as the gradient in ρ^{TD}. There are eight different possible cases, shown schematically in Fig. 6. Cases 5-8 are mirror images of 1-4, respectively.

Equation (62) will cancel an antidiffusion flux whenever it would lead to accentuate a maximum or a minimum, as illustrated in Fig. 6, and will trim it enough not to generate a new maximum or minimum whenever it is not cancelled.

Later in Ref. 2 the raw antidiffusion fluxes were evaluated using ρ_j^T in the raw flux $f_{j+\frac{1}{2}} \equiv \frac{1}{8}(\rho_{j+1}^T - \rho_j^T)$, where

$$\rho_j^T \equiv \rho_j^n - \frac{\varepsilon}{2}(\rho_{j+1}^n - \rho_{j-1}^n) + \frac{\varepsilon^2}{2}(\rho_{j+1}^n - 2\rho_j^n + \rho_{j-1}^n).$$

The corrected flux is expressed as

$$f_{j+\frac{1}{2}}^c = \text{sign}\, f_{j+\frac{1}{2}} \cdot \max\{0, \min[\Delta_{j-\frac{1}{2}} \cdot \text{sign}\, f_{j+\frac{1}{2}}, |f_{j+\frac{1}{2}}|, \Delta_{j+3/2} \cdot \text{sign}\, f_{j+\frac{1}{2}}]\}, \tag{64}$$

where we get sixteen possible cases (twice as many as before, depending whether $f_{j+\frac{1}{2}}$ is parallel to $\Delta_{j+\frac{1}{2}}$ or opposite to it). In Fig. 7 we consider only those cases when $f_{j+\frac{1}{2}}$ is positive, since the other cases are their mirror images.

Again, the flux is cancelled whenever it would accentuate a maximum or minimum. But it is also cancelled in cases 6-8 where it would not in general cause any problems, an unnecessary action. This is due to the fact that $f_{j+\frac{1}{2}}$ is corrected independently of $f_{j-\frac{1}{2}}$ and $f_{j+3/2}$.

Zalesak[5] reexpressed the role of the flux limiter as "guaranteeing that the two antidiffusion fluxes associated with each cell, acting in concert, should not create any ripples." The mathematical formula implementing the above statement is described for 1-D schemes by the following steps:

$$P_j^+ \equiv \text{sum of antidiffusive fluxes "into" grid point } j$$

$$= \max\,(0, f_{j-\frac{1}{2}}) - \min\,(0, f_{j+\frac{1}{2}}) \tag{65}$$

$$Q_j^+ \equiv (\rho_j^{max} - \rho_j^{TD}) \tag{66}$$

$$R_j^+ \equiv \begin{cases} \min\,(1, Q_j^+/P_j^+) & \text{if } P_j^+ > 0 \\ 0 & \text{if } P_j^+ = 0. \end{cases} \tag{67}$$

Similarly,

$$P_j^- \equiv \text{sum of antidiffusive fluxes "out of" grid point } j$$

$$= \max\,(0, f_{j+\frac{1}{2}}) - \min\,(0, f_{j-\frac{1}{2}}) \tag{68}$$

$$Q_j^- \equiv (\rho_j^{TD} - \rho_j^{min}) \tag{69}$$

$$R_j^- \equiv \begin{cases} \min\,(1, Q_j^-/P_j^-) & \text{if } P_j^- > 0 \\ 0 & \text{if } P_j^- = 0, \end{cases} \tag{70}$$

where ρ_j^{max} and ρ_j^{min} are the upper and lower bounds on ρ_j^{n+1}, respectively, which ensure that no ripples form at grid point j. Defining the *correction ratio*

$$C_{j+\frac{1}{2}} \equiv \begin{cases} \min\,(R_{j+1}^+, R_j^-) & \text{if } f_{j+\frac{1}{2}} > 0 \\ \min\,(R_j^+, R_{j+1}^-) & \text{if } f_{j+\frac{1}{2}} < 0. \end{cases} \tag{71}$$

we set

$$f_{j+\frac{1}{2}}^C = C_{j+\frac{1}{2}} f_{j+\frac{1}{2}}. \tag{72}$$

A conservative choice for ρ_j^{max} and ρ_j^{min} is

$$\rho_j^{max} = \max\,(\rho_{j-1}^{TD}, \rho_j^{TD}, \rho_{j+1}^{TD})$$

$$\rho_j^{min} = \min\,(\rho_{j-1}^{TD}, \rho_j^{TD}, \rho_{j+1}^{TD}). \tag{73}$$

This choice will guarantee that no maxima or minima form other than those already existing in the ρ^{TD} distribution. The flux limiter of Eq. (64), however, not only guarantees no ripples, but it also cancels the flux in cases 6-8 of Fig. 7. To reproduce the results of Eq. (64), one should apply the extra limiter

$$f_{j+\frac{1}{2}}^{c} = 0$$

$$\text{if } (f_{j+\frac{1}{2}} \cdot \Delta_{j+\frac{1}{2}} < 0 \text{ and } (f_{j+\frac{1}{2}} \cdot \Delta_{j+3/2} < 0 \text{ or } f_{j+\frac{1}{2}} \cdot \Delta_{j-\frac{1}{2}} < 0)) \tag{74}$$

before Eq. (64).

An extension of Eq. (64) to more than one dimension, however, cannot guarantee that there will be no ripples since it lacks knowledge of $f_{j+3/2}$ and $f_{j-\frac{1}{2}}$ when correcting $f_{j+\frac{1}{2}}$. We are left then with only one safe solution, which is the extension of Eqs. (65) to (74) to multidimensions. Now, going back to Eq. (73), a more tolerant choice would be

$$\rho_j^{max} = \max\,\{\max\,(\rho_{j-1}^{TD}, \rho_{j-1}^{n}),\ \max\,(\rho_j^{TD}, \rho_j^{n}),\ \max\,(\rho_{j+1}^{TD}, \rho_{j+1}^{n})\};$$

$$\rho_j^{min} = \min\,\{\min\,(\rho_{j-1}^{TD}, \rho_{j-1}^{n}),\ \min\,(\rho_j^{TD}, \rho_j^{n}),\ \min\,(\rho_{j+1}^{TD}, \rho_{j+1}^{n})\}. \tag{75}$$

This choice will partially avoid the clipping associated with the flux correction of Eq. (73), as explained in Ref. 5. In summary, by calibrating $(\rho_j^{max}, \rho_j^{min})$ using a guaranteed positive profile, positivity is still preserved after the antidiffusion step is performed.

Now that we have all the definitions and tools necessary for analysis, let us go back to analyzing schemes.

V. A STABLE SIXTH-ORDER DIFFUSION ERROR FOURTH-ORDER PHASE ERROR SCHEME

As mentioned earlier, ETBFCT can be made stable by using $\mu = 1/6 - \alpha\frac{\varepsilon^2}{6}$, where $\alpha \geq 1.056$. Then

$$(|A|^2)''_o = 2[-2(\nu - \mu) + \varepsilon^2] = 2[-2(\frac{2+\alpha}{6}) + 1]\varepsilon^2,$$

yielding

$$|A|^2 = 1 - (\frac{\alpha-1}{3})\varepsilon^2\beta^2 + O(\beta^4), \tag{81}$$

which gives for $\alpha = 1.056$

$$|A|^2 = 1 - \frac{0.056}{3}\varepsilon^2\beta^2 + O(\beta^4),$$

thus giving the scheme a small second-order error, but leaving it essentially fourth order in amplitude.

An alternative is to add a small phoenical diffusion $O(\varepsilon^2)$ to ρ^T. We get then

$$\rho^T_j = \rho^n_j - \frac{\varepsilon}{2}(\rho^n_{j+1} - \rho^n_{j-1}) + \lambda\varepsilon^2(\rho^n_{j+1} - 2\rho^n_j + \rho^n_{j-1});$$

$$\rho^{TD}_j = \rho^T_j + \nu(\rho^n_{j+1} - 2\rho^n_j + \rho^n_{j-1});$$

$$\rho^{n+1}_j = \rho^{TD}_j - \mu(\rho^T_{j+1} - 2\rho^T_j + \rho^T_{j-1}). \tag{82}$$

Assuming $\rho^n_j = \rho^o e^{ikj\delta x}$,

$$A = (1 - \varepsilon t + \lambda\varepsilon^2 d)(1 - \mu d) + \nu d, \tag{83}$$

where $t \equiv i \sin\beta$ and $d \equiv 2(\cos\beta - 1)$. Following the method of analysis described above, we write

$$A_o^t = -\varepsilon,\ A_o^d = (\nu + \lambda\varepsilon^2) - \mu,$$

$$A_o^{td} = \varepsilon\mu,\ A_o^{dd} = -2\lambda\varepsilon^2\mu,\ \text{and}\ A_o^{tdd} = 0$$

Then

$$A_o' = -\ i\varepsilon;$$

$$A_o'' = -\ 2[(\nu + \lambda\varepsilon^2) - \mu];$$

$$A_o''' = -\ i[-\varepsilon + 6\,\varepsilon\mu];$$

$$A_o^{'v} = 2[\nu + \lambda\varepsilon^2 - \mu - 12\lambda\ \varepsilon^2\mu];$$

For a fourth-order diffusion error,

$$(|A|^2)_o'' = 2[-2(\nu + \lambda\varepsilon^2 - \mu) + \varepsilon^2] = 0,$$

yielding

$$\nu + \lambda\varepsilon^2 - \mu = \frac{\varepsilon^2}{2}.$$

Going back to the A_o'', $A_o^{'v}$ expressions, we can rewrite them as

$$A_o'' = -\ \varepsilon^2,$$

$$A_o^{'v} = \varepsilon^2 - 24\lambda\varepsilon^2\mu.$$

For a fourth-order phase error

$$(\log A)_o''' = -i[-\varepsilon + 6\varepsilon\mu] - 3(-i\varepsilon)(-2)(\nu + \lambda\varepsilon^2 - \mu) + 2(-i\varepsilon)^3$$

$$= i\varepsilon[1 - 6(\nu + \lambda\varepsilon^2) + 2\varepsilon^2] = 0,$$

yielding

$$\nu + \lambda\varepsilon^2 = 1/6 + \varepsilon^2/3,$$

which gives

$$\mu = 1/6 - \varepsilon^2/6$$

We can then rewrite A_o''' and $A_o^{'v}$ as

$$A_o''' = i\varepsilon^3,$$

$$A_o^{'v} = \varepsilon^2 - 4\lambda\varepsilon^2(1 - \varepsilon^2).$$

Checking,

$$(|A|^2)_o^{'v} = 2[\varepsilon^2 - 4\lambda\varepsilon^2(1 - \varepsilon^2) - 4\varepsilon^4 + 3\varepsilon^4]$$

$$= 2[1 - 4\lambda)\varepsilon^2(1 - \varepsilon^2)].$$

showing that we can make the scheme sixth-order in diffusion by selecting

$$\lambda = 1/4.$$

In summary,

$$\nu = 1/6 + \varepsilon^2/12,\ \mu = 1/6 - \varepsilon^2/6,\ \lambda = 1/4. \qquad (84)$$

Again, we have to check ^{TD}:

$$\rho_j^{TD} = [1 - 2(\frac{1}{6} + \frac{\varepsilon^2}{2})]\rho_j^n + [\frac{1}{6} + \frac{\varepsilon^2}{3} - \frac{\varepsilon}{2}]\rho_{j+1}^n + [\frac{1}{6} + \frac{\varepsilon^2}{3} + \frac{\varepsilon}{2}]\rho_{j-1}^n.$$

Each quantity in square brackets is ≥ 0 if $|\varepsilon| \leq 1/2$, yielding $\rho_j^{TD} \geq 0$ if $\rho_j^n \geq 0$, thus ensuring positivity. Figure 8 shows $|A|$ and R versus β. Finally, we note that this is still a 5-point scheme.

VI. EXTENSION TO HIGHER ORDERS IN DIFFUSION AND PHASE ERRORS

We seek a combination of transport operator $t(t \equiv i \sin \beta)$ and diffusion operator $d(d \equiv 2(\cos \beta - 1))$ which approaches the analytic solution up to a prescribed order of β. Since the transfer function of the analytic solution is expressed as $A = e^{-i\beta\varepsilon}$,

$$A = \cos \beta\varepsilon - i \sin \beta\varepsilon \tag{85}$$

or

$$A_I = - \sin \beta\varepsilon$$

$$A_R = \cos \beta\varepsilon. \tag{86}$$

Now, we write $\sin \beta\varepsilon$ as

$$\sin \beta\varepsilon = \sin \beta [A_o + A_1(1 - \cos \beta) + A_2(1 - \cos \beta)^2 + \ldots], \tag{87}$$

where A_o, A_1, A_2,... are determined such as to make the series expansion of both sides of Eq. (87) agree up to a prescribed order of β. In other words, the derivatives of both sides with respect to β at $\beta = 0$ have to be equal. We get the following system of algebraic equations:

$$\begin{bmatrix} \varepsilon \\ -\varepsilon^3 \\ \varepsilon^5 \\ \cdot \\ \cdot \\ \cdot \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & \ldots \\ -1 & 3 & 0 & 0 & \ldots \\ 1 & -15 & 30 & 0 & \ldots \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix} \begin{bmatrix} A_o \\ A_1 \\ A_2 \\ \cdot \\ \cdot \\ \cdot \end{bmatrix} \tag{88}$$

solved by "forward substitution" since the matrix of coefficients is already "left-triangular." We solve for A_o first, then for A_1, etc. We get

$$A_o = \varepsilon,\ A_1 = \frac{\varepsilon(1-\varepsilon^2)}{3},\ A_2 = \frac{\varepsilon(4-\varepsilon^2)(1-\varepsilon^2)}{30},\ldots \tag{89}$$

As for the construction of the matrix, the first column is the odd derivatives of $\sin\beta$, the second, those of $\sin\beta(1-\cos\beta)$, the third, those of $\sin\beta(1-\cos\beta)^2, \ldots$ and so on, all at $\beta = 0$. We notice that the even derivatives are all zero. To get these, let $\phi \equiv 1-\cos\beta$, and define K recursively $K_{i+1} \equiv K_i\phi$ where $K_o \equiv \sin\beta$. If we have the derivatives of K_i, those of K_{i+1} will be

$$\begin{aligned} K_{i+1} &= K_i\phi; \\ K'_{i+1} &= K'_i\phi + K_i\phi'; \\ K''_{i+1} &= K''_i\phi + 2K'_i\phi' + K_i\phi'', \end{aligned} \tag{90}$$

and so on. Generally if $(\ )^{(n)} \equiv \left.\frac{d^n(\ )}{d\beta^n}\right|_{\beta=o}$ and $(\ )^{(o)} \equiv (\ )$, we get

$$K_{i+1}^{(n)} = \sum_{m=0}^{n} \binom{n}{m} K_i^{(m)} \phi^{(n-m)} \tag{91}$$

where $\binom{n}{m} = \frac{n!}{(n-m)!m!}$. All we need then is the derivatives of $K_o \equiv \sin\beta$ and $\phi \equiv 1-\cos\beta$ at $\beta = 0$; namely,

$$\begin{aligned} &K_o = 0,\ K'_o = 1,\ K''_o = 0,\ K'''_o = -1,\ldots, \text{ and} \\ &\phi = 0,\ \phi' = 0,\ \phi'' = 1,\ \phi''' = 0,\ \phi^{iv} = -1,\ldots \end{aligned} \tag{92}$$

Now, we write $\cos\beta\varepsilon$ as

$$\cos\beta\varepsilon = B_o + B_1(1-\cos\beta) + B_2(1-\cos\beta)^2 + \ldots \tag{93}$$

where B_o, B_1, B_2,..., are determined such as to make the series expansion of both sides of Eq. (93) agree up to a prescribed order of β. In this case

$$K_o = 1, \; K_o' = K_o'' = K_o''' = \ldots = 0. \tag{94}$$

Using Eq. (91), we get

$$\begin{bmatrix} 1 \\ -\varepsilon^2 \\ \varepsilon^4 \\ \cdot \\ \cdot \\ \cdot \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & \ldots \\ 0 & 1 & 0 & 0 & \ldots \\ 0 & -1 & 6 & 0 & \ldots \\ \cdot & \cdot & \cdot & \cdot & \\ \cdot & \cdot & \cdot & \cdot & \\ \cdot & \cdot & \cdot & \cdot & \end{bmatrix} \begin{bmatrix} B_o \\ B_1 \\ B_2 \\ \cdot \\ \cdot \\ \cdot \end{bmatrix} \tag{95}$$

where we notice again a "left-triangular" coefficients matrix. By "forward substitution" we obtain

$$B_o = 1, \; B_1 = -\varepsilon^2, \; B_2 = \frac{-\varepsilon^2}{6}(1 - \varepsilon^2) \ldots \tag{96}$$

Obviously, we can get Eq. (93) by differentiating Eq. (87) and vice versa, but we need then to continue the expansion one more term and use trigonometric identities. The direct approach followed is, however, preferred, since it enforces a given form on the expansion which is in no way unique, as explained below.

Noticing that $\sin \beta = t/i$ and $1 - \cos \beta = -d/2$, we can write a sixth-order diffusion error, sixth-order phase error scheme, for example, as

$$A_R = 1 + \frac{\varepsilon^2}{2} d - \frac{\varepsilon^2}{24}(1 - \varepsilon^2) d^2$$

$$iA_1 = - \varepsilon t[1 - \frac{1 - \varepsilon^2}{6} d + \frac{1 - \varepsilon^2}{30}(1 - \frac{\varepsilon^2}{4}) d^2]. \tag{97}$$

If we stop at A_1, B_1, we get ETBFCT, which has fourth-order diffusion and phase error. Although t and d are both three-point operators, td^2 is a seven-point formula. An important conclusion follows: We need three points for a second-order diffusion and phase error, five points for a fourth-order error, and so on, adding two points at a time. We can, however, get sixth-order diffusion and fourth-order phase accuracy with only five points since we have to match the sum $|A|^2 = A_I^2 + A_R^2$ up to a prescribed order of β and not A_I and A_R separately. Scheme (82) is an example. Alternatively one can construct a scheme with fourth-order diffusion and sixth-order phase accuracy using only five points since we have to expand $\tan^{-1} \frac{A_I}{A_R}$, not A_I and A_R separately.

Before implementing Eq. (97), it is important to emphasize that the expansion is not unique. For example, we can use the expansions

$$\sin \beta\varepsilon = \sin \beta \, [A_o + A_1(1 - \cos \beta) + A_2(1 - \cos 2\beta) + \ldots.],$$

$$\cos \beta\varepsilon = B_o + B_1(1 - \cos \beta) + B_2(1 - \cos 2\beta) + \ldots \tag{98}$$

We get then

$$\begin{bmatrix} \varepsilon \\ -\varepsilon^3 \\ \varepsilon^5 \\ \cdot \\ \cdot \\ \cdot \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & \ldots \\ -1 & 3 & 12 & \ldots \\ 1 & -15 & -120 & \ldots \\ \cdot & \cdot & \cdot & \\ \cdot & \cdot & \cdot & \\ \cdot & \cdot & \cdot & \end{bmatrix} \begin{bmatrix} A_o \\ A_1 \\ A_2 \\ \cdot \\ \cdot \\ \cdot \end{bmatrix} \tag{99}$$

and

$$\begin{bmatrix} 1 \\ -\varepsilon^2 \\ \varepsilon^4 \\ \cdot \\ \cdot \\ \cdot \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & \cdots \\ 0 & 1 & 4 & \cdots \\ 0 & -1 & -16 & \cdots \\ \cdot & \cdot & \cdot & \\ \cdot & \cdot & \cdot & \\ \cdot & \cdot & \cdot & \end{bmatrix} \begin{bmatrix} B_o \\ B_1 \\ B_2 \\ \cdot \\ \cdot \\ \cdot \end{bmatrix}$$

By solving the two systems (99), (100), we obtain

$$A_o = \varepsilon,\ A_1 = \frac{\varepsilon(9-\varepsilon^2)(1-\varepsilon^2)}{15},\ A_2 = \frac{-\varepsilon(4-\varepsilon^2)(1-\varepsilon^2)}{60} \tag{100}$$

and

$$B_o = 1,\ B_1 = \frac{-\varepsilon^2}{3}(4-\varepsilon^2),\ B_2 = \frac{\varepsilon^2}{2}(1-\frac{\varepsilon^2}{6}). \tag{101}$$

We notice that the matrices are full and the coefficients (A_1, A_2,...); (B_1, B_2,...) are more complex in form than the corresponding coefficients Eq. (89), (96). Moreover, they change if the expansion is extended to higher order. The operator (1 - cos 2β) results from a five-point formula; namely, $\rho_{j+2} - 2\rho_j + \rho_{j-2}$. It is abandoned therefore in favor of the three-point operator formula of Eq. (97) since the latter requires knowledge of only one point outside the boundary.

We rewrite Eq. (97) as

$$A \equiv A_R + iA_I = -\varepsilon t\{1 - (\frac{1-\varepsilon^2}{6})d + (\frac{1-\varepsilon^2}{6})\frac{1}{5}(1-\frac{\varepsilon^2}{4})d^2\}$$
$$+ \{1 + \frac{\varepsilon^2}{2}d - \frac{\varepsilon^2}{4}(\frac{1-\varepsilon^2}{6})d^2\}.$$

Noting that $\rho^{n+1} = A\rho^n$, let us collect the terms in such a way as to ensure positivity at every step. First, $(-\varepsilon t)\rho^n = \rho^T - \rho^n$ where

$$\rho_j^T = \rho_j^n - \frac{\varepsilon}{2}(\rho_{j+1}^n - \rho_{j-1}^n).$$

Then

$$\rho^{n+1} = \rho^n + (\frac{\varepsilon^2}{2} d)\rho^n - [(\frac{1-\varepsilon^2}{6} d)(\frac{\varepsilon^2}{4} d)]\rho^n + \{1-(\frac{1-\varepsilon^2}{6} d)$$

$$+ (\frac{1-\varepsilon^2}{6} d)[\frac{1}{5}(1 - \frac{\varepsilon^2}{4})d]\}(\rho^T - \rho^n), \qquad (102)$$

whence

$$\rho^{n+1} \equiv \rho^T + [(\frac{\varepsilon^2}{2} + \frac{1-\varepsilon^2}{6})d]\rho^n - (\frac{1-\varepsilon^2}{6} d)[\rho^T + (\frac{\varepsilon^2}{4} d)\rho^n]$$

$$+ \{(\frac{1-\varepsilon^2}{6} d)[\frac{1}{5}(1 - \frac{\varepsilon^2}{4})d]\}(\rho^T - \rho^n) \qquad (103)$$

From our earlier experience, the combination

$$\rho^T + (\frac{\varepsilon^2}{2} + \frac{1-\varepsilon^2}{6})d\rho^n$$

is known to be positive for $|\varepsilon| \leq 1/2$. The remaining terms are regarded as antidiffusion. The following scheme is recommended:

$$\rho_j^T = \rho_j^n - \frac{\varepsilon}{2}(\rho_{j+1}^n - \rho_{j-1}^n); \qquad (104a)$$

$$\rho_j^{TA} = \rho_j^T - \frac{1}{5}(1 - \frac{\varepsilon^2}{4})(\rho_{j+1}^T - 2\rho_j^T + \rho_{j-1}^T); \qquad (104b)$$

$$\rho_j^{TAD} = \rho_j^{TA} + \frac{1}{5}(1 + \varepsilon^2)(\rho_{j+1}^n - 2\rho_j^n + \rho_{j-1}^n); \qquad (104c)$$

$$\rho_j^{TD} = \rho_j^T + (\frac{1}{6} + \frac{\varepsilon^2}{3})(\rho_{j+1}^n - 2\rho_j^n + \rho_{j-1}^n); \qquad (104d)$$

$$\rho_j^{n+1} = \rho_j^{TD} - (\frac{1-\varepsilon^2}{6})(\rho_{j+1}^{TAD} - 2\rho_j^{TAD} + \rho_{j-1}^{TAD})^*, \qquad (104e)$$

where the asterisk of Eq. (104e) means that the antidiffusive fluxes in this step are to be corrected. It is worth noticing that if ρ^{TAD} is taken as ρ^T, we obtain a fourth-order diffusion, fourth-order phase algorithm. If

$$\rho^{TAD} \equiv \rho^T + \frac{\varepsilon^2}{4} d\rho^n ,$$

we get a sixth-order diffusion, fourth-order phase, and finally,

$$\rho^{TAD} \equiv \rho^T + \frac{1}{5}(1 + \varepsilon^2) d\rho^n$$

yields a fourth-order diffusion, sixth-order phase error scheme. The amplitude and phase error versus β are shown in Fig. 9.

VII. PHYSICAL ASPECTS

The conservation of mass, momentum, and energy applied to a system are expressed as

$$\frac{d}{dt}\int_{\mathcal{V}^f(t)} \rho(\vec{x},t)\,d\mathcal{V} = 0 \tag{111}$$

$$\frac{d}{dt}\int_{\mathcal{V}^f(t)} \rho(\vec{x},t)\vec{u}(\vec{x},t)\,d\mathcal{V} = \int_{\mathcal{V}^f(t)} \rho(\vec{x},t)\vec{G}(\vec{x},t)\,d\mathcal{V} + \int_{S^f(t)} \vec{T}(\vec{n},\vec{x},t)\,dS \tag{112}$$

and

$$\frac{d}{dt}\int_{\mathcal{V}^f(t)} \rho(\vec{x},t)\left\{e(\vec{x},t) + \frac{|\vec{u}(\vec{x},t)|^2}{2}\right\}d\mathcal{V} = \int_{\mathcal{V}^f(t)} \rho(\vec{x},t)\vec{G}(\vec{x},t)\cdot\vec{u}(\vec{x},t)\,d\mathcal{V}$$

$$+ \int_{S^f(t)} \vec{T}(\vec{n},\vec{x},t)\cdot\vec{u}(\vec{x},t)\,dS + \int_{S^f(t)} \vec{q}\cdot\vec{n}\,dS \tag{113}$$

where e and G are the internal energy and body force per unit mass, $\vec{T}$ is the stress on an element of surface dS with unit normal $\vec{n}$, and $\vec{q}$ is the flux of energy through the surface, for example, heat flux. The integrations are carried out over $\mathcal{V}^f(t)$, $S^f(t)$, where the superscript indicates that the control volume moves with the fluid. We notice that all the terms contributing to the balance of any of the conserved quantities are volume or surface integrals.

In the case of an inviscid fluid

$$\vec{T}(\vec{n},\vec{x},t) = -\,p(\vec{x},t)\vec{n}. \tag{114}$$

The surface integrals $\int_{S^f} \vec{T}dS$ and $\int_{S^f} \vec{T}\cdot\vec{u}dS$ reduce then to $\int_{S^f} p\vec{n}dS$ and $\int_{S^f} p\vec{u}\cdot\vec{n}dS$ which yield $\int_{\forall^f}$ grad $p d\forall$ and $\int_{\forall^f}$ div $(p\vec{u})d\forall$, respectively, when we apply the divergence theorem.

Recalling Reynold's transport theorem

$$\frac{d}{dt}\int_{\forall^*(t)} \chi(\vec{x},t)\,d\forall = \int_{\forall^*(t)} \frac{\partial\chi}{\partial t}\,d\forall + \int_{S^*(t)} \chi\,\vec{u}^*\cdot\vec{n}dS \qquad (115)$$

where $\forall^*(t)$ is a control volume whose surface elements dS move with arbitrary velocity $\vec{u}^*$. Notice that the two integrals on the RHS are over space and therefore depend only on the instantaneous position of the control volume. Consequently, the integration can be carried out over any control volume which happens to coincide with $\forall^*$ at this instant, whether it is fixed or moving with another velocity. Denoting the fluid velocity by $\vec{u}^f$ and the control surface velocity by $\vec{u}^g$ we get, using Eq. (115)

$$\frac{d}{dt}\int_{\forall^f} \chi\,d\forall = \int_{\forall^f} \frac{\partial\chi}{\partial t}\,d\forall + \int_{S^f} \chi\,\vec{u}^f\cdot\vec{n}dS$$

$$\frac{d}{dt}\int_{\forall^g} \chi\,d\forall = \int_{\forall^g} \frac{\partial\chi}{\partial t}\,d\forall + \int_{S^g} \chi\,\vec{u}^g\cdot\vec{n}dS \qquad (116)$$

If $\forall^g$ coincide with $\forall^f$ at time t, we get

$$\frac{d}{dt}\int_{\forall^f} \chi\,d\forall = \frac{d}{dt}\int_{\forall^g} \chi\,d\forall + \int_{S^g} (\vec{u}^f - \vec{u}^g)\cdot\vec{n}dS \qquad (117)$$

When $G = 0$ and $q = 0$, Eqs. (111) through (113) become

$$\frac{d}{dt}\int_{\forall^g} \rho d\forall + \int_{S^g} \rho(\vec{u}^f - \vec{u}^g)\cdot\vec{n}dS = 0; \tag{118}$$

$$\frac{d}{dt}\int_{\forall^g} \rho\vec{u}^f d\forall + \int_{S^g} \rho\vec{u}^f[(\vec{u}^f - \vec{u}^g)\cdot\vec{n}]dS = -\int_{S^g} p\vec{n}dS; \tag{119}$$

$$\frac{d}{dt}\int_{\forall^g} \rho(e + \frac{|\vec{u}^f|^2}{2})d\forall + \int_{S^g} \rho(e + \frac{|\vec{u}^f|^2}{2})(\vec{u}^f - \vec{u}^g)\cdot\vec{n}dS = -\int_{S^g} p\vec{u}^f\cdot\vec{n}dS. \tag{120}$$

Using the divergence theorem we can get the differential form of the conservation equations. However, it is far more convenient to use the integral form, because a numerical scheme based on the integral form is already conservative, since the fluxes leaving one control volume have to enter an adjacent one, and discontinuities can be propagated in principle without any smoothing, since one can always integrate a profile including a discontinuity, in contrast with differentiation. Consider Fig. 10, representing a uniform fixed one-dimensional grid and a continuous density profile incorporating one discontinuity. If we know the mass in the hatched cell and the velocity at interfaces A and B, Eq. (118) will give us the rate of change of mass within the cell, and hence the mass itself after an infinitesimal time δt. But we have to get the density at A and B and the velocity for the next time step. We must have recourse then to "averaging" procedures to get the density from a known cell mass and "interpolation" procedures to get the values of the interfaces from the cell average values. Through these two procedures, errors are introduced. Finally, we have to use a finite grid in any case.

Equations (118) to (120) can be written in a reduced form as

$$\frac{d}{dt}\int_{\forall^g} \rho^* d\forall + \int_{S^g} \rho^* (\vec{u}^f - \vec{u}^g)\cdot\vec{n}dS = -\int_{S^g} T^* dS + \int_{\forall^g} G^* d\forall$$

where ρ^* is a generalized density (ρ^* denotes ρ, $\rho\vec{u}^f$ and $E \equiv \rho(e + \frac{|\vec{u}^f|^2}{2})$ in Eqs. (118) to (120), respectively), T^* is a generalized surface stress ($T^* = 0$, $p\vec{n}$, $p\vec{u}^f\cdot\vec{n}$), while G^* denotes a generalized body force ($G^* = 0$ in Eqs. (118) to (120)). The two integrals on the RHS are referred to as source terms.

A naive "finite-integral" form solution can be written as

$$\begin{bmatrix}\text{mass within}\\ \text{control volume}\\ \text{at } t + \delta t\end{bmatrix} = \begin{bmatrix}\text{mass within}\\ \text{control volume}\\ \text{at } t\end{bmatrix} - \begin{bmatrix}\text{net outgoing}\\ \text{mass flux through}\\ \text{control surface}\end{bmatrix} + [\text{source terms}].$$

As will be explained next, the above formula is supplemented with diffusion flux terms (actually diffusion and antidiffusion) to improve its accuracy.

ACCURACY

The above mathematical analysis was carried out assuming a fixed uniform grid and $\frac{\partial\rho}{\partial t} + u_o\frac{\partial\rho}{\partial x} = 0$, where $u_o \equiv$ constant. We notice also the absence of any source term (inhomogeneous part of a conservation equation). The analytical solution was found out to be

$$\rho^{n+1} = A\rho^n$$

where $A = e^{-i\beta\varepsilon}$, then was expanded to get a numerical scheme that matches it up to a prescribed order of β. In this context the numerical scheme is an approximate solution of the whole PDE, in contrast to schemes which approximate $\frac{\partial}{\partial x}$ *alone by a finite difference* and $\frac{\partial}{\partial t}$ alone. By getting a solution of the PDE as a whole, we mix the time and space derivatives for a higher order scheme. To see that, let us expand $\rho(t + \delta t, x)$ in a Taylor series:

$$\rho(t + \delta t, x) = \rho(t) + \delta t \left.\frac{\partial \rho}{\partial t}\right|_x + \frac{\delta t^2}{2!} \left.\frac{\partial^2 \rho}{\partial t^2}\right|_x + \ldots \tag{121}$$

From the PDE

$$\frac{\partial \rho}{\partial t} = - u_o \frac{\partial \rho}{\partial x} \tag{122a}$$

$$\frac{\partial^2 \rho}{\partial t^2} = \frac{\partial}{\partial t}\left(\frac{\partial}{\partial t}\right) = \frac{\partial}{\partial t}\left(-u_o \frac{\partial \rho}{\partial x}\right) = - u_o \frac{\partial}{\partial x}\left(\frac{\partial \rho}{\partial t}\right) - u_o{}^2 \frac{\partial^2 \rho}{\partial x^2} . \tag{122b}$$

Substituting Eqs. (122) into (121) we obtain

$$\rho(t + \delta t, x) = \rho(t) - u_o \delta t \frac{\partial \rho}{\partial x} + \frac{u_o{}^2 \delta t^2}{2} \frac{\partial^2 \rho}{\partial x^2} + \ldots, \tag{123}$$

showing that we can get a better solution in the time domain (of higher order in δt) by adding to $[\rho(t) - u_o \delta t \frac{\partial \rho}{\partial x}]$ a diffusion term, $\frac{u_o{}^2 \delta t^2}{2} \frac{\partial^2 \rho}{\partial x^2}$, a purely spatial derivative. Notice that $\frac{u_o^2 (\delta t)^2}{2}$ is equivalent to $\frac{\varepsilon^2}{2}$, the coefficient of $d\rho^n$ in the schemes discussed earlier. The remaining terms appear when we try to express $\frac{\partial \rho}{\partial x}$ and $\frac{\partial^2 \rho}{\partial x^2}$ in terms of finite differences accurately.

A scheme which splits the time and space domains, on the other hand, treats Eq. (122a) as an ODE, where the right-hand side is assumed to be a function of time. A second-order Runge-Kutta explicit scheme can be written as

$$\rho(t + \delta t,x) = \rho(t,x) - u_o\delta t \left.\frac{\partial\rho}{\partial x}\right|_{t + \frac{\partial t}{2},\, x} \qquad (124)$$

where $\left.\frac{\partial\rho}{\partial x}\right|_{t + \frac{\partial t}{2},\, x}$ is obtained by first getting a provisional value of the density at $t + \delta t/2$ using a lower-order scheme

$$\rho(t + \frac{\delta t}{2},x) = \rho(t,x) - u_o \frac{\delta t}{2} \left.\frac{\partial\rho}{\partial x}\right|_{t,x} \qquad (125)$$

then getting $\left.\frac{\partial\rho}{\partial x}\right|_{t + \frac{\partial t}{2},\, x}$ by differentiating $\rho(t + \frac{\delta t}{2},x)$ spatially, with the result

$$\left.\frac{\partial\rho}{\partial x}\right|_{t + \frac{\delta t}{2},\, x} = \left.\frac{\partial\rho}{\partial x}\right|_{t,x} - u_o \frac{\delta t}{2} \left.\frac{\partial^2\rho}{\partial x^2}\right|_{t,x} .$$

Upon substituting in Eq. (124), this yields Eq. (123) again. One can deduce therefore that up to a given order, schemes which mix the time and space domains and those which split them are equivalent. A warning, however, is in order here: A concept derived for a split time-space scheme cannot be applied directly to one that mixes both domains. For example, using a half point density in Eq. (123), i.e., the scheme

$$\rho(t + \frac{\delta t}{2},x) = \rho(t,x) - u_o \frac{\delta t}{2} \left.\frac{\partial\rho}{\partial x}\right|_{t,x} + \frac{u_o^{\,2}\delta t^2}{8} \left.\frac{\partial^2\rho}{\partial x^2}\right|_{t,x} \qquad (126a)$$

$$\rho(t + \delta t,x) = \rho(t,x) - u_o\delta t \left.\frac{\partial\rho}{\partial x}\right|_{t + \frac{\delta t}{2},x} + \frac{u_o^{\,2}\delta t^2}{2} \left.\frac{\partial^2\rho}{\partial x^2}\right|_{t + \frac{\delta t}{2},x} \qquad (126b)$$

will cause a decrease in accuracy instead of improving it, as can be seen from differentiating Eq. (126a) with respect to x and substituting in Eq. (126b). The key point is that Eq. (123) is a solution of the PDE as a whole.

In summary, the schemes derived in earlier sections are solutions of the conservation equations if u^f = constant, $u^g = 0$, and source terms = 0.

If these are not satisfied, a correction that preserves the order of the scheme should be adopted. Here we split the two effects:

(1) u^f variable and source terms are variable $\neq 0$

(2) $u^g \neq 0$

and treat each separately.

GRID MOTION

According to the above splitting, we need to consider a case where $u^f = 0$ and source terms vanish, but $u^g \neq 0$. This is a static field, where the density and energy are constants. Equations (118) and (120) reduce then to

$$\frac{d}{dt}\int_{V^g} dV = \int_{S^g} \vec{u}^g \cdot \vec{n}dS \tag{127}$$

This exhibits the formula for an accurate scheme when the grid is moving: the rate of change of volume equals the rate of sweeping by the moving surface, as illustrated in Fig. 11. Here we can achieve an infinite-order accuracy in δt by defining a mean control area S^{mean} such that

$$\int_{S^{mean}} \vec{u}^g \delta t \cdot \vec{n}dS = \text{swept volume}$$

Let us consider the three cases of 1-D geometry; namely, planar, cylindrical, and spherical symmetries, denoted from now on by $\alpha = 1$, 2, and 3, respectively.

In the planar case, the area is independent of the radius, so that

$$A_L^{n+\frac{1}{2}} = A_R^{n+\frac{1}{2}} = 1, \tag{128}$$

where L and R denote the left and right interfaces of the control cell, respectively.

In cylindrical 1-D geometry, the volume swept by the interface is

$$\Delta V_B = \pi[(r_B^{n+1})^2 - (r_B^n)^2],$$

where B indicates L or R. Here the depth of the cell being considered is taken equal to unity. Since $u^g \delta t = r_B^{n+1} - r_B^n$, the average area is

$$A_B^{n+\frac{1}{2}} \equiv \frac{\Delta V_B}{u^g \delta t} = \pi \frac{[(r_B^{n+1})^2 - (r_B^n)^2]}{r_B^{n+1} - r_B^n} = \pi(r_B^{n+1} + r_B^n) \tag{129}$$

One can define then average radii

$$r_B^{n+\frac{1}{2}} \equiv \frac{1}{2}(r_B^n + r_B^{n+1}), \tag{130}$$

since $A_B^{n,n+\frac{1}{2},n+1} = 2\pi r_B^{n,n+\frac{1}{2},n+1}$.

Finally, in spherical geometry, the swept volume is

$$\Delta V = \frac{4}{3} \pi[(r_B^{n+1})^3 - (r_B^n)^3],$$

yielding

$$A_B^{n+\frac{1}{2}} \equiv \frac{\Delta V}{r_B^{n+1} - r_B^n} = \frac{4}{3} \pi[(r_B^n)^2 + (r_B^n)(r_B^{n+1}) + (r_B^{n+1})^2], \tag{131}$$

whence

$$r_B^{n+\frac{1}{2}} = \{\frac{1}{3}[(r_B^n)^2 + (r_B^n)(r_B^{n+1}) + (r_B^{n+1})^2]\}^{\frac{1}{2}}, \tag{132}$$

since

$$A_B^{n,n+\frac{1}{2},n+\frac{1}{2}} = 4\pi(r_B^{n,n+\frac{1}{2},n+1})^2 .$$

Equations (128), (129), and (131) should be used as the proper interface areas when evaluating the fluxes and surface forces. To complete the formulation, when body forces are present, the volume used should be that confined between the average interfaces. It can be arbitrarily selected for $\alpha = 1$, and is defined as

$$\forall^{n+\frac{1}{2}} = \pi[(r_R^{n+\frac{1}{2}})^2 - (r_L^{n+\frac{1}{2}})^2] \tag{133}$$

for $\alpha = 2$, and

$$\forall^{n+\frac{1}{2}} = \frac{4}{3}\pi[(r_R^{n+\frac{1}{2}})^3 - (r_L^{n+\frac{1}{2}})^3] \tag{134}$$

for $\alpha = 3$. This choice will ensure a proper balance between surface and body forces.

Variable Velocity Field and Source Terms

To account for these two effects, the fluid velocity and source terms used in the "finite-integral" solution should be evaluated at some intermediate time between t^n, t^{n+1} so as to preserve the accuracy of the scheme. Since we split the effects of grid motion, variable velocity field and source terms, the above intermediate values should be derived from an ODE solver of a consistent order in δt. For a fourth-order (diffusion and phase error) accurate scheme, for example, we need a second-order-accurate explicit ODE solver. In other words, for the system of Eqs. (118) to (120), we advance the time one-half step using $\vec{u}^f = \vec{u}^n$ and $p = p^n$ to get $\rho^{n+\frac{1}{2}}$, $(\rho\vec{u}^f)^{n+\frac{1}{2}}$, $E^{n+\frac{1}{2}}$. We define $\vec{u}^{n+\frac{1}{2}} \equiv (\rho\vec{u}^f)^{n+\frac{1}{2}}/\rho^{n+\frac{1}{2}}$ and $p^{n+\frac{1}{2}} \equiv p(\rho^{n+\frac{1}{2}}, e^{n+\frac{1}{2}})$ where $p(\rho,e)$ is the equation of state and

$$e^{n+\frac{1}{2}} = (E^{n+\frac{1}{2}}/\rho^{n+\frac{1}{2}}) - \frac{|\vec{u}^{n+\frac{1}{2}}|^2}{2} .$$

Then we advance the system a whole time step using $\vec{u}^f = \vec{u}^{n+\frac{1}{2}}$ and $p = p^{n+\frac{1}{2}}$. As explained earlier, we need not and should not update ρ, $\rho\vec{u}^f$ and E, during the full time step, since the scheme is already a solution of the whole PDE. For a sixth-order-accurate scheme, we need a fourth-order ODE solver and so on.

Example of an Algorithm

Let us implement the scheme

$$\rho_j^T = \rho_j^n - \frac{\varepsilon}{2}(\rho_{j+1}^n - \rho_{j-1}^n) + \frac{\varepsilon^2}{4}(\rho_{j+1}^n - 2\rho_j^n + \rho_{j-1}^n);$$

$$\rho_j^{TD} = \rho_j^T + (\frac{1}{6} + \frac{\varepsilon^2}{12})(\rho_{j+1}^n - 2\rho_j^n + \rho_{j-1}^n);$$

$$\rho_j^{n+1} = \rho_j^{TD} - (\frac{1}{6} - \frac{\varepsilon^2}{6})(\rho_{j+1}^T - 2\rho_j^T + \rho_{j-1}^T), \qquad (135)$$

a stable, fourth-order phase error, sixth-order diffusion error scheme, where ρ denotes either of ρ, $\rho\vec{u}^f$, or E.

If we have N cells whose interfaces are at radii $(r_{1/2}^n, r_{3/2}^n, \ldots, r_{N+1/2}^n)$ at time t^n, moving to $(r_{1/2}^{n+1}, r_{3/2}^{n+1}, \ldots)$ at t^{n+1}, let us denote the cell centers by the subscripts $j = 1, 2, \ldots, N$, located at

$$r_j^{n,n+1} \equiv \begin{cases} \frac{1}{2}(r_{j-1/2}^{n,n+1} + r_{j+1/2}^{n,n+1}) & \text{for } \alpha = 1,2 \\ \{\frac{1}{3}[(r_{j-1/2}^{n,n+1})^2 + (r_{j-1/2}^{n,n+1})(r_{j+1/2}^{n,n+1}) + (r_{j+1/2}^{n,n+1})^2]\}^{\frac{1}{2}} & \text{for } \alpha = 3. \end{cases} \qquad (136)$$

The volume of the j^{th} cell per unit angle is given by

$$
\forall_j^{n,n+1} = \begin{cases} r_{j+1/2}^{n,n+1} - r_{j-1/2}^{n,n+1}, & \alpha = 1 \\ \frac{1}{2}[(r_{j+1/2}^{n,n+1})^2 - (r_{j-1/2}^{n,n+1})^2], & \alpha = 2 \\ \frac{1}{3}[(r_{j+1/2}^{n,n+1})^3 - (r_{j-1/2}^{n,n+1})^3, & \alpha = 3 \end{cases} \tag{137}
$$

Denoting the mean interface radii by $r_{j+\frac{1}{2}}^{n+\frac{1}{2}}$, Eqs. (128), (130), and (132) imply for $j = 0,\ldots,N$,

$$
r_{j+\frac{1}{2}}^{n+\frac{1}{2}} = \begin{cases} (r_{j+\frac{1}{2}}^{n} + r_{j+\frac{1}{2}}^{n+1})/2 & \alpha = 1,\ 2 \\ \left[\dfrac{(r_{j+\frac{1}{2}}^{n})^2 + (r_{j+\frac{1}{2}}^{n})(r_{j+\frac{1}{2}}^{n+1}) + (r_{j+\frac{1}{2}}^{n+1})^2}{3}\right]^{\frac{1}{2}}, & \alpha = 3 \end{cases} \tag{138}
$$

giving, according to Eqs. (128), (129), and (131), mean interface area per unit angle

$$
A_{j+\frac{1}{2}}^{n+\frac{1}{2}} = \begin{cases} 1 \\ r_{j+\frac{1}{2}}^{n+\frac{1}{2}} \\ (r_{j+\frac{1}{2}}^{n+\frac{1}{2}})^2 \end{cases} \tag{139}
$$

and mean cell volume per unit angle

$$
\forall_j^{n+\frac{1}{2}} = \begin{cases} (r_{j+\frac{1}{2}}^{n+\frac{1}{2}}) - (r_{j-\frac{1}{2}}^{n+\frac{1}{2}}) \\ \frac{1}{2}[(r_{j+\frac{1}{2}}^{n+\frac{1}{2}})^2 - (r_{j-\frac{1}{2}}^{n+\frac{1}{2}})^2] \\ \frac{1}{3}[(r_{j+\frac{1}{2}}^{n+\frac{1}{2}})^3 - (r_{j-\frac{1}{2}}^{n+\frac{1}{2}})^3] \end{cases} \tag{140}
$$

for $\alpha = 1, 2, 3$, respectively. We write Eq. (135a) in the form

$$\mathcal{V}_j^{n+1}\rho_j^T = \mathcal{V}_j^n\rho_j^n - \delta t(\rho_{j+\frac{1}{2}}^n\ A_{j+\frac{1}{2}}^{n+\frac{1}{2}}\ \delta U_{j+\frac{1}{2}}^{n+\frac{1}{2}}) + \delta t(\rho_{j-\frac{1}{2}}^n\ A_{j-\frac{1}{2}}^{n+\frac{1}{2}}\ \delta U_{j-\frac{1}{2}}^{n+\frac{1}{2}})$$

$$+ \lambda_{j+\frac{1}{2}}^{n+\frac{1}{2}}\ \mathcal{V}_{j+\frac{1}{2}}^n(\rho_{j+\frac{1}{2}}^n - \rho_j^n) - \lambda_{j-\frac{1}{2}}^{n+\frac{1}{2}}\ \mathcal{V}_{j-\frac{1}{2}}^n(\rho_j^n - \rho_{j-1}^n) + \text{source}\ _j^{n+\frac{1}{2}}, \tag{141}$$

where

$$\rho_{j+\frac{1}{2}}^n = \frac{1}{2}(\rho_j^n + \rho_{j+1}^n) \tag{142}$$

for j = 1,..., N-1, while

$$\rho_{\frac{1}{2}}^n = \frac{1}{2}(\rho_L^n + \rho_1^n)\quad ,\quad \rho_{N-\frac{1}{2}}^n = \frac{1}{2}(\rho_N^n + \rho_R^n),$$

where L and R denote left and right guard cells, respectively. The difference $\delta U_{j+\frac{1}{2}}$ between the fluid and grid velocities is given by

$$\delta U_{j+\frac{1}{2}}^{n+\frac{1}{2}}\ \delta t = U_{j+\frac{1}{2}}^{n+\frac{1}{2}}\ \delta t - U_{j+\frac{1}{2}}^g \delta t = U_{j+\frac{1}{2}}^{n+\frac{1}{2}}\ \delta t - (r_{j+\frac{1}{2}}^{n+1} - r_{j+\frac{1}{2}}^n), \tag{143}$$

while the diffusion coefficient is

$$\lambda_{j+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{1}{4}(\varepsilon_{j+\frac{1}{2}}^{n+\frac{1}{2}})^2, \tag{144}$$

where

$$\varepsilon_{j+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{\delta U_{j+\frac{1}{2}}^{n+\frac{1}{2}}\ A_{j+\frac{1}{2}}^{n+\frac{1}{2}}\ \delta t}{2}\left(\frac{1}{\mathcal{V}_j^n} + \frac{1}{\mathcal{V}_{j+1}^n}\right). \tag{145}$$

The velocity at the interfaces satisfies

$$U_{j+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{1}{2}(U_j^{n+\frac{1}{2}} + U_{j+1}^{n+\frac{1}{2}}) \tag{146}$$

for j = 1,..., N-1, while

$$U_{\frac{1}{2}}^{n+\frac{1}{2}} = U_L^{n+\frac{1}{2}}, \; U_{N+\frac{1}{2}}^{n+\frac{1}{2}} = U_R^{n+\frac{1}{2}}.$$

The volumes $\Psi_{j+\frac{1}{2}}^{n}$ are defined as

$$\Psi_{j+\frac{1}{2}}^{n} = \frac{1}{2}(\Psi_j^n + \Psi_{j+1}^n) \tag{147}$$

for $j = 1, \ldots, N-1$, and

$$\Psi_{\frac{1}{2}}^{n} = \Psi_1^n, \; \Psi_{N+\frac{1}{2}}^{n} = \Psi_N^n.$$

Equation (135b) then adds the main diffusion, giving

$$\Psi_j^{n+1}\rho_j^{TD} = \Psi_j^{n+1}\rho_j^{T} + \nu_{j+\frac{1}{2}}^{n+\frac{1}{2}}\,\Psi_{j+\frac{1}{2}}^{n}(\rho_{j+1}^n - \rho_j^n) - \nu_{j-\frac{1}{2}}^{n+\frac{1}{2}}\,\Psi_{j-\frac{1}{2}}^{n}(\rho_j^n - \rho_{j-1}^n) \tag{148}$$

where

$$\nu_{j+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{1}{6} + \frac{(\varepsilon_{j+\frac{1}{2}}^{n+\frac{1}{2}})^2}{12}\;. \tag{149}$$

Finally, the antidiffusive fluxes are evaluated according to

$$F_{j+\frac{1}{2}} = \mu_{j+\frac{1}{2}}^{n+\frac{1}{2}}\,\Psi_{j+\frac{1}{2}}^{n+1}(\rho_{j+1}^T - \rho_j^T), \tag{150}$$

where

$$\mu_{j+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{1}{6} - \frac{(\varepsilon_{j+\frac{1}{2}}^{n+\frac{1}{2}})^2}{6}\;, \tag{151}$$

and then corrected using one of the flux limiters Eq. (64) or Eqs. (65)-(75). Let us select Eq. (64) on account of its simplicity. The corrected fluxes are given by

$$F_{j+\frac{1}{2}}^{C} = \text{sign}\,(F_{j+\frac{1}{2}})\cdot\max\{0, \min[\text{sign}\,(F_{j+\frac{1}{2}})\cdot\Psi_{j+\frac{1}{2}}^{n+1}\cdot(\rho_{j+2}^{TD} - \rho_{j+1}^{TD}),$$

$$|F_{j+\frac{1}{2}}|, \; \text{sign}\,(F_{j+\frac{1}{2}})\cdot\Psi_{j-\frac{1}{2}}^{n+1}\cdot(\rho_j^{TD} - \rho_{j-1}^{TD})]\} \tag{152}$$

whence

$$\rho_j^{n+1} = \rho_j^{TD} - \frac{1}{\forall_j^{n+1}} (F^c_{j+\frac{1}{2}} - F^c_{j-\frac{1}{2}}). \tag{153}$$

As for the source terms, they are summations over the surface or the volume of the cell. Let us consider first $[-\int_{S^g} pn \, dS]$, which yields [- grad p]. In cartesian coordinates, following the diagram of Fig. 12,

$$\text{source}_j^{n+\frac{1}{2}} = p_{j-\frac{1}{2}}^{n+\frac{1}{2}} A_{j-\frac{1}{2}}^{n+\frac{1}{2}} - p_{j+\frac{1}{2}}^{n+\frac{1}{2}} A_{j+\frac{1}{2}}^{n+\frac{1}{2}} \tag{154}$$

where

$$p_{j+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{1}{2}(p_j^{n+\frac{1}{2}} + p_{j+1}^{n+\frac{1}{2}}) \tag{155}$$

for j = 1,..., N-1, while $p_{\frac{1}{2}}^{n+\frac{1}{2}} = p_L^{n+\frac{1}{2}}$ and $p_{N+\frac{1}{2}}^{n+\frac{1}{2}} = p_R^{n+\frac{1}{2}}$.

In cylindrical geometry, following Fig. 13, we have

$$\text{source}_j^{n+\frac{1}{2}} = p_{j-\frac{1}{2}}^{n+\frac{1}{2}} A_{j-\frac{1}{2}}^{n+\frac{1}{2}} - p_{j+\frac{1}{2}}^{n+\frac{1}{2}} A_{j+\frac{1}{2}}^{n+\frac{1}{2}} + p_j^{n+\frac{1}{2}}(r_{j+\frac{1}{2}}^{n+\frac{1}{2}} - r_{j-\frac{1}{2}}^{n+\frac{1}{2}})$$

and since

$$r_{j+\frac{1}{2}}^{n+\frac{1}{2}} - r_{j-\frac{1}{2}}^{n+\frac{1}{2}} = \frac{(r_{j+\frac{1}{2}}^{n+\frac{1}{2}})^2 - (r_{j-\frac{1}{2}}^{n+\frac{1}{2}})^2}{r_{j+\frac{1}{2}}^{n+\frac{1}{2}} + r_{j-\frac{1}{2}}^{n+\frac{1}{2}}} = \frac{\forall_j^{n+\frac{1}{2}}}{r_j^{n+\frac{1}{2}}},$$

where from Eq. (136)

$$r_j^{n+\frac{1}{2}} = \frac{1}{2}(r_{j+\frac{1}{2}}^{n+\frac{1}{2}} + r_{j-\frac{1}{2}}^{n+\frac{1}{2}}) \tag{156}$$

for $\alpha = 2$, we can rewrite the expression for $\text{source}_j^{n+\frac{1}{2}}$ as

$$\text{source}_j^{n+\frac{1}{2}} = p_{j-\frac{1}{2}}^{n+\frac{1}{2}} A_{j-\frac{1}{2}}^{n+\frac{1}{2}} - p_{j+\frac{1}{2}}^{n+\frac{1}{2}} A_{j+\frac{1}{2}}^{n+\frac{1}{2}} + \frac{p_j^{n+\frac{1}{2}}}{r_j^{n+\frac{1}{2}}} \forall_j^{n+\frac{1}{2}}, \tag{157}$$

where we notice that $p_j^{n+\frac{1}{2}}/r_j^{n+\frac{1}{2}}$ acts as a body force per unit volume per unit angle.

In spherical geometry,

$$\text{source}_j^{n+\frac{1}{2}} = p_{j-\frac{1}{2}}^{n+\frac{1}{2}} A_{j-\frac{1}{2}}^{n+\frac{1}{2}} - p_{j+\frac{1}{2}}^{n+\frac{1}{2}} A_{j+\frac{1}{2}}^{n+\frac{1}{2}} + p_j^{n+\frac{1}{2}}[(r_{j+\frac{1}{2}}^{n+\frac{1}{2}})^2 - (r_{j-\frac{1}{2}}^{n+\frac{1}{2}})^2] = p_{j-\frac{1}{2}}^{n+\frac{1}{2}} A_{j-\frac{1}{2}}^{n+\frac{1}{2}} - p_{j+\frac{1}{2}}^{n+\frac{1}{2}} A_{j+\frac{1}{2}}^{n+\frac{1}{2}} + \frac{2p_j^{n+\frac{1}{2}}}{(r_j^{n+\frac{1}{2}})^2/r_{j,\alpha=2}^{n+\frac{1}{2}}} V_j^{n+\frac{1}{2}} ,$$

where from Eq. (136),

$$r_j^{n+\frac{1}{2}} = \frac{1}{3}[(r_{j-\frac{1}{2}}^{n+\frac{1}{2}})^2 + (r_{j-\frac{1}{2}}^{n+\frac{1}{2}})(r_{j+\frac{1}{2}}^{n+\frac{1}{2}}) + (r_{j+\frac{1}{2}}^{n+\frac{1}{2}})]^{\frac{1}{2}} \tag{159}$$

for $\alpha = 3$, and

$$r_{j,\alpha=2}^{n+\frac{1}{2}} = \frac{r_{j+\frac{1}{2}}^{n+\frac{1}{2}} + r_{j-\frac{1}{2}}^{n+\frac{1}{2}}}{2}$$

Again, $\dfrac{2p_j^{n+\frac{1}{2}}}{(r_j^{n+\frac{1}{2}})^2/r_{j,\alpha=2}^{n+\frac{1}{2}}}$ acts as a body force per unit volume per unit angle.

Next we consider $[-\int_{S^g} p\vec{u}\cdot\vec{n}dS]$, which gives rise to the term [- div (pu)].

For the three geometries, we get

$$\text{source}_j^{n+\frac{1}{2}} = p_{j-\frac{1}{2}}^{n+\frac{1}{2}} U_{j-\frac{1}{2}}^{n+\frac{1}{2}} A_{j-\frac{1}{2}}^{n+\frac{1}{2}} - p_{j+\frac{1}{2}}^{n+\frac{1}{2}} U_{j+\frac{1}{2}}^{n+\frac{1}{2}} A_{j+\frac{1}{2}}^{n+\frac{1}{2}} \tag{160}$$

In summary, all we need for the source terms is a routine to multiply by the frontal area for the surface integrals, or cell volume in the case volume integrals.

Finally, $U_j^{n+\frac{1}{2}}$ and source $_j^{n+\frac{1}{2}}$ are obtained by first advancing the whole system of Eqs. (136)-(160) a half time step using U_j^n, source $_j^n$, then a whole time step using

$$U_j^{n+\frac{1}{2}}\Big|_{t\to t+\delta t} = U_j^{n+1}\Big|_{t\to t+\delta t/2} \tag{161}$$

and

$$\text{source}\,_j^{n+\frac{1}{2}}\Big|_{t\to t+\delta t} = \text{source}\,_j^{n+1}\Big|_{t\to t+\delta t/2}. \tag{162}$$

XI. TWO-DIMENSIONAL TRANSPORT

Now let us consider the two-dimensional equivalent of Eq. (2),

$$\frac{\partial\rho}{\partial t} + u_1 \frac{\partial\rho}{\partial x} + u_2 \frac{\partial\rho}{\partial y} = 0, \tag{201}$$

whose analytic solution is

$$\rho(x,y,t) = \rho(x - u_1 t, y - u_2 t, 0), \tag{202}$$

a wave propagating with velocity $\vec{u} = (u_1, u_2)$. Assuming an initial density $\rho(x,y,0) = F(x,y)$, we Fourier analyze $F(x,y)$ in space on a rectangle $L_1 \times L_2$ with periodic boundary conditions:

$$F(\vec{r}) = \sum_{\vec{k}=-\infty}^{\infty} \hat{\rho}_{\vec{k}} e^{-i\vec{k}\cdot\vec{r}}, \tag{203a}$$

where $\vec{r} = (x,y)$, and $\vec{k} = (k_1, k_2)$ is assumed to be normalized, i.e., $\vec{k}$ denotes $2\pi(\frac{k_1}{L_1}, \frac{k_2}{L_2})$. Notice that the summation of (203a) is actually a double summation.

$$F(x,y) = \sum_{k_1=-\infty}^{\infty} \sum_{k_2=-\infty}^{\infty} \hat{\rho}_{k_1,k_2} e^{i(k_1 x + k_2 y)}. \tag{203b}$$

To gain insight, let us consider only one wave component of Eq. (203),

$$F(\vec{r}) = \sin \vec{k}\cdot\vec{r} \tag{204a}$$

or

$$F(x,y) = \text{six } 2\pi(\frac{k_1 x}{L_1} + \frac{k_2 y}{L_2}). \tag{204b}$$

Figure 21 shows the resulting waves for different values of (L_1, L_2), (k_1, k_2). From Eq. (204b), $F(x,y)$ is constant along lines of constant

$(\frac{k_1 x}{L_1} + \frac{k_2 y}{L_2})$. For example, the nodes of the wave coincide with the lines

$$\frac{k_1 x}{L_1} + \frac{k_2 y}{L_2} = 0,\ \frac{1}{2},\ 1,\ \frac{3}{2},\ 2, \ldots \tag{205}$$

which are normal to the wave vector $\vec{k}$.

To find the wave length for a given (k_1,k_2), we first go back to the one-dimensional case. For a system of length L and periodic boundary conditions, the harmonics $\sin 2\pi\frac{kx}{L}$ and $\cos 2\pi\frac{ky}{L}$ are admitted, where $k = 0, 1, 2, \ldots, \infty$. With each of these is associated a wave length λ defined as the distance between two successive "even" nodes. Since $\sin 2\pi\frac{kx}{L} = 0$ at $\frac{2\pi kx}{L} = 0, \pi, 2\pi, 3\pi, \ldots$, λ is obtained from $\frac{2\pi k\lambda}{L} = 2\pi$, yielding

$$\lambda = \frac{L}{k} . \tag{206}$$

We get therefore wave lengths ∞, L, $\frac{L}{2}$, $\frac{L}{3}$, $\frac{L}{4}, \ldots$, where the longest finite wave length equals L, the system length. In two-dimensional, the wave length for a given k is defined analogously as the distance between two points on successive "even" node lines, projected on the direction of $\vec{k}$. From Eq. (204b),

$$F(x,0) = \sin 2\pi \frac{k_1 x}{L_1}$$

which, as explained above, yields $\lambda_x = \frac{L_1}{k_1}$ where λ_x is the wave length along the x-direction, which when projected on $k = 2\pi(\frac{k_1}{L_1}, \frac{k_2}{L_2})$ yields λ:

$$\lambda = \frac{(\frac{L_1}{k_1},0)\cdot(\frac{k_1}{L_1}, \frac{k_2}{L_2})}{\sqrt{(\frac{k_1}{L_1})^2 + (\frac{k_2}{L_2})^2}} = \frac{1}{\sqrt{(\frac{k_1}{L_1})^2 + (\frac{k_2}{L_2})^2}} = \frac{2\pi}{|\vec{k}|}, \tag{207a}$$

where

$$|\vec{k}| = \sqrt{\left(\frac{2\pi k_1}{L_1}\right)^2 + \left(\frac{2\pi k_2}{L_2}\right)^2}$$

or

$$\lambda = \frac{1}{\sqrt{\left(\frac{1}{\lambda_x}\right)^2 + \left(\frac{1}{\lambda_y}\right)^2}} \tag{207b}$$

N w we find all the wavelengths along a given direction $\frac{k_1}{L_1} : \frac{k_2}{L_2} =$ constant c. Noticing that k_1, k_2 for periodic boundary conditions can take only integer values, the waves along a given direction correspond to

$k_1^{(n)} = nk_1^{(1)}$, $k_2^{(n)} = nk_2^{(1)}$ $(n = 1,2,\ldots,\infty)$ where $k_1^{(1)}$, $k_2^{(1)}$ are the smallest integers that satisfy

$$\frac{k_1^{(1)}/L_1}{k_2^{(1)}/L_2} = c$$

From Eq. (207a)

$$\lambda_n = \frac{1}{\sqrt{\left(\frac{nk_1^{(1)}}{L_1}\right)^2 + \left(\frac{nk_2^{(1)}}{L_2}\right)^2}} = \frac{\lambda_1}{n}, \tag{208}$$

where

$$\lambda_1 = \frac{1}{\sqrt{\left(\frac{k_1^{(1)}}{L_1}\right)^2 + \left(\frac{k_2^{(1)}}{L_2}\right)^2}}. \tag{209}$$

Along a given direction we have wave lengths $\lambda_1, \frac{\lambda_1}{2}, \frac{\lambda_1}{3}, \ldots, \frac{\lambda_1}{\infty}$.

Consider, for example, Fig. 21(b), where $L_1 = 2$, $L_2 = 1$. Along direction

$(1/2,\ 1)$, $k_1^{(1)} = k_2^{(1)} = 1$, whence $\lambda_1 = 1/\sqrt{(\frac{1}{2})^2 + 1} = 2/\sqrt{5}$. The maximum system length along this direction being $\sqrt{(\frac{1}{2})^2 + 1} = \frac{\sqrt{5}}{2}$, $\frac{\lambda_1}{L_{\frac{1}{2},1}} = \frac{2/\sqrt{5}}{\sqrt{5}/2} = \frac{4}{5}$, showing that because of the periodic boundary condition independently in each direction the longest wave length is only 80 percent of the maximum system length in the direction $(\frac{1}{2},1)$, in contrast to one-dimensional cases where $\lambda_1 = L$. For the case of Fig. 21(a), λ_1 is 50 percent of the system length.

From Eq. (202),

$$\rho(x,y,t) = \sum_{k_1=-\infty}^{\infty} \sum_{k_2=-\infty}^{\infty} \hat{\hat{\rho}}_{k_1,k_2} e^{i[k_1(x - u_1t) + k_2(y - u_2t)]}$$

$$= \sum_{k_1} \sum_{k_2} \hat{\rho}_{k_1,k_2}(t)\ e^{i(k_1x + k_2y)} \tag{210a}$$

or

$$\rho(\vec{r},t) = \sum_{\vec{k}=-\infty}^{\infty} \hat{\hat{\rho}}_k e^{i\vec{k}\cdot(\vec{r} - \vec{u}t)} = \sum \hat{\rho}_{\vec{k}}\ e^{i\vec{k}\cdot\vec{r}} \tag{210b}$$

where

$$\hat{\rho}_{k_1,k_2}(t) = \hat{\hat{\rho}}_{k_1,k_2} e^{-i(k_1u_1 + k_2u_2)t} \tag{211a}$$

or

$$\hat{\rho}_{\vec{k}}(t) = \hat{\hat{\rho}}_{\vec{k}}\ e^{-i\vec{k}\cdot\vec{u}t} \tag{211b}$$

Thus each harmonic independently advances uniformly in phase without changing its magnitude, as shown in Fig. (22).

We notice that the different harmonics advance in the direction $\vec{u}$, which is generally different from that of k, as illustrated in Fig. (23). They keep their front normal to $\vec{k}$ and therefore the projection of $\vec{u}$ on $\vec{k}$ is the speed of advance. This adds extra requirements that were not invoked in the one-dimensional case, namely:

1. The scheme should keep the wave front a straight line; otherwise distortion of profiles occurs.
2. It should also keep the wave front normal to $\vec{k}$; otherwise "scattering" occurs, namely waves with different $|\vec{k}|$ but the same direction $(k_1:k_2)$ will come out in different directions, causing scattering of the transported profile.

As will be proved later, the speed of propagation $\vec{V}$ of a numerical scheme differs from $\vec{u}$ not only in magnitude as in one dimension but also in direction, providing one more source of error. If the above two requirements are satisfied, however, only $\vec{k}\cdot(\vec{V} - \vec{u})$ contributes to the phase error.

Now suppose ϕ is known at all times only on a set of $(N_1 + 1)\cdot(N_2 + 1)$ discrete grid points with separation $\delta x = \frac{L_1}{N_1}$, $\delta y = \frac{L_2}{N_2}$, namely, $x_i = i\delta x$ $(i = 0,1,\ldots, N_1 - 1)$, $y_j = j\delta y$ $(j = 0,1,\ldots N_2 - 1)$, the origin being a member of the set. According to periodicity assumption $\phi_{o,j} = \phi_{N_1,j}$, $\phi_{i,o} = \phi_{i,N_2}$; hence we can have only $\frac{N_1N_2}{2} + 1$ different harmonics. Let

$$f(x,y) = \sum_{k_1 = \frac{-N_1}{2}}^{\frac{N_1}{2}} \sum_{k_2 = \frac{-N_2}{2}}^{\frac{N_2}{2}} \hat{\phi}_{k_1,k_2} e^{i(k_1x + k_2y)} . \tag{212}$$

Since

$$e^{i(k_1 x + k_2 y)}\Big|_{k_1 = \frac{N_1}{2}} = e^{i(\frac{2\pi}{L_1}(\frac{N_1}{2}) i\delta x + \frac{2\pi k_2}{L_2} j\delta y)} = e^{i(i\pi + 2\pi \frac{k_2}{L_2} j\delta y)}$$

$$= e^{i[i\pi + 2\pi \frac{k_2}{L_2} j\delta y) - 2\pi i]} = e^{i(-i\pi + \frac{2\pi k_2}{L_2} j\delta y)}$$

$$= e^{i[\frac{2\pi}{L_1}(\frac{-N_1}{2}) i\delta x + \frac{2\pi k_2}{L_2} j\delta y]} = e^{i(k_1 x + k_2 y)}\Big|_{k_1 = \frac{-N_1}{2}}$$

for all i, and similarly

$$e^{i(k_1 x + k_2 y)}\Big|_{k_2 = \frac{-N_2}{2}} = e^{i(k_1 x + k_2 y)}\Big|_{k_2 = \frac{N_2}{2}}$$

for all j, Eq. (212) can be rewritten as

$$f(x,y) = \sum_{k_I = \frac{-N_1}{2} + 1}^{\frac{N_1}{2}} \sum_{k_2 = \frac{-N_2}{2} + 1}^{\frac{N_1}{2}} \hat{\rho}_{k_1,k_2} e^{i(k_1 x + k_2 y)},$$

showing that $\vec{k}$ space structure contains only $N_1 \times N_2$ independent points (see Fig. 24). The amplitudes $\hat{\delta}_{k_1,k_2}$ can be obtained from

$$\rho^0_{i,j} = \sum_{k_1 = \frac{-N_1}{2} + 1}^{\frac{N_1}{2}} \sum_{k_2 = \frac{-N_2}{2} + 1}^{\frac{N_2}{2}} \hat{\rho}_{k_1,k_2} e^{i(\frac{2\pi k_1 i\delta x}{L_1} + \frac{2\pi k_2 j\delta y}{L_2})} \tag{214}$$

for $i = 0,1,2,\ldots, N_1-1$, and $j = 0,1,2,\ldots, N_2-1$.

In terms of sines and cosines, Eq. (213) can be written as

$$f(x,y) = A_{o,o} + \left(\sum_{k_1=1}^{\frac{N_1}{2}-1} \sum_{k_2=1}^{\frac{N_2}{2}-1} A_{k_1,k_2} \cos\left(\frac{2\pi k_1 x}{L_1} + \frac{2\pi k_2 y}{L_2}\right) \right.$$

$$+ B_{k_1,k_2} \sin\left(\frac{2\pi k_1 x}{L_1} + \frac{2\pi k_2 y}{L_2}\right) + C_{k_1,k_2} \cos\left(\frac{2\pi k_1 x}{L_1} - \frac{2\pi k_2 y}{L_2}\right)$$

$$\left. + D_{k_1,k_2} \sin\left(\frac{2\pi k_1 x}{L_1} - \frac{2\pi k_2 y}{L_2}\right) \right) + \sum_{k_1=1}^{\frac{N_1}{2}-1} \left(A_{k_1,o} \cos\left(\frac{2\pi k_1 x}{L_1}\right) \right.$$

$$\left. + B_{k_1,o} \left(\sin \frac{2\pi k_1 x}{L_1}\right) \right) + A_{\frac{N_1}{2},o} \cos\left(\frac{\pi N_1 x}{L_1}\right) + \sum_{k_2=1}^{\frac{N_2}{2}-1} \left(A_{o,k_2} \cos\left(\frac{2\pi k_2 y}{L_2}\right) \right.$$

$$\left. + B_{o,k_2} \sin\left(\frac{2\pi k_2 y}{L_2}\right) \right) + A_{o,\frac{N_2}{2}} \cos\left(\frac{\pi N_2 y}{L_2}\right) + A_{\frac{N_1}{2},\frac{N_2}{2}} \cos\left(\frac{\pi N_1 x}{L_1} + \frac{\pi N_2 y}{L_2}\right), \tag{215}$$

where

$$\hat{\delta}_{k_1,k_2} = \begin{cases} \dfrac{A_{k_1,k_2} - iB_{k_1,k_2}}{2} & \text{for } k_1 > 0,\ k_2 > 0 \\[2ex] \dfrac{A_{k_1,k_2} + iB_{k_1,k_2}}{2} & \text{for } k_1 < 0,\ k_2 < 0 \\[2ex] \dfrac{C_{k_1,k_2} - iD_{k_1,k_2}}{2} & \text{for } k_1 > 0,\ k_2 < 0 \\[2ex] \dfrac{C_{k_1,k_2} + iD_{k_1,k_2}}{2} & \text{for } k_1 < 0,\ k_2 > 0 \end{cases}$$

Again, we have in Eq. (215) $N_1 \times N_2$ coefficients: A_{k_1,k_2} ($k_1 = 0,1,\ldots,\frac{N_1}{2}$ and $k_2 = 0,1,\ldots,\frac{N_2}{2}$), B_{k_1,k_2} ($k_1 = 0,1,\ldots,\frac{N_1}{2} - 1$ and $k_2 = 0,1,\ldots,\frac{N_2}{2} - 1$), C_{k_1,k_2}, D_{k_1,k_2} ($k_1 = 1,2,\ldots,\frac{N_1}{2} - 1$ and $k_2 = 1,2,\ldots,\frac{N_2}{2} - 1$) that can be determined from the system of equations $f(x_i,x_j) \equiv \rho^o_{i,j}$.

Going back to Fig. 24 let us count the different harmonics. The harmonics are considered equal if they have the same magnitude $|\vec{k}| \equiv \sqrt{(\frac{2\pi k_1}{L_1})^2 + (\frac{2\pi k_2}{L_2})^2}$ and are aligned, i.e., $\frac{k_1}{L_1} : \frac{k_2}{L_2}$ = constant. The number of the harmonics is almost half the space of Fig. 24 since (k_1,k_2) is equivalent to $(-k_1,-k_2)$ and $(k_1,-k_2)$ is equivalent to $(-k_1,k_2)$. For example: a and b in Fig. 24 are equivalent. Figure 25 shows the independent harmonics selected to match the choice in Eq. (215). The number of the harmonics is therefore, $\frac{N_1 N_2}{2} + 1$.

If we count the maximum number of wave lengths, we get an even smaller number, since according to Eq. (207a), $\lambda = \frac{2\pi}{|\vec{k}|}$. Two harmonics such as a and b in Fig. 25 will give the same value for $|\vec{k}|$. The maximum number of wave lengths is therefore $(\frac{N_1}{2} + 1)\cdot(\frac{N_2}{2} + 1)$, corresponding to the positive quadrant of Fig. 25. This is an upper limit. This is because the number of wave lengths can be less if the ratio $\delta x/\delta y$ is a rational number. As explained above, decomposition in two directions puts a limit on the longest finite wave length λ in a given direction. Discretization, on the other hand, puts a limit on the shortest wave length in a given direction since it reduces n in Eq. (208). The largest value occurs for $k_1 = \frac{N_1}{2}$, $k_2 = \frac{N_2}{2}$. If $k_1^{(1)}$, $k_2^{(2)}$ are the smallest integers for a given direction, the shortest wave length along this direction corresponds to

$$n = \underset{\text{integer}}{\min} \left(\frac{N_1/2}{k_1^{(1)}}, \frac{N_2/2}{k_2^{(2)}}\right). \tag{216}$$

Assuming $\rho(x,y,0) = f(x,y)$, i.e., assuming the density in between the grid points values $\rho^o_{i,j}$ to be $f(x,y)$, Eq. (202) predicts the density at time t as

$$\rho(x,y,t) = \sum_{k_1=\frac{-N_1}{2}+1}^{\frac{N_1}{2}} \sum_{k_2=\frac{-N_2}{2}+1}^{\frac{N_2}{2}} \hat{\hat{\rho}}_{k_1,k_2} e^{i[k_1(x-u_1t) + k_2(y-u_2t)]}$$

$$= \sum_{k_1} \sum_{k_2} \hat{\rho}_{k_1,k_2}(t) e^{i(k_1x + k_2y)}$$

where $\hat{\rho}_{k_1,k_2}(t) = \hat{\hat{\rho}}_{k_1,k_2} e^{-i(k_1u_1t + k_2u_2t)}$. Since we are only concerned with $\rho(x_i,y_j,t)$, let $x = x_i = i\delta x$, $y = y_j = j\delta y$. We then get

$$\rho(x_i,y_j,t) = \sum_{k_1=\frac{-N_1}{2}+1}^{\frac{N_1}{2}} \sum_{k_2=\frac{-N_2}{2}+1}^{\frac{N_2}{2}} \hat{\rho}_k(t) e^{i(k_1 i\delta x + k_2 j\delta y)}.$$ If the time is also discretized, let $t^n \equiv n\delta t$, $\rho^n_{i,j} \equiv \rho(x_i,y_j,t^n)$ and $\hat{\rho}^n_{k_1,k_2} \equiv \hat{\rho}_{k_1,k_2}(t^n)$.

Then $$\rho^n_{i,j} = \sum_{k_1} \sum_{k_2} \hat{\rho}^n_{k_1,k_2} e^{i(k_1 i\delta x + k_2 j\delta y)} \tag{217}$$

where

$$\hat{\rho}^n_{k_1,k_2} = \hat{\hat{\rho}}_{k_1,k_2} e^{-i(k_1u_1 + k_2u_2)n\delta t} \tag{218}$$

We define $A(k_1,k_2)$ as

$$A(k_1,k_2) = \frac{\rho^{n+1}_{k_1,k_2}}{\rho^{n}_{k_1,k_2}} .$$

Equation (218) expresses the analytic solution as

$$A(k_1,k_2) = e^{-i(k_1u_1\delta t + k_2u_2\delta t)}. \tag{219}$$

If we denote $\frac{u_1\delta t}{\delta x}$ by ε_x, $\frac{u_2\delta t}{\delta y}$ by ε_y, $k_1\delta x$ by β_x, and $k_2\delta y$ by β_y, Eq. (219) reduces to

$$A(k_1,k_2) = e^{-i(\varepsilon_x\beta_x + \varepsilon_y\beta_y)} \tag{220}$$

Now let us analyze a fully two-dimensional scheme, a direct extension of the one-dimensional scheme

$$\rho^T_j = \rho^n_j - \frac{\varepsilon}{2}(\rho^n_{j+1} - \rho^n_{j-1})$$

$$\rho^{TD}_j = \rho^T_j + \nu(\rho^n_{j+1} - 2\rho^n_j + \rho^n_{j-1})$$

$$\rho^{n+1}_j = \rho^{TD}_j - \mu(\rho^T_{j+1} - 2\rho^T_j + \rho^T_{j-1}), \tag{221}$$

namely,

$$\rho^{Tx}_{i,j} = \rho^n_{i,j} - \frac{\varepsilon_x}{2}(\rho^n_{i+1,j} - \rho^n_{i-1,j}); \tag{222a}$$

$$\rho^{Ty}_{i,j} = \rho^n_{i,j} - \frac{\varepsilon_y}{2}(\rho^n_{i,j+1} - \rho^n_{i,j-1}); \tag{222b}$$

$$\rho^{T}_{i,j} = \rho^n_{i,j} - \frac{\varepsilon_x}{2}(\rho^n_{i+1,j} - \rho^n_{i-1,j}) - \frac{\varepsilon_y}{2}(\rho^n_{i,j+1} - \rho^n_{i,j-1}); \tag{222c}$$

$$\rho^{TD}_{i,j} = \rho^T_{i,j} + \nu_x(\rho^n_{i+1,j} - 2\rho^n_{i,j} + \rho^n_{i-1,j}) + \nu_y(\rho^n_{i,j+1} - 2\rho^n_{i,j} + \rho^n_{i,j-1}); \tag{222d}$$

$$\rho^{n+1}_{i,j} = \rho^{TD}_{i,j} - \mu_x(\rho^{Tx}_{i+1,j} - 2\rho^{Tx}_{i,j} + \rho^{Tx}_{i-1,j}) - \mu_y(\rho^{Ty}_{i,j+1} - 2\rho^{Ty}_{i,j} + \rho^{Ty}_{i,j-1}). \tag{222e}$$

Again as in one-dimension, after Fourier-analyzing the initial density profile, i.e., after we have gotten the $\{\hat{\rho}_{k_1,k_2}\}$, the problem is reduced to propagation of the complex harmonics $e^{i(k_1x + k_2y)}$. Since for the linear problem Eq. (201), each harmonic propagates independently, we can get $A(k_1,k_2)$ by assuming only one harmonic:

$$\rho^n_{i,j} = \rho^o e^{i(k_1 i\delta x + k_2 j\delta y)} = \rho^o e^{i(i\beta_x + j\beta_y)}, \tag{223}$$

then using

$$A(k_1,k_2) = \frac{\rho^{n+1}_{i,j}}{\rho^n_{i,j}} . \tag{224}$$

Substituting Eq. (223) into (222a) we get

$$\rho^{Tx}_{i,j} = \rho^o e^{i(k_1 i\delta x + k_2 j\delta y)} - \frac{\varepsilon_x}{2}\{\rho^o e^{i[k_1(i+1)\delta x + k_2 j\delta y]} - \rho^o e^{i[k_1(i-1)\delta x + k_2 j\delta y)}\} \tag{225}$$

hence

$$\frac{\rho^{Tx}_{i,j}}{\rho^n_{i,j}} = 1 - \frac{\varepsilon_x}{2}(e^{i\beta_x} - e^{-i\beta_x}) = 1 - i\,\varepsilon_x \sin\beta_x \tag{226a}$$

Similarly Eq. (222b) gives

$$\frac{\rho^{Ty}_{i,j}}{\rho^n_{i,j}} = 1 - i\,\varepsilon_y \sin\beta_y. \tag{226b}$$

Denoting $i \sin\beta_x$ by t_x and $i \sin\beta_y$ by t_y, Eq. (222c) gives

$$\frac{\rho^{T}_{i,j}}{\rho^n_{i,j}} = 1 - \varepsilon_x t_x - \varepsilon_x t_x \tag{226c}$$

Substituting Eq. (223) into (222d)

$$\frac{\rho^{TD}_{i,j}}{\rho^{n}_{i,j}} = \frac{\rho^{T}_{i,j}}{\rho^{n}_{i,j}} + \nu_x(e^{i\beta_x} - 2 + e^{-i\beta_x}) + \nu_y(e^{i\beta_y} - 2 + e^{-i\beta_y})$$

$$= \frac{\rho^{T}_{i,j}}{\rho^{n}_{i,j}} + \nu_x d_x + \nu_y d_y, \tag{226d}$$

where $d_x \equiv 2(\cos\beta_x - 1)$ and $d_y \equiv 2(\cos\beta_y - 1)$. Finally, Eq. (222e) yields with Eqs. (226c) and (226d)

$$A(\beta_x,\beta_y) = \frac{\rho^{n+1}_{i,j}}{\rho^{n}_{i,j}} = (1 - \varepsilon_x t_x - \varepsilon_y t_y) + \nu_x d_x + \nu_y d_y - \mu_x d_x(1 - \varepsilon_x t_x)$$

$$- \mu_y d_y(1 - \varepsilon_y t_y) \tag{226e}$$

From which

$$\rho^{n+1}_{i,j} = A(\beta_x,\beta_y)\rho^{o} e^{i(i\beta_x + j\beta_y)}$$

We notice that the coefficient of $e^{i(i\beta_x + j\beta_y)}$ is independent of i and j, i.e., independent of x,y. Consequently, $\rho^{n+1}_{i,j}$ have the same wave front inclination and shape as $\rho^{n}_{i,j}$; i.e., along the lines of $k_1x + k_2y$ = constant, $\rho^{n+1}_{i,j}$ = constant. Finally, this is a nine-point explicit scheme, as illustrated in Fig. 26, which shows the points involved in determining $\rho^{n+1}_{i,j}$.

XII. AMPLITUDE AND PHASE ANALYSIS

We write A as $A = |A|e^{i\theta}$, where $|A|$ is the amplitude and θ is the phase angle. To classify the order of the scheme we need to expand $|A|$ and θ in a power series in β_x and β_y.

PHASE ERRORS

In the two-dimensional case we have $A = A(t_x,t_y,d_x,d_y)$ where t_x,d_x are functions of β_x, while t_y,d_y are functions of β_y. Since $\log A = \log |A| + i(\theta)$,

$$\theta = \mathrm{Im}\ (\log A). \tag{229}$$

Expanding θ in a power series of β_x, β_y near $\beta_x,\beta_y = 0$, we get

$$\theta = \theta_o + (\theta_o^x\beta_x + \theta_o^y\beta_y) + (\theta_o^{xx}\frac{\beta_x^2}{2} + \theta_o^{xy}\beta_x\beta_y + \theta_o^{yy}\frac{\beta_y^2}{2}) \tag{230}$$

$$+ (\theta_o^{xxx}\frac{\beta_x^3}{6} + \theta_o^{xxy}\frac{\beta_x^2\beta_y}{2} + \theta_o^{xyy}\frac{\beta_x\beta_y^2}{2} + \theta_o^{yyy}\frac{\beta_y^3}{6}) + \ldots, \tag{230}$$

where $\theta_o^x \equiv (\partial\theta/\partial\beta_x)$ at $\beta_x = 0$, while $\theta_o^y \equiv (\partial\theta/\partial\beta_y)$ at $\beta_y = 0$, etc.

We therefore need the derivatives of log A. Noticing that $A(\beta_x,\beta_y = 0) = 1$ we get

$$(\log A)_o^x = A_o^x \tag{231a}$$

$$(\log A)_o^y = A_o^y; \tag{231b}$$

$$(\log A)_o^{xx} = A_o^{xx} - (A_o^x)^2; \tag{232a}$$

$$(\log A)_o^{xy} = A_o^{xy} - A_o^xA_o^y; \tag{232b}$$

$$(\log A)_o^{yy} = A_o^{yy} - (A_o^y)^2 \tag{232c}$$

$$(\log A)_o^{xxx} = A_o^{xxx} - 3A_o^{xx}A_o^x + 2(A_o^x)^3; \tag{233a}$$

$$(\log A)_o^{xxy} = A_o^{xxy} - 2A_o^{xy}A_o^x - A_o^{xx}A_o^y + 2(A_o^x)^2A_o^y; \tag{233b}$$

$$(\log A)_o^{xyy} = A_o^{xyy} - 2A_o^{xy}A_o^y - A_o^xA_o^{yy} + 2A_o^x(A_o^y)^2; \tag{233c}$$

$$(\log A)_o^{yyy} = A_o^{yyy} - 3A_o^{yy}A_o^y + 2(A_o^y)^3; \tag{233d}$$

and so on.

Denoting $\frac{\partial(\ )}{\partial t_x}\Big|\beta_x,\beta_y = 0$ by $(\ )_o^{t_x}$, $\frac{\partial(\ )}{\partial d_x}\Big|\beta_x,\beta_y = 0$ by $(\ )_o^{d_x}$, so on, confining our scope to schemes of second degree in the operators t_x, t_y, d_x, or d_y, and using the chain rule of differentiation we get

$$A_o^x = A_o^{t_x}\, t'_{xo} + A_o^{d_x}\, d'_{xo}; \tag{235a}$$

$$A_o^y = A_o^{t_y}\, t'_{yo} + A_o^{d_y}\, d'_{yo}; \tag{235b}$$

$$A_o^{xx} = t''_{xo}\, A_o^{t_x} + d''_{xo}A_o^{d_x} + t'^2_{xo}A_o^{t_xt_x} + 2t'_{xo}d'_{xo}A_o^{t_xd_x} + d'^2_{xo}A_o^{d_xd_x}; \tag{236a}$$

$$A_o^{xy} = t'_{xo}t'_{yo}A_o^{t_xt_y} + t'_{xo}d'_{yo}A_o^{t_xd_y} + d'_{xo}t'_{yo}A_o^{d_xt_y} + d'_{xo}d'_{yo}A_o^{d_xd_y}; \tag{236b}$$

$$A_o^{yy} = t''_{yo}A_o^{t_y} + d''_{yo}A_o^{d_y} + t'^2_{yo}A_o^{t_yt_y} + 2t'_{yo}d'_{yo}A_o^{t_yd_y} + d'^2_{yo}A_o^{d_yd_y}; \tag{236c}$$

$$A_o^{xxx} = t'''_{xo}A_o^{t_x} + d'''_{xo}A_o^{d_x} + 3t'_{xo}t''_{xo}A_o^{t_xt_x}$$

$$+ 3(t'_{xo}d''_{xo} + t''_{xo}d'_{xo})A_o^{t_xd_x} + 3d'_{xo}d''_{xo}A_o^{d_xd_x}; \tag{237a}$$

$$A_o^{xxy} = t''_{xo}t'_{yo}A_o^{t_xt_y} + t''_{xo}d'_{yo}A_o^{t_xd_y} + d''_{xo}t'_{yo}A_o^{d_xt_y} + d''_{xo}d'_{yo}A_o^{d_xd_y}; \tag{237b}$$

$$A_o^{xyy} = t'_{xo} t''_{yo} A_o^{t_x t_y} + t'_{xo} d''_{yo} A_o^{t_x d_y} + d'_{xo} t''_{yo} A_o^{d_x t_y} + d'_{xo} d''_{yo} A_o^{d_x d_y}; \tag{237c}$$

$$\begin{aligned} A_o^{yyy} = {} & t'''_{yo} A_o^{t_y} + d'''_{yo} A_o^{d_y} + 3t'_{yo} t''_{yo} A_o^{t_y t_y} \\ & + 3(t'_{yo} d''_{yo} + t''_{yo} d'_{yo}) A_o^{t_y d_y} + 3d'_{yo} d''_{yo} A_o^{d_y d_y}. \end{aligned} \tag{237d}$$

Finally,

$$\begin{aligned} A_o^{xxxx} = {} & t^{iv}_{xo} A_o^{t_x} + d^{iv}_{xo} A_o^{d_x} + (4t'_{xo} t'''_{xo} + 3t''^{2}_{xo}) A_o^{t_x t_x} + (4t'''_{xo} d'_{xo} \\ & + 6t''_{xo} d''_{xo} + 4t'_{xo} d'''_{xo}) A_o^{t_x d_x} + (4d'_{xo} d'''_{xo} + 3d''^{2}_{xo}) A_o^{d_x d_x}; \end{aligned} \tag{239a}$$

$$A_o^{xxxy} = t'''_{xo} (t'_{yo} A_o^{t_x t_y} + d'_{yo} A_o^{t_x d_y}) + d'''_{xo} (t'_{yo} A_o^{d_x t_y} + d'_{yo} A_o^{d_x d_y}); \tag{239b}$$

$$A_o^{xxyy} = t''_{xo} t''_{yo} A_o^{t_x t_y} + d''_{xo} d''_{yo} A_o^{d_x d_y} + t''_{xo} d''_{yo} A_o^{t_x d_y} + d''_{xo} t''_{yo} A_o^{d_x t_y}; \tag{239c}$$

$$A_o^{xyyy} = t'''_{yo} (t'_{xo} A_o^{t_x t_y} + d'_{xo} A_o^{d_x t_y}) + d'''_{yo} (t'_{xo} A_o^{t_x d_y} + d'_{xo} A_o^{d_x d_y}); \tag{239d}$$

$$\begin{aligned} A_o^{yyyy} = {} & t^{iv}_{yo} A_o^{t_y} + d^{iv}_{yo} A_o^{d_y} + (4t'_{yo} t'''_{yo} + 3t''^{2}_{yo}) A_o^{t_y t_y} - (4t'''_{yo} d'_{yo} \\ & + 6t''_{yo} d''_{yo} + 4t'_{yo} d'''_{yo}) A_o^{t_y d_y} + (4d'_{yo} d'''_{yo} + 3d''^{2}_{yo}) A_o^{d_y d_y}; \end{aligned} \tag{239e}$$

Going back to the definitions of t_x, t_y, d_x, and d_y,

$$\begin{aligned} & t_{xo} = t_{yo} = 0; \\ & t'_{xo} = t'_{yo} = i; \\ & t''_{xo} = t''_{yo} = 0; \\ & t'''_{xo} = t'''_{yo} = -i; \\ & t^{iv}_{xo} = t^{iv}_{yo} = 0; \end{aligned} \tag{240a}$$

$$d_{xo} = d_{yo} = 0;$$

$$d'_{xo} = d'_{yo} = 0;$$

$$d''_{xo} = d''_{yo} = -2; \qquad (240b)$$

$$d'''_{xo} = d'''_{yo} = 0;$$

$$d^{iv}_{xo} = d^{iv}_{yo} = 2.$$

Substituting into Eqs. (235)-(239) and assuming $A^{t_x t_x} = A^{t_y t_y} = 0$, we get

$$A_o = 1; \qquad (241)$$

$$A_o^x = iA_o^{t_x}, \quad A_o^y = iA_o^{t_y}; \qquad (242)$$

$$A_o^{xx} = -2A_o^{d_x}, \quad A_o^{xy} = -A_o^{t_x t_y}, \quad A_o^{yy} = -2A_o^{d_y}; \qquad (243)$$

$$A_o^{xxx} = -i(A_o^{t_x} + 6A_o^{t_x d_x}); \qquad (244a)$$

$$A_o^{xxy} = -2i A_o^{t_y d_x}; \qquad (244b)$$

$$A_o^{xyy} = -2i A_o^{t_x d_y}; \qquad (244c)$$

$$A_o^{yyy} = -i(A_o^{t_y} + 6A_o^{t_y d_y}); \qquad (244d)$$

and

$$A_o^{xxxx} = 2(A_o^{d_x} + 6A_o^{d_x d_x}); \qquad (245a)$$

$$A_o^{xxxy} = A_o^{t_x t_y}; \qquad (245b)$$

$$A_o^{xxyy} = 4A_o^{d_x d_y} \qquad (245c)$$

$$A_o^{xyyy} = A_o^{t_x t_y}; \qquad (245d)$$

$$A_o^{yyyy} = 2(A_o^{d_y} + 6A_o^{d_y d_y}). \tag{245e}$$

It is worth noticing that Eqs. (241)-(244) are valid for schemes of higher degree in the operators t_x, t_y, d_x, and d_y, as long as $A^{t_x t_x} = A^{t_y t_y} = 0$, i.e., as long as composite transport is excluded. With the above equations, Eqs. (231)-(233) yield

$$(\log A)_o^{x} = iA_o^{t_x}, \quad (\log A)_o^{y} = iA_o^{t_y}; \tag{246}$$

$$(\log A)_o^{xx} = -2A_o^{d_x} + (A_o^{t_x})^2; \tag{247a}$$

$$(\log A)_o^{xy} = -A_o^{t_x t_y} + A_o^{t_x} A_o^{t_y}; \tag{247b}$$

$$(\log A)_o^{yy} = -2A_o^{d_y} + (A_o^{t_y})^2; \tag{247c}$$

$$(\log A)_o^{xxx} = -iA_o^{t_x}(1 - 6A_o^{d_x}) - i[6A_o^{t_x d_x} + 2(A_o^{t_x})^3]; \tag{248a}$$

$$(\log A)_o^{xxy} = -2i(A_o^{d_x t_y} - A_o^{d_x} A_o^{t_y}) + 2iA_o^{t_x}(A_o^{t_x t_y} - A_o^{t_x} A_o^{t_y}); \tag{248b}$$

$$(\log A)_o^{xyy} = -2i(A_o^{d_y t_x} - A_o^{d_y} A_o^{t_x}) + 2iA_o^{t_y}(A_o^{t_x t_y} - A_o^{t_x} A_o^{t_y}); \tag{248c}$$

$$(\log A)_o^{yyy} = -iA_o^{t_y}(1 - 6A_o^{d_y}) - i[6A_o^{t_y d_y} + 2(A_o^{t_y})^3]. \tag{248d}$$

Only the odd derivatives are imaginary. Therefore, Eq. (229) implies

$$\theta = \left[\frac{(\log A)_o^{x}}{i}\beta_x + \frac{(\log A)_o^{y}}{i}\beta_y\right] + \left[\frac{(\log A)_o^{xxx}}{i}\frac{\beta_x^3}{6} + \frac{(\log A)_o^{xxy}}{i}\frac{\beta_x^2\beta_y}{2} + \frac{(\log A)_o^{xyy}}{i}\frac{\beta_x\beta_y^2}{2} + \frac{(\log A)_o^{yyy}}{i}\frac{\beta_y^3}{6}\right] + \ldots \tag{249}$$

<u>Example</u>:

Let us analyze the phase error associated with Eq. (226e),

$$A = (1 - \varepsilon_x t_x - \varepsilon_y t_y) + \nu_x d_x + \nu_y d_y - \mu_x d_x(1 - \varepsilon_x t_x) - \mu_y d_y(1 - \varepsilon_y t_y).$$

By direct differentiation we get

$$A_o^{t_x} = \varepsilon_x, \quad A_o^{t_y} = -\,\varepsilon_y; \tag{250}$$

$$A_o^{d_x} = \nu_x - \mu_x, \quad A_o^{d_y} = \nu_y - \mu_y;$$

$$A_o^{t_x t_x} = 0, \quad A_o^{t_x d_x} = \varepsilon_x \mu_x, \quad A_o^{d_x d_x} = 0;$$

$$A_o^{t_y t_y} = 0, \quad A_o^{t_y d_y} = \varepsilon_y \mu_y, \quad A_o^{d_y d_y} = 0;$$

$$A_o^{t_x t_y} = 0, \quad A_o^{t_x d_y} = 0, \quad A_o^{t_y d_x} = 0, \quad A_o^{d_x d_y} = 0;$$

whence

$$\frac{(\log A)_o^x}{i} = -\,\varepsilon_x, \quad \frac{(\log A)_o^y}{i} = -\,\varepsilon_y; \tag{251}$$

$$\frac{(\log A)_o^{xxx}}{i} = 6\varepsilon_x\left(\frac{1}{6} - \nu_x + \frac{\varepsilon_x^2}{3}\right) \tag{252a}$$

$$\frac{(\log A)_o^{xxy}}{i} = -\,2\varepsilon_y(\nu_x - \mu_x - \varepsilon_x^2); \tag{252b}$$

$$\frac{(\log A)_o^{xxy}}{i} = -\,2\varepsilon_x(\nu_y - \mu_y - \varepsilon_y^2); \tag{252c}$$

$$\frac{(\log A)_o^{yyy}}{i} = 6\varepsilon_y\left(\frac{1}{6} - \nu_y + \frac{\varepsilon_y^2}{3}\right). \tag{252d}$$

Substituting in Eq. (249), we get

$$\theta = -\,\varepsilon_x\beta_x\left[1 + \left(\nu_x - \frac{1}{6} - \frac{\varepsilon_x^2}{3}\right)\beta_x^2 + (\nu_y - \mu_y - \varepsilon_y^2)\beta_y^2 + \ldots\right]$$

$$-\,\varepsilon_y\beta_y\left[1 + \left(\nu_y - \frac{1}{6} - \frac{\varepsilon_y^2}{3}\right)\beta_y^2 + (\nu_x - \mu_x - \varepsilon_x^2)\beta_x + \ldots\right].$$

Noting that $\varepsilon_x\beta_x = (\frac{u_1\delta t}{\delta x})(k_1\delta x) = u_1k_1\delta t$ and $\varepsilon_y\beta_y = u_2k_2\delta t$, we can rewrite the above equation as

$$\vartheta = -\vec{k}\cdot\vec{V}\delta t, \tag{253}$$

where $\vec{k} = (k_1,k_2)$, $\vec{V} = (v_1,v_2)$. If $\vec{U} = (u_1,u_2)$,

$$v_1 = u_1[1 + (\nu_x - \frac{1}{6} - \frac{\varepsilon_x^2}{3})\,\beta_x^2 + (\nu_y - \mu_y - \varepsilon_y^2)\beta_y^2 + \ldots];$$

and

$$v_2 = u_2\,[1 + (\nu_y - \frac{1}{6} - \frac{\varepsilon_y^2}{3})\beta_y^2 + (\nu_x - \mu_x - \varepsilon_x^2)\beta_x^2 + \ldots]. \tag{254b}$$

Ccomparing Eq. (253) to the analytical solution, we find

$$\vartheta_{analytic} = -\vec{k}\cdot\vec{U}\delta t \tag{255}$$

as is obvious from Eqs. (211).

Following Eq. (19b), we define a relative phase error matrix, R, such that

$$\vec{V} = \vec{U} + R\vec{U}, \tag{256}$$

where R, given by Eqs. (254), in this scheme is

$$R = \begin{pmatrix} (\nu_x - \frac{1}{6} - \varepsilon_x^2/3)\beta_x^2 + (\nu_y - \mu_y - \varepsilon_y^2)\beta_y^2 \ldots & 0 \\ 0 & (\nu_y - \frac{1}{6} - \varepsilon_y^2/3)\beta_y^2 + (\nu_x - \mu_x - \varepsilon_x^2)\beta_x^2 + \ldots \end{pmatrix}, \tag{257}$$

Thus we can reduce the phase error to fourth order by selecting

$$\nu_{\substack{x\\y}} = \frac{1}{6} + \varepsilon_{\substack{x\\y}}^2/3; \tag{258a}$$

$$\nu_{\substack{x\\y}} - \mu_{\substack{x\\y}} = \varepsilon_{\substack{x\\y}}^2 . \tag{258b}$$

Solving Eqs. (258a, b), we get

$$\mu_{\substack{x\\y}} = \frac{1}{6} - \frac{2}{3}\,\varepsilon^2_{\substack{x\\y}} \,. \tag{258c}$$

AMPLITUDE ANALYSIS

Following the analysis of the one-dimensional case, since $|A|^2 = A\bar{A}$ we have

$$(|A|^2)_o = 1;$$

$$(|A|^2)^x_o = A^x_o\overline{A_o} + A_o\overline{A^x_o}$$

$$(|A|^2)^y_o = A^y_o\overline{A_o} + A_o\overline{A^y_o}, \tag{259}$$

and so on. Noticing from Eqs. (241)-(245) that odd derivatives are purely imaginary while even ones are real, we get after substituting in Eqs. (259)

$$(|A|^2)_o = 1; \tag{260}$$

$$(|A|^2)^{xx}_o = 2[A^{xx}_o + (\frac{A^x_o}{i})^2]; \tag{261a}$$

$$(|A|^2)^{xy}_o = 2[A^{xy}_o + \frac{A^x_o}{i}\,\frac{A^y_o}{i}]; \tag{261b}$$

$$(|A|^2)^{yy}_o = 2[A^{yy}_o + (\frac{A^y_o}{i})^2]; \tag{261c}$$

$$(|A|^2)^{xxxx}_o = 2[A^{xxxx}_o + 4(\frac{A^x_o}{i})(\frac{A^{xxx}_o}{i}) + 3(A^{xx}_o)^2]; \tag{262a}$$

$$(|A|^2)^{xxxy}_o = 2(A^{xxxy}_o + (\frac{A^{xxx}_o}{i})(\frac{A^y_o}{i}) + 3(\frac{A^{xxy}_o}{i})(\frac{A^x_o}{i}) + (3A^{xx}_oA^{xy}_o]; \tag{262b}$$

$$(|A|^2)^{xxyy}_o = 2[A^{xxyy}_o + (\frac{A^{xxy}_o}{i})(\frac{A^y_o}{i}) + A^{xx}_oA^{yy}_o$$
$$+ 2(\frac{A^{xyy}_o}{i})(\frac{A^x_o}{i}) + 2(A^{xy}_o)^2]; \tag{262c}$$

$$(|A|^2)_o^{xyyy} = 2[A_o^{xyyy} + (\frac{A_o^x}{i})(\frac{A_o^{yyy}}{i}) + 3(\frac{A_o^{xyy}}{i})(\frac{A_o^y}{i}) + 3A_o^{xy}A_o^{yy}]; \tag{262d}$$

$$(|A|^2)_o^{yyyy} = 2[A_o^{yyyy} + 4(\frac{A_o^y}{i})(\frac{A_o^{yyy}}{i}) + 3(A_o^{yy})^2], \tag{262e}$$

while the odd derivative vanishes. Consequently, the expansion of $|A|^2$ takes the form

$$\begin{aligned} |A|^2 = (|A|^2)_o &+ [(|A|^2)_o^{xx}\frac{\beta_x^2}{2} + (|A|^2)_o^{xy}\beta_x\beta_y + (|A|^2)_o^{yy}\frac{\beta_y^2}{2}] \\ &+ [(|A|^2)_o^{xxxx}\frac{\beta_x^4}{24} + (|A|^2)_o^{xxxy}\frac{\beta_x^3\beta_y}{6} + (|A|^2)_o^{xxyy}\frac{\beta_x^2\beta_y^2}{4} \\ &+ (|A|^2)_o^{xyyy}\frac{\beta_x\beta_y^3}{6} + (|A|^2)_o^{yyyy}\frac{\beta_y^4}{24}] + \ldots \end{aligned} \tag{263}$$

Example:

Using Eqs. (250), Eqs. (241)-(243) yield

$$A_o = 1;$$

$$\frac{A_o^x}{i} = -\epsilon_x, \quad \frac{A_o^y}{i} = -\epsilon_y;$$

$$A_o^{xx} = -2(\nu_x - \mu_x) = -2\epsilon_x^2;$$

$$A_o^{xy} = 0;$$

$$A_o^{yy} = -2(\nu_y - \mu_y) = -2\epsilon_y^2,$$

which when substituted into Eqs. (260), (261) give

$$(|A|^2)_o = 1;$$

$$(|A|^2)_o^{xx} = -2\epsilon_x^2;$$

$$(|A|^2)_o^{xy} = 2\varepsilon_x\varepsilon_y;$$

$$(|A|^2)_o^{yy} = -\,2\varepsilon_y^2.$$

Equation (263) then expresses the amplitude expansion as

$$|A|^2 = 1 - (\varepsilon_x^2\beta_x^2 - 2\varepsilon_x\varepsilon_y\,\beta_x\beta_y + \varepsilon_y^2\beta_y^2) + \ldots$$

$$|A|^2 = 1 = -\,|\,\varepsilon_x\beta_x - \varepsilon_y\beta_y\,|^2 + \ldots, \tag{264}$$

showing that the diffusion of the scheme is second-order.

POSITIVITY

From Eqs. (223) and using Eq. (258a),

$$\rho_{i,j}^{TD} = \rho_{i,j}^{n}[1 - 2(\frac{1}{6} + \frac{\varepsilon_x^2}{3}) - 2(\frac{1}{6} + \frac{\varepsilon_y^2}{3})]$$

$$+ \rho_{i+1,j}^{n}[(\frac{1}{6} + \frac{\varepsilon_x^2}{3}) - \frac{\varepsilon_x}{2}] + \rho_{i-1,j}^{n}[\frac{1}{6} + \frac{\varepsilon_x^2}{3}) + \frac{\varepsilon_x}{2}]$$

$$+ \rho_{i,j+1}^{n}[(\frac{1}{6} + \frac{\varepsilon_y^2}{3}) - \frac{\varepsilon_y}{2}] + \rho_{i,j-1}^{n}[(\frac{1}{6} + \frac{\varepsilon_y^2}{3}) + \frac{\varepsilon_y}{2}]$$

Each of the square brackets is ≥ 0 for $|\varepsilon_x|,|\varepsilon_y| \leq \frac{1}{2}$. Consequently, $\rho_{i,j}^{TD} \geq 0$ if all $\rho_{i,j}^{n} \geq 0$. Now we get

$$\rho_{i,j}^{n+1} = \rho_{i,j}^{TD} - \mu_x(\rho_{i+1,j}^{T_x} - 2\rho_{i,j}^{T_x} + \rho_{i-1,j}^{T_x})^* - \mu_y(\rho_{i,j+1}^{T_y} - 2\rho_{i,j}^{T_y} + \rho_{i,j-1}^{T_y})^*$$

The asterisks denote the fact that the antidiffusion fluxes are trimmed enough such that $\rho_{i,j}^{n+1}$ is limited by the sign of $\rho_{i,j}^{TD}$. Then $\rho_{i,j}^{n+1} \geq 0$.

STABILITY

Equation (264) proves the stability of the scheme near $\beta_x = \beta_y = 0$. For the scheme to be completely stable, however, we must have $|A| \leq 1$ for $0 \leq \beta_x, \beta_y \leq \pi$. Let us check A, at the largest values admitted for ε_x, ε_y, namely 1/2.

From Eq. (226e)

$$A_R = 1 - 2(\nu_x - \mu_x)(1 - \cos\beta_x) - 2(\nu_y - \mu_y)(1 - \cos\beta_y); \tag{266a}$$

$$\begin{aligned} A_I = &- \varepsilon_x \sin\beta_x\,[1 + 2\mu_x(1 - \cos\beta_x)] \\ &- \varepsilon_y \sin\beta_y\,[1 + 2\mu_y(1 - \cos\beta_y)] \end{aligned} \tag{266b}$$

Substituting for $\nu_{\substack{x\\y}} - \mu_{\substack{x\\y}}$ from Eq. (258b), and $\mu_{\substack{x\\y}}$ from Eq. (258c), we get

$$A_R = 1 - 2\varepsilon_x^2(1 - \cos\beta_x) - 2\varepsilon_y^2(1 - \cos\beta_y); \tag{267a}$$

$$\begin{aligned} A_I = &- \varepsilon_x \sin\beta_x\,[1 + \tfrac{1}{4}(1 - 4\varepsilon_x^2)(1 - \cos\beta_x)] \\ &- \varepsilon_y \sin\beta_y\,[1 + \tfrac{1}{4}(1 - 4\varepsilon_y^2)(1 - \cos\beta_y)]. \end{aligned} \tag{267b}$$

At ε_x, $\varepsilon_y = 1/2$, $\mu_x = \mu_y = 0$; Eqs. (267) reduce to

$$A_R = 1 - \frac{1}{2}(1 - \cos\beta_x) - \frac{1}{2}(1 - \cos\beta_y);$$

$$A_I = -\frac{1}{2}(\sin\beta_x + \sin\beta_y).$$

Noticing that $1 - \cos\beta = 2\sin^2(\beta/2)$ and $\sin\beta = 2\sin(\beta/2)\cos(\beta/2)$, we get

$$A_R = 1 - \sin^2(\beta_x/2)\ \sin^2(\beta_y/2);$$

$$A_I = -\ [\sin\ (\beta_x/2)\ \cos\ (\beta_x/2) + \sin\ (\beta_y/2)\ \cos\ (\beta_y/2)],$$

yielding

$$|A|^2 = A_R^2 + A_I^2 = 1 + \sin^4 \frac{\beta_x}{2} + \sin^4 \frac{\beta_y}{2} + 2\sin^2 \frac{\beta_x}{2} \sin^2 \frac{\beta_y}{2}$$

$$- 2(\sin^2 \frac{\beta_x}{2} + \sin^2 \frac{\beta_y}{2}) + \sin^2 \frac{\beta_x}{2} \cos^2 \frac{\beta_x}{2} + \sin^2 \frac{\beta_y}{2} \cos^2 \frac{\beta_y}{2}$$

$$+ 2 \sin \frac{\beta_x}{2} \sin \frac{\beta_y}{2} \cos \frac{\beta_x}{2} \cos \frac{\beta_y}{2}.$$

Collecting the terms containing $\sin^2 \frac{\beta_x}{2}$, we have

$$- \sin^2 \frac{\beta_x}{2}[(1 - \sin^2 \frac{\beta_y}{2}) + (1 - \cos^2 \frac{\beta_x}{2})] = - \sin^2 \frac{\beta_x}{2}[\cos^2 \frac{\beta_y}{2}$$

$$+ \sin^2 \frac{\beta_x}{2}] = - \sin^2 \frac{\beta_x}{2} \cos^2 \frac{\beta_y}{2} - \sin^4 \frac{\beta_x}{2}.$$

Similarly $\sin^2 \frac{\beta_y}{2}$ terms yield $- \sin^2 \frac{\beta_y}{2} \cos^2 \frac{\beta_x}{2} - \sin^4 \frac{\beta_y}{2}$, resulting in

$$|A|^2 = 1 - (\sin^2 \frac{\beta_x}{2} \cos^2 \frac{\beta_y}{2} - 2 \sin \frac{\beta_x}{2} \sin \frac{\beta_y}{2} \cos \frac{\beta_x}{2} \cos \frac{\beta_y}{2}$$

$$+ \sin^2 \frac{\beta_y}{2} \cos^2 \frac{\beta_x}{2}) = 1 - (\sin \frac{\beta_x}{2} \cos \frac{\beta_y}{2} - \sin \frac{\beta_y}{2} \cos \frac{\beta_x}{2})^2$$

$$= 1 - \sin^2(\frac{\beta_x}{2} - \frac{\beta_y}{2}) = \cos^2(\frac{\beta_x}{2} - \frac{\beta_y}{2}).$$

Consequently,

$$|A|_{\epsilon_x=\epsilon_y=\frac{1}{2}} = \cos\ (\frac{\beta_x}{2} - \frac{\beta_y}{2}) \le 1, \tag{268}$$

showing the scheme to be stable at $\epsilon_x, \epsilon_y = \frac{1}{2}$. The value $|A|$ for smaller values of ϵ_x, ϵ_y was evalu ted numerically and found always to satisfy ≤ 1. Hence the scheme is completely stable.

It is worth noticing the diagonal symmetry of Eqs. (264), (268). In fact, on the β_x, β_y plane, $|A|$ looks like a wave with front parallel to the $\beta_x = \beta_y$ diagonal, as illustrated in Fig. 27.

XIII. RECTANGULAR GRID MOTION

Consider a system of points tagged by the double indices i, j;

$$x_{i,j} = x(i,j,t); \tag{270a}$$

$$y_{i,j} = y(i,j,t). \tag{270b}$$

Figure 28 illustrates the grid formed by Eq. (270) at a given time t. The pair of numbers at each point indicates (i,j). For a strictly rectangular grid at all times (which includes Langrangian grid motion),

$$x_{i,j} = x(i,t); \tag{271a}$$

$$y_{i,j} = y(j,t). \tag{271b}$$

which we therefore denote from now on by

$$x_{i} = x(i,t); \tag{272a}$$

$$y_{j} = y(j,t). \tag{272b}$$

This leads to a mesh as in Fig. 29.

XIV. GEOMETRICAL ASPECTS

We consider seven geometries. (These by no means cover the whole spectrum of two-dimensional systems.) In cartesian geometry, we have x-y (x-z or y-z); in cylindrical geometry, r-z, r-ϕ, and z-ϕ, and finally in spherical geometry r-θ, r-ϕ, and θ-ϕ. Figure 30 illustrates a finite control volume in each of the different cases.

As explained earlier, when the grid moves the control surface area in the integral form of the conservation equations should be an average surface area defined as

$$\int_{S^{mean}} (\vec{u}^g \delta t \cdot \vec{n})\, dS = \text{swept volume}.$$

In one-dimensional cases, the above definition reduces to defining $A_{interface} = \frac{\text{swept volume}}{u^g \delta t}$. In two dimensions, however, this is not enough. We have to find a path between the old grid and the new one such that we can construct a mean cell having its surfaces equal to the average areas and corners located on the above path.

1. Cartesian Coordinates

Figure 31 illustrates the location of cell (i,j) at times t^n and $t^{n+1} = t^n + \delta t$. The left and right interfaces are denoted by (i - 1/2, j), (i,j + 1/2, j), respectively, and the bottom and top ones by (i,j - 1/2), (i,j + 1/2). We notice here that since all i ± 1/2, j interfaces (different j's) move as a whole, the grid velocity is independent of j. It is therefore denoted by $u^g_{i\pm\frac{1}{2}}$ without a j index. The same is true for $v^g_{j\pm\frac{1}{2}}$.

In cartesian geometry, it is obvious that the path needed is a straight line between the new and old corners of the cell, and the mean cell is halfway between the old cell and the new one.

The volume swept by interface (i ± 1/2, j) is given by the product (average base) x (height):

$$\Delta V_{i\pm\frac{1}{2},j} = \frac{(y^n_{j+\frac{1}{2}} - y^n_{j-\frac{1}{2}}) + (y^{n+1}_{j+\frac{1}{2}} - y^{n+1}_{j-\frac{1}{2}})}{2} [x^{n+1}_{i\pm\frac{1}{2}} - x^n_{i\pm\frac{1}{2}}]$$

$$= \frac{1}{2}(A^n_j + A^{n+1}_j)^2 (x^{n+1}_{i\pm\frac{1}{2}} - x^n_{i\pm\frac{1}{2}}),$$

where we notice again that the i index is omitted from $A_{i\pm\frac{1}{2},j}$ since all the $A_{i\pm\frac{1}{2},j}$ interfaces (different i's) are equal. The above equation can be written as

$$\Delta V_{i\pm\frac{1}{2},j} = [(\frac{y^n_{j\pm\frac{1}{2}} + y^{n+1}_{j+\frac{1}{2}}}{2}) - (\frac{y^n_{j-\frac{1}{2}} + y^{n+1}_{j-\frac{1}{2}}}{2})](x^{n+1}_{i\pm\frac{1}{2}} - x^n_{i\pm\frac{1}{2}}) \tag{286}$$

showing that the mean area is halfway between old and new. The grid velocity $u^g_{i\pm\frac{1}{2}}$ in this case is considered constant,

$$u^g_{i\pm\frac{1}{2}} = \frac{x^{n+1}_{i\pm\frac{1}{2}} - x^n_{i\pm\frac{1}{2}}}{\delta t}, \tag{287}$$

and the mean area is

$$A^{n+\frac{1}{2}}_j = y^{n+\frac{1}{2}}_{j+\frac{1}{2}} - y^{n+\frac{1}{2}}_{j-\frac{1}{2}} = \frac{A^n_j + A^{n+1}_j}{2}, \tag{288a}$$

where

$$y^{n+\frac{1}{2}}_{j\pm\frac{1}{2}} = \frac{1}{2}(y^n_{j\pm\frac{1}{2}} + y^{n+1}_{j\pm\frac{1}{2}}). \tag{288b}$$

Similarly,

$$A_i^{n+\frac{1}{2}} = x_{i+\frac{1}{2}}^{n+\frac{1}{2}} - x_{i-\frac{1}{2}}^{n+\frac{1}{2}} = \frac{A_i^n + A_i^{n+1}}{2} , \tag{289a}$$

where

$$x_{i\pm\frac{1}{2}}^{n+\frac{1}{2}} = \frac{1}{2}(x_{i\pm\frac{1}{2}}^{n} + x_{i\pm\frac{1}{2}}^{n+1}) . \tag{289b}$$

The mean cell colume is

$$\mathcal{V}_{i,j}^{n+\frac{1}{2}} = (y_{j+\frac{1}{2}}^{n+\frac{1}{2}} - y_{j-\frac{1}{2}}^{n+\frac{1}{2}})(x_{i+\frac{1}{2}}^{n+\frac{1}{2}} - x_{i-\frac{1}{2}}^{n+\frac{1}{2}}) . \tag{290}$$

2. Cylindrical (r-z) Coordinates

Let us derive the required path between the corners of old and new cells such that the corners of the mean cell fall on that path. Figure 32 illustrates the old and new cells. Figure 33 shows the volume swept by interfact (i,j ± 1/2):

$$\mathcal{V}_{i,j\pm\frac{1}{2}} = \int_{z_{j\pm\frac{1}{2}}^{n}}^{z_{j\pm\frac{1}{2}}^{n+1}} \pi r_{i\pm\frac{1}{2}}^2 \, dz_{j\pm\frac{1}{2}} - \int_{z_{j\pm\frac{1}{2}}^{n}}^{z_{j\pm\frac{1}{2}}^{n+1}} \pi r_{i-\frac{1}{2}}^2 \, dz_{j\pm\frac{1}{2}} , \tag{291}$$

where it is obvious that a linear average can be obtained if $r_{i\pm\frac{1}{2}}^2$ is assumed to be linear in $z_{j\pm\frac{1}{2}}$. Let

$$\frac{(r_{i\pm\frac{1}{2}})^2 - (r_{i\pm\frac{1}{2}}^n)^2}{(r_{i\pm\frac{1}{2}}^{n+1})^2 - (r_{i\pm\frac{1}{2}}^n)^2} = \frac{z_{j\pm\frac{1}{2}} - z_{j\pm\frac{1}{2}}^n}{z_{j\pm\frac{1}{2}}^{n+1} - z_{j\pm\frac{1}{2}}^n} , \tag{292a}$$

i.e., a parabolic path. The above formula can be written concisely as

$$\frac{\Delta r_{i\pm\frac{1}{2}}^2}{\Delta R_{i\pm\frac{1}{2}}^2} = \frac{\Delta z_{j\pm\frac{1}{2}}}{\Delta Z_{j\pm\frac{1}{2}}} , \tag{292b}$$

yielding

$$r^2_{i\pm\frac{1}{2}} = (r^n_{i\pm\frac{1}{2}})^2 + \frac{\Delta z_{j\pm\frac{1}{2}}}{\Delta Z_{j\pm\frac{1}{2}}} \Delta R^2_{i\pm\frac{1}{2}}. \tag{292c}$$

Substituting (292c) into (291), we get

$$\Delta \mathbf{V}_{i,j\pm\frac{1}{2}} = \pi \Delta Z_{j\pm\frac{1}{2}} \int_0^1 (r^2_{i+\frac{1}{2}} - r^2_{i-\frac{1}{2}})\, d\left(\frac{\Delta z_{j\pm\frac{1}{2}}}{\Delta Z_{j\pm\frac{1}{2}}}\right)$$

$$= \pi \Delta Z_{j\pm\frac{1}{2}} \left[\frac{(r^n_{i+\frac{1}{2}} + (r^{n+1}_{i+\frac{1}{2}})^2}{2} + \frac{(r^n_{i-\frac{1}{2}})^2 + (r^{n+1}_{i-\frac{1}{2}})^2}{2}\right],$$

yielding a mean area

$$A_i^{n+\frac{1}{2}} = \frac{\Delta \mathbf{V}_{i,j\pm\frac{1}{2}}}{\Delta Z_{j\pm\frac{1}{2}}} = \pi[(r^{n+\frac{1}{2}}_{i+\frac{1}{2}})^2 - (r^{n+\frac{1}{2}}_{i-\frac{1}{2}})^2] = \frac{A_i^n + A_i^{n+1}}{2}, \tag{293a}$$

where

$$r^{n+\frac{1}{2}}_{i\pm\frac{1}{2}} = \left(\frac{(r^n_{i\pm\frac{1}{2}})^2 + (r^n_{i\pm\frac{1}{2}})^2}{2}\right)^{\frac{1}{2}} \tag{293b}$$

This shows the advantage of the parabolic path (292a), namely

$$\frac{\Delta z_{j\pm\frac{1}{2}}}{\Delta Z_{j\pm\frac{1}{2}}} = \frac{\Delta r^2_{i\pm\frac{1}{2}}}{\Delta R^2_{i\pm\frac{1}{2}}} = 1/2, \tag{293c}$$

i.e., the average area $A_i^{n+\frac{1}{2}}$ is halfway along z between the old and new ones, at

$$z^{n+\frac{1}{2}}_{j\pm\frac{1}{2}} = \frac{z^n_{j\pm\frac{1}{2}} + z^{n+1}_{j\pm\frac{1}{2}}}{2}. \tag{293d}$$

Following the nomenclature of Fig. 34, the volume swept by the interface $i\pm\frac{1}{2},j$ is

$$\Delta V_{i\pm\frac{1}{2},j} = \int_{r^{n}_{i\pm\frac{1}{2}}}^{r^{n+1}_{i\pm\frac{1}{2}}} 2\pi r_{i\pm\frac{1}{2}}(z_{j+\frac{1}{2}} - z_{j-\frac{1}{2}})dr_{i\pm\frac{1}{2}}$$

$$= \int_{r^{n}_{i\pm\frac{1}{2}}}^{r^{n+1}_{i\pm\frac{1}{2}}} \pi(z_{j+\frac{1}{2}} - z_{j-\frac{1}{2}})dr^{2}_{i\pm\frac{1}{2}}. \qquad (294)$$

But

$$z_{j\pm\frac{1}{2}} = z^{n}_{j\pm\frac{1}{2}} + \Delta z_{j\pm\frac{1}{2}}, \qquad (295)$$

yielding

$$\Delta V_{i\pm\frac{1}{2},j} = \int_{r^{n}_{i\pm\frac{1}{2}}}^{r^{n+1}_{i\pm\frac{1}{2}}} \pi[(z^{n}_{j+\frac{1}{2}} - z^{n}_{j-\frac{1}{2}}) + (\frac{\Delta z_{j+\frac{1}{2}}}{\Delta Z_{j+\frac{1}{2}}}\Delta Z_{j+\frac{1}{2}} - \frac{\Delta z_{j-\frac{1}{2}}}{\Delta Z_{j-\frac{1}{2}}}\Delta Z_{j-\frac{1}{2}})]dr^{2}_{i\pm\frac{1}{2}}$$

which, with (292b) gives

$$\Delta V_{i\pm\frac{1}{2},j} = \pi\Delta R^{2}_{i\pm\frac{1}{2}} \int_{0}^{1} [(z^{n}_{j+\frac{1}{2}} - z^{n}_{j-\frac{1}{2}})$$

$$+ \frac{\Delta r^{2}_{i+\frac{1}{2}}}{\Delta R^{2}_{i+\frac{1}{2}}}(\Delta Z_{j+\frac{1}{2}} - \Delta Z_{j-\frac{1}{2}})]d\frac{\Delta r^{2}_{i\pm\frac{1}{2}}}{\Delta R^{2}_{i\pm\frac{1}{2}}}$$

$$= \pi\Delta R^{2}_{i\pm\frac{1}{2}}[z^{n+\frac{1}{2}}_{j+\frac{1}{2}} + z^{n+\frac{1}{2}}_{j-\frac{1}{2}}]. \qquad (296)$$

Now to be able to construct a rectangular mean cell with its four corners on the parabolic paths of Eq. (292a), the quantities $A^{n+\frac{1}{2}}_{i\pm\frac{1}{2},j}$ have to be also half way between old and new, i.e.,

$$A^{n+\frac{1}{2}}_{i\pm\frac{1}{2},j} = 2\pi r^{n+\frac{1}{2}}_{i\pm\frac{1}{2}} [z^{n+\frac{1}{2}}_{j+\frac{1}{2}} - z^{n+\frac{1}{2}}_{j-\frac{1}{2}}], \tag{297}$$

where we notice that the interface area is dependent on both i,j, in contrast to the cartesian case. With Eq. (296), Eq. (297) yields

$$A^{n+\frac{1}{2}}_{i\pm\frac{1}{2},j} = \frac{\Delta V_{i\pm\frac{1}{2}}}{\Delta R^2_{i\pm\frac{1}{2}}/2r^{n+\frac{1}{2}}_{i\pm\frac{1}{2}}} \tag{298}$$

whence, if $u^g_{i\pm\frac{1}{2}}$ denotes the average velocity of the grid during t,

$$u^g_{i\pm\frac{1}{2}}\delta t = \frac{(r^{n+1}_{i\pm\frac{1}{2}})^2 - (r^n_{i\pm\frac{1}{2}})^2}{2r^{n+\frac{1}{2}}_{i\pm\frac{1}{2}}} \tag{299}$$

where, as is clear from Eq. (293a), it was assumed that

$$v^g_{j\pm\frac{1}{2}}\delta t = \Delta Z_{j\pm\frac{1}{2}} = z^{n+1}_{j\pm\frac{1}{2}} - z^n_{j\pm\frac{1}{2}}. \tag{300}$$

The difference between the form of (299) and that of (300) is attributed to the parabolic path of the corner. If the grid velocity $v^g_{j\pm\frac{1}{2}}$ is a constant during δt, we evaluate $u^g_{i\pm\frac{1}{2}}$ at $t^{n+\frac{1}{2}} = t^n + \frac{\delta t}{2}$ from (292c)

$$2r_{i\pm\frac{1}{2}} \frac{dr_{i\pm\frac{1}{2}}}{dt} = \frac{\Delta R^2_{i\pm\frac{1}{2}}}{\Delta Z_{j\pm\frac{1}{2}}} \frac{d\Delta z_{j\pm\frac{1}{2}}}{dt} = \frac{\Delta R^2_{i\pm\frac{1}{2}}}{\Delta Z_{j\pm\frac{1}{2}}} \frac{dz_{j\pm\frac{1}{2}}}{dt},$$

whence

$$u^g_{i\pm\frac{1}{2}} = \frac{\Delta R^2_{i\pm 1}}{2r_{i\pm\frac{1}{2}}} \frac{v^g_{j\pm\frac{1}{2}}}{\Delta Z_{j\pm\frac{1}{2}}} = \frac{\Delta R^2_{i\pm\frac{1}{2}}}{2r_{i\pm\frac{1}{2}}\delta t}, \tag{301}$$

using Eq. (300). Since $v^g_{j\pm\frac{1}{2}}$ = const., $(\Delta z_{j\pm\frac{1}{2}}/\Delta Z_{j\pm\frac{1}{2}})_{t + \frac{\delta t}{2}} = 1/2$.

Consequently, from (292c)

$$r^2_{i\pm\frac{1}{2}}\Big|_{t+\frac{\delta t}{2}} = \frac{1}{2}[(r^n_{i\pm\frac{1}{2}})^2 + (r^{n+1}_{i\pm\frac{1}{2}})^2] = (r^{n+\frac{1}{2}}_{i\pm\frac{1}{2}})^2,$$

thus reproducing Eq. (299) when substituted in Eq. (301). A more general definition of the average interface is therefore

$$\begin{bmatrix}\text{mean}\\ \text{interface}\\ \text{area}\end{bmatrix} = \frac{\text{swept volume}}{(\text{velocity of interface at } t^n + \frac{\delta t}{2}).\delta t} \tag{302}$$

where the denominator is approximately but not quite exactly equal to the distance the interface is shifted. Finally, the mean cell volume is

$$\forall_{i,j}^{n+\frac{1}{2}} = \pi[(r_{i+\frac{1}{2}}^{n+\frac{1}{2}})^2 - (r_{i+\frac{1}{2}}^{n+\frac{1}{2}})^2][z_{j+\frac{1}{2}}^{n+\frac{1}{2}} - z_{j-\frac{1}{2}}^{n+\frac{1}{2}}]. \tag{303}$$

3. Spherical r-θ Coordinates

Figure 35 illustrates cell i,j at t^n and t^{n+1}. Consider Fig. 36 showing the motion of interface $i,j\pm\frac{1}{2}$. The volume swept by interface $i,j\pm\frac{1}{2}$ is

$$\Delta\forall_{i,j\pm\frac{1}{2}} = \int_{\theta_{j\pm\frac{1}{2}}^{n}}^{\theta_{j\pm\frac{1}{2}}^{n+1}} \frac{2\pi}{3}(r_{i+\frac{1}{2}}^3 - r_{i-\frac{1}{2}}^3)\sin\theta_{j\pm\frac{1}{2}}\, d\theta_{j\pm\frac{1}{2}}$$

$$= \int_{\theta_{j\pm\frac{1}{2}}^{n}}^{\theta_{j\pm\frac{1}{2}}^{n+1}} \frac{2\pi}{3}(r_{i+\frac{1}{2}}^3 - r_{i-\frac{1}{2}}^3)d(-\cos\theta_{j\pm\frac{1}{2}}), \tag{304}$$

showing that we can get a linear average if $r_{i\pm\frac{1}{2}}^3$ is assumed to be a linear function of $(-\cos\theta_{j\pm\frac{1}{2}})$. Let

$$\frac{(r_{i\pm\frac{1}{2}})^3 - (r_{i\pm\frac{1}{2}}^n)^3}{(r_{i\pm\frac{1}{2}}^{n+1})^3 - (r_{i\pm\frac{1}{2}}^n)^3} = \frac{\cos\theta_{j\pm\frac{1}{2}}^n - \cos\theta_{j\pm\frac{1}{2}}}{\cos\theta_{j\pm\frac{1}{2}}^n - \cos\theta_{j\pm\frac{1}{2}}^{n+1}}, \tag{305a}$$

or in a more concise form,

$$\frac{\Delta r^3_{i\pm\frac{1}{2}}}{\Delta R^3_{i\pm\frac{1}{2}}} = \frac{\Delta(-\cos\theta_{j\pm\frac{1}{2}})}{\Delta(-\cos\Theta_{j\pm\frac{1}{2}})} \; . \tag{305b}$$

This yields

$$r^3_{i\pm\frac{1}{2}} = (r^n_{i\pm\frac{1}{2}})^3 + \frac{\Delta(-\cos\theta_{j\pm\frac{1}{2}})}{\Delta(-\cos\Theta_{j\pm\frac{1}{2}})}\,\Delta R^3_{i\pm\frac{1}{2}} . \tag{305c}$$

Substituting into Eq. (304) we get

$$\begin{aligned}
\Delta\mathcal{V}_{i,j\pm\frac{1}{2}} &= \frac{2\pi}{3}\Delta(-\cos\Theta_{j\pm\frac{1}{2}})\int_0^1 [(r^{n3}_{i+\frac{1}{2}} - r^{n3}_{i-\frac{1}{2}}) \\
&\quad + \frac{\Delta(-\cos\theta_{j\pm\frac{1}{2}})}{\Delta(-\cos\Theta_{j\pm\frac{1}{2}})}(\Delta R^3_{i+\frac{1}{2}} - \Delta R^3_{i-\frac{1}{2}})]\,d\,\frac{\Delta(-\cos\theta_{j\pm\frac{1}{2}})}{\Delta(-\cos\Theta_{j\pm\frac{1}{2}})} \\
&= \frac{2\pi}{3}(\cos\theta^n_{j\pm\frac{1}{2}} - \cos\theta^{n+1}_{j\pm\frac{1}{2}})[\frac{(r^n_{i+\frac{1}{2}})^3 + (r^{n+1}_{i+\frac{1}{2}})^3}{2} \\
&\quad - \frac{(r^n_{i-\frac{1}{2}})^3 + (r^{n+1}_{i-\frac{1}{2}})^3}{2}] .
\end{aligned} \tag{306}$$

We notice that the mean interface $i,j\pm\frac{1}{2}$ is halfway on a cosine scale between $\theta^n_{j\pm\frac{1}{2}}$, $\theta^{n+1}_{j\pm\frac{1}{2}}$ or on a cubic scale between $r^n_{i\pm\frac{1}{2}}$, $r^{n+1}_{i\pm\frac{1}{2}}$. As for interface $(i\pm\frac{1}{2},j)$, it sweeps a volume (see Fig. 37),

$$\begin{aligned}
\Delta\mathcal{V}_{i\pm\frac{1}{2},j} &= \int_{r^n_{i\pm\frac{1}{2}}}^{r^{n+1}_{i\pm\frac{1}{2}}} 2\pi r^2_{i\pm\frac{1}{2}}(\cos\theta_{j-\frac{1}{2}} - \cos\theta_{j+\frac{1}{2}})\,dr_{i\pm\frac{1}{2}} \\
&= \int_{r^n_{i\pm\frac{1}{2}}}^{r^{n+1}_{i\pm\frac{1}{2}}} \frac{2\pi}{3}(\cos\theta_{j-\frac{1}{2}} - \cos\theta_{j+\frac{1}{2}})\,dr^3_{i\pm\frac{1}{2}} .
\end{aligned} \tag{307}$$

But $\cos\theta_{j\pm\frac{1}{2}} = \cos\theta^n_{j\pm\frac{1}{2}} + \Delta(-\cos\theta_{j\pm\frac{1}{2}})$, yielding

$$\Delta\forall_{i\pm\frac{1}{2},j} = \frac{2\pi}{3}\int_{r^n_{i\pm\frac{1}{2}}}^{r^{n+1}_{i\pm\frac{1}{2}}} [(\cos\theta^n_{j-\frac{1}{2}} - \cos\theta^n_{j+\frac{1}{2}}) + \frac{\Delta(-\cos\theta_{j\pm\frac{1}{2}})}{\Delta(-\cos\Theta_{j\pm\frac{1}{2}})}\{\Delta(-\cos\Theta_{j-\frac{1}{2}})$$

$$- \Delta(-\cos\Theta_{j+\frac{1}{2}})\}]\ dr^3_{i\pm\frac{1}{2}},$$

which with Eq. (305b) results in

$$\Delta\forall_{i\pm\frac{1}{2},j} = \frac{2\pi}{3}\Delta R^3_{i\pm\frac{1}{2}}\int_0^1 [(\cos\theta^n_{j-\frac{1}{2}} - \cos\theta^{n+1}_{j+\frac{1}{2}})$$

$$+ \frac{\Delta r^3_{i\pm\frac{1}{2}}}{\Delta R^3_{i\pm\frac{1}{2}}}\{\Delta(-\cos\Theta_{j-\frac{1}{2}}) - \Delta(-\cos\Theta_{j+\frac{1}{2}})\}]\ d\,\frac{\Delta r^3_{i\pm\frac{1}{2}}}{\Delta R^3_{i\pm\frac{1}{2}}}$$

$$= \frac{2\pi}{3}\ \Delta R^3_{i\pm\frac{1}{2}}\ [\frac{\cos\theta^n_{j-\frac{1}{2}} + \cos\theta^{n+1}_{j-\frac{1}{2}}}{2} - \frac{\cos\theta^n_{j+\frac{1}{2}} + \cos\theta^{n+1}_{j+\frac{1}{2}}}{2}]. \qquad (308)$$

Here we notice that interface $i\pm\frac{1}{2},j$ is halfway on a cubic scale between $r^n_{i\pm\frac{1}{2}}$, $r^{n+1}_{i\pm\frac{1}{2}}$ or on a cosine scale between $\theta^n_{j\pm\frac{1}{2}}$, $\theta^{n+1}_{j\pm\frac{1}{2}}$. Consequently, we can construct a mean cell having its corners on the paths of Eq. (305a). Let

$$r^{n+\frac{1}{2}}_{i\pm\frac{1}{2}} \equiv \left(\frac{(r^n_{i\pm\frac{1}{2}})^3 + (r^{n+1}_{i\pm\frac{1}{2}})^3}{2}\right)^{1/3} \qquad (309)$$

and

$$\cos\theta^{n+\frac{1}{2}}_{j\pm\frac{1}{2}} \equiv \frac{\cos\theta^n_{j\pm\frac{1}{2}} + \cos\theta^{n+1}_{j\pm\frac{1}{2}}}{2}\ . \qquad (310)$$

Eqs. (306) and (308) can be written then as

$$\Delta\forall_{i,j\pm\frac{1}{2}} = \frac{2\pi}{3}(\cos\theta^n_{j\pm\frac{1}{2}} - \cos\theta^{n+1}_{j\pm\frac{1}{2}})[(r^{n+\frac{1}{2}}_{i+\frac{1}{2}})^3 - (r^{n+\frac{1}{2}}_{i-\frac{1}{2}})^3] \qquad (311)$$

and

$$\Delta\Psi_{i\pm\frac{1}{2},j} = \frac{2\pi}{3}(\cos\theta^{n+\frac{1}{2}}_{j-\frac{1}{2}} - \cos\theta^{n+\frac{1}{2}}_{j+\frac{1}{2}})[(r^{n+1}_{i\pm\frac{1}{2}})^3 - (r^{n}_{i\pm\frac{1}{2}})^3], \tag{312}$$

respectively. Now in order to be able to construct the average cell, $A_{i,j\pm\frac{1}{2}}$ and $A_{i\pm\frac{1}{2},j}$ should take the forms

$$A^{n+\frac{1}{2}}_{i,j\pm\frac{1}{2}} = \pi[(r^{n+\frac{1}{2}}_{i+\frac{1}{2}})^2 - (r^{n+\frac{1}{2}}_{i-\frac{1}{2}})^2] \sin\theta^{n+\frac{1}{2}}_{j\pm\frac{1}{2}}, \tag{313a}$$

forcing the choice

$$v^g_{i,j\pm\frac{1}{2}}\,\delta t = \frac{\Delta\Psi_{i,j\pm\frac{1}{2}}}{A^{n+\frac{1}{2}}_{i,j\pm\frac{1}{2}}} = \frac{2}{3}\,\frac{(r^{n+\frac{1}{2}}_{i+\frac{1}{2}})^3 - (r^{n+\frac{1}{2}}_{i-\frac{1}{2}})^3}{(r^{n+\frac{1}{2}}_{i+\frac{1}{2}})^2 - (r^{n+\frac{1}{2}}_{i-\frac{1}{2}})^2}\,\frac{\cos\theta^{n}_{j\pm\frac{1}{2}} - \cos\theta^{n+1}_{j\pm\frac{1}{2}}}{\sin\theta^{n+\frac{1}{2}}_{j\pm\frac{1}{2}}}, \tag{313b}$$

and

$$A^{n+\frac{1}{2}}_{i\pm\frac{1}{2},j} = 2\pi(r^{n+\frac{1}{2}}_{i\pm\frac{1}{2}})^2(\cos\theta^{n+\frac{1}{2}}_{j-\frac{1}{2}} - \cos\theta^{n+\frac{1}{2}}_{j+\frac{1}{2}}), \tag{314a}$$

forcing the choice

$$u^g_{i\pm\frac{1}{2}}\,\delta t = \frac{\Delta\Psi_{i\pm\frac{1}{2},j}}{A^{n+\frac{1}{2}}_{i\pm\frac{1}{2},j}} = \frac{(r^{n+1}_{i\pm\frac{1}{2}})^3 - (r^{n}_{i\pm\frac{1}{2}})^3}{3(r^{n+\frac{1}{2}}_{i\pm\frac{1}{2}})^2}\,. \tag{314b}$$

To complete the formulation, it remains to check the consistency of the two velocities $u^g_{i\pm\frac{1}{2}}$, $v^g_{i,j\pm\frac{1}{2}}$, namely that they occur at the same instant. Differentiating (305a) with respect to time and taking $r_{i\pm\frac{1}{2}}$, $\theta_{j\pm\frac{1}{2}}$ at the moment when they are halfway i.e., $r^{n+\frac{1}{2}}_{i\pm\frac{1}{2}}$, $\theta^{n+\frac{1}{2}}_{j\pm\frac{1}{2}}$, we get

$$\frac{3(r^{n+\frac{1}{2}}_{i\pm\frac{1}{2}})^2(dr_{i\pm\frac{1}{2}}/dt)^{n+\frac{1}{2}}}{(r^{n+1}_{i\pm\frac{1}{2}})^3 - (r^{n}_{i\pm\frac{1}{2}})^3} = \frac{\sin\theta^{n+1}_{j\pm\frac{1}{2}}(d\theta_{j\pm\frac{1}{2}}/dt)^{n+\frac{1}{2}}}{\cos\theta^{n}_{j\pm\frac{1}{2}} - \cos\theta^{n+1}_{j\pm\frac{1}{2}}}\,.$$

Recognizing that $(dr_{i\pm\frac{1}{2}}/dt)^{n+\frac{1}{2}} = u^g_{i\pm\frac{1}{2}}$, the velocity of the grid at $t^n + \frac{\delta t}{2}$, from Eq. (314b) and the above equation we obtain

$$\left(\frac{d\theta_{j\pm\frac{1}{2}}}{dt}\right)^{n+\frac{1}{2}}\cdot\,\delta t = \frac{\cos\theta^{n}_{j\pm\frac{1}{2}} - \cos\theta^{n+1}_{j\pm\frac{1}{2}}}{\sin\theta^{n+\frac{1}{2}}_{j\pm\frac{1}{2}}}\,, \tag{315}$$

whence from Eq. (313b), the velocity of the grid at $t^n + \frac{\delta t}{2}$,

$$v^{g}_{i,j\pm\frac{1}{2}} = \frac{2}{3}\,\frac{(r^{n+\frac{1}{2}}_{i+\frac{1}{2}})^3 - (r^{n+\frac{1}{2}}_{i-\frac{1}{2}})^3}{(r^{n+\frac{1}{2}}_{i+\frac{1}{2}})^2 - (r^{n+\frac{1}{2}}_{i-\frac{1}{2}})^2}\left(\frac{d\theta_{j\pm\frac{1}{2}}}{dt}\right)^{n+\frac{1}{2}} \tag{316}$$

Recognizing $(\frac{d\theta_{j\pm\frac{1}{2}}}{dt})$ as the angular velocity at $t^n + \delta t/2$ of the interface $i,j\pm\frac{1}{2}$ [from Eq. (315) obviously independent of index i as expected after the discussion in the section "Rectangular Grid Motion"], we can define an average radius for the interface $i,j\pm\frac{1}{2}$ (independent of j) as

$$R^{n+\frac{1}{2}}_{i} = \frac{\frac{1}{3}[(r^{n+\frac{1}{2}}_{i+\frac{1}{2}})^2 + (r^{n+\frac{1}{2}}_{i+\frac{1}{2}})(r^{n+\frac{1}{2}}_{i-\frac{1}{2}}) + (r^{n+\frac{1}{2}}_{i-\frac{1}{2}})^2]}{\frac{1}{2}[(r^{n+\frac{1}{2}}_{i+\frac{1}{2}}) + (r^{n+\frac{1}{2}}_{i-\frac{1}{2}})]} \tag{317}$$

Finally, the mean cell volume is

$$\forall^{n+\frac{1}{2}}_{i,j} = \frac{2\pi}{3}[(r^{n+\frac{1}{2}}_{i+\frac{1}{2}})^3 - (r^{n+\frac{1}{2}}_{i-\frac{1}{2}})^3](\cos\theta^{n+\frac{1}{2}}_{j-\frac{1}{2}} - \cos\theta^{n+\frac{1}{2}}_{j+\frac{1}{2}}). \tag{318}$$

Coordinate cases 4-7 will be treated in a later report.

XV. SOURCE TERMS

As explained earlier, source terms are integrated either over cell volume or over cell interface area. The volumes and areas used are those of the mean cell. The balance of source terms is the main reason for the necessity of a closed mean cell construction, i.e., the ability to construct a closed cell whose corners are on the paths between old and new cell corners. For example, if we try to solve a hydrostatic pressure problem in cylindrical r-z coordinates, the momentum equation is nothing but the balance of the body gravity force and the pressure force on the top and bottom surfaces. If the mid-cell interfaces compose a closed surface enclosing the midway cell which happens to have a volume consistent with the interface areas, force balance is already guaranteed (provided the pressures are correct).

Let us consider the difference form of $-\int_{s_g} p\vec{n}ds$ (yielding - grad p) in the three coordina[illegible] ases considered above. The resulting forces along the x, y directions are

$$F_{x_{i,j}} = (p^{n+\frac{1}{2}}_{i-\frac{1}{2},j} - p^{n+\frac{1}{2}}_{i+\frac{1}{2},j})A^{n+\frac{1}{2}}_{i}; \qquad (321a)$$

$$F_{y_{i,j}} = (p^{n+\frac{1}{2}}_{i,j-\frac{1}{2}} - p^{n+\frac{1}{2}}_{i,j+\frac{1}{2}})A^{n+\frac{1}{2}}_{j}; \qquad (321b)$$

respectively, where

$$p^{n+\frac{1}{2}}_{i+\frac{1}{2},j} = \frac{p^{n+\frac{1}{2}}_{i,j} + p^{n+\frac{1}{2}}_{i+1,j}}{2} \qquad (322a)$$

and

$$p^{n+\frac{1}{2}}_{i,j+\frac{1}{2}} = \frac{p^{n+\frac{1}{2}}_{i,j} + p^{n+\frac{1}{2}}_{i,j+1}}{2} \ . \tag{322b}$$

In cylindrical r-z coordinates,

$$F_{r_{i,j}} = p^{n+\frac{1}{2}}_{i-\frac{1}{2},j}\, A^{n+\frac{1}{2}}_{i-\frac{1}{2},j} - p^{n+\frac{1}{2}}_{i+\frac{1}{2},j}\, A^{n+\frac{1}{2}}_{i+\frac{1}{2},j} + 2\pi\, p^{n+\frac{1}{2}}_{i,j}(r^{n+\frac{1}{2}}_{i+\frac{1}{2}} - r^{n+\frac{1}{2}}_{i-\frac{1}{2}})(z^{n+\frac{1}{2}}_{j+\frac{1}{2}} - z^{n+\frac{1}{2}}_{j-\frac{1}{2}}),$$

which with Eq. (303) yields

$$F_{r_{i,j}} = p^{n+\frac{1}{2}}_{i-\frac{1}{2},j}\, A^{n+\frac{1}{2}}_{i-\frac{1}{2},j} - p^{n+\frac{1}{2}}_{i+\frac{1}{2},j}\, A^{n+\frac{1}{2}}_{i+\frac{1}{2},j} + \frac{p^{n+\frac{1}{2}}_{i,j}\, V^{n+\frac{1}{2}}_{i,j}}{r^{n+\frac{1}{2}}_{i}}, \tag{323a}$$

where

$$r^{n+\frac{1}{2}}_{i} \equiv \frac{r^{n+\frac{1}{2}}_{i+\frac{1}{2}} + r^{n+\frac{1}{2}}_{i-\frac{1}{2}}}{2} \ . \tag{324}$$

We notice that $p^{n+\frac{1}{2}}_{i,j}/r^{n+\frac{1}{2}}_{i}$ acts as a body force per unit volume. The force in the z-direction is

$$F_{z_{i,j}} = (p^{n+\frac{1}{2}}_{i,j-\frac{1}{2}} - p^{n+\frac{1}{2}}_{i,j+\frac{1}{2}})A^{n+\frac{1}{2}}_{i} \ . \tag{323b}$$

In spherical r-θ coordinates, as illustrated in Fig. 38, the pressure acting on the hatched area creates a resultant force normal to the axis from which θ is measured, which in turn gives rise to a radial component F'_r and a tangential component F'_θ. This situation, namely, the creation of a body-force-like component, occurs whenever the area of parallel surfaces of the cell are not equal. This is bound to happen whenever the interface area depends on both indices i,j. A simple way to evaluate the force generated is the "pressure x projected area" since this area is the difference between the areas of these parallel surfaces. The radial force is therefore

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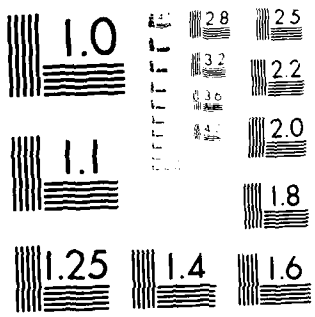

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$$F_{r_{i,j}} = p^{n+\frac{1}{2}}_{i-\frac{1}{2},j}\, A^{n+\frac{1}{2}}_{i-\frac{1}{2},j} - p^{n+\frac{1}{2}}_{i+\frac{1}{2},j}\, A^{n+\frac{1}{2}}_{i+;,j} + F'_{r_{i,j}} ,$$

where

$$F'_{r_{i,j}} = p^{n+\frac{1}{2}}_{i,j}\, (A^{n+\frac{1}{2}}_{i+\frac{1}{2},j} - A^{n+\frac{1}{2}}_{i-\frac{1}{2},j}) = 2\pi\, p^{n+\frac{1}{2}}_{i,j}\, [(r^{n+\frac{1}{2}}_{i+\frac{1}{2}})^2$$

$$- (r^{n+\frac{1}{2}}_{i-\frac{1}{2}})^2](\cos\theta^{n+\frac{1}{2}}_{j-\frac{1}{2}} - \cos\theta^{n+\frac{1}{2}}_{j+\frac{1}{2}}) = \frac{2p^{n+\frac{1}{2}}_{i,j}\, \mathcal{V}^{n+\frac{1}{2}}_{i,j}}{R^{n+\frac{1}{2}}_{i}} ;$$

R_i was defined earlier in Eq. (317). Thus

$$F_{r_{i,j}} = p^{n+\frac{1}{2}}_{i-\frac{1}{2},j}\, A^{n+\frac{1}{2}}_{i-\frac{1}{2},j} - p^{n+\frac{1}{2}}_{i+\frac{1}{2},j}\, A^{n+\frac{1}{2}}_{i+\frac{1}{2},j} + \frac{2p^{n+\frac{1}{2}}_{i,j}\, \mathcal{V}^{n+\frac{1}{2}}_{i,j}}{R^{n+\frac{1}{2}}_{i}} . \qquad (325)$$

As for the tangential direction,

$$F_{\theta_{i,j}} = p^{n+\frac{1}{2}}_{i,j-\frac{1}{2}}\, A^{n+\frac{1}{2}}_{i,j+\frac{1}{2}} - p^{n+\frac{1}{2}}_{i,j+\frac{1}{2}}\, A^{n+\frac{1}{2}}_{i,j+\frac{1}{2}} + F'_{\theta_{i,j}} ,$$

where

$$F'_{\theta_{i,j}} = p^{n+\frac{1}{2}}_{i,j}\, (A^{n+\frac{1}{2}}_{i,j+\frac{1}{2}} - A^{n+\frac{1}{2}}_{i,j-\frac{1}{2}}) = \pi\, p^{n+\frac{1}{2}}_{i,j}\, [(r^{n+\frac{1}{2}}_{i+\frac{1}{2}})^2$$

$$- (r^{n+\frac{1}{2}}_{i-\frac{1}{2}})^2](\sin\theta^{n+\frac{1}{2}}_{j+\frac{1}{2}} - \sin\theta^{n+\frac{1}{2}}_{j-\frac{1}{2}}) .$$

If we note that

$$\sin\theta^{n+\frac{1}{2}}_{j+\frac{1}{2}} - \sin\theta^{n+\frac{1}{2}}_{j-\frac{1}{2}} = 2\sin\left(\frac{\theta^{n+\frac{1}{2}}_{j+\frac{1}{2}} - \theta^{n+\frac{1}{2}}_{j-\frac{1}{2}}}{2}\right) \cos\left(\frac{\theta^{n+\frac{1}{2}}_{j+\frac{1}{2}} + \theta^{n+\frac{1}{2}}_{j-\frac{1}{2}}}{2}\right)$$

and

$$\cos\theta^{n+\frac{1}{2}}_{j-\frac{1}{2}} - \cos\theta^{n+\frac{1}{2}}_{j+\frac{1}{2}} = 2\sin\left(\frac{\theta^{n+\frac{1}{2}}_{j+\frac{1}{2}} + \theta^{n+\frac{1}{2}}_{j-\frac{1}{2}}}{2}\right) \sin\left(\frac{\theta^{n+\frac{1}{2}}_{j+\frac{1}{2}} + \theta^{n+\frac{1}{2}}_{j-\frac{1}{2}}}{2}\right)$$

and using Eq. (318), F'_{θ} can be expressed as

$$F'_{\theta\,i,j} = \frac{p^{n+\frac{1}{2}}_{i,j}\, v^{n+\frac{1}{2}}_{i,j}}{R^{n+\frac{1}{2}}_{i} \tan \theta^{n+\frac{1}{2}}_{j}},$$

where

$$\theta^{n+\frac{1}{2}}_{j} = \frac{\theta^{n+\frac{1}{2}}_{j+\frac{1}{2}} + \theta^{n+\frac{1}{2}}_{j-\frac{1}{2}}}{2}\,. \tag{326}$$

Thus

$$F_{\theta\,i,j} = p^{n+\frac{1}{2}}_{i,j-\frac{1}{2}}\, A^{n+\frac{1}{2}}_{i,j-\frac{1}{2}} - p^{n+\frac{1}{2}}_{i,j+\frac{1}{2}}\, A^{n+\frac{1}{2}}_{i,j+\frac{1}{2}} + \frac{p^{n+\frac{1}{2}}_{i,j}\, v^{n+\frac{1}{2}}_{i,j}}{R^{n+\frac{1}{2}}_{i} \tan \theta^{n+\frac{1}{2}}_{j}}\,,$$

Next, let us consider the difference form of $-\int_{s^g} p\vec{u}\cdot\vec{n}ds$ [yielding $-$ div($p\vec{u}$)].

For the three coordinate systems considered above, the power added to the cell (i,j) is

$$P_{i,j} = p^{n+\frac{1}{2}}_{i-\frac{1}{2},j}\, u^{n+\frac{1}{2}}_{i-\frac{1}{2},j}\, A^{n+\frac{1}{2}}_{i-\frac{1}{2},j} - p^{n+\frac{1}{2}}_{i+\frac{1}{2},j}\, u^{n+\frac{1}{2}}_{i+\frac{1}{2},j}\, A^{n+\frac{1}{2}}_{i+\frac{1}{2},j}$$

$$+ p^{n+\frac{1}{2}}_{i,j-\frac{1}{2}}\, v^{n+\frac{1}{2}}_{i,j-\frac{1}{2}}\, A^{n+\frac{1}{2}}_{i,j-\frac{1}{2}} - p^{n+\frac{1}{2}}_{i,j+\frac{1}{2}}\, v^{n+\frac{1}{2}}_{i,j+\frac{1}{2}}\, A^{n+\frac{1}{2}}_{i,j+\frac{1}{2}}, \tag{328}$$

where

$$u^{n+\frac{1}{2}}_{i+\frac{1}{2},j} = \frac{u^{n+\frac{1}{2}}_{i,j} + u^{n+\frac{1}{2}}_{i+1,j}}{2} \tag{329a}$$

and

$$v^{n+\frac{1}{2}}_{i,j+\frac{1}{2}} = \frac{v^{n+\frac{1}{2}}_{i,j} + v^{n+\frac{1}{2}}_{i,j+1}}{2}. \tag{329b}$$

The forces (F_x,F_y), (F_r,F_z), and (F_r,F_θ), and the power P constitute a sample of the source terms encountered in treating generalized continuity equations. These are denoted by source$^{n+\frac{1}{2}}_{i,j}$ in the next section.

XVI. ALGORITHM

We describe the implementation of the scheme of Eqs. (223). The program and calling sequence are listed in the Appendix.

Assume a rectangular grid in two dimensions denoted by the coordinates x, y (not necessarily cartesian; for example $x \equiv r$, $y \equiv \theta$ yield spherical coordinates). Let the interfaces coordinates be $x_{1/2}, x_{3/2}, \ldots, x_{N_x+1/2}$; $y_{1/2}, y_{3/2}, \ldots, y_{N_y+1/2}$ (see Fig. 39).

The cell centers are located midway between the interfaces and are denoted by a pair of indices (i,j), corresponding to (x,y), respectively. The cell volumes are given by

$$\mathcal{V}^{n,n+1}_{i,j} = \begin{cases} \begin{array}{c}\text{cartesian}\\ \text{x-y}\end{array} : (y^{n,n+1}_{j+\frac{1}{2}} - y^{n,n+1}_{j-\frac{1}{2}})(x^{n,n+1}_{i+\frac{1}{2}} - x^{n,n+1}_{i-\frac{1}{2}}); \\ \\ \begin{array}{c}\text{cylindrical}\\ \text{r-z}\end{array} : [(x^{n,n+1}_{i+\frac{1}{2}})^2 - (x^{n,n+1}_{i-\frac{1}{2}})^2][y^{n,n+1}_{j+\frac{1}{2}} - y^{n,n+1}_{j-\frac{1}{2}}] \\ \\ \begin{array}{c}\text{spherical}\\ \text{r-}\theta\end{array} : \frac{2\pi}{3}[(x^{n,n+1}_{i+\frac{1}{2}})^3 - (x^{n,n+1}_{i-\frac{1}{2}})^3][\cos y^{n,n+1}_{j-\frac{1}{2}} - \cos y^{n,n+1}_{j+\frac{1}{2}}]; \end{cases}$$

We have then

$$\mathcal{V}^{n+1}_{i,j}\, \rho^{T_x}_{i,j} = \mathcal{V}^{n}_{i,j}\, \rho^{n}_{i,j} - \delta t(\rho^{n}_{i+\frac{1}{2},j}\, A^{n+\frac{1}{2}}_{i+\frac{1}{2},j}\, \delta U^{n+\frac{1}{2}}_{i+\frac{1}{2},j})$$

$$+ \delta t(\rho^{n}_{i-\frac{1}{2},j}\, A^{n+\frac{1}{2}}_{i-\frac{1}{2},j}\, \delta U^{n+\frac{1}{2}}_{i-\frac{1}{2},j}) + \text{source}^{\,n+\frac{1}{2}}_{i,j} \qquad (332a)$$

and

$$\mathbf{v}^{n+1}_{i,j}\ \rho^{T_y}_{i,j} = \mathbf{v}^{n}_{i,j}\ \rho^{n}_{i,j} - \delta t(\rho^{n}_{i,j+\frac{1}{2}}\ A^{n+\frac{1}{2}}_{i,j+\frac{1}{2}}\ \delta V^{n+\frac{1}{2}}_{i,j+\frac{1}{2}})$$

$$+ \delta t(\rho^{n}_{i,j-\frac{1}{2}}\ A^{n+\frac{1}{2}}_{i,j-\frac{1}{2}}\ \delta V^{n+\frac{1}{2}}_{i,j-\frac{1}{2}}) + \text{source}^{\ n+\frac{1}{2}}_{i,j} \qquad (332b)$$

for $(i = 1,\ldots,N_x)$ and $(j = 1,\ldots,N_y)$, where

$$\rho^{n}_{i+\frac{1}{2},j} = \frac{\rho^{n}_{i,j} + \rho^{n}_{i+1,j}}{2} \qquad (33a)$$

for $i = 1,\ldots,N_x - 1$ and $j = 1,\ldots,N_y$, while

$$\rho^{n}_{i,j+\frac{1}{2}} = \frac{\rho^{n}_{i,j} + \rho^{n}_{i,j+1}}{2} \qquad (333b)$$

for $i = 1,\ldots,N_x$ and $j = 1,\ldots,N_y - 1$. The boundary values $\rho^{n}_{\frac{1}{2},j}$, $\rho^{n}_{N_x+\frac{1}{2},j}$ are obtained from

$$\rho^{n}_{\frac{1}{2},j} = \frac{\rho^{n}_{1,j} + \rho^{n}_{L,j}}{2};$$

$$\rho^{n}_{N_x+\frac{1}{2},j} = \frac{\rho^{n}_{N_x,j} + \rho^{n}_{R,j}}{2},$$

for $(j = 1,\ldots,N_y)$ where L and R denote left and right boundaries, respectively, while

$$\rho^{n}_{i,\frac{1}{2}} = \frac{\rho^{n}_{i,1} + \rho^{n}_{i,B}}{2};$$

$$\rho^{n}_{i,N_y+\frac{1}{2}} = \frac{\rho^{n}_{i,N_y} + \rho^{n}_{i,T}}{2},$$

for $(i = 1,\ldots,N_x)$ where B and T denote bottom and top boundaries, respectively. The mean interface areas $A^{n+\frac{1}{2}}_{i+\frac{1}{2},j}$ and $A^{n+\frac{1}{2}}_{i,j+\frac{1}{2}}$ are given by

$$A^{n+\frac{1}{2}}_{i+\frac{1}{2},j} = y^{n+\frac{1}{2}}_{j+\frac{1}{2}} - y^{n+\frac{1}{2}}_{j-\frac{1}{2}} \tag{334a}$$

and

$$A^{n+\frac{1}{2}}_{i,j+\frac{1}{2}} = x^{n+\frac{1}{2}}_{i+\frac{1}{2}} - x^{n+\frac{1}{2}}_{i-\frac{1}{2}}, \tag{334b}$$

where

$$y^{n+\frac{1}{2}}_{j+\frac{1}{2}} = \frac{y^{n}_{j+\frac{1}{2}} + y^{n+1}_{j+\frac{1}{2}}}{2} \tag{335a}$$

and

$$x^{n+\frac{1}{2}}_{i+\frac{1}{2}} = \frac{x^{n}_{i+\frac{1}{2}} + x^{n+1}_{i+\frac{1}{2}}}{2} \tag{335b}$$

for cartesian x-y coordinates; by

$$A^{n+\frac{1}{2}}_{i+\frac{1}{2},j} = 2\pi\ x^{n+\frac{1}{2}}_{i+\frac{1}{2}}(y^{n+\frac{1}{2}}_{j+\frac{1}{2}} - y^{n+\frac{1}{2}}_{j-\frac{1}{2}}) \tag{336a}$$

and

$$A^{n+\frac{1}{2}}_{i,j+\frac{1}{2}} = \pi[(x^{n+\frac{1}{2}}_{i+\frac{1}{2}})^2 - (x^{n+\frac{1}{2}}_{i-\frac{1}{2}})^2], \tag{336b}$$

where

$$y^{n+\frac{1}{2}}_{j+\frac{1}{2}} = \frac{y^{n}_{j+\frac{1}{2}} + y^{n+1}_{j+\frac{1}{2}}}{2} \tag{337a}$$

and

$$x^{n+\frac{1}{2}}_{i+\frac{1}{2}} = \left[\frac{(x^{n}_{i+\frac{1}{2}})^2 + (x^{n+1}_{i+\frac{1}{2}})^2}{2}\right]^{\frac{1}{2}} \tag{337b}$$

for cylindrical r-z coordinates; and by

$$A^{n+\frac{1}{2}}_{i+\frac{1}{2},j} = 2\pi(x^{n+\frac{1}{2}}_{i+\frac{1}{2}})^2[\cos y^{n+\frac{1}{2}}_{j-\frac{1}{2}} - \cos y^{n+\frac{1}{2}}_{j+\frac{1}{2}}] \tag{338a}$$

and

$$A^{n+\frac{1}{2}}_{i,j+\frac{1}{2}} = \pi[(x^{n+\frac{1}{2}}_{i+\frac{1}{2}})^2 - (x^{n+\frac{1}{2}}_{i-\frac{1}{2}})^2] \sin y^{n+\frac{1}{2}}_{j+\frac{1}{2}}, \tag{338b}$$

where

$$y^{n+\frac{1}{2}}_{j+\frac{1}{2}} = \arccos\, [\tfrac{1}{2}\{\cos y^{n}_{j+\frac{1}{2}} + \cos y^{n+1}_{j+\frac{1}{2}}\}] \tag{339a}$$

and

$$x^{n+\frac{1}{2}}_{i+\frac{1}{2}} \left[\frac{(x^{n}_{i+\frac{1}{2}})^3 + (x^{n+1}_{i+\frac{1}{2}})^3}{2}\right]^{1/3} \tag{339b}$$

for spherical r-θ coordinates. Finally,

$$\delta U^{n+\frac{1}{2}}_{i+\frac{1}{2},j} = u^{n+\frac{1}{2}}_{i+\frac{1}{2},j} - u^{g}_{i+\frac{1}{2},j} \tag{340a}$$

and

$$\delta V^{n+\frac{1}{2}}_{i,j+\frac{1}{2}} = v^{n+\frac{1}{2}}_{i,j+\frac{1}{2}} - v^{g}_{i,j+\frac{1}{2}} \tag{341a}$$

The grid velocities $u^{g}_{i+\frac{1}{2},j}$, $v^{g}_{i,j+\frac{1}{2}}$ are given by

$$u^{g}_{i+\frac{1}{2},j} = \frac{x^{n+1}_{i+\frac{1}{2}} - x^{n}_{i+\frac{1}{2}}}{\delta t} \tag{341b}$$

$$v^{g}_{i,j+\frac{1}{2}} = \frac{y^{n+1}_{j+\frac{1}{2}} - y^{n}_{j+\frac{1}{2}}}{\delta t}$$

for cartesian x-y coordinates; by

$$u^{g}_{i+\frac{1}{2},j} = \frac{(x^{n+1}_{i+\frac{1}{2}})^2 - (x^{n}_{i+\frac{1}{2}})^2}{2\, x^{n+\frac{1}{2}}_{i+\frac{1}{2}}\, \delta t} \tag{342a}$$

$$v^g_{i,j+\frac{1}{2}} = \frac{y^{n+1}_{j+\frac{1}{2}} - y^n_{j+\frac{1}{2}}}{\delta t} \tag{342b}$$

for cylindrical r-z coordinates; and by

$$u^g_{i+\frac{1}{2},j} = \frac{(x^{n+1}_{i+\frac{1}{2}})^3 - (x^n_{i+\frac{1}{2}})^3}{3(x^{n+\frac{1}{2}}_{i+\frac{1}{2}})^2 \ \delta t} \tag{343a}$$

$$v^g_{i,j+\frac{1}{2}} = \frac{x^{n+\frac{1}{2}}_i}{\delta t} \ \frac{\cos y^n_{j+\frac{1}{2}} - \cos y^{n+1}_{j+\frac{1}{2}}}{\sin y^{n+\frac{1}{2}}_{j+\frac{1}{2}}} \tag{343b}$$

for spherical r-θ coordinates, where

$$x^{n+\frac{1}{2}}_i = \frac{2}{3} \ \frac{(x^{n+\frac{1}{2}}_{i+\frac{1}{2}})^2 + (x^{n+\frac{1}{2}}_{i+\frac{1}{2}})(x^{n+\frac{1}{2}}_{i-\frac{1}{2}}) + (x^{n+\frac{1}{2}}_{i-\frac{1}{2}})^2}{x^{n+\frac{1}{2}}_{i+\frac{1}{2}} + x^{n+\frac{1}{2}}_{i-\frac{1}{2}}} \ . \tag{344}$$

Equations (334)-(344) are valid for $i = 0, 1, \ldots, N_x$ and $j = 0, 1, \ldots, N_y$. Equations (332) yield $\rho^{Tx}_{i,j}$ and $\rho^{Ty}_{i,j}$, which are used later to evaluate the antidiffusion fluxes. The transported and diffused densities are then obtained from

$$\begin{aligned} \mathcal{V}^{n+1}_{i,j} \rho^{TD}_{i,j} = {} & \mathcal{V}^{n+1}_{i,j} \rho^{T}_{i,j} + \nu_{i+\frac{1}{2},j} \mathcal{V}^{n+1}_{i+\frac{1}{2},j} (\rho^n_{i+1,j} - \rho^n_{i,j}) \\ & - \nu_{i-\frac{1}{2},j} \mathcal{V}^{n+1}_{i-\frac{1}{2},j} (\rho^n_{i,j} - \rho^n_{i-1,j}) + \nu_{i,j+\frac{1}{2}} \mathcal{V}^{n+1}_{i,j+\frac{1}{2}} (\rho^n_{i,j+1} \\ & - \rho^n_{i,j}) - \nu_{i,j-\frac{1}{2}} \mathcal{V}^{n+1}_{i,j-\frac{1}{2}} (\rho^n_{i,j} - \rho^n_{i,j-1}) \end{aligned} \tag{346}$$

for $i = 1, \ldots, N_x$ and $j = 1, \ldots, N_y$, where

$$\nu_{i+\frac{1}{2},j} = \frac{1}{6} + \frac{1}{3} \epsilon^2_{i+\frac{1}{2},j} \tag{347a}$$

and

$$\nu_{i,j+\frac{1}{2}} = \frac{1}{6} + \frac{1}{3}\,\varepsilon^2_{i,j+\frac{1}{2}}, \tag{347b}$$

while

$$\Psi^{n+1}_{i+\frac{1}{2},j} = \frac{1}{2}(\Psi^{n+1}_{i,j} + \Psi^{n+1}_{i+1,j}) \tag{348a}$$

for $i = 1,\ldots,N_x - 1$ and $j = 1,\ldots,N_y$. Similarly,

$$\Psi_{i,j+\frac{1}{2}} = \frac{1}{2}(\Psi^{n+1}_{i,j} + \Psi^{n+1}_{i,j+1}) \tag{348b}$$

for $i = 1,\ldots,N_x$ and $j = 1,\ldots,N_y - 1$. At the boundaries,

$$\Psi^{n+1}_{\frac{1}{2},j} = \Psi^{n+1}_{1,j} \quad \text{and} \quad \Psi^{n+1}_{N_x+\frac{1}{2},j} = \Psi^{n+1}_{N_x,j} \tag{349a}$$

for $j = 1,\ldots,N_y$, while

$$\Psi^{n+1}_{i,\frac{1}{2}} = \Psi^{n+1}_{i,1} \quad \text{and} \quad \Psi^{n+1}_{i,N_y+\frac{1}{2}} = \Psi^{n+1}_{i,N_y} \tag{349b}$$

for $i = 1,\ldots,N_x$. The dimensionless velocities $\varepsilon_{i+\frac{1}{2},j}$, $\varepsilon_{i,j+\frac{1}{2}}$ are obtained from

$$\varepsilon_{i+\frac{1}{2},j} = \frac{\delta U^{n+\frac{1}{2}}_{i+\frac{1}{2},j}\; A^{n+\frac{1}{2}}_{i+\frac{1}{2},j}\,\delta t}{2}\left(\frac{1}{\Psi^{n+1}_{i,j}} + \frac{1}{\Psi^{n+1}_{i+1,j}}\right) \tag{350a}$$

for $i = 0,\ldots,N_x$ and $j = 1,\ldots,N_y$ using (349a) and

$$\varepsilon_{i,j+\frac{1}{2}} = \frac{\delta V^{n+\frac{1}{2}}_{i,j+\frac{1}{2}}\; A^{n+\frac{1}{2}}_{i,j+\frac{1}{2}}\;\delta t}{2}\left(\frac{1}{\Psi^{n+1}_{i,j}} + \frac{1}{\Psi^{n+1}_{i,j+1}}\right) \tag{350b}$$

for $i = 1,\ldots,N_x$ and $j = 0,\ldots,N_y$ using (349b). The antidiffusion fluxes are then evaluated according to

$$F_{i+\frac{1}{2},j} = \mu_{i+\frac{1}{2},j} \, V^{n+1}_{i+\frac{1}{2},j} \, (\rho^{Tx}_{i+1,j} - \rho^{Tx}_{i,j}) \tag{351a}$$

and

$$F_{i,j+\frac{1}{2}} = \mu_{i,j+\frac{1}{2}} \, V^{n+1}_{i,j+\frac{1}{2}} (\rho^{Ty}_{i,j+1} - \rho^{Ty}_{i,j}), \tag{351b}$$

where

$$\mu_{i+\frac{1}{2},j} = \frac{1}{6} - \frac{2}{3} \varepsilon^2_{i+\frac{1}{2},j}$$

and

$$\mu_{i,j+\frac{1}{2}} = \frac{1}{6} - \frac{2}{3} \varepsilon^2_{i,j+\frac{1}{2}}.$$

FLUX CORRECTION

The flux correction adopted here is that of Zalesak[5] in multi-dimensions. It "guarantees that the four antidiffusion fluxes, associated with each cell, acting in concert, do not create any ripples." In our notation it takes the following form:

1. A flux is cancelled if it is opposite to the local gradient of ρ^{TD} along the same direction, and if opposite to either or both adjacent gradients of ρ^{TD}, i.e., $F_{i+\frac{1}{2},j} = 0$ if

$$[F_{i+\frac{1}{2},j}(\rho^{TD}_{i+1,j} - \rho^{TD}_{i,j}) < 0] \text{ and } \{[F_{i+\frac{1}{2},j}(\rho^{TD}_{i+2,j} - \rho^{TD}_{i+1,j}) < 0] \text{ or } [F_{i+\frac{1}{2},j}(\rho^{TD}_{i,j} - \rho^{TD}_{i-1,j}) < 0]\} \tag{352a}$$

and $F_{i,j+\frac{1}{2}} = 0$ if

$$[F_{i,j+\frac{1}{2}}(\rho^{TD}_{i,j+1} - \rho^{TD}_{i,j}) < 0] \text{ and } \{[F_{i,j+\frac{1}{2}}(\rho^{TD}_{i,j+2} - \rho^{TD}_{i,j+1}) < 0] \text{ or } [F_{i,j+\frac{1}{2}}(\rho^{TD}_{i,j} - \rho^{TD}_{i,j-1}) < 0]\}. \tag{352b}$$

2. Evaluate the total in- and out-fluxes and their upper bounds. Let $P^+_{i,j}$ equal the sum of all antidiffusive fluxes "into" grid point (i,j):

$$P^+_{i,j} = \max(0, F_{i-\frac{1}{2},j}) - \min(0, F_{i+\frac{1}{2},j}) + \max(0, F_{i,j-\frac{1}{2}}) - \min(0, F_{i,j+\frac{1}{2}}). \tag{353a}$$

Next we evaluate the upper bound $Q^+_{i,j}$ on $P^+_{i,j}$:

$$Q^+_{i,j} = (\rho^{max}_{i,j} - \rho^{TD}_{i,j})\forall^{n+1}_{i,j}. \tag{354a}$$

The limiting ratio $R^+_{i,j}$ is thus estimated as

$$R^+_{i,j} = \begin{cases} \min(1, Q^+_{i,j}/P^+_{i,j}) & \text{if } P^+_{i,j} > 0 \\ 0 & \text{if } P^+_{i,j} = 0 \end{cases} \tag{355a}$$

Figure 40 illustrates the bounding process. Similarly, an upper bound $Q^-_{i,j}$ is placed on the "outgoing" fluxes.

$$P^-_{i,j} = \max(0, F_{i+\frac{1}{2},j}) - \min(0, F_{i-\frac{1}{2},j}) + \max(0, F_{i,j+\frac{1}{2}}) - \min(0, F_{i,j-\frac{1}{2}}) \tag{353b}$$

$$Q^-_{i,j} = (\rho^{TD}_{i,j} - \rho^{min}_{i,j})\forall^{n+1}_{i,j} \tag{354b}$$

$$R^-_{i,j} = \begin{cases} \min\left(1, \dfrac{Q^-_{i,j}}{P^-_{i,j}}\right) & \text{if } P^-_{i,j} > 0 \\ 0 & \text{if } P^-_{i,j} = 0 \end{cases} \tag{355b}$$

In the above $\rho^{max}_{i,j}$, $\rho^{min}_{i,j}$ are the upper and lower bounds, respectively, on $\rho^{n+1}_{i,j}$, chosen so as to guarantee no ripples formation at grid point (i,j). Finally, since each flux leaves a cell to enter an adjacent one,

3. The fluxes correction factors are defined as

$$C_{i+\frac{1}{2},j} = \begin{cases} \min\ (R^{+}_{i+1,j},\ R^{-}_{i,j}) & \text{if } F_{i+\frac{1}{2},j} \geq 0 \\ \min\ (R^{-}_{i+1,j},\ R^{+}_{i,j}) & \text{if } F_{i+\frac{1}{2},j} < 0 \end{cases} \tag{356a}$$

and

$$C_{i,j+\frac{1}{2}} = \begin{cases} \min\ (R^{+}_{i,j+1},\ R^{-}_{i,j}) & \text{if } F_{i,j+\frac{1}{2}} \geq 0 \\ \min\ (R^{-}_{i,j+1},\ R^{+}_{i,j}) & \text{if } F_{i,j+\frac{1}{2}} < 0. \end{cases} \tag{356b}$$

The corrected fluxes are given by

$$F^{C}_{i+\frac{1}{2},j} = C_{i+\frac{1}{2},j}\ F_{i+\frac{1}{2},j}; \tag{357a}$$

$$F^{C}_{i,j+\frac{1}{2}} = C_{i,j+\frac{1}{2}}\ F_{i,j+\frac{1}{2}}, \tag{357b}$$

4. For ρ^{max}_{j} and ρ^{min}_{j}, two choices are presented. A conservative choice would be

$$\rho^{max}_{i,j} = \max\ (\rho^{TD}_{i-1,j},\ \rho^{TD}_{i,j-1},\ \rho^{TD}_{i,j},\ \rho^{TD}_{i+1,j},\ \rho^{TD}_{i,j+1}); \tag{358a}$$

$$\rho^{min}_{i,j} = \min\ (\rho^{TD}_{i-1,j},\ \rho^{TD}_{i,j-1},\ \rho^{TD}_{i,j},\ \rho^{TD}_{i+1,j},\ \rho^{TD}_{i,j+1}). \tag{358b}$$

A more tolerant choice that gets rid of the problems of "clipping" and "terracing" partially is

$$\rho^{max}_{i,j} = \max\ (\rho^{a}_{i-1,j},\ \rho^{a}_{i,j-1},\ \rho^{a}_{i,j}\ ,\ \rho^{a}_{i+1,j},\ \rho^{a}_{i,j+1}), \tag{359a}$$

where

$$\rho^{a}_{i,j} = \max\ (\rho^{TD}_{i,j}, \rho^{n}_{i,j}),$$

and

$$\rho^{min}_{i,j} = \min\ (\rho^{b}_{i-1,j}, \rho^{b}_{i,j-1}, \rho^{b}_{i,j}, \rho^{b}_{i+1,j}, \rho^{b}_{j+1}), \tag{359b}$$

where

$$\rho^{b}_{i,j} = \min\ (\rho^{TD}_{i,j}, \rho^{n}_{i,j}).$$

ANTIDIFFUSION AND HALF-STEP UPDATING

The corrected antidiffusion fluxes are added

$$\forall^{n+1}_{i,j}\ \rho^{n+1}_{i,j} = \forall^{n+1}_{i,j}\ \rho^{TD}_{i,j} - (F^{c}_{i+\frac{1}{2},j} - F^{c}_{i-\frac{1}{2},j}) - (F^{c}_{i,j+\frac{1}{2}} - F^{c}_{i,j-\frac{1}{2}}) \tag{360}$$

thus giving the new density $\rho^{n+1}_{i,j}$.

Finally, it remains to specify $u^{n+\frac{1}{2}}_{i+\frac{1}{2},j}$ and $v^{n+\frac{1}{2}}_{i,j+\frac{1}{2}}$ in equations (340) and the source terms denoted by "*source* $^{n+\frac{1}{2}}_{i,j}$." First, the velocities at the interfaces are obtained from

$$u^{n+\frac{1}{2}}_{i+\frac{1}{2},j} = \frac{u^{n+\frac{1}{2}}_{i,j} + u^{n+\frac{1}{2}}_{i+1,j}}{2} \tag{361a}$$

for $i = 1,\ldots,N_x - 1$ and $j = 1,\ldots,N_y$ while

$$u^{n+\frac{1}{2}}_{\frac{1}{2},j} = \frac{u^{n+\frac{1}{2}}_{i,j} + u_L}{2}$$

$$u^{n+\frac{1}{2}}_{N_x+\frac{1}{2},j} = \frac{u^{n+\frac{1}{2}}_{N_x,j} + u_R}{2}$$

and

$$v_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{v_{i,j}^{n+\frac{1}{2}} + v_{i,j+1}^{n+\frac{1}{2}}}{2} \tag{361b}$$

for $i = 1,\ldots,N_x$ and $j = 1,\ldots,N_y - 1$ while

$$v_{i,\frac{1}{2}}^{n+\frac{1}{2}} = \frac{v_{i,1}^{n+\frac{1}{2}} + v_B}{2}$$

$$v_{i,N_y+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{v_{i,N_y}^{n+\frac{1}{2}} + v_T}{2}$$

As for the source terms they were defined earlier, Eqs. (321) through (329). Next, to get $u_{i,j}^{n+\frac{1}{2}}, v_{i,j}^{n+\frac{1}{2}}$, and source $_{i,j}^{n+\frac{1}{2}}$, we advance our system of conservation equations ½ time step using $u_{i,j}^{n}$, $v_{i,j}^{n}$, source $_{i,j}^{n}$, then

$$u_{i,j}^{n+\frac{1}{2}} \Big|_{t^n \to t^n + \delta t} = u_{i,j}^{n+1} \Big|_{t^n \to t^n + \frac{\delta t}{2}}$$

$$v_{i,j}^{n+\frac{1}{2}} \Big|_{t^n \to t^n + \delta t} = v_{i,j}^{n+1} \Big|_{t^n \to t^n + \frac{\delta t}{2}}$$

$$\text{source}_{i,j}^{n+\frac{1}{2}} \Big|_{t^n \to t^n + \delta t} = \text{source}_{i,j}^{n+1} \Big|_{t^n \to t^n + \frac{\delta t}{2}} .$$

XVII. TWO-DIMENSIONAL TIME SPLITTING VERSUS FUL Y TWO-DIMENSIONAL ALGORITHMS

Going back to Eq. (202),

$$A(\beta_x,\beta_y) = e^{-i(\varepsilon_x\beta_x + \varepsilon_y\beta_y)} = e^{-i\varepsilon_x\beta_x} e^{-i\varepsilon_y\beta_y} = A(\beta_x)A(\beta_y) \tag{362}$$

If $\rho^n_{i,j} = e^{i\vec{k}\cdot\vec{x}}$, where $\vec{x} = (i\delta x, j\delta y)$, the analytic solution of $\frac{\partial\rho}{\partial t} + \vec{u}\cdot\nabla\rho = 0$, according to Eq. (362), yields

$$\rho^{n+1}_{i,j} = A(\beta_y)A(\beta_x)\rho^n_{i,j} \tag{363}$$

where $\vec{u} = (u,v)$ is constant and the two operators $A(\beta_x)$ and $A(\beta_y)$ are commutable. Noticing that

$$\rho^x_{i,j} = A(\beta_x)\rho^n_{i,j} \tag{364a}$$

is the analytic solution of $\frac{\partial\rho}{\partial t} + u\,\frac{\partial\rho}{\partial x} = 0$, whereas

$$\rho^{n+1}_{i,j} = A(\beta_y)\rho^x_{i,j} \tag{364b}$$

is the analytic solution of $\frac{\partial\rho}{\partial t} + v\,\frac{\partial\rho}{\partial y} = 0$ for an initial density $\rho^x_{i,j}$, equation (363) invokes time splitting as an exact solution for the linear PDE. If we derive a numerical scheme by expanding $A(\beta_x,\beta_y)$ in terms of $\sin\beta_x$, $\cos\beta_x$, $\sin\beta_y$ and $\cos\beta_y$ such that both $A(\beta_x,\beta_y)$ and its expansion agree up to a prescribed order of β_x and β_y, we obviously end with a time splitting scheme, in which each of the x and y operators agrees with $A(\beta_x)$ and $A(\beta_y)$ up to a prescribed order of β_x and β_y, respectively.

Alternatively, if a 1-D scheme is n - order in phase error and m - order in diffusion error, namely

$$|A| = 1 + O(\beta^m) \tag{365}$$

and

$$\theta = \theta_{exact} + O(\beta^{n+1}) \tag{365b}$$

where $|A|$ and θ are the amplitude and angle of the scheme transfer function A, i.e., $A = |A|\ e^{i\theta}$, using a time-splitted version of the one-dimensional scheme to solve a two-dimensional, x-y problem, gives $|A|\ e^{i\theta} = A \equiv A_x A_y$ $= (|A_x|e^{i\theta}x)(|A_y|e^{i\theta}y)$. Thus,

$$|A| = |A_x|\cdot|A_y| = (1 + O(\beta_x^m))(1 + O(\beta_y^m)) = 1 + O(\beta_x^m) + O(\beta_y^m) \tag{366a}$$

and

$$\theta = \theta_x + \theta_y = [\theta_{x\ exact} + O(\beta_x^{n+1})] + [\theta_{y\ exact} + O(\beta_y^{n+1})]$$

$$= \theta_{exact} + O(\beta_x^{n+1}) + O(\beta_y^{n+1}) \tag{366b}$$

showing the two-dimensional scheme to be of the same order as the one-dimensional one. Moreover, the errors in both $|A|$ and θ are free from mixed frequencies, such as $O(\beta_x^{n_1}\beta_y^{n_2})$ where $n_1 + n_2 = m$ or $n + 1$.

Although time-splitting appears to be the perfect solution, physically unacceptable results are produced when dealing with incompressible or nearly incompressible flow fields, or when a differential identity, such as divergence free property or irrotationality, is to be strictly enforced. Moreover, because the antidiffusion fluxes are corrected in each direction independently of the other, unnecessary "clipping" occurs. Namely, the flux corrector may cancel a flux that would produce a ripple in one direction, which actually is safe in two-dimensions due to the growth or decay of the adjacent cells in the other direction.

Going back to the problems arising in incompressible flows, let's consider a case where $\vec{U} = \vec{U}(x,y)$, independent of time, satisfying $\nabla \cdot \vec{U} = 0$. For simplicity assume $u = u_o + Cx$ and $v = v_o - Cy$. Figure 41 illustrates the velocities at the interfaces of a cell, when $\delta x = \delta y = 1$, $C = 0.1$.

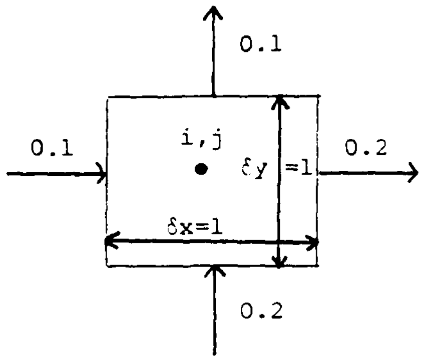

Fig. 41

Using a simple-transport scheme with time splitting

$$\mathcal{V}_{i,j}\, \rho^{x}_{i,j} = \mathcal{V}_{i,j}\, \rho^{o}_{i,j} - (u_{i+\frac{1}{2},j}\, \rho^{o}_{i+\frac{1}{2},j} - u_{i-\frac{1}{2},j}\, \rho^{o}_{i-\frac{1}{2},j})\delta y \delta t \qquad (367a)$$

$$\mathcal{V}_{i,j}\, \rho^{1}_{i,j} = \mathcal{V}_{i,j}\, \rho^{x}_{i,j} - (v_{i,j+\frac{1}{2}}\, \rho^{x}_{i,j+\frac{1}{2}} - v_{i,j-\frac{1}{2}}\, \rho^{x}_{i,j-\frac{1}{2}})\delta x \delta t \qquad (367b)$$

where 0,1 stands for $t = 0, \delta t$, respectively. Assuming a uniform initial density $\rho^{o} = 1$, and $\delta t = 1$, Eq. (367a) gives $(1)\cdot(\rho^{x}_{i,j}) = (1)\cdot(1) - ((0.2)\cdot(1) - (0.1)\cdot(1))\cdot(1)\cdot(1)$ yielding $\rho_{i,j} = 0.9$. Since $u = u(x)$, $v = v(y)$, $\rho^{x}_{i,j} = 0.9$ for all j's and since u,v are linear, it is also true for all i's. Then, from Eq. (367b), we obtain $(1)\cdot(\rho^{1}_{i,j}) = (1)\cdot(0.9) - ((0.1)\cdot(0.9) - (0.2)\cdot(0.9))\cdot(1)\cdot(1)$ yielding $\rho^{1}_{i,j} = 0.99$. After n time steps, it is obvious that $\rho^{n}_{i,j} = (0.99)^{n}$ for all i and j. Generally, $\rho^{n}_{i,j} = \rho^{o}_{i,j}(1-C^{2})^{n}$. In other words, the density keeps on uniformly distributed but decreases with time continuously.

An equivalent fully two-dimensional scheme would be

$$V_{i,j}\,\rho^{1}_{i,j} = V_{i,j}\,\rho^{o}_{i,j} - (u_{i+\frac{1}{2},j}\,\rho^{o}_{i+\frac{1}{2},j} - u_{i-\frac{1}{2},j}\,\rho^{o}_{i-\frac{1}{2},j})\,\delta y\delta t$$

$$- (v_{i,j+\frac{1}{2}}\,\rho^{o}_{i+\frac{1}{2}} - v_{i,j-\frac{1}{2}}\,\rho^{o}_{i,j-\frac{1}{2}})\,\delta x\delta t \qquad (368)$$

which gives $\rho^{1}_{i,j} = 1$, i.e. conserves the mass.

The discrepancy obviously lies in the assumption of $\vec{U}$ = const while ρ is varying when deriving Eq. (362). In terms of transfer functions, the scheme of Eqs. (367) is written as $A = (1 - \varepsilon_x t_x)(1 - \varepsilon_y t_y)$ whereas that of Eq. (368) takes the form $A = 1 - \varepsilon_x t_x - \varepsilon_y t_y$.

The difference is obviously in the term "$\varepsilon_x \varepsilon_y t_x t_y$" which as will be shown later is essential for high order diffusion. In the next section, we try to cast a time-splitted scheme into a fully two-dimensional form. A detailed explanation of the problems involved is given.

FULLY TWO-DIMENSIONAL VERSIONS OF TIME-SPLITTED SCHEMES

Going back to the fourth order phase and diffusion scheme

$$A = (1 - \varepsilon t)(1 - \mu d) + \nu d \qquad (370)$$

where $\nu = \frac{1}{6} + \frac{\varepsilon^2}{3}$ and $\mu = \frac{1-\varepsilon^2}{6}$. The two-dimensional, splitted version of Eq. (370)

$$A = [(1 - \varepsilon_x t_x)(1 - \mu_x d_x) + \nu_x d_x]\cdot[(1 - \varepsilon_y t_y)(1 - \mu_y d_y) + \nu_y d_y] \qquad (371a)$$

or

$$A = (1 - \varepsilon_x t_x + \nu_x d_x)(1 - \varepsilon_y t_y + \nu_y d_y) - \mu_x d_x (1 - \varepsilon_x t_x)(1 - \varepsilon_y t_y + \nu_y d_y)$$

$$- \mu_y d_y (1 - \varepsilon_y t_y)(1 - \varepsilon_x t_x + \nu_x d_x) - \mu_x \mu_y d_x d_y (1 - \varepsilon_x t_x)(1 - \varepsilon_y t_y) \qquad (371b)$$

can be written as

$$A^{TD} = 1 - \varepsilon_x t_x \left(1 - \frac{\varepsilon_y t_y}{2} + \frac{\nu_y d_y}{2}\right) - \varepsilon_y t_y \left(1 - \frac{\varepsilon_x t_x}{2} + \frac{\nu_x d_x}{2}\right)$$

$$+ \nu_x d_x \left(1 - \frac{\varepsilon_y t_y}{2} + \frac{\nu_y d_y}{2}\right) + \nu_y d_y \left(1 - \frac{\varepsilon_x t_x}{2} + \frac{\nu_x d_x}{2}\right) \qquad (372a)$$

which is ≥ 0 for $|\varepsilon_x|, |\varepsilon_y| \leq \frac{1}{2}$, therefore ensuring positivity of ρ^{TD} if $\rho^n \geq 0$. Then,

$$A = A^{TD} - \mu_x d_x^* (1 - \varepsilon_x t_x)[1 - \varepsilon_y t_y + \nu_y d_y - \frac{1}{2} \mu_y d_y (1 - \varepsilon_y t_y)]$$

$$- \mu_y d_y^* (1 - \varepsilon_y t_y)[1 - \varepsilon_x t_x + \nu_x d_x - \frac{1}{2} \mu_x d_x (1 - \varepsilon_x t_x)] \qquad (372b)$$

where the asterisks denote the operators which fluxes are to be corrected. This will allow us to correct the x and y antidiffusion fluxes simultaneously, thus avoiding unnecessary clipping. But that does not solve the problems associated with divergence free flow fields, for example, because of the term "$\varepsilon_x \varepsilon_y t_x t_y$." Moreover, we notice that the form of Eq. (372) is in no way unique.

Although Eqs. (366) show in a clear simple way that $A \equiv A_x A_y$ is fourth order in phase and diffusion, let us analyze it using Eqs. (246) to (248), Eqs. (260)-(262) with Eqs. (241)-(244). The purpose is to determine which terms are responsible for the fourth order diffusion, fourth order phase error, positivity, stability, and so on. We notice that $A^{t_x t_x} = 0$, $A^{t_y t_y} = 0$, making Eqs. (241)-(244) valid.

Differentiating Eq. (371a), we get

$$A^{t_{\substack{x\\y}}} = -\,\varepsilon_{\substack{x\\y}}(1 - \mu_{\substack{x\\y}} d_{\substack{x\\y}})\, A_{\substack{y\\x}} \tag{374}$$

$$A^{d_{\substack{x\\y}}} = [(\nu_{\substack{x\\y}} - \mu_{\substack{x\\y}}) + \varepsilon_{\substack{x\\y}}\mu_{\substack{x\\y}}t_{\substack{x\\y}}]A_{\substack{y\\x}} \tag{375}$$

$$A^{t_{\substack{x\\y}}d_{\substack{x\\y}}} = \varepsilon_{\substack{x\\y}}\mu_{\substack{x\\y}}A_{\substack{y\\x}} \tag{376}$$

$$A^{t_{\substack{x\\y}}d_{\substack{y\\x}}} = -\,\varepsilon_{\substack{x\\y}}(1 - \mu_{\substack{x\\y}}d_{\substack{x\\y}})[(\nu_{\substack{y\\x}} - \mu_{\substack{y\\x}}) + \varepsilon_{\substack{y\\x}}\mu_{\substack{y\\x}}t_{\substack{y\\x}}] \tag{377}$$

$$A^{t_x t_y} = \varepsilon_x\varepsilon_y(1 - \mu_x d_x)(1 - \mu_y d_y) \tag{378a}$$

$$A^{d_x d_y} = [(\nu_x - \mu_x) + \varepsilon_x\mu_x t_x][(\nu_y - \mu_y) + \varepsilon_y\mu_y t_y] \tag{378b}$$

At $\beta_x = \beta_y = 0$, $t_x = t_y = 0$, and $d_x = d_y = 0$, thus $A_x = A_y = 1$, yielding

$$A_o^{t_{\substack{x\\y}}} = -\,\varepsilon_{\substack{x\\y}} \tag{379}$$

$$A_o^{d_{\substack{x\\y}}} = \nu_{\substack{x\\y}} - \mu_{\substack{x\\y}} \tag{380}$$

$$A_o^{t_{\substack{x\\y}}d_{\substack{x\\y}}} = \varepsilon_{\substack{x\\y}}\mu_{\substack{x\\y}} \tag{381}$$

$$A_o^{t_{\substack{x\\y}}d_{\substack{y\\x}}} = -\,\varepsilon_{\substack{x\\y}}(\nu_{\substack{y\\x}} - \mu_{\substack{y\\x}}) \tag{382}$$

$$A_o^{t_x t_y} = \varepsilon_x\varepsilon_y \tag{383a}$$

$$A_o^{d_x d_y} = (\nu_x - \mu_x)(\nu_y - \mu_y) \tag{383b}$$

Substituting into Eqs. (246) and (248), we get

$$(\log A)_o^{\substack{x\\y}} = -\, i\varepsilon_{\substack{x\\y}} \tag{384}$$

$$\begin{aligned}(\log A)_o^{\substack{xxx\\yyy}} &= i\varepsilon_{\substack{x\\y}}[1 - 6(\nu_{\substack{x\\y}} - \mu_{\substack{x\\y}})] - i[6\varepsilon_{\substack{x\\y}}\mu_{\substack{x\\y}} - 2\varepsilon_{\substack{x\\y}}^3] \\ &= 6i\varepsilon_{\substack{x\\y}}\left(\frac{1}{6} + \frac{\varepsilon_{\substack{x\\y}}^2}{3} - \nu_{\substack{x\\y}}\right)\end{aligned} \tag{385}$$

showing A_xA_y to be fourth order in phase error, but more importantly, that the cross terms of Eqs. (382) and (393a), which do not appear in one-dimension, are essential to the fourth order phase. More specifically, these cross terms reduce the dependence of phase error on ν and μ to dependence on ν only, leaving μ free to be adjusted for a high order diffusion.

$A_o^{d_xd_y}$ in Eq. (383b) is not used in either (384) or (385) and therefore can take any value without affecting the phase error.

Now we can construct the simplest fourth order phase error scheme. Such a scheme has to satisfy Eqs. (379) to (382) plus Eq. (383a) giving,

$$\begin{aligned}A = {} & (1 - \varepsilon_xt_x)(1 - \varepsilon_yt_y) + (\nu_x - \mu_x)d_x + (\nu_y - \mu_y)dy + \varepsilon_xt_x\mu_xd_x \\ & + \varepsilon_yt_y\mu_yd_y - \varepsilon_xt_x(\nu_y - \mu_y)d_y - \varepsilon_yt_y(\nu_x - \mu_x)d_x\end{aligned} \tag{386}$$

where the integration constant was selected as unity to satisfy consistency, i.e., $A(\beta_x, \beta_y = 0) = 1$. Eq. (386) can be written as

$$\begin{aligned}A = {} & (1 - \varepsilon_xt_x)(1-\varepsilon_yt_y) + \nu_xd_x(1 - \varepsilon_yt_y) + \nu_yd_y(1 - \varepsilon_xt_x) \\ & - \mu_xd_x(1 - \varepsilon_xt_x - \varepsilon_yt_y) - \mu_yd_y(1 - \varepsilon_xt_x - \varepsilon_yt_y)\end{aligned} \tag{387}$$

Since $A_o^{d_x d_y}$ does not affect the phase error order, we can assign a value for it that would ensure positivity. We add to the terms of Eq. (387) "$\nu_x \nu_y d_x d_y$," yielding

$$A = (1 - \varepsilon_x t_x + \nu_x d_x)(1 - \varepsilon_y t_y + \nu_y d_y) - \mu_x d_x (1 - \varepsilon_x t_x - \varepsilon_y t_y)$$

$$- \mu_y d_y (1 - \varepsilon_x t_x - \varepsilon_y t_y) \qquad (388)$$

Now, substituting Eqs. (379) to (383) into Eqs. (242) and (243), we get

$$A_o^{\substack{x\\y}} = - i\varepsilon_{\substack{x\\y}} \qquad (389)$$

$$A_o^{\substack{xx\\yy}} = - 2(\nu_{\substack{x\\y}} - \mu_{\substack{x\\y}}) \qquad (390a)$$

$$A_o^{xy} = - \varepsilon_x \varepsilon_y \qquad (390b)$$

which when substituted into Eqs. (261), yield

$$(|A|^2)_o^{\substack{xx\\yy}} = 2[-2(\nu_{\substack{x\\y}} - \mu_{\substack{x\\y}}) + \varepsilon_{\substack{x\\y}}^2] = 0 \qquad (391a)$$

$$(|A|^2)_o^{xy} = 2[- \varepsilon_x \varepsilon_y + \varepsilon_x] = 0 \qquad (391b)$$

showing $A_x A_y$ to be fourth order in diffusion error.

Notice that $A_o^{t_x t_y} = \varepsilon_x \varepsilon_y$, is essential for fourth order diffusion (already satisfied by the scheme of Eq. (388)).

The simplest fourth order (phase and diffusion error) positive scheme is therefore that of Eq. (388). It is, however, unstable. For instance,

$$A_R = 1 + (\nu_x - \mu_x)d_x + (\nu_y - \mu_y)d_y + \nu_x\nu_y d_x d_y + \varepsilon_x\varepsilon_y t_x t_y \tag{392a}$$

while

$$A_I = -\varepsilon_x t_x[1 - \mu_x d_x + (\nu_y - \mu_y)d_y] - \varepsilon_y t_y[1 - \mu_y d_y + (\nu_x - \mu_x)d_x] \tag{392b}$$

At $\varepsilon_x = \varepsilon_y = \frac{1}{2}$ and $\beta_x = \beta_y = \pi/2$, $d_x = d_y = -2$, and $t_x = t_y = i$, yielding

$$A_R = 1 - \frac{1}{4} - \frac{1}{4} + \frac{1}{4} - \frac{1}{4} = \frac{1}{2} \tag{393a}$$

$$A_I = -\frac{1}{2}[1 + \frac{1}{4} - \frac{1}{4}] - \frac{1}{2}[1 + \frac{1}{4} - \frac{1}{4}] = -1 \tag{393b}$$

Since we know that A of Eq. (372) is stable, let's try to approach it in steps. First, we try

$$A = (1 - \varepsilon_x t_x + \nu_x d_x)(1 - \varepsilon_y t_y + \nu_y d_y) - \mu_x d_x(1 - \varepsilon_x t_x)(1 - \varepsilon_y t_y)$$

$$- \mu_y d_y(1 - \varepsilon_y t_y)(1 - \varepsilon_x t_x) \tag{394}$$

thus adding "$-(\mu_x d_x + \mu_y d_y)(\varepsilon_x\varepsilon_y t_x t_y)$" to the real part, becoming then

$$A_R = 1/2 - 1/8 = 3/8 \tag{395}$$

still unstable. Next, we try

$$A = (1 - \varepsilon_x t_x + \nu_x d_x)(1 - \varepsilon_y t_y + \nu_y d_y) - \mu_x d_x(1 - \varepsilon_x t_x)(1 - \varepsilon_y t_y + \nu_y d_y)$$

$$- \mu_y d_y(1 - \varepsilon_y t_y)(1 - \varepsilon_x t_x + \nu_x d_x) \tag{396}$$

This will add "$-(\mu_x\nu_y + \mu_y\nu_x)d_x d_y$" to the real part and "$(\varepsilon_x t_x\mu_x\nu_y + \varepsilon_y t_y\mu_y\nu_x)d_x d_y$" to the imaginary one. We get then

$$A_R = \frac{3}{8} - \frac{1}{4} = \frac{1}{8} \tag{397a}$$

$$A_I = -1 + \frac{1}{8} = -\frac{7}{8} \tag{397b}$$

whence $|A|^2 = (\frac{7}{8})^2 + (\frac{1}{8})^2 = \frac{50}{64} < 1$, showing Eq. (396) to be too stable at $\beta_x = \beta_y = \frac{\pi}{2}$. Moreover, it is not phoenical; $A \neq 1$ at $\varepsilon_x = \varepsilon_y = 0$. These two effects can be avoided by picking

$$A = (1 - \varepsilon_x t_x + \nu_x d_x)(1 - \varepsilon_y t_y + \nu_y d_y) - \mu_x d_x(1 - \varepsilon_x t_x)(1 - \varepsilon_y t_y + \frac{1}{2}\nu_y d_y)$$

$$- \mu_y d_y(1 - \varepsilon_y t_y)(1 - \varepsilon_x t_x + \frac{1}{2}\nu_x d_x) \tag{398}$$

yielding

$$A_R = \frac{3}{8} - \frac{1}{2} \times \frac{1}{4} = \frac{1}{4} \tag{399a}$$

$$A_I = -1 + \frac{1}{2} \times \frac{1}{8} = -\frac{15}{16} \tag{399b}$$

whence $|A|^2 = (\frac{15}{16})^2 + (\frac{1}{4})^2 = \frac{241}{256} < 1$, closer to 1, therefore promising a smaller net diffusion and phoenical since $A = 1$ at $\varepsilon_x = \varepsilon_y = 0$.

Noticing that the added terms to Eq. (388) are triple operators ($t_x t_y d_x$, $t_x t_y d_y$, $t_x d_x d_y$, $t_y d_x d_y$) they have no effect on $(\log A)_o'''$. Eq. (398) is still fourth order in phase error. Furthermore, upon expanding $|A|^2$, we get

$$|A|^2 = 1 + \frac{1}{12}\{\varepsilon_x^2(1 - \varepsilon_x^2)\beta_x^4 + [\varepsilon_x^2(1 - \varepsilon_y^2)$$

$$+ \varepsilon_y^2(1 - \varepsilon_x^2)]\beta_x^2\beta_y^2 + \varepsilon_y^2(1 - \varepsilon_y^2)\beta_y^4\} + \dots \tag{400}$$

showing diffusion error to be of fourth order. The scheme is, however, slightly unstable near $\beta_x = \beta_y = 0$, since the fourth order coefficient is positive. We notice also the presence of a term "$\beta_x^2\beta_y^2$" in Eq. (400) (also in the phase error expansion), which does not show in the expansion of Eq. (372) (according to Eq. (366), making the scheme of Eq. (398) slightly inferior to that of Eq. (372).

Upon comparing Eq. (398) to (372), it is obvious that Eq. (372) cannot be much simplified; at least without sacrificing stability or phoenicity. Whichever we use, the n° of operations involved in evaluating ρ^{n+1} is much larger than that in the fully two-dimensional scheme of Eq. (226e). Moreover, the n° of two-dimensional arrays required to store the intermediate values is enormcus.

Since the only advantage of Eqs. (372), the fully two-dimensional version of the time-splitted scheme of Eq. (371b) is the reduced clipping associated with the flux limiter, we conclude that time splitting is the sensible answer. We abandon, therefore, trials to cast the time-splitted scheme in fully two-dimensional versions.

XVIII. IMPROVING DIFFUSION ERROR OF THE FULLY TWO-DIMENSIONAL SCHEME

Now that we have classified the terms responsible for the fourth order phase, diffusion, etc., in the time-splitted scheme, let's go back to the fully two-dimensional scheme and study the terms preventing us from reaching a fourth order diffusion error. As explained earlier, the term "$\varepsilon_x \varepsilon_y t_x t_y$" is essential to reduce the dependence of the phase error to one on ν alone, thus leaving μ free to be adjusted for a high order diffusion. A closer look reveals, however, that the above conclusion is an indirect one. The direct conclusion is that "$\varepsilon_x \varepsilon_y t_x t_y$" is needed to cancel "$\varepsilon_x \beta_x \varepsilon_y \beta_y$" resulting from squaring the imaginary part. Specifically, any scheme has to incorporate the combination $(\varepsilon_x t_x + \varepsilon_y t_y)$ leading to $i(\varepsilon_x \sin \beta_x + \varepsilon_y \sin \beta_y)$ which is approximated by $i(\varepsilon_x \beta_x + \varepsilon_y \beta_y)$. To cancel it, a term including $\sin \beta_x \sin \beta_y$ is needed. Besides $t_x t_y$, the above term can also result from $\cos(\beta_x \pm \beta_y)$, i.e. diagonal diffusion $(\rho^n_{i+1,j\pm 1} - 2\rho^n_{i,j} + \rho^n_{i-1,j\mp 1})$. Admitting diagonal terms is outside the scope of this article and is left out to an upcoming one. However, we emphasize that there is a stability problem caused by the imaginary part $iA_I = -[\varepsilon_x t_x(1 - \mu_x d_x) + \varepsilon_y t_y(1 - \mu_y d_y)]$ which amplitude is already larger than unity for $\varepsilon_x = \varepsilon_y = \frac{1}{2}$, $\beta_x = \beta_y = \frac{\pi}{2}$ unless $\mu_x = \mu_y = 0$ there, in which case we have a large residual diffusion. Adding just a diagonal diffusion can't help, since it only adds to the real part.

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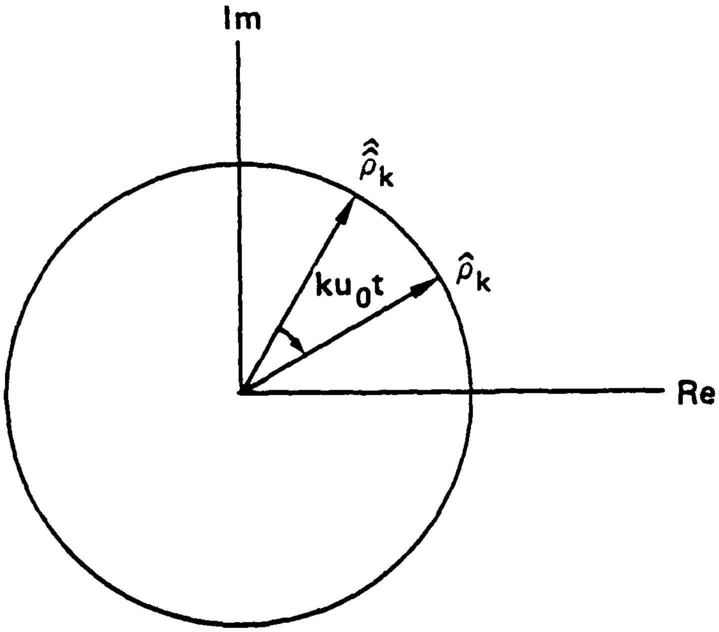
FIGURES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$\hat{\hat{\rho}}_k$
$\hat{\rho}_k$
ku_0t
Re

Fig. 1

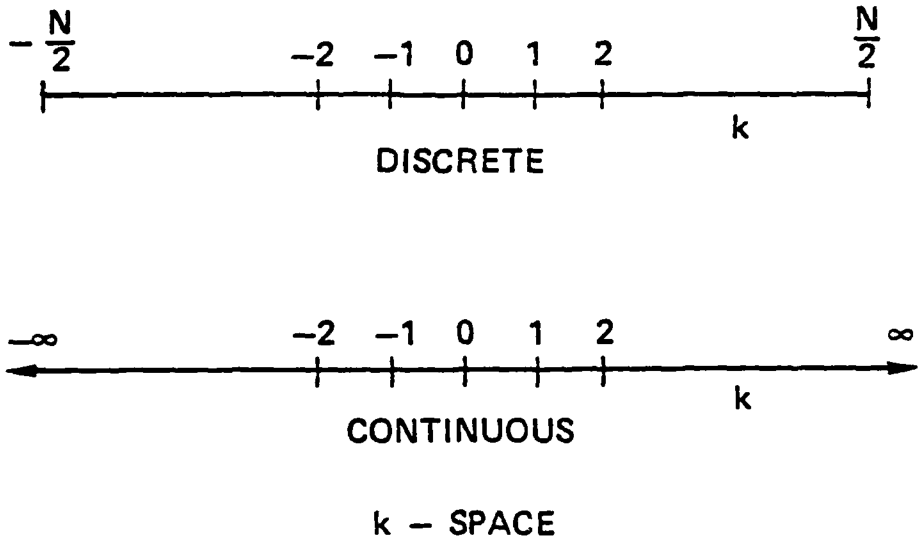

$-\frac{N}{2}$
−2 −1 0 1 2
$\frac{N}{2}$
k
DISCRETE
−∞
−2 −1 0 1 2
∞
k
CONTINUOUS
k − SPACE

Fig. 2

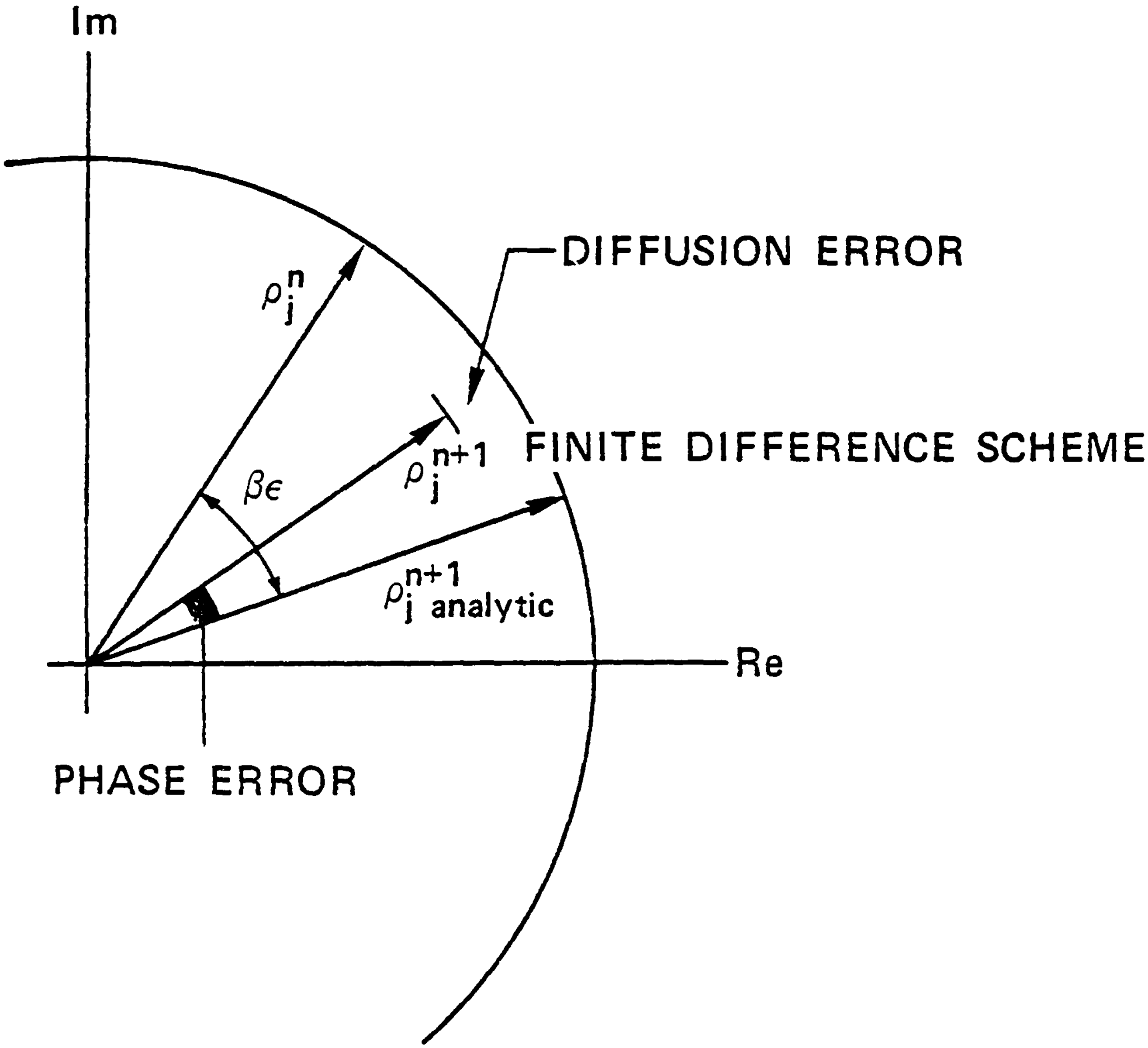

Im
DIFFUSION ERROR
ρ_j^n
FINITE DIFFERENCE SCHEME
ρ_j^{n+1}
$\beta\epsilon$
$\rho_{j\ \text{analytic}}^{n+1}$
Re
PHASE ERROR

Fig. 3

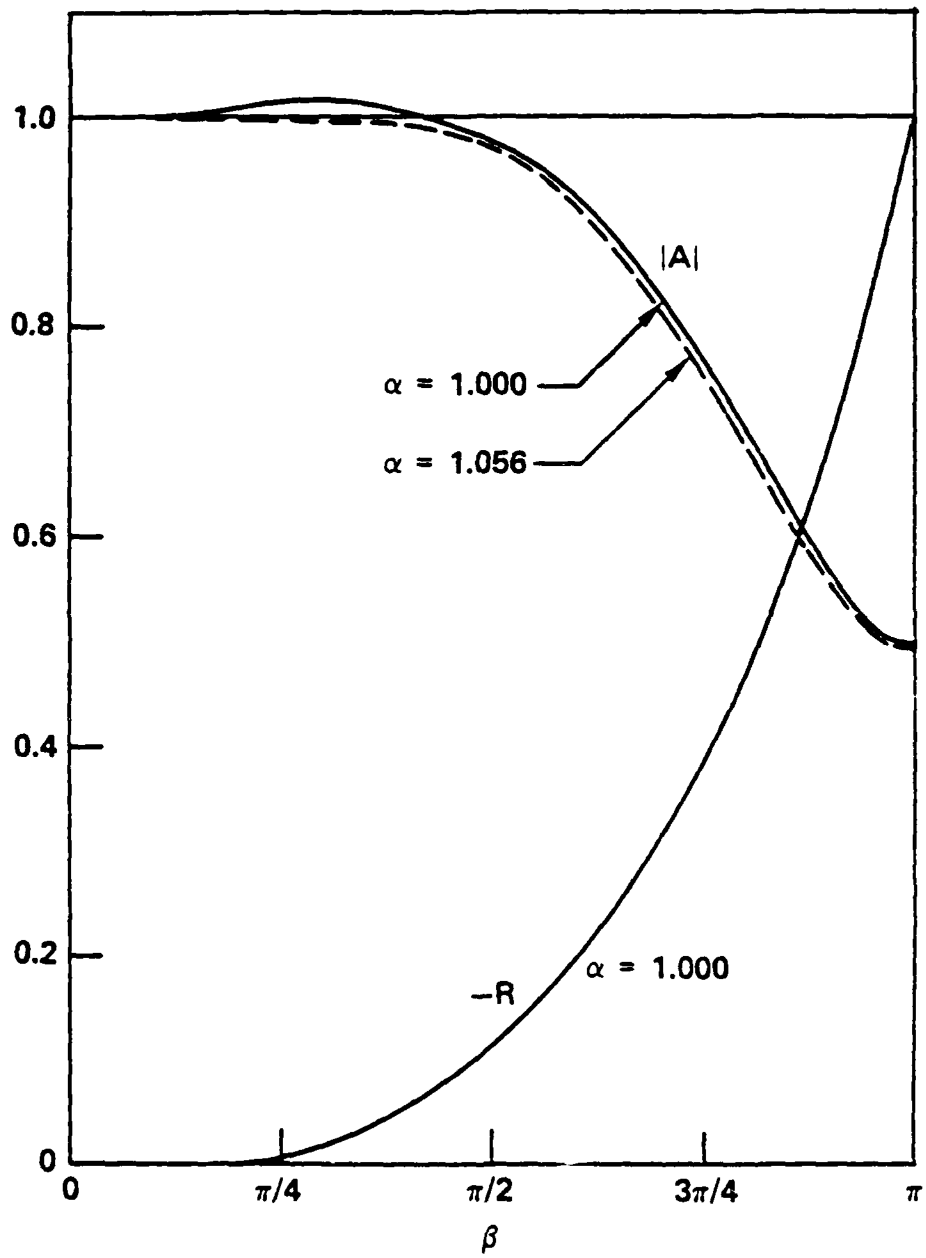


Fig. 4

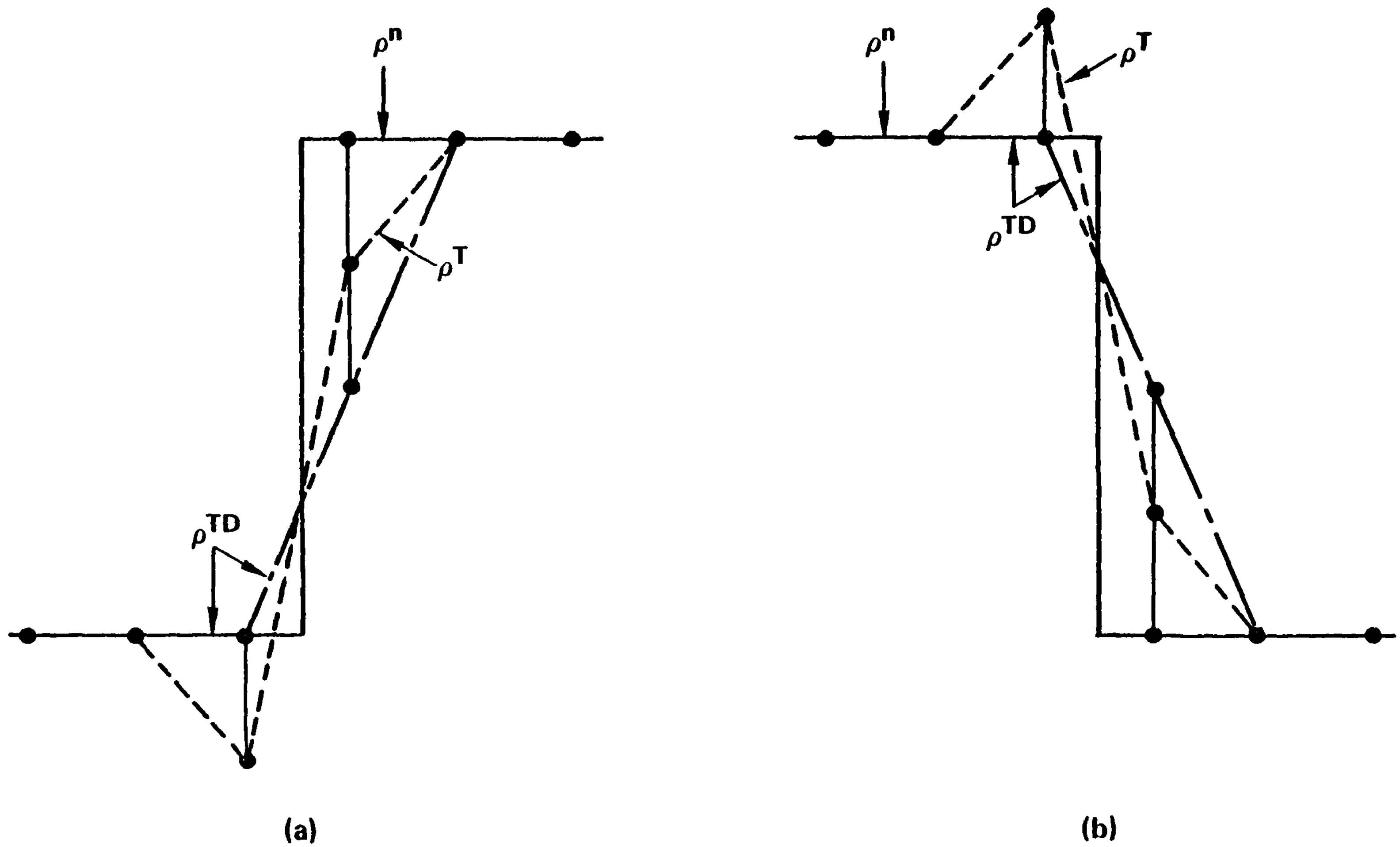
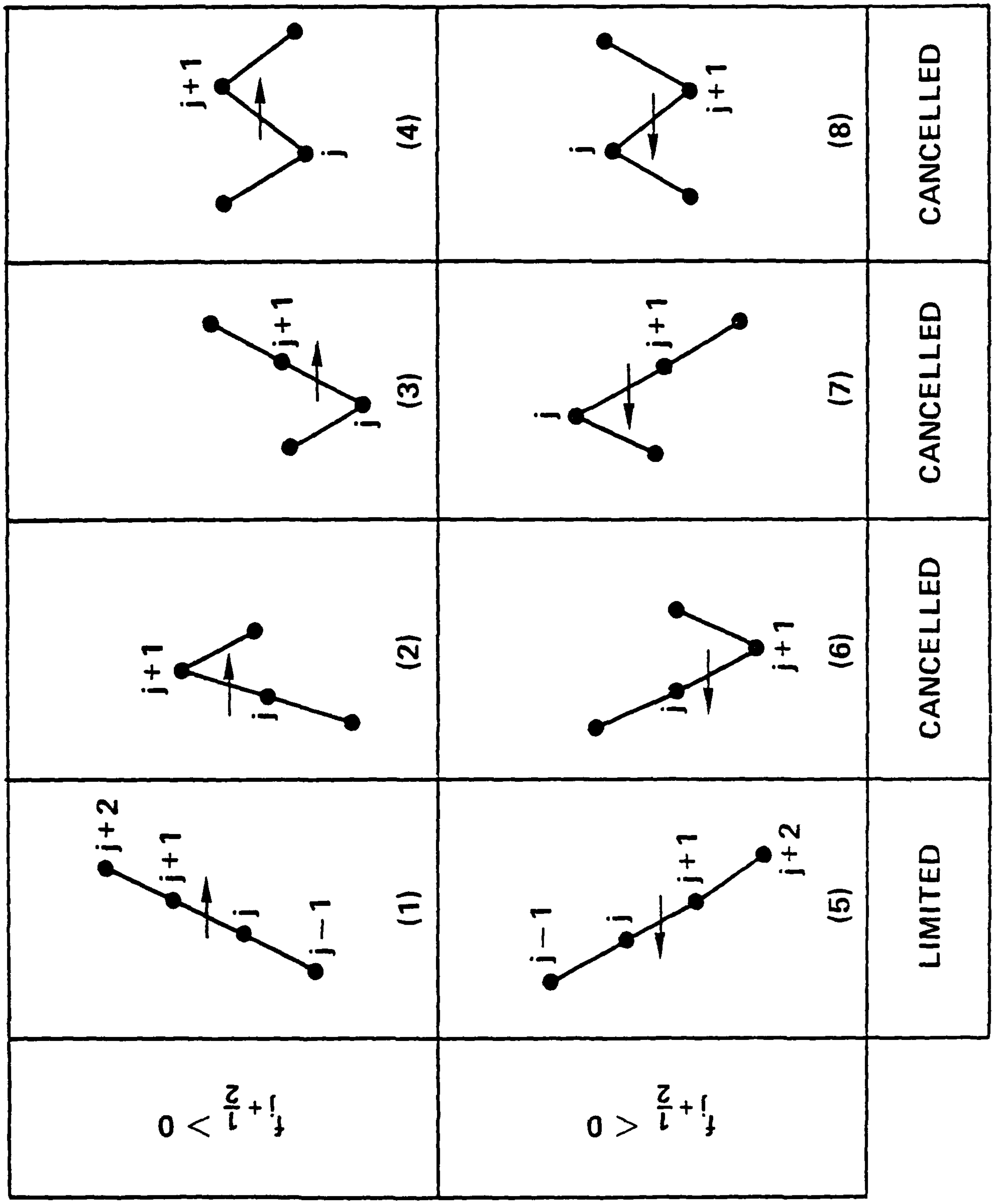
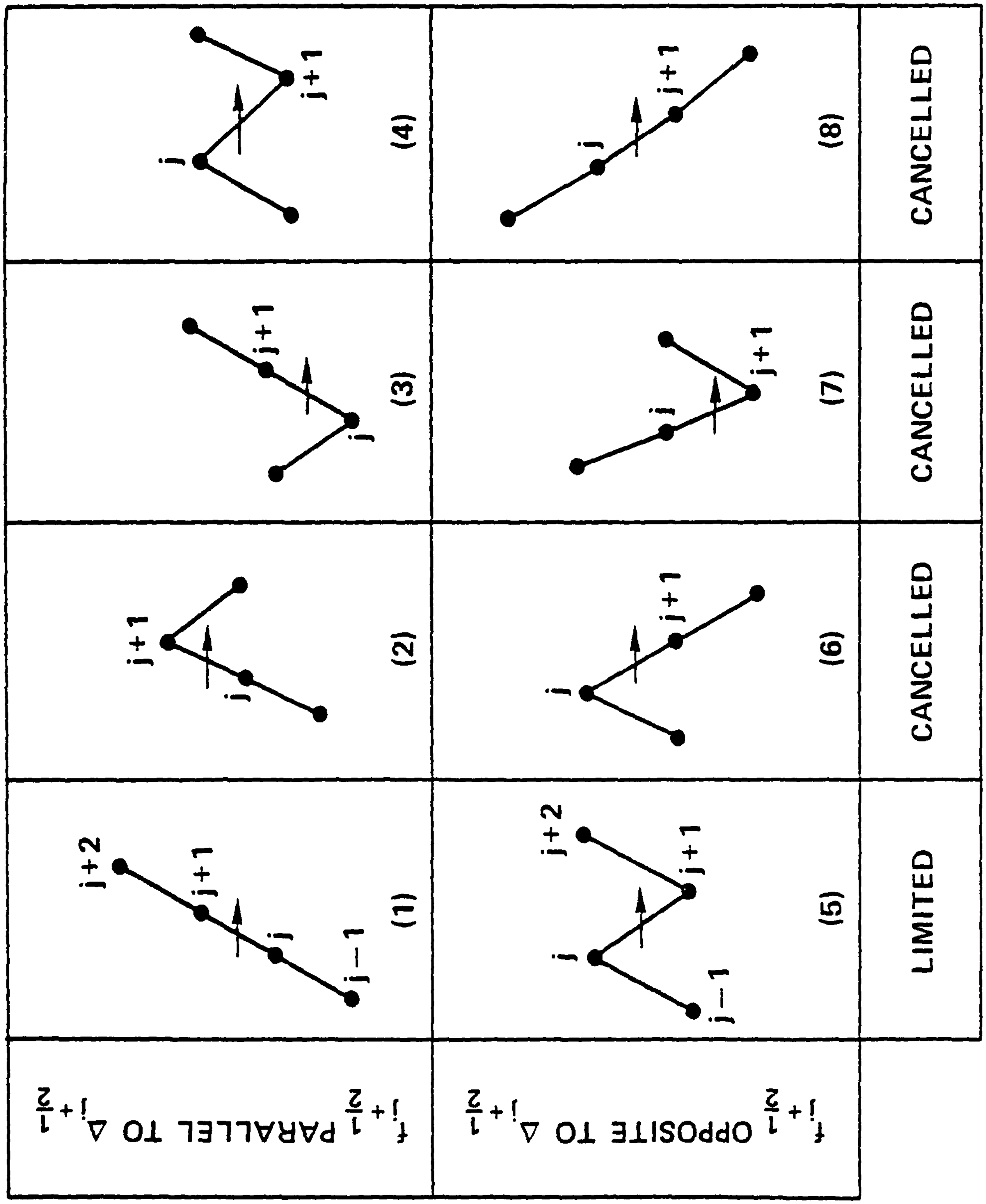


Fig. 5



$f_{j+\frac{1}{2}} > 0$
$f_{j+\frac{1}{2}} < 0$
j−1
j
j+1
j+2
(1)
(2)
(3)
(4)
(5)
(6)
(7)
(8)
LIMITED
CANCELLED
CANCELLED
CANCELLED

Fig. 6



$f_{j+\frac{1}{2}}$ PARALLEL TO $\Delta_{j+\frac{1}{2}}$
$f_{j+\frac{1}{2}}$ OPPOSITE TO $\Delta_{j+\frac{1}{2}}$
j−1
j
j+1
j+2
(1)
(2)
(3)
(4)
(5)
(6)
(7)
(8)
LIMITED
CANCELLED
CANCELLED
CANCELLED

Fig. 7

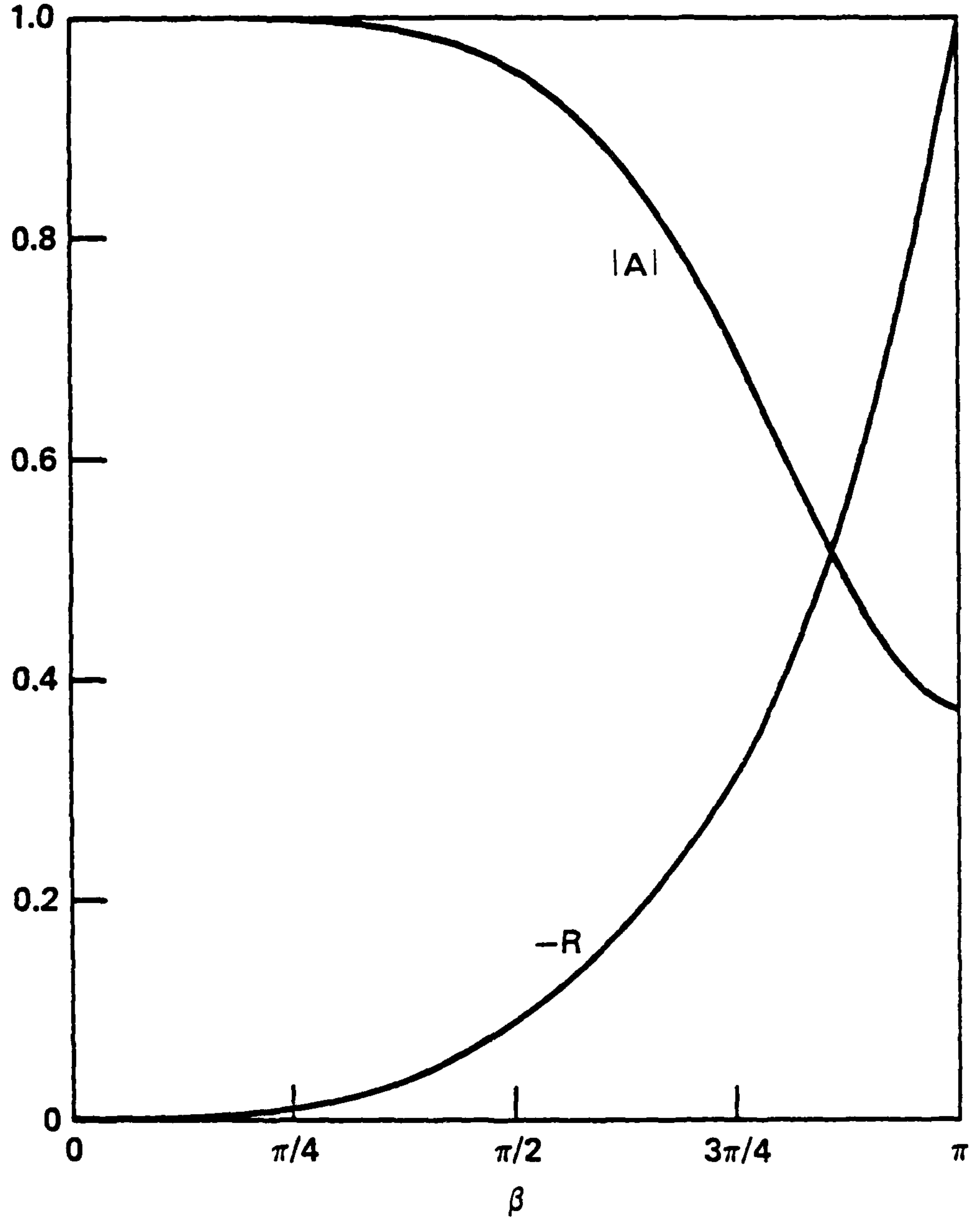


Fig. [illegible]

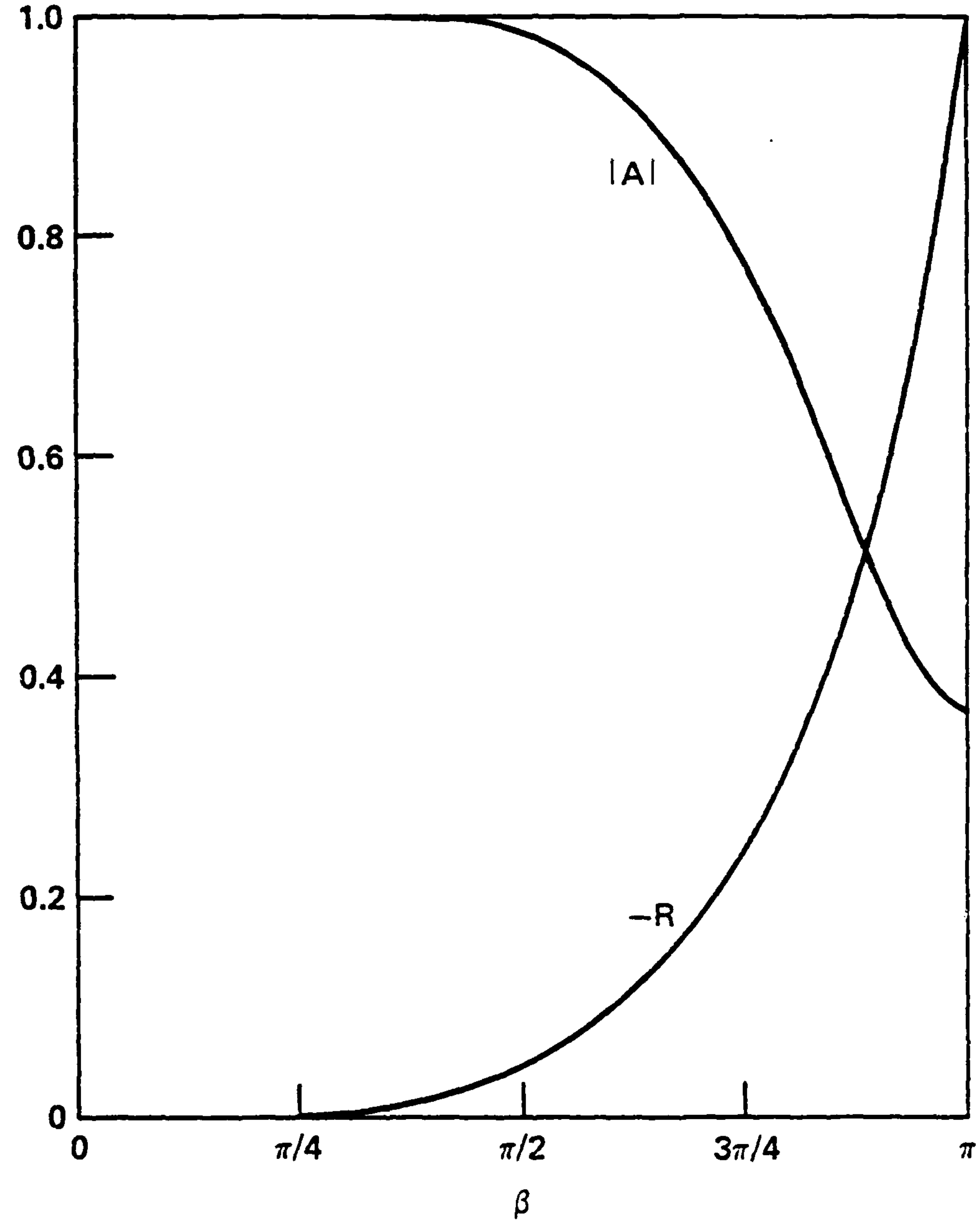


Fig. [illegible]

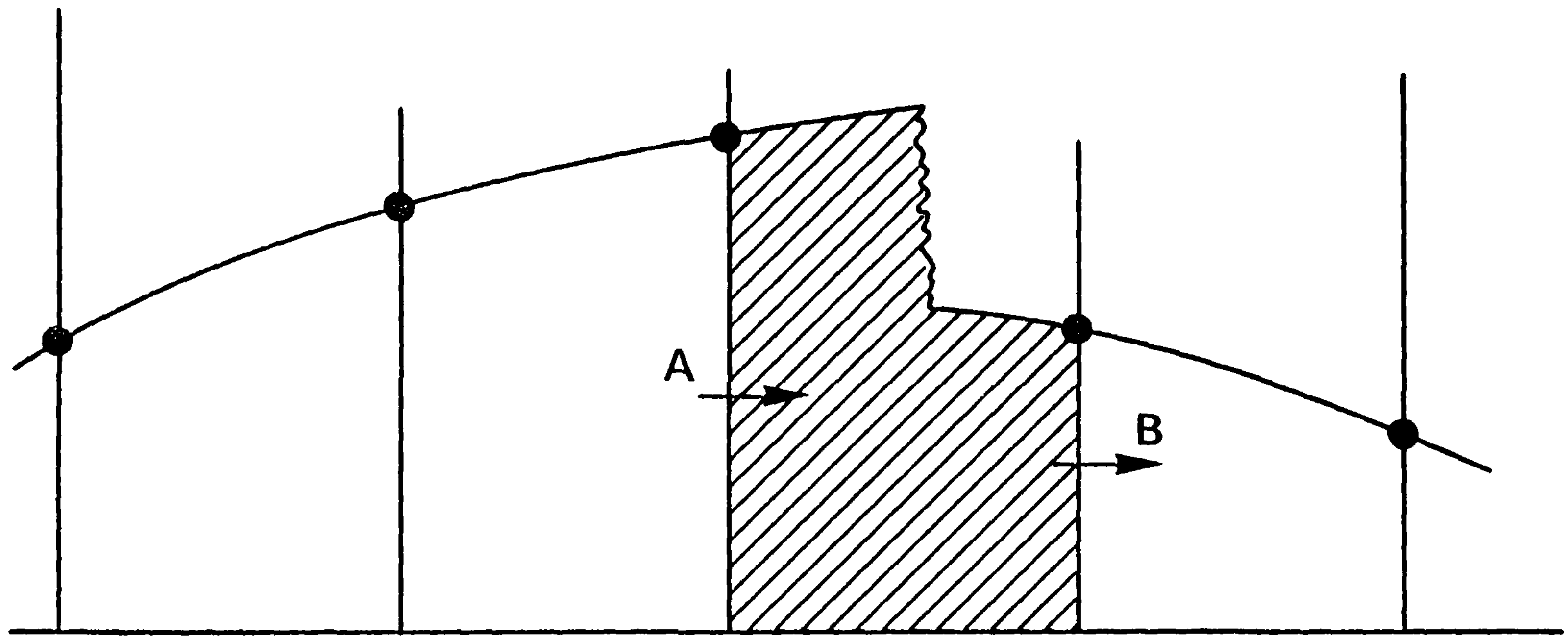


Fig. 10

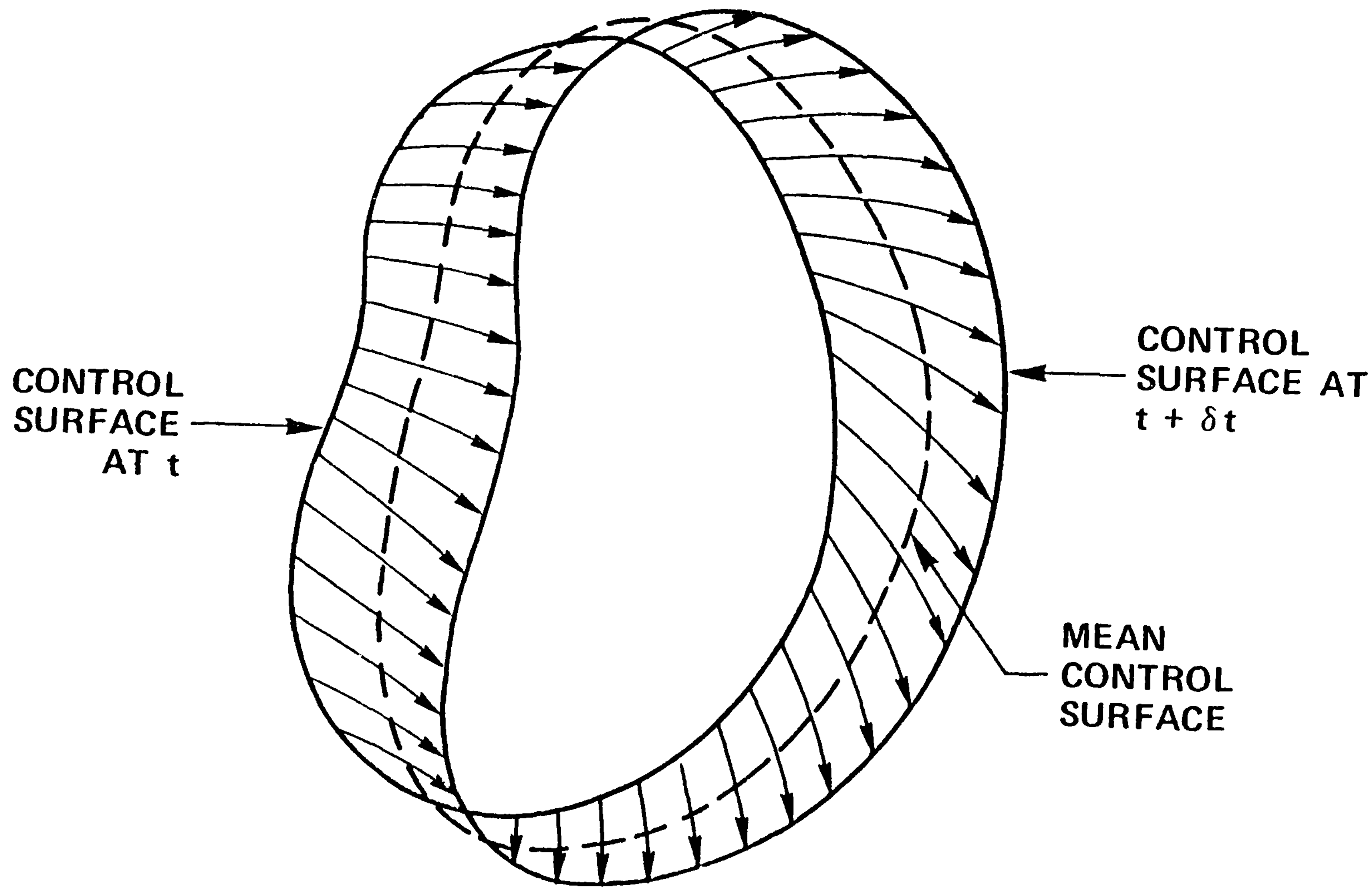
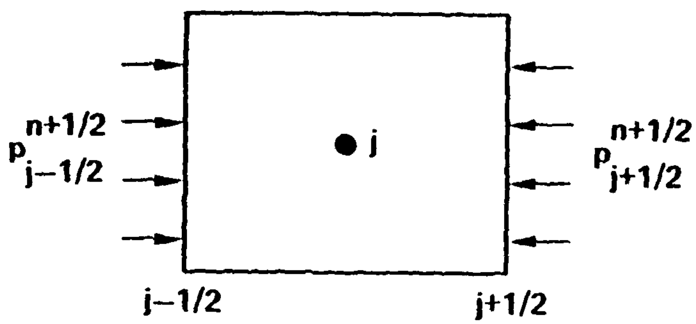
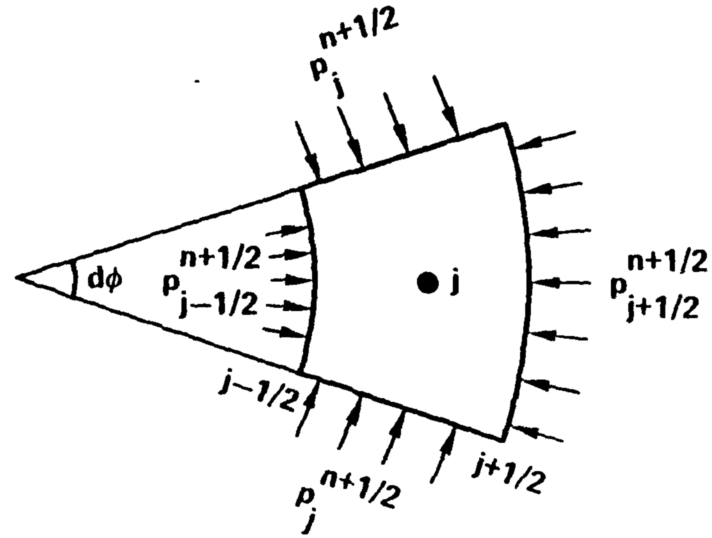

CONTROL
SURFACE
AT t
CONTROL
SURFACE AT
t + δt
MEAN
CONTROL
SURFACE

Fig. 11



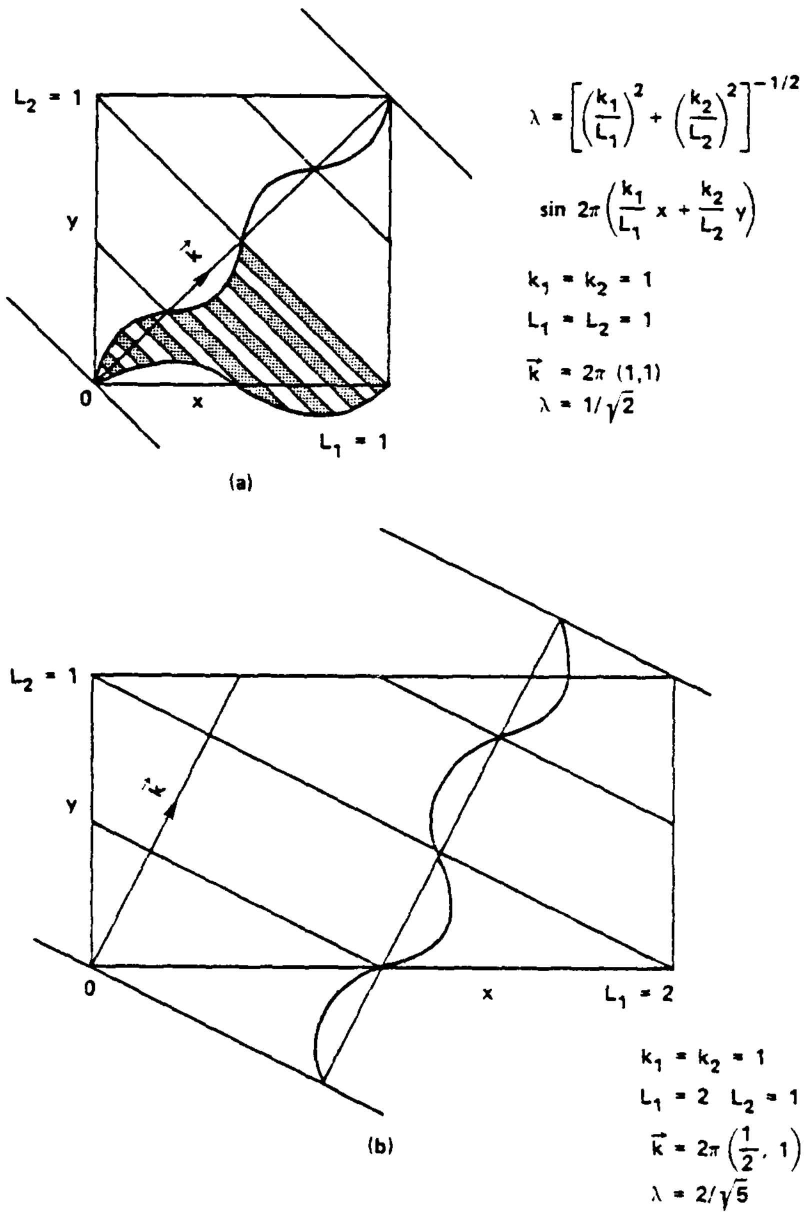
$p_{j-1/2}^{n+1/2}$
j
$p_{j+1/2}^{n+1/2}$
j–1/2
j+1/2

Fig 12



$p_{j}^{n+1/2}$
dφ
$p_{j-1/2}^{n+1/2}$
j
$p_{j+1/2}^{n+1/2}$
j–1/2
$p_{j}^{n+1/2}$
j+1/2

Fig. 13



$L_2 = 1$
y
$\vec{k}$
0
x
$L_1 = 1$
$\lambda = \left[\left(\frac{k_1}{L_1}\right)^2 + \left(\frac{k_2}{L_2}\right)^2\right]^{-1/2}$
$\sin 2\pi\left(\frac{k_1}{L_1}x + \frac{k_2}{L_2}y\right)$
$k_1 = k_2 = 1$
$L_1 = L_2 = 1$
$\vec{k} = 2\pi\ (1,1)$
$\lambda = 1/\sqrt{2}$
(a)
$L_2 = 1$
y
$\vec{k}$
0
x
$L_1 = 2$
$k_1 = k_2 = 1$
$L_1 = 2 \quad L_2 = 1$
$\vec{k} = 2\pi\left(\frac{1}{2}, 1\right)$
$\lambda = 2/\sqrt{5}$
(b)

Fig. 21

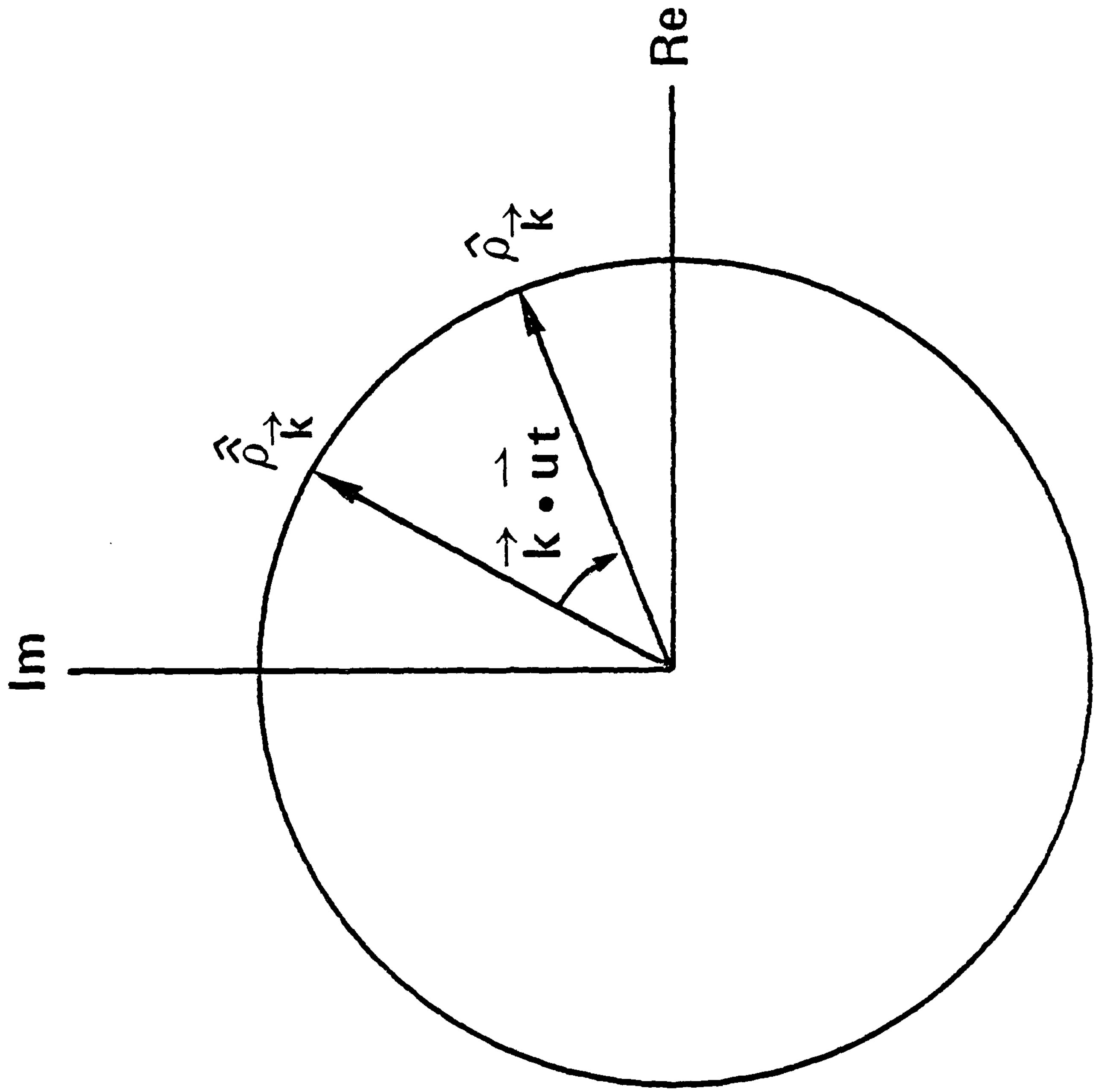


Fig. 22

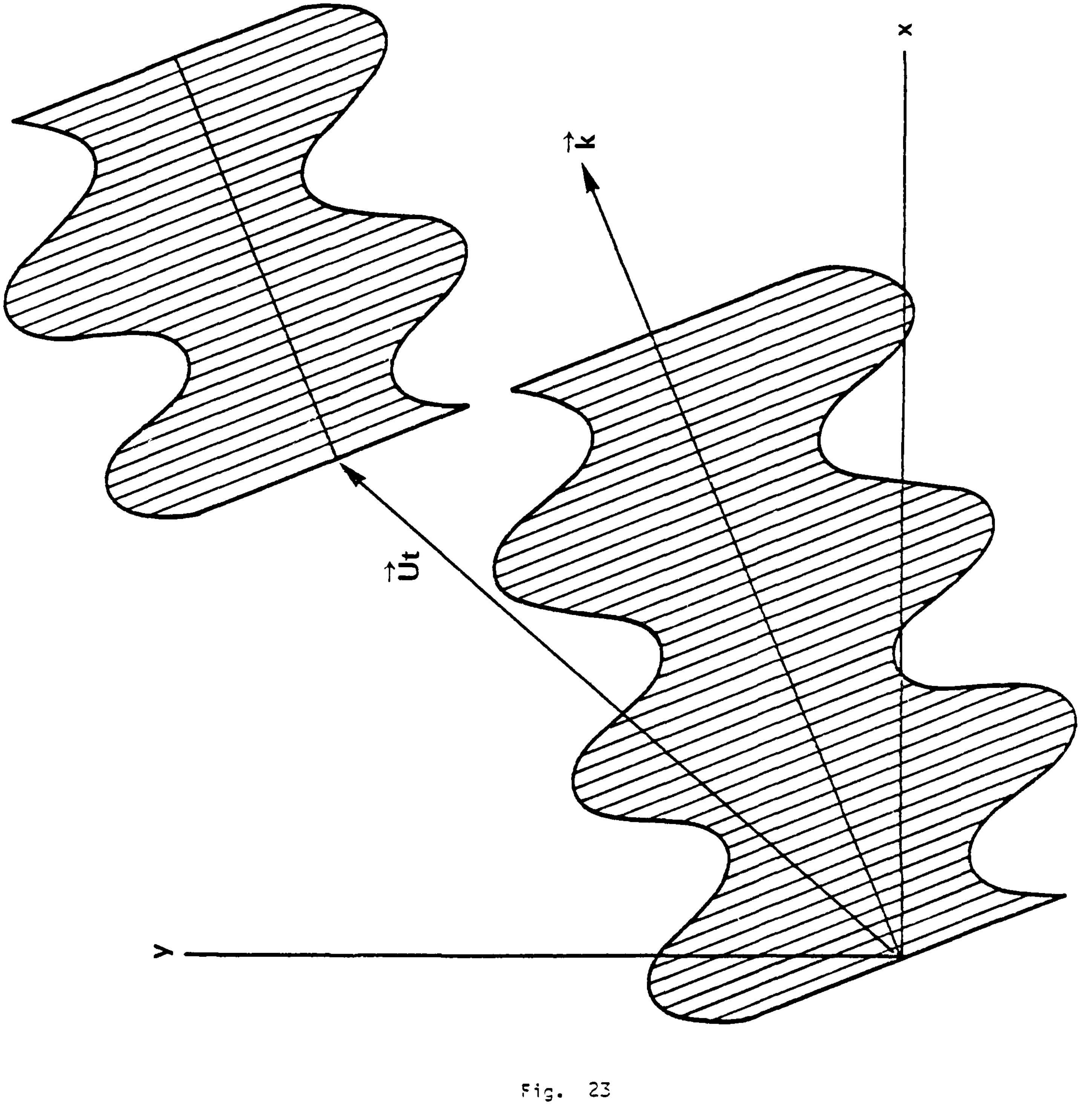


Fig. 23

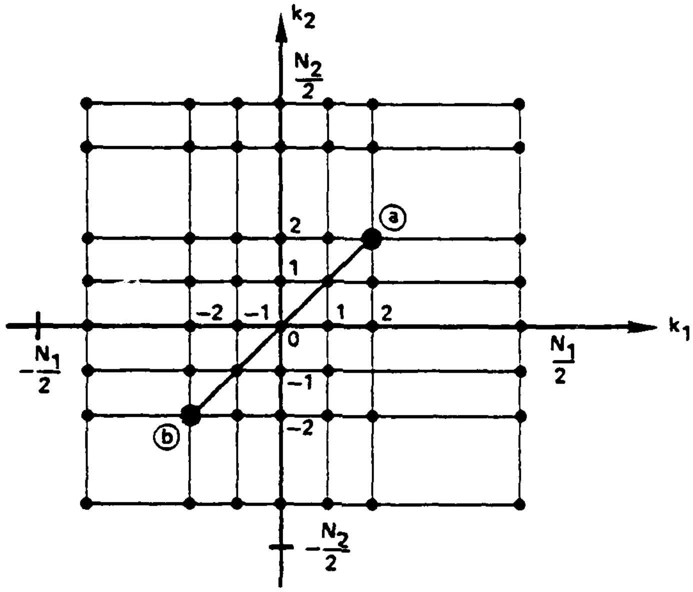


Fig. 24

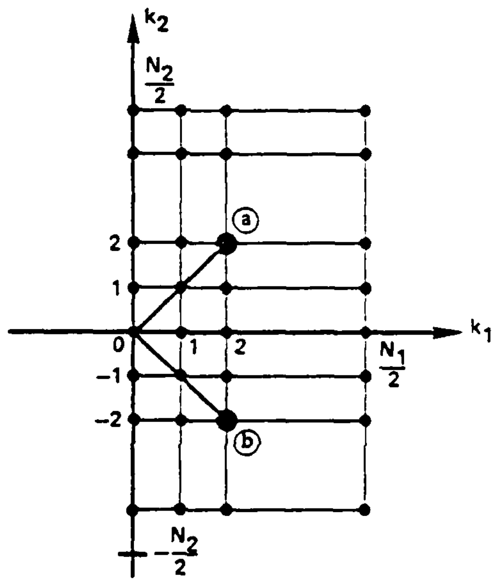


Fig. 25

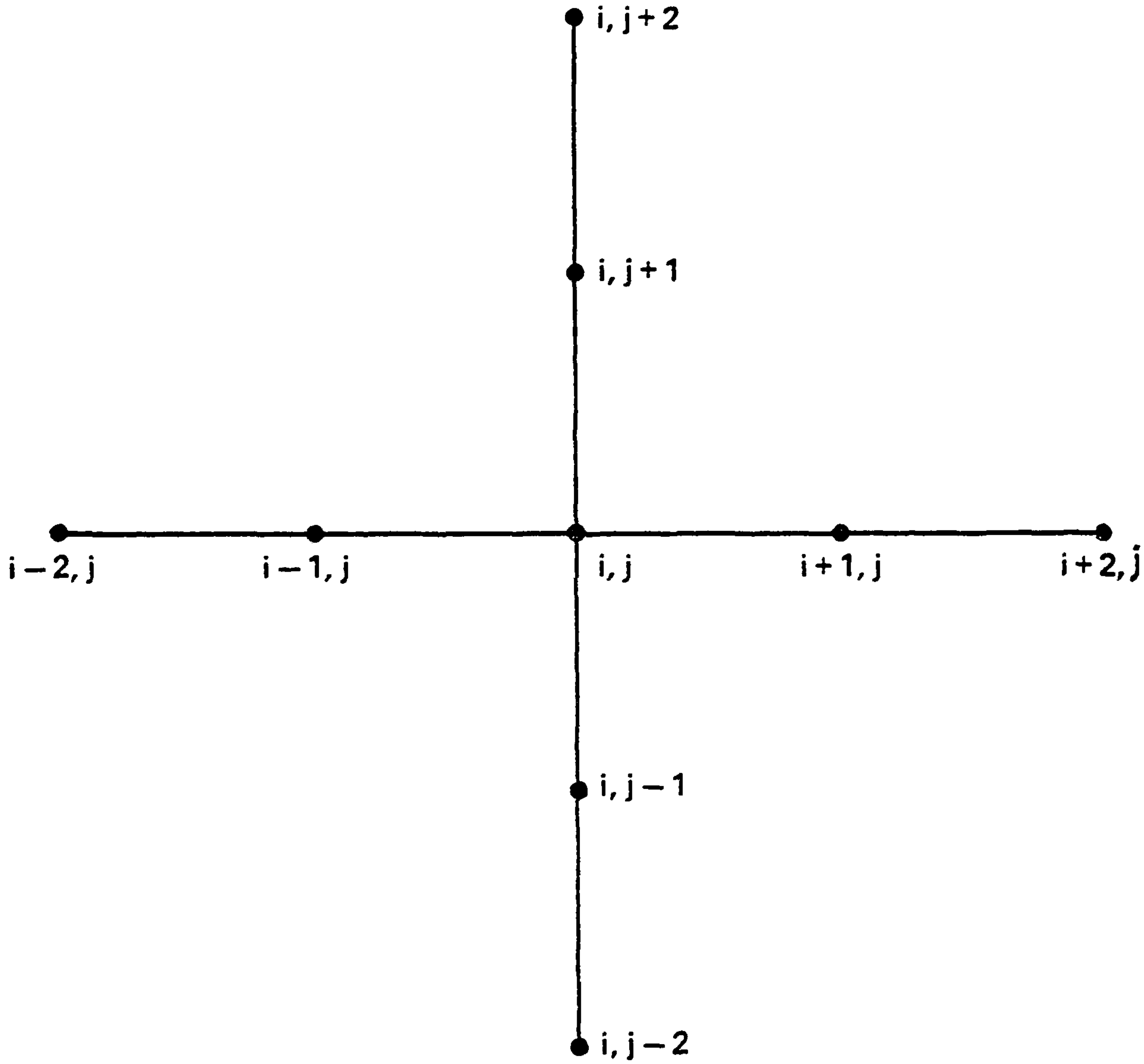


Fig. 26

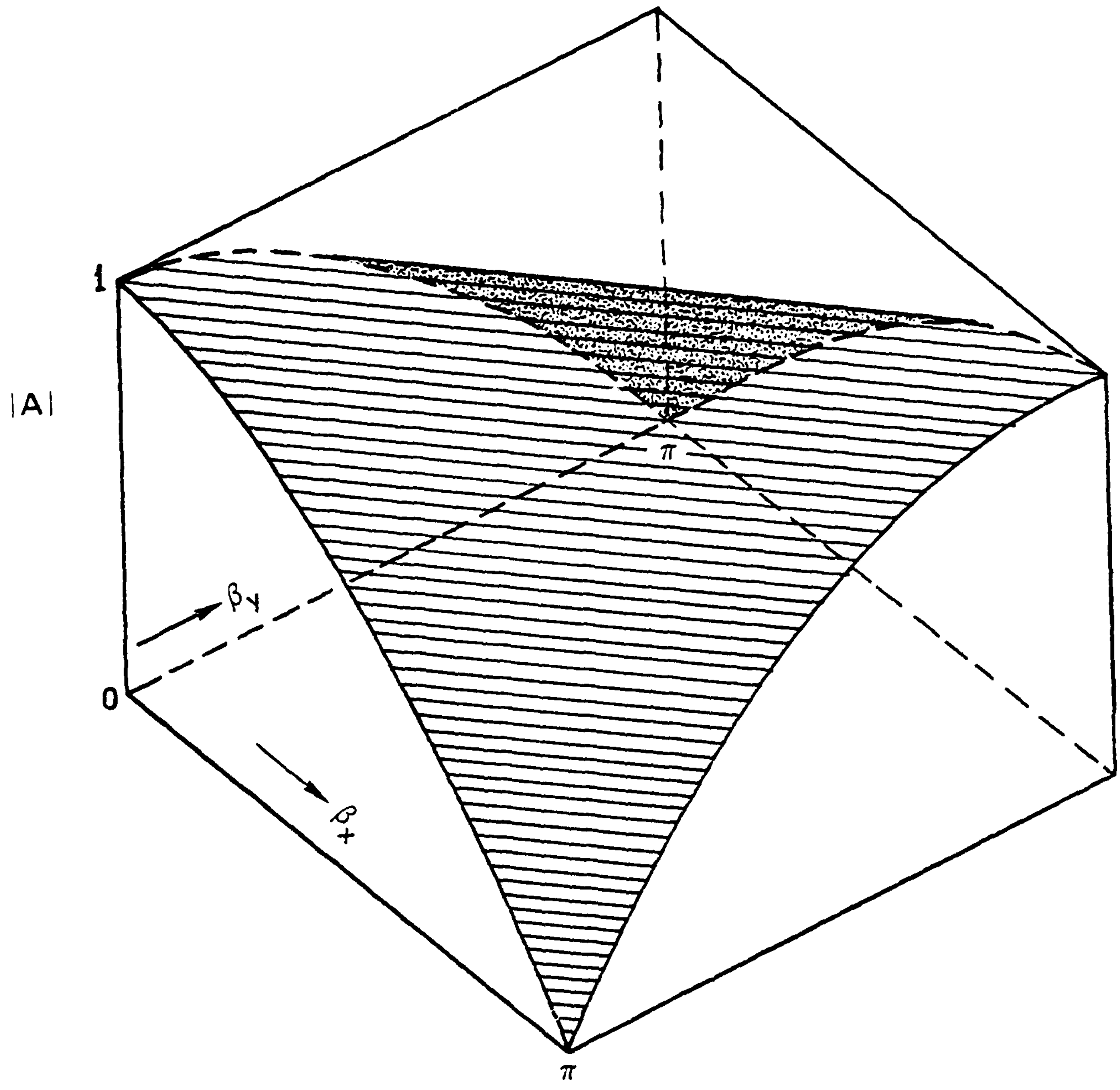


Fig. 27

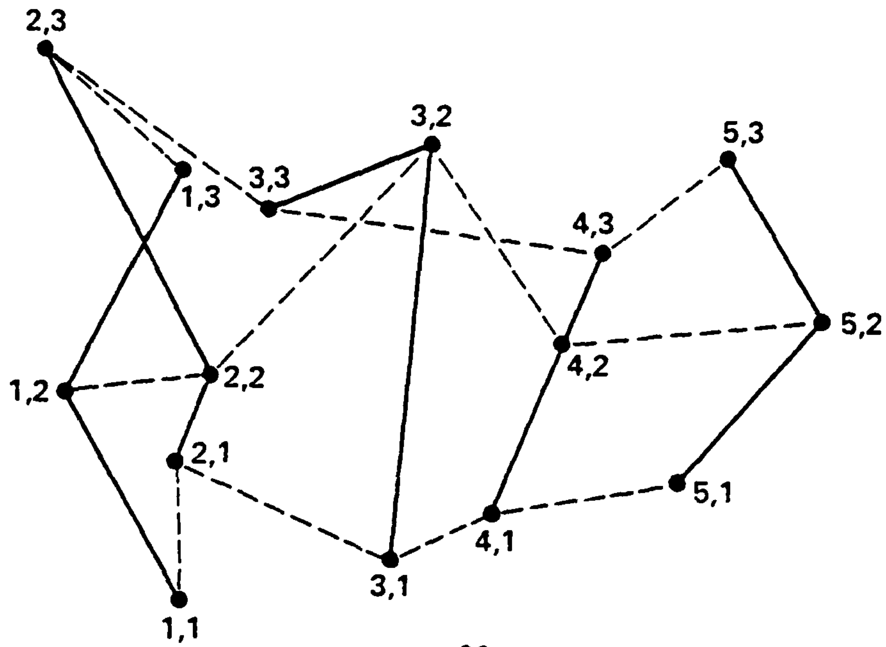

2,3
3,2
5,3
1,3
3,3
4,3
5,2
4,2
1,2
2,2
2,1
5,1
4,1
3,1
1,1

Fig. 28

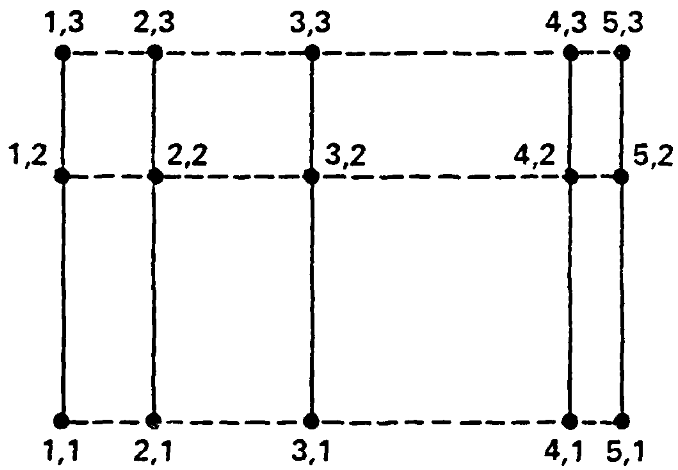

1,3
2,3
3,3
4,3
5,3
1,2
2,2
3,2
4,2
5,2
1,1
2,1
3,1
4,1
5,1

Fig. 29

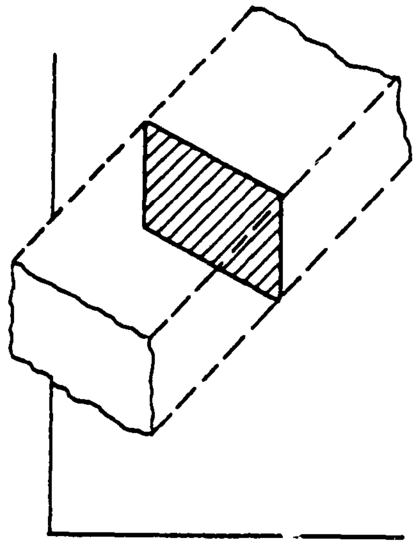


Fig. 30-1

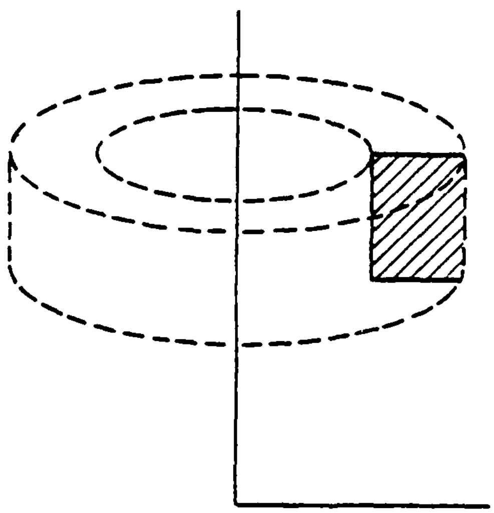


Fig. 30-2

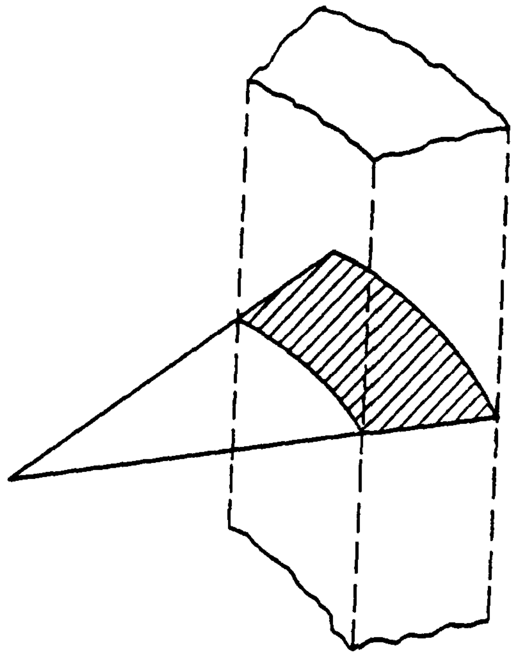


Fig. 30-3

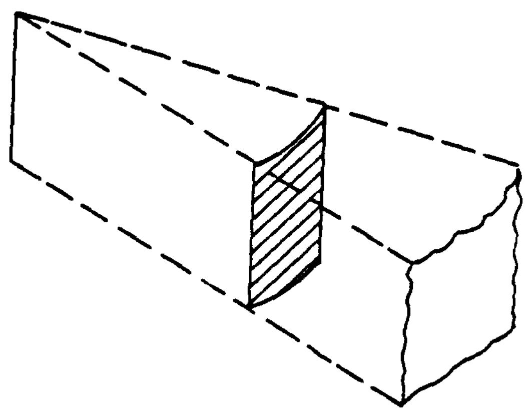


Fig. 30-4

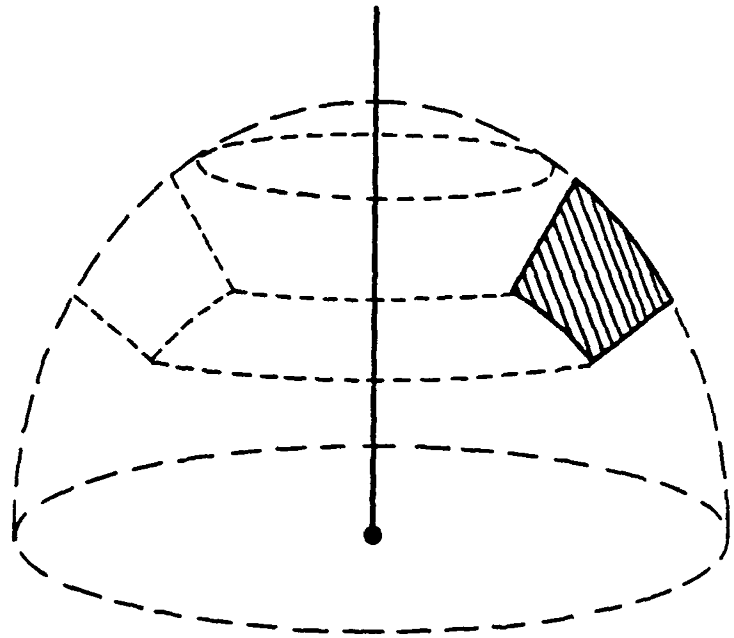


Fig. 30-5

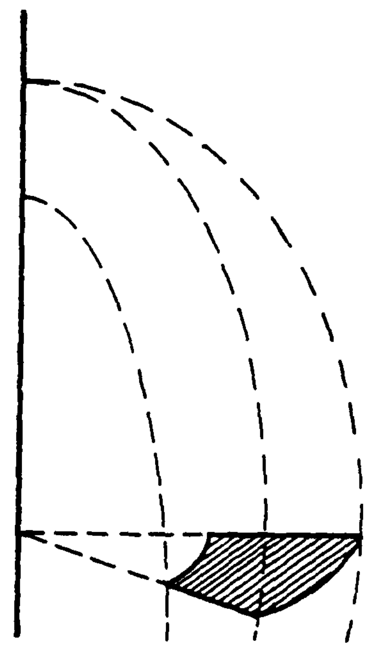


Fig. 30-6

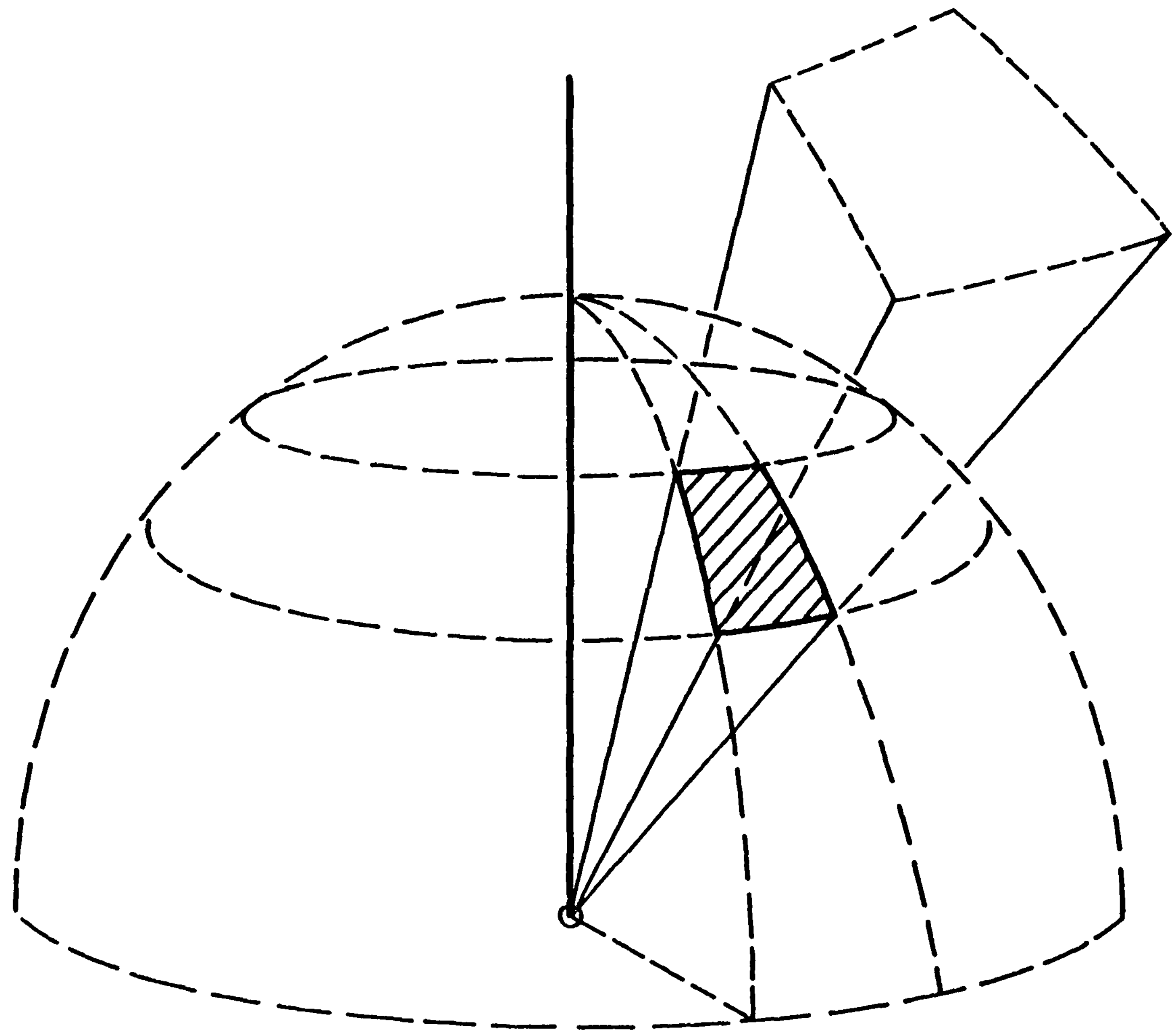


Fig. 30-7

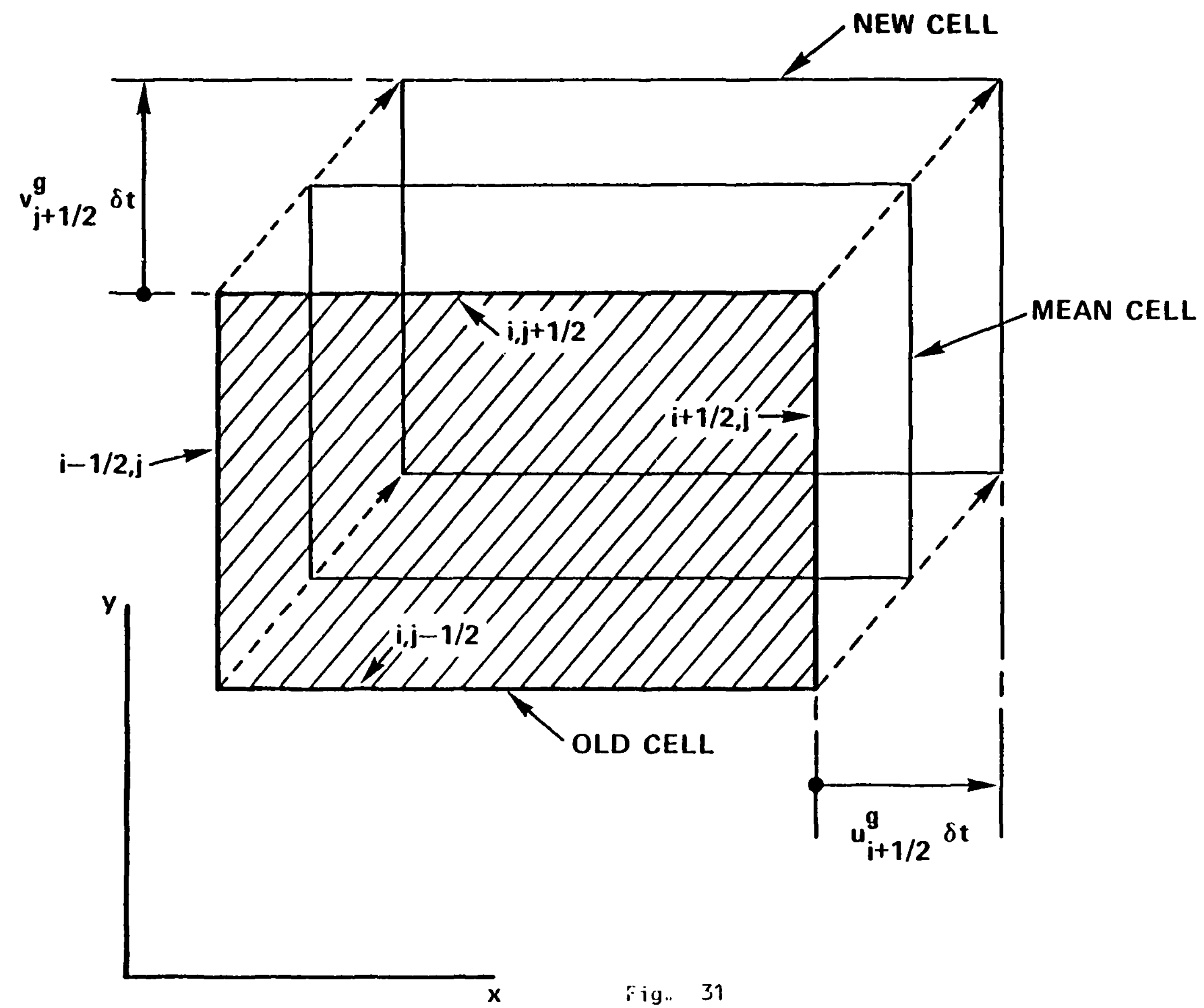
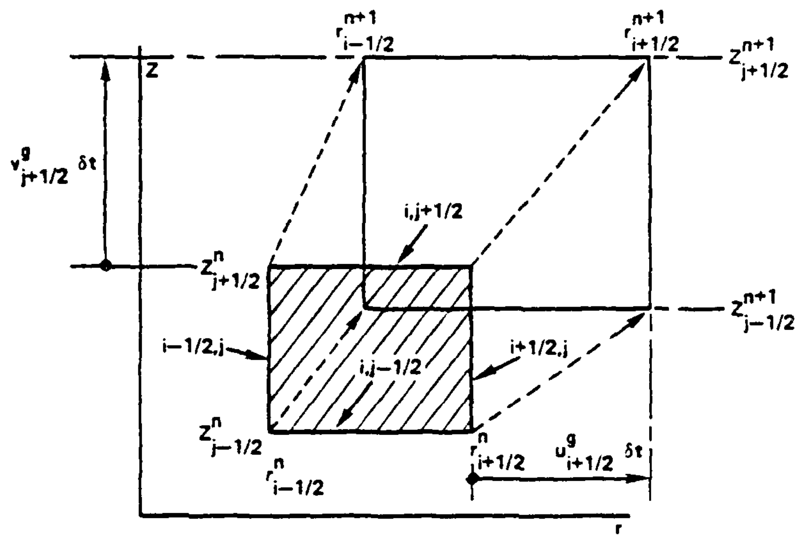
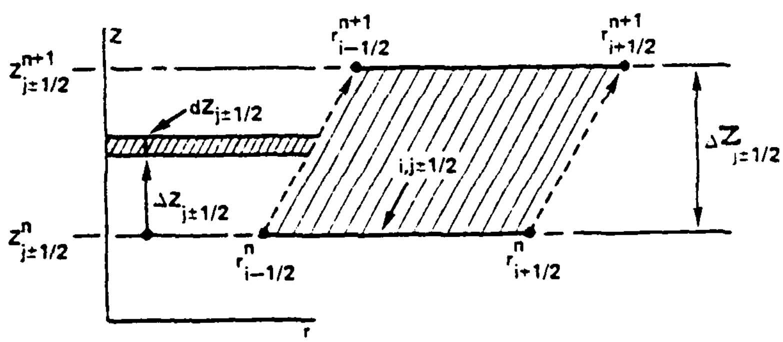

NEW CELL
MEAN CELL
OLD CELL
$v^g_{j+1/2}\ \delta t$
$u^g_{i+1/2}\ \delta t$
i,j+1/2
i+1/2,j
i−1/2,j
i,j−1/2
y
x

Fig. 31



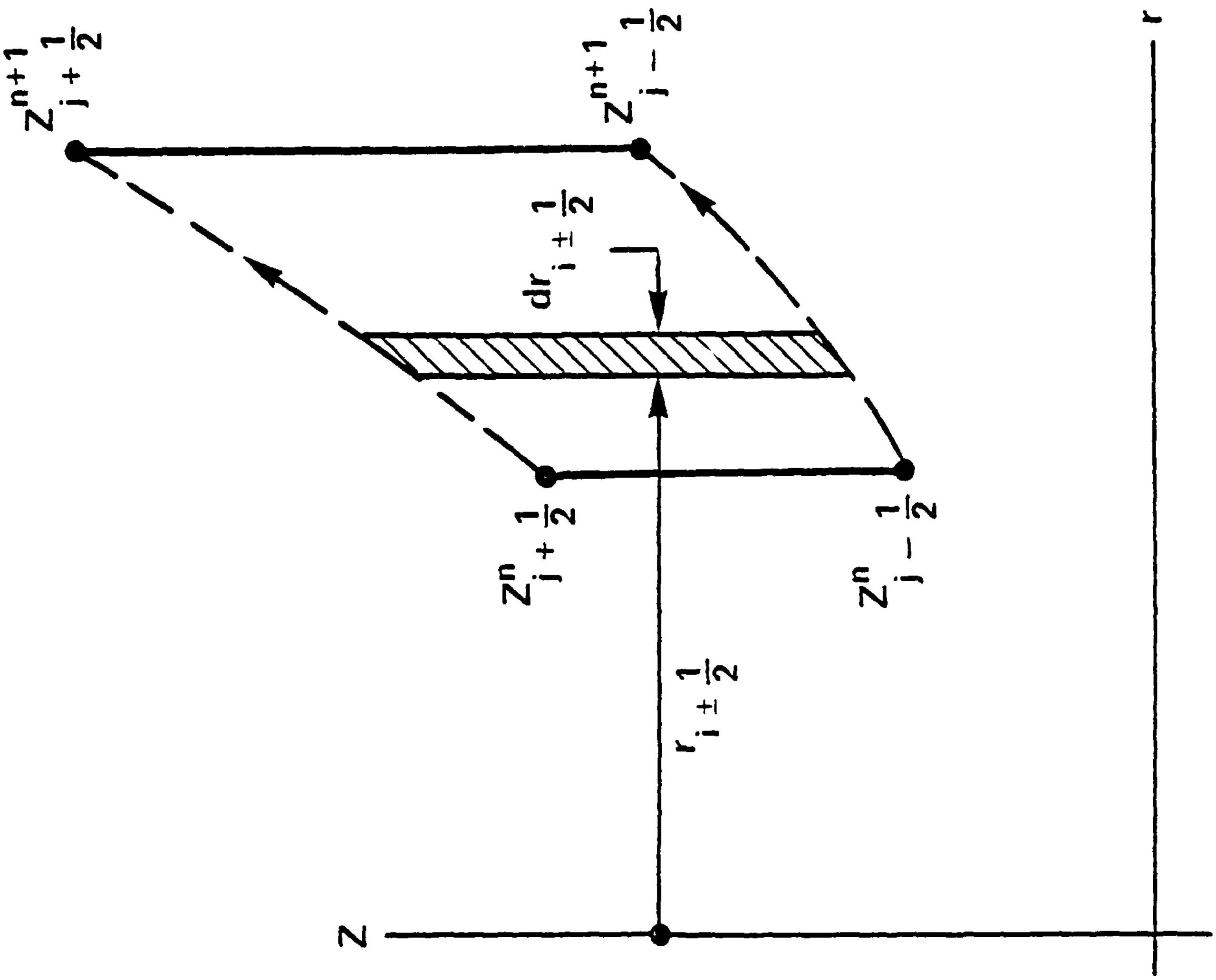
$r^{n+1}_{i-1/2}$
$r^{n+1}_{i+1/2}$
$Z^{n+1}_{j+1/2}$
Z
$v^{g}_{j+1/2}\ \delta t$
i,j+1/2
$Z^{n}_{j+1/2}$
$Z^{n+1}_{j-1/2}$
i−1/2,j
i,j−1/2
i+1/2,j
$Z^{n}_{j-1/2}$
$r^{n}_{i-1/2}$
$r^{n}_{i+1/2}$
$u^{g}_{i+1/2}\ \delta t$
r

Fig. 32



Z
$r^{n+1}_{i-1/2}$
$r^{n+1}_{i+1/2}$
$Z^{n+1}_{j\pm1/2}$
$dZ_{j\pm1/2}$
$\Delta Z_{j\pm1/2}$
i,j±1/2
$\Delta Z_{j\pm1/2}$
$Z^{n}_{j\pm1/2}$
$r^{n}_{i-1/2}$
$r^{n}_{i+1/2}$
r

Fig. 33



$Z^{n+1}_{j+\frac{1}{2}}$
$Z^{n+1}_{j-\frac{1}{2}}$
$dr_{i\pm\frac{1}{2}}$
$Z^{n}_{j+\frac{1}{2}}$
$Z^{n}_{j-\frac{1}{2}}$
$r_{i\pm\frac{1}{2}}$
Z
r

Fig. 34

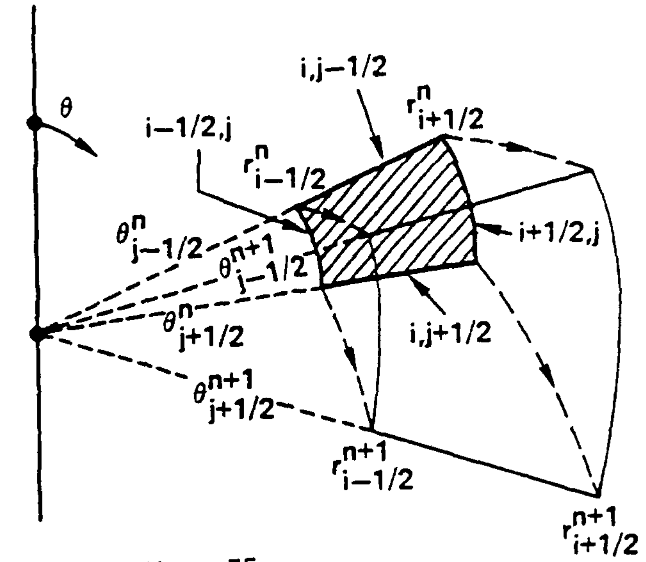

θ
i,j−1/2
$r^{n}_{i+1/2}$
i−1/2,j
$r^{n}_{i-1/2}$
$\theta^{n}_{j-1/2}$
$\theta^{n+1}_{j-1/2}$
i+1/2,j
$\theta^{n}_{j+1/2}$
i,j+1/2
$\theta^{n+1}_{j+1/2}$
$r^{n+1}_{i-1/2}$
$r^{n+1}_{i+1/2}$

Fig. 35

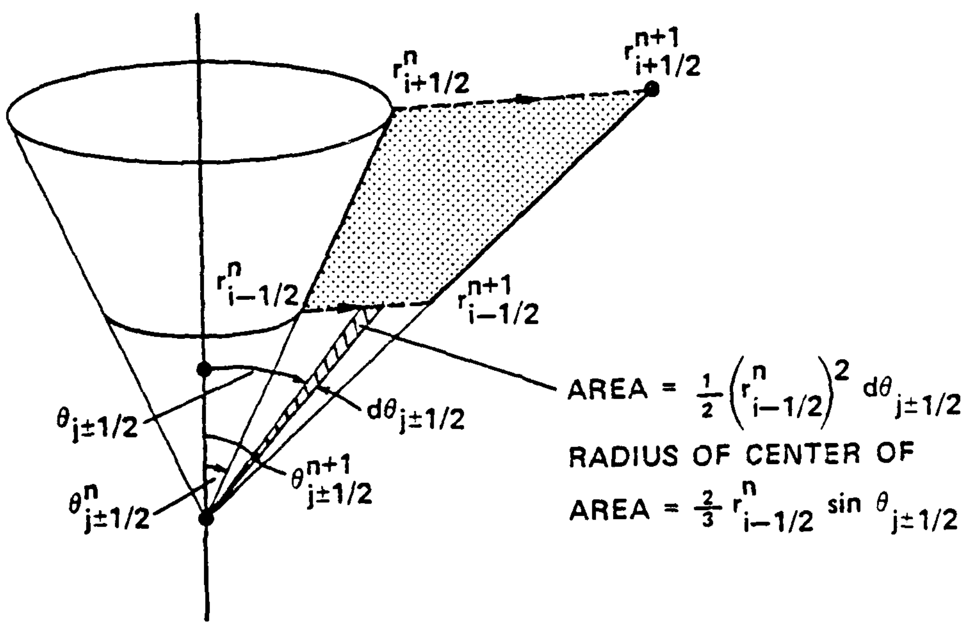

$r^{n}_{i+1/2}$
$r^{n+1}_{i+1/2}$
$r^{n}_{i-1/2}$
$r^{n+1}_{i-1/2}$
AREA = $\frac{1}{2}\left(r^{n}_{i-1/2}\right)^2 d\theta_{j\pm1/2}$
$\theta_{j\pm1/2}$
$d\theta_{j\pm1/2}$
RADIUS OF CENTER OF
AREA = $\frac{2}{3} r^{n}_{i-1/2} \sin \theta_{j\pm1/2}$
$\theta^{n+1}_{j\pm1/2}$
$\theta^{n}_{j\pm1/2}$

Fig. 36

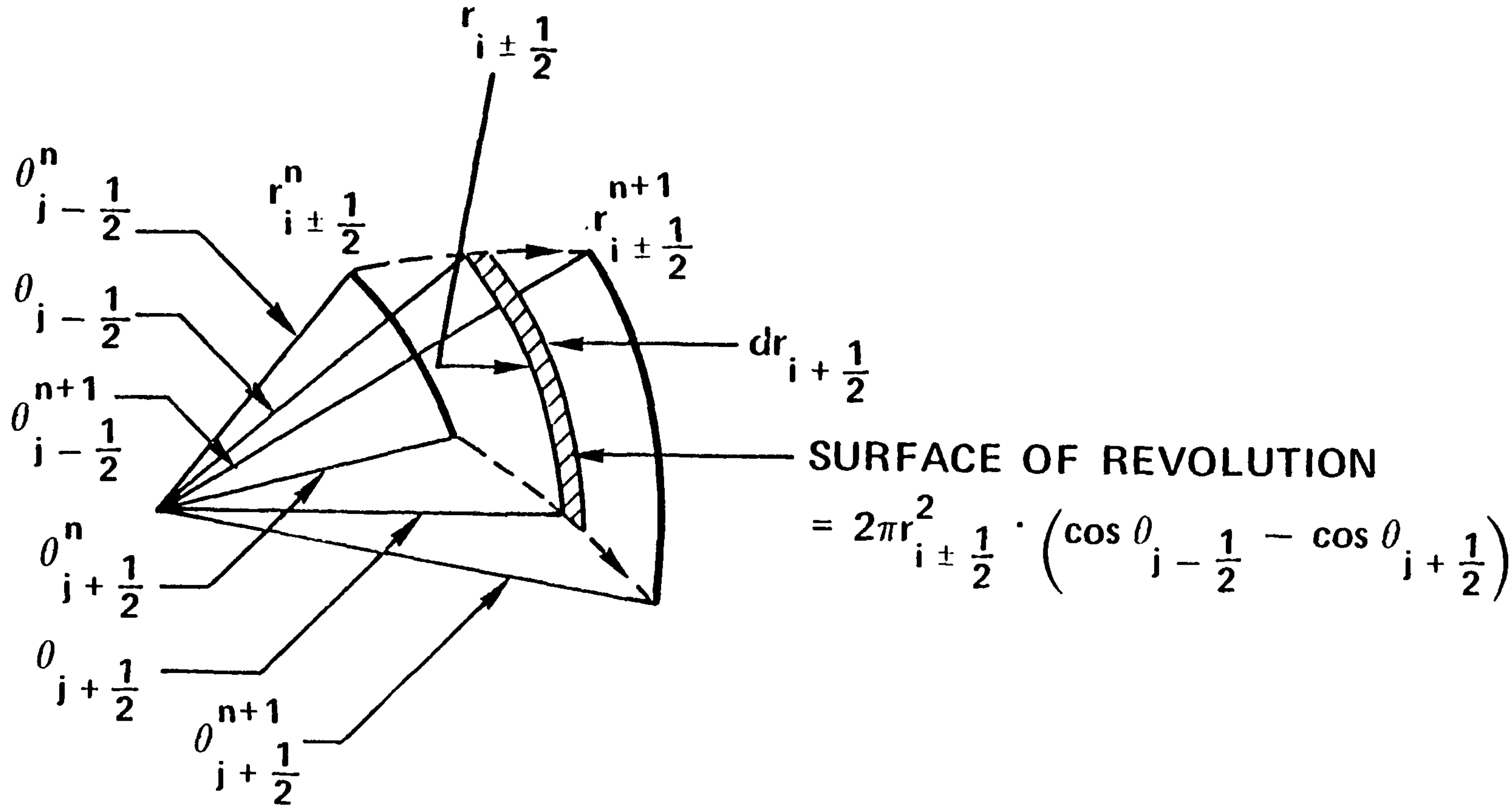

$\theta^{n}_{j-\frac{1}{2}}$
$\theta_{j-\frac{1}{2}}$
$\theta^{n+1}_{j-\frac{1}{2}}$
$\theta^{n}_{j+\frac{1}{2}}$
$\theta_{j+\frac{1}{2}}$
$\theta^{n+1}_{j+\frac{1}{2}}$
$r^{n}_{i\pm\frac{1}{2}}$
$r_{i\pm\frac{1}{2}}$
$r^{n+1}_{i\pm\frac{1}{2}}$
$dr_{i+\frac{1}{2}}$
SURFACE OF REVOLUTION
$= 2\pi r^2_{i\pm\frac{1}{2}} \cdot \left(\cos\theta_{j-\frac{1}{2}} - \cos\theta_{j+\frac{1}{2}}\right)$

Fig. 37

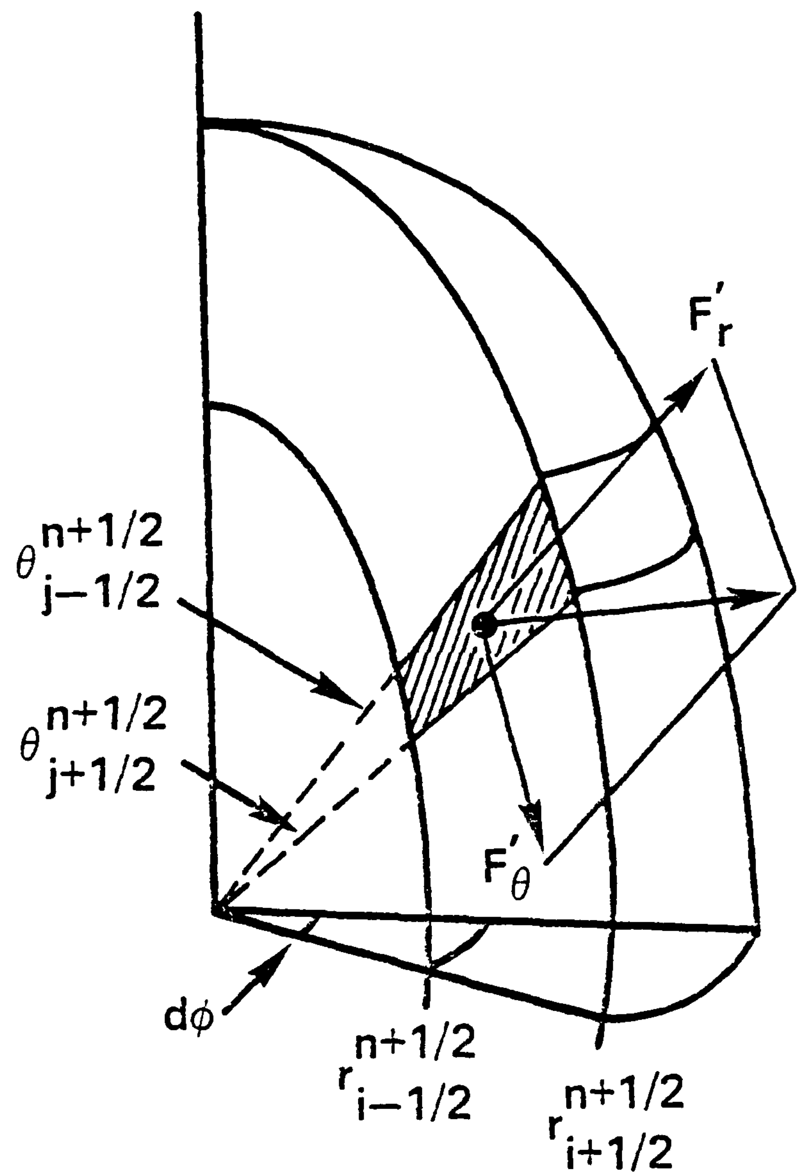


Fig. 30

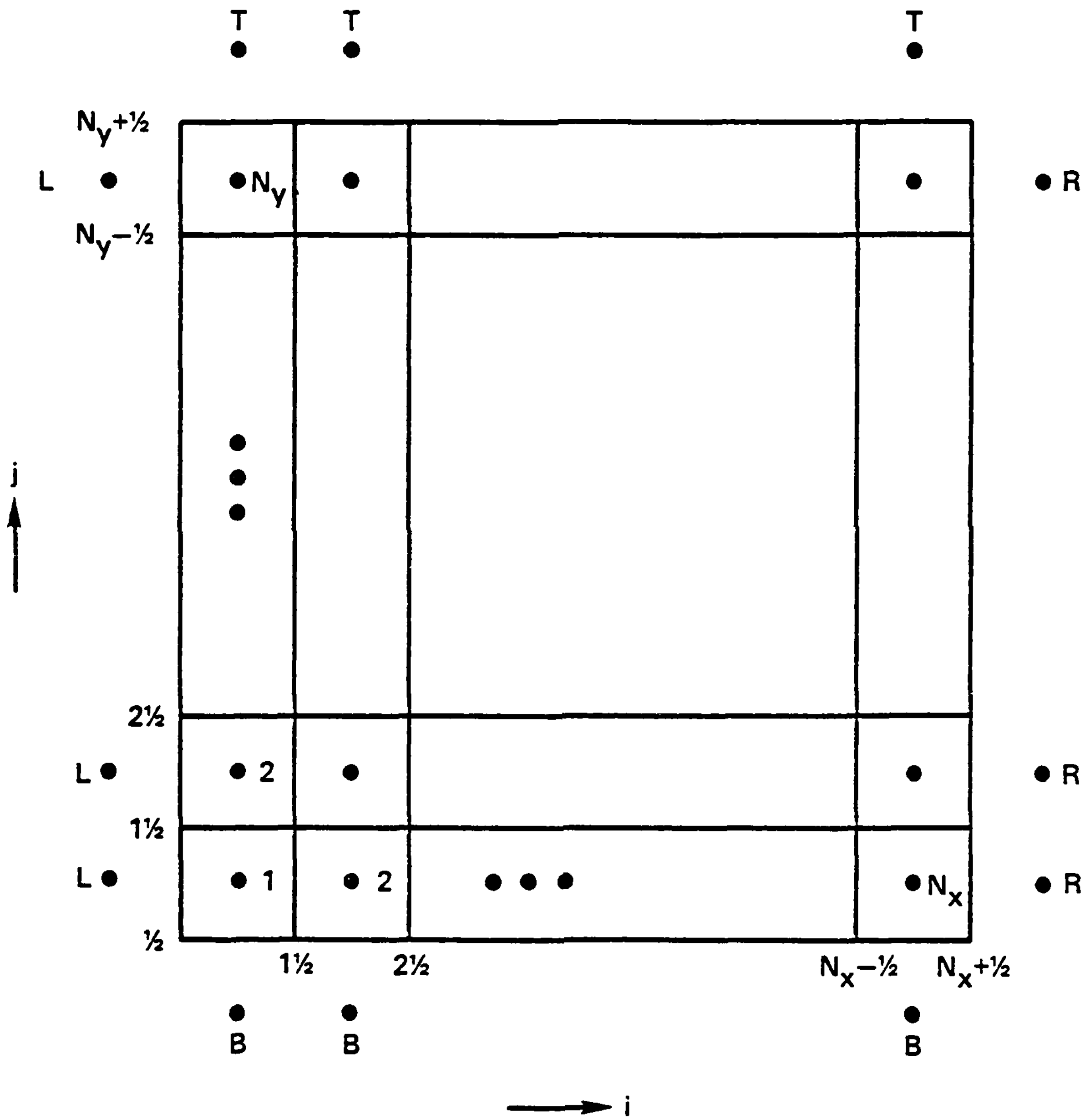
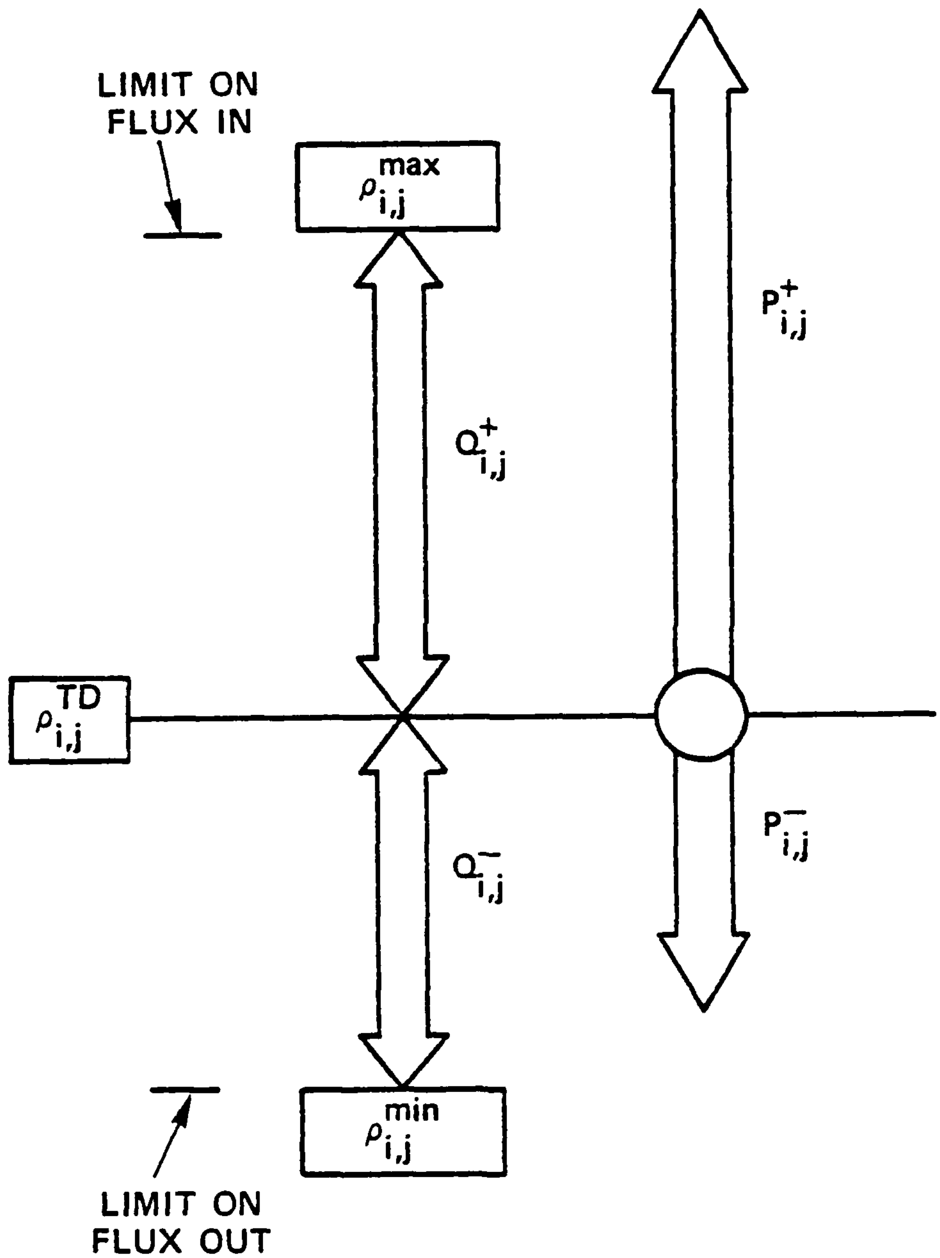


Fig. 39



LIMIT ON FLUX IN
$\rho_{i,j}^{max}$
$P_{i,j}^{+}$
$Q_{i,j}^{+}$
$\rho_{i,j}^{TD}$
$P_{i,j}^{-}$
$Q_{i,j}^{-}$
$\rho_{i,j}^{min}$
LIMIT ON FLUX OUT

Fig. 40

APPENDIX

```
      SUBROUTINE FCT2D(RHO,KO,KN,KR,SNKRNZ,
     &          LBC,RHOLBC,RBC,RHORBC,BBC,RHOBBC,TBC,RHOTBC)
C
C
C     ORIGINATOR :   RAAFAT  H.  GUIRGUIS
C
C     DESCRIPTION :
C     -----------
C
C     A FULLY 2-D ROUTINE THAT SOLVES GENERALIZED CONTINUITY EQUATIONS
C     OF THE FORM
C
C         D RHO / D T = - DIV( RHO * V ) - SOURCES
C
C     WHERE RHO IS THE GENERALIZED DENSITY, AND V IS THE FLUID VELOCITY.
C     FOR SECOND ORDER ACCURACY, IT IS ADVISABLE TO ADVANCE HALF A
C     TIME STEP USING THE VELOCITY AND SOURCE TERMS AT THE BEGINNING
C     OF THE TIME STEP, THEN ADVANCE A WHOLE TIME STEP USING THE
C     HALF-POINT VELOCITY AND SOURCE TERMS.   USING THE HALF POINT
C     DENSITY IS NOT RECOMMENDED.   IT IS, HOWEVER, INCLUDED AS AN
C     OPTION, BY ALTERNATING (KO,KN) BETWEEN (1,2) FOR THE HALF TIME
C     STEP, AND (2,1) FOR THE WHOLE TIME STEP.
C     THE OLD, (KO), AND NEW, (KN), DENSITIES ( AT THE BEGINNING AND END
C     OF THE TIME STEP, RESPECTIVELY ) ARE STORED IN A 2-LEVEL 2-D ARRAY
C     ( 3-D ARRAY ).   THE MASS AND DIFFUSION FLUXES ARE EVALUATED USING
C     KO DENSITY, WHEREAS KN DENSITY DETERMINES THE ANTI-DIFFUSION
C     FLUXES.   IT IS ADVISABLE TO SET KO = 1, KN = 2, UNLESS THE HALF
C     POINT DENSITY IS TO BE USED DURING THE WHOLE TIME STEP.   THEN
C     KO = 2, KN = 1  FOR THE WHOLE TIME STEP.
C     KR DETERMINES THE LOCATION OF THE RESULTING DENSITY.   IT IS
C     ADVISABLE TO SET KR = 2 , 1 , FOR THE HALF AND WHOLE TIME STEPS,
C     RESPECTIVELY.   THIS CHOICE ELIMINATES THE NEED TO COPY THE NEW
C     DENSITY ON THE OLD ARRAY, IN PREPARATION FOR A NEW TIME STEP.
C     SNKRNZ IS A LOGICAL VARIABLE WHICH, WHEN SET TO .TRUE., TELLS THE
C     ROUTINE TO USE THE CORRECTION FACTORS OF THE LAST SNKRNZ = .FALSE.
C     CALL, TO LIMIT THE ANTI-DIFFUSION FLUXES.   IF SET TO .FALSE., THE
C     CORRECTION FACTORS ARE EVALUATED FROM THE CURRENT VARIABLES AND
C     USED IN THE LIMITING PROCESS.
C     LBC, RHOLBC, RBC, RHORBC, BBC, RHOBBC, TBC, RHOTBC, ARE DEFINED
C     BELOW.
C
C     (1)   A PARTICULAR GEOMETRY IS SELECTED BY A CALL TO ENTRY
C           SETGOM :
C               CALL SETGOM( 4HCART, 1HX, 1HY, NX, NY )
C           OR ..,1HX, 1HZ,... OR ..., 1HZ, 1HY,...,ASSUMES CARTESIAN
C           COORDINATES.   ORDER OF THE 2 COORDINATES IS IMMATERIAL ONLY
C           FOR THIS CASE.
C               CALL SETGOM( 3HCYL, 1HR, 1HZ, NX, NY )
C               CALL SETGOM( 3HCYL, 1HR, 3HFYE, NX, NY )
C               CALL SETGOM( 3HCYL, 1HZ, 3HFYE, NX, NY )
C           FOR THE 3 TYPICAL CYLINDRICAL COORDINATES.
C               CALL SETGOM( 3HSPH, 1HR, 4HCETA, NX, NY )
```

```
C               CALL SETGOM( 3HSPH, 1HR, 3HFYE, NX, NY )
C               CALL SETGOM( 3HSPH, 4HCETA, 3HFYE, NX, NY )
C          FOR THE 3 TYPICAL SPHERICAL COORDINATES.
C          NX, NY, ARE THE NUMBERS OF CELLS CENTERS ALONG THE 2
C          COORDINATES, IN THE PRESCRIBED ORDER.   IF THE LITERAL
C          CONSTANTS DESCRIBING THE GEOMETRY ARE MISS-SPELLED, AN ERROR
C          MESSAGE IS ISSUED, AND EXECUTION STOPPED.
C          NOTE : THE 2 COORDINATES ARE GENERALLY DENOTED BY (X,Y).   IN
C          SPHERICAL R-FYE GEOMETRY, FOR EXAMPLE, X MEANS R, WHILE
C          Y MEANS FYE.
C
C     (2)  THE LEFT, RIGHT, BOTTOM, AND TOP BOUNDARIES ARE EXTENDED
C          1 CELL BEYOND THE LAST GRID POINT, YIELDING (NX+2)*(NY+2)
C          CELLS.   THE DENSITY OF AN EXTRA LEFT CELL = LBC * (DENSITY
C          OF ADJACENT CELL ON SAME ROW) + RHOLBC.   BY ADJUSTING THE
C          VALUES OF THE TWO 1-D REAL ARRAYS ( OF DIMENSION NY+2 ) LBC
C          AND RHOLBC, VARIOUS TYPES OF BOUNDARIES CAN BE SIMULATED.
C          SIMILAR RELATIONS APPLY FOR RIGHT, BOTTOM, AND TOP
C          BOUNDARIES, DENOTED BY R, B, AND T, RESPECTIVELY.   NOTE
C          THAT BOTTOM AND TOP ARRAYS ARE NX+2 CELLS LONG.
C
C     (3)  ALL THE BOUNDARIES ARE CONSIDERED PERMEABLE TO DIFFUSION AND
C          ANTI-DIFFUSION FLUXES, UNLESS A CALL TO ENTRY SOLDFY INFORMS
C          THE ROUTINE OTHERWISE.   ANY OF
C               CALL SOLDFY( 4HLEFT, KSTRT, KEND )
C               CALL SOLDFY( 4HRITE, KSTRT, KEND )
C               CALL SOLDFY( 4HBOTM, KSTRT, KEND )
C               CALL SOLDFY( 3HTOP, KSTRT, KEND )
C          MAKES THE LEFT, RIGHT, BOTTOM, OR TOP BOUNDARIES IMPERMEABLE
C          TO BOTH DIFFUSION AND ANTI-DIFFUSION FLUXES FROM CELL
C          NUMBER KSTRT TO CELL NUMBER KEND, INCLUSIVE.
C          NOTE : CELL 1 IS NOW THE EXTRA CELL BEYOND THE BOUNDARY,
C          CONFINING CELLS 2 TO NX+1, OR NY+1.
C          ANY NUMBER OF CALLS TO SOLDFY IS ALLOWED, MAKING
C          IT POSSIBLE TO SOLIDIFY UNCONNECTED PATCHES ALONG EACH
C          BOUNDARY.   EACH TIME SOLDFY IS CALLED, A MESSAGE EXPLAINING
C          THE ACTION TAKEN IS ISSUED.
C
C     (4)  CALLS TO ENTRY PRODIC, FOR EXAMPLE,
C               CALL PRODIC( 1 , 1HX )
C          INFORM THE ROUTINE TO TREAT THE 1 ST OR 2 ND COORDINATE AS
C          PERIODIC.   THE SECOND ARGUMENT IS JUST TO GENERATE A LABEL;
C          THE MESSAGE " X COORDINATE PERIODIC " IS ISSUED.   SIMILARLY,
C               CALL PRODIC( 2 , 3HFYE )
C          MAKES THE 2 ND COORDINATE PERIODIC, AND THE MESSAGE " FYE
C          COORDINATE PERIODIC " ISSUED.
C          IF THE PERIODIC CALL IS MADE FOR A COORDINATE THAT SHOULDN'T
C          BE PERIODIC, A WARNING MESSAGE IS ISSUED, THEN EXECUTION
C          PROCEEDS.
C
```

```
C      (5)  THE GRID IS INITIALIZED BY A CALL TO ENTRY ORIGRD:
C                CALL ORIGRD( XGN, YGN )
C           WHERE XGN, YGN ARE TWO 1-D REAL ARRAYS OF DIMENSIONS NX+1,
C           NY+1, CONTAINING THE LOCATIONS OF X, Y INTERFACES.
C           ORIGRD WILL THEN CONSIDER THESE AS THE INITIAL LOCATIONS.
C           AT THE BEGINNING OF EACH TIME STEP
C                CALL NGRID( XGN, YGN )
C           WILL EVALUATE VOLUME, MEAN INTERFACE AREA,... OF CELLS,
C           WHEREAS
C                CALL OGRID( XGN, YGN )
C           AT THE END OF EACH TIME STEP, RESET THE OLD ARRAYS
C           FOR THE NEXT TIME STEP.
C
C      (6)  IT IS ASSUMED THAT THE GRID IS MOVING, UNLESS CALLS TO ENTRY
C           FIXGRD FIX ONE OR BOTH OF THE COORDINATES GRIDS.
C                CALL FIXGRD( 1 , 1HX )
C           INFORMS THE ROUTINE THAT THE 1 ST COORDINATE GRID IS FIXED.
C           THE SECOND ARGUMENT IS JUST TO GENERATE A LABEL; THE MESSAGE
C           "X GRID FIXED " IS ISSUED.   SIMILARLY,
C                CALL FIXGRD( 2 , 1HZ )
C           FIXES THE 2 ND COORDINATE GRID AND ISSUES THE MESSAGE " Z
C           GRID FIXED ".   IF BOTH COORDINATES GRIDS ARE FIXED, CALL
C           NGRID, THEN OGRID, ONLY ONCE AFTER INITIALIZATION.
C
C      (7)  A PARTICULAR ANTI-DIFFUSION FLUX CORRECTOR IS SELECTED BY A
C           CALL TO ENTRY SETLMT :
C                CALL SETLMT( 5HBORIS, 4HBOOK )
C           INVOKES BORIS-BOOK FLUX LIMITER, WHILE
C                CALL SETLMT( 7HZALESAK, 1H )
C           INVOKES ZALESAK FLUX LIMITER.   THE ARGUMENTS REFER TO THE
C           ORIGINATORS OF THE FLUX LIMITER.   IF THE LITERAL CONSTANTS
C           DESCRIBING A LIMITER ARE MISS-SPELLED, AN ERROR MESSAGE IS
C           ISSUED, AND EXECUTION STOPPED.
C
C      (8)  A TIME STEP STARTS BY A CALL TO ENTRY NGRID, FOLLOWED BY
C                CALL VOLFLX( U, V, DT )
C           WHERE U,V ARE TWO 2-D REAL ARRAYS OF DIMENSIONS (NX+2)*(NY+2)
C           CONTAINING THE COMPONENTS OF VELOCITY VECTOR AT THE CELLS
C           CENTERS.   DT IS THE TIME STEP.
C
C      (9)  BEFORE EACH CALL TO FCT2D, THE SOURCE TERM IS DETERMINED
C           BY A SEQUENCE OF CALLS :
C                CALL CLRSRC
C           CLEARS THE SOURCE TERM WHICH REMAINS ZERO UNTIL ANY OF THE
C           NEXT CALLS IS DONE.   EACH CALL ADDS TO THE SOURCE TERM.
C           ANY NUMBER OF CALLS IS ALLOWED, TO FORM THE TOTAL VALUE OF
C           THE SOURCE TERM.
C                CALL SORCES( 3HBDF, SORCE, DT )
C           ADDS A BODY TYPE FORCE, WHERE SORCE IS A 2-D REAL ARRAY OF
C           DIMENSION (NX+2)*(NY+2) CONTAINING THE BODY FORCES PER UNIT
C           VOLUME.
```

```
C               CALL SORCES( 4HXGRD, SORCE, DT )
C               CALL SORCES( 4HYGRD, SORCE, DT )
C          ADDS THE X OR Y COMPONENTS OF THE GRADIENT OF THE QUANTITY
C          IN ARRAY SORCE.
C               CALL SORCES( 3HDIV, SORCE, DT )
C          ADDS THE DIVERGENCE OF THE QUANTITY IN SORCE.   ENTRY SORCES
C          DETERMINES WHICH FORM OF GRADIENT OR DIVERGENCE TO USE
C          ACCORDING TO THE GEOMETRY.   ALTERNATIVELY, ONE CAN
C          SEPARATELY CALL ENTRY BODY FOR BODY FORCES, XGRAD OR YGRAD
C          FOR THE GRADIENT IN CARTESIAN COORDINATES, RCGRAD OR YGRAD
C          FOR THE GRADIENT IN CYLINDRICAL R-Z GEOMETRY,... OR XGRAD AND
C          YGRAD FOR DIVERGENCE IN CARTESIAN GEOMETRY, RCDIV AND YGRAD
C          DIVERGENCE IN CYLINDRICAL R-Z GEOMETRY,...
C
C     (10) THE TIME STEP ENDS BY A CALL TO OGRID
C
C     (11) FOR 2 ND ORDER ACCURACY, STEPS (8) , (9) ARE PERFORMED TWICE.
C          ONCE WITH DT= TIME STEP / 2 FOR THE HALF TIME STEP, THEN
C          DT= TIME STEP FOR THE WHOLE TIME STEP.
C
C         ENTRIES ...
C         ENTRY NGRID(XGN,YGN)
C         ENTRY OGRID(XGN,YGN)
C         ENTRY ORIGRD(XGN,YGN)
C         ENTRY VOLFLX(U,V,DT)
C         ENTRY SORCES(SRCTYP,SORCE,DT)
C         ENTRY CLRSRC
C         ENTRY BODY(SORCE,DT)
C         ENTRY XGRAD(SORCE,DT)
C         ENTRY YGRAD(SORCE,DT)
C         ENTRY RCGRAD(SORCE,DT)
C         ENTRY RCDIV(SORCE,DT)
C         ENTRY SETGOM(GOMTRY,CRD1,CRD2,N1,N2)
C         ENTRY PRODIC(CRDNT,CRD)
C         ENTRY SETLMT(LMTR1,LMTR2)
C         ENTRY FIXGRD(CRNT,CRD)
C         ENTRY SOLDFY(BONDRY,KSTRT,KEND)
C
C
C         CALLS TO ...
C         SUBROUTINE NUMU(NI,NJ,EPS,NUV,MUV)
C
```

```
C       DECLARATIONS :
C       ------------
C
            PARAMETER      NPX=100,NPY=100
            PARAMETER      NP1X=NPX+1,NP1Y=NPY+1
            PARAMETER      NP2X=NPX+2,NP2Y=NPY+2
C
C
            INTEGER   GEOM,CRDNT
C
            INTEGER   IFLX(NP2X,NP2Y)
C
C
            LOGICAL   LSRC
            LOGICAL   SNKRNZ
            LOGICAL   XCHNG,YCHNG
            LOGICAL   XPRDC,YPRDC
C
C
            REAL      TEXT(20)
            REAL      LMTR1(2),LMTR2(2)
            REAL      TGM(3),TCRD(6),TLM1(2,4),TLM2(2,4)
C
            REAL      LBC(NP2Y),RHOLBC(NP2Y)
            REAL      RBC(NP2Y),RHORBC(NP2Y)
            REAL      BBC(NP2X),RHOBBC(NP2X)
            REAL      TBC(NP2X),RHOTBC(NP2X)
C
            REAL      PRMBLL(NP2Y),PRMBLR(NP2Y),PRMBLB(NP2X),PRMBLT(NP2X)
C
            REAL      XGO(NP1X),XGN(NP1X),YGO(NP1Y),YGN(NP1Y)
            REAL      XG(NP1X),DXG(NP1X),YG(NP1Y),DYG(NP1Y)
            REAL      DXGO(NP2X),DXGN(NP2X),DYGO(NP2Y),DYGN(NP2Y)
            REAL      RDXGN(NP2X),RDYGN(NP2Y)
            REAL      DXGNH(NP1X),RDXGNH(NP1X),DYGNH(NP1Y),RDYGNH(NP1Y)
            REAL      AX(NPX),AY(NPY)
            REAL      SQ(NP1X),SQO(NP1X),SQN(NP1X)
C
            REAL      RHO(NP2X,NP2Y,2)
            REAL      U(NP2X,NP2Y),ADUDT(NP1X,NPY)
            REAL      V(NP2X,NP2Y),ADVDT(NPX,NP1Y)
            REAL      CELMAS(NPX,NPY),SOURCE(NP2X,NP2Y),SORCE(NP2X,NP2Y)
C
            REAL      TEMP1(NP2X,NP2Y),TEMP2(NP2X,NP2Y)
            REAL      TEMP3(NP1X,NP1Y),TEMP4(NP1X,NP1Y)
            REAL      TEMP5(NP2X,NP2Y),TEMP6(NP2X,NP2Y)
C
            REAL      OLDVOL(NP2X,NP2Y),RVOL(NP2X,NP2Y)
            REAL      AVXVL(NP1X,NP1Y),RAVXVL(NP1X,NP1Y)
            REAL      AVYVL(NP1X,NP1Y),RAVYVL(NP1X,NP1Y)
C
            REAL      XMSFLX(NP1X,NP1Y),YMSFLX(NP1X,NP1Y)
            REAL      XDFFLX(NP2X,NP2Y),YDFFLX(NP2X,NP2Y)
            REAL      XNTFLX(NP1X,NP1Y),YNTFLX(NP1X,NP1Y)
C
```

```
      REAL      EPSX(NP1X,NP1Y),NUX(NP2X,NP2Y),MUX(NP2X,NP2Y)
      REAL      EPSY(NP1X,NP1Y),NUY(NP2X,NP2Y),MUY(NP2X,NP2Y)
      REAL      NUXVOL(NP2X,NP2Y),MUXVOL(NP2X,NP2Y)
      REAL      NUYVOL(NP2X,NP2Y),MUYVOL(NP2X,NP2Y)
C
      REAL      MXFLX(NP2X,NP2Y),MNFLX(NP2X,NP2Y)
      REAL      FLXIN(NP2X,NP2Y),FLXOUT(NP2X,NP2Y)
      REAL      RHOMX(NP2X,NP2Y),RHOMN(NP2X,NP2Y)
      REAL      MXIN(NP2X,NP2Y),MXOUT(NP2X,NP2Y)
      REAL      DIFF(NP2X,NP2Y),FLX(NP2X,NP2Y)
C
      REAL      RIN(NP2X,NP2Y),ROUT(NP2X,NP2Y)
      REAL      XFLXCR(NP2X,NP2Y),YFLXCR(NP2X,NP2Y)
C
C
      EQUIVALENCE   (TEMP1,FLXIN,RIN)
      EQUIVALENCE   (TEMP2,FLXOUT,ROUT)
      EQUIVALENCE   (TEMP3,XMSFLX,XNTFLX,AVXVL,RAVXVL,EPSX)
      EQUIVALENCE   (TEMP4,YMSFLX,YNTFLX,AVYVL,RAVYVL,EPSY)
      EQUIVALENCE   (TEMP5,XDFFLX,YDFFLX,NUX,NUXVOL,NUY,NUYVOL)
      EQUIVALENCE   (TEMP5,OLDVOL,RVOL,DIFF,MXFLX,FLX,IFLX)
      EQUIVALENCE   (TEMP6,SOURCE,MUX,MUXVOL,MUY,MUYVOL)
      EQUIVALENCE   (TEMP6,RHOMX,RHOMN,MXIN,MXOUT,MNFLX)
      EQUIVALENCE   (TEMP6,XFLXCR,YFLXCR)
C
C
      DATA TEXT(1),TEXT(2),TEXT(3)/4H   M,4HISS-,4HSPEL/
      DATA TEXT(4),TEXT(5)/4HLING,4H OF /
      DATA TEXT(9),TEXT(10),TEXT(11)/4H IDE,4HNTIF,4HIER /
      DATA TEXT(12),TEXT(13),TEXT(14)/4H  GE,4HOMET,4HRY  /
      DATA TEXT(15),TEXT(16),TEXT(17)/4HFLUX,4H LIM,4HITER/
      DATA TEXT(18),TEXT(19),TEXT(20)/4HSOUR,4HCE T,4HYPE /
C
      DATA TGM(1),TGM(2),TGM(3)/4HCART,4HCYL ,4HSPH /
C
      DATA TCRD(1),TCRD(2),TCRD(3)/4HX   ,4HY   ,4HZ   /
      DATA TCRD(4),TCRD(5),TCRD(6)/4HR   ,4HCETA,4HFYE /
C
      DATA TBND(1),TBND(2)/4HLEFT,4HRITE/
      DATA TBND(3),TBND(4)/4HBOTM,4HTOP /
C
      DATA LMTR1,LMTR2/4*4H    /
      DATA TLM1(1,1),TLM1(2,1)/4HBORI,4HS   /
      DATA TLM2(1,1),TLM2(2,1)/4HBOOK,4H    /
      DATA TLM1(1,2),TLM1(2,2)/4HZALE,4HSAK /
      DATA TLM2(1,2),TLM2(2,2)/4H    ,4H    /
C
      DATA BDF/3HBDF/,XGRD,YGRD/4HXGRD,4HYGRD/,DIV/3HDIV/
C
C
```

```
C      FORMATS :
C      --------
C
   10     FORMAT(///5X,7HWARNING,5X,11A4)
   20     FORMAT(///5X,7HWARNING,5X,A4,2X,22HSHOULD NOT BE PERIODIC)
   30     FORMAT(///5X,24HALL BOUNDARIES PERMEABLE)
   40     FORMAT(///5X,A4,2X,19HCOORDINATE PERIODIC)
   50     FORMAT(///5X,A4,2X,10HGRID FIXED)
   60     FORMAT(///5X,A4,2X,22HBOUNDARY SOLID BETWEEN,
     &        2X,4HCELL,2X,I4,2X,3HAND,2X,I4)
   70     FORMAT(///5X,25HGEOMETRY NOT INCLUDED YET)
C
C
```

```
C     EVALUATE OLD CELL MASS "CELMAS"
          DO 110 J=1,NY
          DO 110 I=1,NX
          OLDVOL(I,J)=DXGO(I+1)*DYGO(J+1)
  110     CELMAS(I,J)=RHO(I+1,J+1,1)*OLDVOL(I,J)
C
C     ADD SOURCE TERM "SOURCE" WHEN APPROPRIATE
          IF(.NOT.LSRC) GO TO 125
C
C
          DO 120 J=1,NY
          DO 120 I=1,NX
  120     CELMAS(I,J)=CELMAS(I,J)-SOURCE(I,J)
C
  125     CONTINUE
C
C
C     EVALUATE X-CONVECTION FLUX "XMSFLX"
          DO 130 J=1,NY
          DO 130 I=1,NXP1
          TEMP3(I,J)=RHO(I+1,J+1,KO)+RHO(I,J+1,KO)
          TEMP5(I,J)=0.5*ADUDT(I,J)
  130     XMSFLX(I,J)=TEMP3(I,J)*TEMP5(I,J)
C
C     EVALUATE Y-CONVECTION FLUX "YMSFLX"
          DO 140 J=1,NYP1
          DO 140 I=1,NX
          TEMP4(I,J)=RHO(I+1,J+1,KO)+RHO(I+1,J,KO)
          TEMP6(I,J)=0.5*ADVDT(I,J)
  140     YMSFLX(I,J)=TEMP4(I,J)*TEMP6(I,J)
C
C     EVALUATE X AND Y TRANSPORTED DENSITIES
          DO 150 J=1,NY
          DO 150 I=1,NX
          TEMP5(I,J)=XMSFLX(I,J)-XMSFLX(I+1,J)
          TEMP6(I,J)=YMSFLX(I,J)-YMSFLX(I,J+1)
          TEMP3(I,J)=CELMAS(I,J)+TEMP5(I,J)
          TEMP4(I,J)=CELMAS(I,J)+TEMP6(I,J)
          CELMAS(I,J)=TEMP3(I,J)+TEMP6(I,J)
          RVOL(I,J)=RDXGN(I+1)*RDYGN(J+1)
          RHO(I+1,J+1,KN)=TEMP3(I,J)*RVOL(I,J)
  150     TEMP4(I,J)=TEMP4(I,J)*RVOL(I,J)
C
C     EVALUATE X-TRANSPORTED DENSITY AT LEFT AND RIGHT BOUNDARIES
          DO 170 J=2,NYP1
          RHO(1,J,KN)=LBC(J)*RHO(IL,J,KN)+RHOLBC(J)
  170     RHO(NXP2,J,KN)=RBC(J)*RHO(IR,J,KN)+RHORBC(J)
C
```

```
C      EVALUATE "EPSX"
           DO 180 J=1,NY
           DO 180 I=1,NXP1
           RAVXVL(I,J)=RDXGNH(I)*RDYGN(J+1)
  180      EPSX(I,J)=RAVXVL(I,J)*ADUDT(I,J)
C
C      EVALUATE X DIFFUSION AND ANTI-DIFFUSIONTEOEFFICIENTS "NUX", "MUX"
           CALL NUMU(NXP1,NY,EPSX,NUX,MUX)
C
C      CANCEL THE DIFFUSION AND ANTI-DIFFUSION X-FLUXES THROUGH SOLID
C      PORTIONS OF LEFT AND RIGHT BOUNDARIES
           DO 185 J=1,NY
           NUX(1,J)=NUX(1,J)*PRMBLL(J+1)
           MUX(1,J)=MUX(1,J)*PRMBLL(J+1)
           NUX(NXP1,J)=NUX(NXP1,J)*PRMBLR(J+1)
  185      MUX(NXP1,J)=MUX(NXP1,J)*PRMBLR(J+1)
C
C      EVALUATE X DIFFUSION AND ANTI-DIFFUSION FLUXES "XDFFLX" , "XNTFLX"
           DO 190 J=1,NY
           DO 190 I=1,NXP1
           AVXVL(I,J)=DXGNH(I)*DYGN(J+1)
           NUXVOL(I,J)=NUX(I,J)*AVXVL(I,J)
           MUXVOL(I,J)=MUX(I,J)*AVXVL(I,J)
           TEMP3(I,J)=RHO(I+1,J+1,KO)-RHO(I,J+1,KO)
           XDFFLX(I,J)=NUXVOL(I,J)*TEMP3(I,J)
           TEMP3(I,J)=RHO(I+1,J+1,KN)-RHO(I,J+1,KN)
  190      XNTFLX(I,J)=MUXVOL(I,J)*TEMP3(I,J)
C
C      ADD X-DIFFUSION TO "CELMAS"
           DO 200 J=1,NY
           DO 200 I=1,NX
           RHO(I+1,J+1,KN)=TEMP4(I,J)
           TEMP6(I,J)=XDFFLX(I+1,J)-XDFFLX(I,J)
  200      CELMAS(I,J)=CELMAS(I,J)+TEMP6(I,J)
C
C      EVALUATE Y-TRANSPORTED DENSITY AT BOTTOM AND TOP BOUNDARIES
           DO 210 I=1,NXP2
           RHO(I,1,KN)=BBC(I)*RHO(I,JB,KN)+RHOBBC(I)
  210      RHO(I,NYP2,KN)=TBC(I)*RHO(I,JT,KN)+RHOTBC(I)
C
C      EVALUATE "EPSY"
           DO 220 J=1,NYP1
           DO 220 I=1,NX
           RAVYVL(I,J)=RDXGN(I+1)*RDYGNH(J)
  220      EPSY(I,J)=RAVYVL(I,J)*ADVDT(I,J)
C
C      EVALUATE Y DIFFUSION AND ANTI-DIFFUSION COEFFICIENTS "NUY", "MUY"
           CALL NUMU(NX,NYP1,EPSY,NUY,MUY)
C
```

```
C     CANCEL THE DIFFUSION AND ANTI-DIFFUSION Y-FLUXES THROUGH SOLID
C     PORTIONS OF BOTTOM AND TOP BOUNDARIES
          DO 225 I=1,NX
          NUY(I,1)=NUY(I,1)*PRMBLB(I+1)
          MUY(I,1)=MUY(I,1)*PRMBLB(I+1)
          NUY(I,NYP1)=NUY(I,NYP1)*PRMBLT(I+1)
  225     MUY(I,NYP1)=MUY(I,NYP1)*PRMBLT(I+1)
C
C     EVALUATE Y DIFFUSION AND ANTI-DIFFUSION FLUXES "YDFFLX" , "YNTFLX"
          DO 230 J=1,NYP1
          DO 230 I=1,NX
          AVYVL(I,J)=DXGN(I+1)*DYGNH(J)
          NUYVOL(I,J)=NUY(I,J)*AVYVL(I,J)
          MUYVOL(I,J)=MUY(I,J)*AVYVL(I,J)
          TEMP4(I,J)=RHO(I+1,J+1,KO)-RHO(I+1,J,KO)
          YDFFLX(I,J)=NUYVOL(I,J)*TEMP4(I,J)
          TEMP4(I,J)=RHO(I+1,J+1,KN)-RHO(I+1,J,KN)
  230     YNTFLX(I,J)=MUYVOL(I,J)*TEMP4(I,J)
C
C     ADD Y-DIFFUSION TO "CELMAS"
          DO 240 J=1,NY
          DO 240 I=1,NX
          TEMP6(I,J)=YDFFLX(I,J+1)-YDFFLX(I,J)
  240     CELMAS(I,J)=CELMAS(I,J)+TEMP6(I,J)
C
C     IF SYNCHRONIZATION OF ANTI-DIFFUSION FLUXES IS SPECIFIED, SKIP
C     EVALUATION OF CORRECTION FACTORS
          IF(SNKRNZ) GO TO 445
C
C
C     EVALUATE TRANSPORTED-DIFFUSED DENSITY
          DO 250 J=1,NY
          DO 250 I=1,NX
          RVOL(I,J)=RDXGN(I+1)*RDYGN(J+1)
  250     RHO(I+1,J+1,KN)=CELMAS(I,J)*RVOL(I,J)
C
C     EVALUATE TRANSPORTED-DIFFUSED DENSITY AT BOTTOM AND TOP BOUNDARIES
          DO 260 I=2,NXP1
          TEMP1(I,1)=1.0
          TEMP2(I-1,NYP1)=1.0
          RHO(I,1,KN)=BBC(I)*RHO(I,JB,KN)+RHOBBC(I)
  260     RHO(I,NYP2,KN)=TBC(I)*RHO(I,JT,KN)+RHOTBC(I)
C
C     EVALUATE TRANSPORTED-DIFFUSED DENSITY AT LEFT AND RIGHT BOUNDARIES
          DO 270 J=2,NYP1
          TEMP1(1,J)=1.0
          TEMP2(NXP1,J-1)=1.0
          RHO(1,J,KN)=LBC(J)*RHO(IL,J,KN)+RHOLBC(J)
  270     RHO(NXP2,J,KN)=RBC(J)*RHO(IR,J,KN)+RHORBC(J)
C
C
```

```
C     CANCEL THE ANTI-DIFFUSION X-FLUX IF IT IS OPPOSITE TO ITS LOCAL
C     TRANSPORTED-DIFFUSED DENSITY GRADIENT AND ANY OF THE ADJACENT ONES
          DO 280 J=1,NY
          DO 280 I=1,NXP1
  280     DIFF(I,J)=RHO(I+1,J+1,KN)-RHO(I,J+1,KN)
C
          DO 290 J=1,NY
          DO 290 I=1,NX
          TEMP1(I+1,J+1)=XOR(XNTFLX(I+1,J),DIFF(I,J))
  290     TEMP2(I,J)=XOR(XNTFLX(I,J),DIFF(I+1,J))
C
          DO 300 J=1,NY
          DO 300 I=1,NXP1
          TEMP5(I,J)=XOR(XNTFLX(I,J),DIFF(I,J))
          TEMP6(I,J)=OR(TEMP1(I,J+1),TEMP2(I,J))
          FLX(I,J)=AND(TEMP5(I,J),TEMP6(I,J))
          FLX(I,J)=COMPL(FLX(I,J))
          IFLX(I,J)=LSHF(IFLX(I,J),-31)
          FLX(I,J)=FLOAT(IFLX(I,J))
  300     XNTFLX(I,J)=XNTFLX(I,J)*FLX(I,J)
C
C     IF X-COORDINATE IS PERIODIC AND EITHER LEFT OR RIGHT BOUNDARY'S
C     ANTI-DIFFUSION FLUX IS CANCELLED, CANCEL THE OTHER
          IF(.NOT.XPRDC) GO TO 305
C
          DO 304 J=1,NY
          XNTFLX(1,J)=AND(XNTFLX(1,J),XNTFLX(NXP1,J))
  304     XNTFLX(NXP1,J)=XNTFLX(1,J)
C
  305     CONTINUE
C
C
C     CANCEL THE ANTI-DIFFUSION Y-FLUX IF IT IS OPPOSITE TO ITS LOCAL
C     TRANSPORTED-DIFFUSED DENSITY GRADIENT AND ANY OF THE ADJACENT ONES
          DO 310 J=1,NYP1
          DO 310 I=1,NX
  310     DIFF(I,J)=RHO(I+1,J+1,KN)-RHO(I+1,J,KN)
C
          DO 320 J=1,NY
          DO 320 I=1,NX
          TEMP1(I+1,J+1)=XOR(YNTFLX(I,J+1),DIFF(I,J))
  320     TEMP2(I,J)=XOR(YNTFLX(I,J),DIFF(I,J+1))
C
          DO 330 J=1,NYP1
          DO 330 I=1,NX
          TEMP5(I,J)=XOR(YNTFLX(I,J),DIFF(I,J))
          TEMP6(I,J)=OR(TEMP1(I+1,J),TEMP2(I,J))
          FLX(I,J)=AND(TEMP5(I,J),TEMP6(I,J))
          FLX(I,J)=COMPL(FLX(I,J))
          IFLX(I,J)=LSHF(IFLX(I,J),-31)
          FLX(I,J)=FLOAT(IFLX(I,J))
  330     YNTFLX(I,J)=YNTFLX(I,J)*FLX(I,J)
C
```

```
C     IF Y-COORDINATE IS PERIODIC AND EITHER BOTTOM OR TOP BOUNDARY'S
C     ANTI-DIFFUSION FLUX IS CANCELLED, CANCEL THE OTHER
          IF(.NOT.YPRDC) GO TO 335
C
          DO 334 I=1,NX
          YNTFLX(I,1)=AND(YNTFLX(I,1),YNTFLX(I,NYP1))
  334     YNTFLX(I,NYP1)=YNTFLX(I,1)
C
  335     CONTINUE
C
C
C     EVALUATE NET INCOMING "FLXIN", OUTGOING "FLXOUT" ANTI-DIFFUSION
          DO 340 J=1,NY
          DO 340 I=1,NXP1
          TEMP5(I,J)=ASHF(XNTFLX(I,J),-31)
          MNFLX(I,J)=AND(XNTFLX(I,J),TEMP5(I,J))
          TEMP5(I,J)=XOR(XNTFLX(I,J),TEMP5(I,J))
  340     MXFLX(I,J)=AND(XNTFLX(I,J),TEMP5(I,J))
C
          DO 350 J=1,NY
          DO 350 I=1,NX
          FLXIN(I+1,J+1)=1.E-50+MXFLX(I,J)
          FLXOUT(I+1,J+1)=1.E-50-MNFLX(I,J)
          FLXIN(I+1,J+1)=FLXIN(I+1,J+1)-MNFLX(I+1,J)
  350     FLXOUT(I+1,J+1)=FLXOUT(I+1,J+1)+MXFLX(I+1,J)
C
          DO 360 J=1,NYP1
          DO 360 I=1,NX
          TEMP5(I,J)=ASHF(YNTFLX(I,J),-31)
          MNFLX(I,J)=AND(YNTFLX(I,J),TEMP5(I,J))
          TEMP5(I,J)=XOR(YNTFLX(I,J),TEMP5(I,J))
  360     MXFLX(I,J)=AND(YNTFLX(I,J),TEMP5(I,J))
C
          DO 370 J=1,NY
          DO 370 I=1,NX
          FLXIN(I+1,J+1)=FLXIN(I+1,J+1)+MXFLX(I,J)
          FLXOUT(I+1,J+1)=FLXOUT(I+1,J+1)-MNFLX(I,J)
          FLXIN(I+1,J+1)=FLXIN(I+1,J+1)-MNFLX(I,J+1)
  370     FLXOUT(I+1,J+1)=FLXOUT(I+1,J+1)+MXFLX(I,J+1)
C
C
          GO TO (375,385) ILMTR
C
  375     CONTINUE
C     IF BORIS-BOOK FLUX LIMITER IS REQUESTED, USE TRANSPORTED-DIFFUSED
C     DENSITY TO BOUND NEW DENSITY
          DO 380 J=1,NYP2
          DO 380 I=1,NXP2
  380     TEMP5(I,J)=RHO(I,J,KN)
C
          GO TO 395
C
```

```
  385     CONTINUE
C      IF ZALESAK FLUX LIMITER IS REQUESTED, USE MAXIMUM OF OLD AND
C      TRANSPORTED-DIFFUSED DENSITY AS UPPER BOUND FOR NEW DENSITY
          DO 390 J=1,NYP2
          DO 390 I=1,NXP2
  390     TEMP5(I,J)=AMAX1(RHO(I,J,KO),RHO(I,J,KN))
C
  395     CONTINUE
C
          DO 400 J=2,NYP1
C      EVALUATE MAXIMUM ADMISSIBLE ANTI-DIFFUSION INTO CELL "MXIN", AND
C      IN TURN CORRECTION FACTOR "RIN"
          DO 400 I=2,NXP1
          TEMP6(I,J)=AMAX1(TEMP5(I,J),TEMP5(I-1,J))
          TEMP6(I,J)=AMAX1(TEMP6(I,J),TEMP5(I+1,J))
          TEMP6(I,J)=AMAX1(TEMP6(I,J),TEMP5(I,J-1))
          RHOMX(I,J)=AMAX1(TEMP6(I,J),TEMP5(I,J+1))
          TEMP6(I,J)=RHOMX(I,J)-RHO(I,J,KN)
          TEMP6(I,J)=TEMP6(I,J)*DXGN(I)
          MXIN(I,J)=TEMP6(I,J)*DYGN(J)
          TEMP6(I,J)=MXIN(I,J)/FLXIN(I,J)
  400     RIN(I,J)=AMIN1(1.0,TEMP6(I,J))
C
          GO TO (415,405) ILMTR
C
  405     CONTINUE
C      IF ZALESAK FLUX LIMITER IS REQUESTED, USE MINIMUM OF OLD AND
C      TRANSPORTED-DIFFUSED DENSITY AS LOWER BOUND FOR NEW DENSITY
          DO 410 J=1,NYP2
          DO 410 I=1,NXP2
  410     TEMP5(I,J)=AMIN1(RHO(I,J,KO),RHO(I,J,KN))
C
  415     CONTINUE
C      EVALUATE MAXIMUM ADMISSIBLE ANTI-DIFFUSION OUT OF CELL "MXOUT",
C      AND IN TURN CORRECTION FACTOR "ROUT"
          DO 420 J=2,NYP1
          DO 420 I=2,NXP1
          TEMP6(I,J)=AMIN1(TEMP5(I,J),TEMP5(I-1,J))
          TEMP6(I,J)=AMIN1(TEMP6(I,J),TEMP5(I+1,J))
          TEMP6(I,J)=AMIN1(TEMP6(I,J),TEMP5(I,J-1))
          RHOMN(I,J)=AMIN1(TEMP6(I,J),TEMP5(I,J+1))
          TEMP6(I,J)=RHO(I,J,KN)-RHOMN(I,J)
          TEMP6(I,J)=TEMP6(I,J)*DXGN(I)
          MXOUT(I,J)=TEMP6(I,J)*DYGN(J)
          TEMP6(I,J)=MXOUT(I,J)/FLXOUT(I,J)
  420     ROUT(I,J)=AMIN1(1.0,TEMP6(I,J))
C
```

```
C       IF A COORDINATE IS NOT PERIODIC, "RIN", ROUT " ARE ASSUMED TO BE
C       CONTINUOUS THROUGH ITS NORMAL BOUNDARY
            DO 430 I=2,NXP1
            RIN(I,1)=RIN(I,JB)
            RIN(I,NYP2)=RIN(I,JT)
            ROUT(I,1)=ROUT(I,JB)
  430       ROUT(I,NYP2)=ROUT(I,JT)
C
            DO 440 J=2,NYP1
            RIN(1,J)=RIN(IL,J)
            RIN(NXP2,J)=RIN(IR,J)
            ROUT(1,J)=ROUT(IL,J)
  440       ROUT(NXP2,J)=ROUT(IR,J)
C
  445       CONTINUE
C
C
C       LIMIT ANTI-DIFFUSION FLUXES USING MINIMUM OF ADJACENT CELLS'
C       MAXIMUM  ADMISSIBLE FLUXES
            DO 450 J=1,NY
            DO 450 I=1,NXP1
            FLX(I,J)=XNTFLX(I,J)
            IFLX(I,J)=LSHF(IFLX(I,J),-31)
            FLX(I,J)=FLOAT(IFLX(I,J))
            RHO(I+1,J+1,KN)=AMIN1(RIN(I,J+1),ROUT(I+1,J+1))
            XFLXCR(I,J)=FLX(I,J)*RHO(I+1,J+1,KN)
            RHO(I+1,J+1,KN)=AMIN1(RIN(I+1,J+1),ROUT(I,J+1))
            FLX(I,J)=1.0-FLX(I,J)
            FLX(I,J)=FLX(I,J)*RHO(I+1,J+1,KN)
            XFLXCR(I,J)=XFLXCR(I,J)+FLX(I,J)
  450       XNTFLX(I,J)=XNTFLX(I,J)*XFLXCR(I,J)
C
            DO 460 J=1,NYP1
            DO 460 I=1,NX
            FLX(I,J)=YNTFLX(I,J)
            IFLX(I,J)=LSHF(IFLX(I,J),-31)
            FLX(I,J)=FLOAT(IFLX(I,J))
            RHO(I+1,J+1,KN)=AMIN1(RIN(I+1,J),ROUT(I+1,J+1))
            YFLXCR(I,J)=FLX(I,J)*RHO(I+1,J+1,KN)
            RHO(I+1,J+1,KN)=AMIN1(RIN(I+1,J+1),ROUT(I+1,J))
            FLX(I,J)=1.0-FLX(I,J)
            FLX(I,J)=FLX(I,J)*RHO(I+1,J+1,KN)
            YFLXCR(I,J)=YFLXCR(I,J)+FLX(I,J)
  460       YNTFLX(I,J)=YNTFLX(I,J)*YFLXCR(I,J)
C
C
```

```
C     ADD CORRECTED ANTI-DIFFUSION FLUXES AND EVALUATE NEW DENSITY
          DO 470 J=1,NY
          DO 470 I=1,NX
          TEMP5(I,J)=XNTFLX(I,J)-XNTFLX(I+1,J)
          TEMP6(I,J)=YNTFLX(I,J)-YNTFLX(I,J+1)
          CELMAS(I,J)=CELMAS(I,J)+TEMP5(I,J)
          CELMAS(I,J)=CELMAS(I,J)+TEMP6(I,J)
          RVOL(I,J)=RDXGN(I+1)*RDYGN(J+1)
  470     RHO(I+1,J+1,KR)=CELMAS(I,J)*RVOL(I,J)
C
C     EVALUATE NEW DENSITY AT BOTTOM AND TOP BOUNDARIES
          DO 490 I=2,NXP1
          RHO(I,1,KR)=BBC(I)*RHO(I,JB,KR)+RHOBBC(I)
  490     RHO(I,NYP2,KR)=TBC(I)*RHO(I,JT,KR)+RHOTBC(I)
C
C     EVALUATE NEW DENSITY AT LEFT AND RIGHT BOUNDARIES
          DO 500 J=2,NYP1
          RHO(1,J,KR)=LBC(J)*RHO(IL,J,KR)+RHOLBC(J)
  500     RHO(NXP2,J,KR)=RBC(J)*RHO(IR,J,KR)+RHORBC(J)
C
          RETURN
C
C
C
```

```
      ENTRY NGRID(XGN,YGN)
C     --------------------
C
C     EVALUATE AVERAGE ( BETWEEN OLD AND NEW ) INTERFACE VELOCITY AND AREA
C     AND NEW AND AVERAGE VOLUME COMPONENTS.
C     IF X-GRID OR Y-GRID IS NOT MOVING, USE ITS OLD VALUES.
C     INTERFACE VOLUME IS CONSIDERED AVERAGE OF ADJACENT CELLS' VOLUMES.
C
C
      GO TO (510,520,530,540,550,560,570) GEOM
C
C
  510 CONTINUE
C
C     CARTESIAN COORDINATES
C
      IF(.NOT.XCHNG) GO TO 513
C
      DO 511 I=1,NXP1
      XG(I)=0.5*(XGN(I)+XGO(I))
  511 DXG(I)=XGN(I)-XGO(I)
C
      DO 512 I=2,NXP1
      DXGN(I)=XGN(I)-XGN(I-1)
      AX(I-1)=XG(I)-XG(I-1)
  512 RDXGN(I)=1.0/DXGN(I)
C
  513 CONTINUE
      IF(.NOT.YCHNG) GO TO 580
C
      DO 516 J=1,NYP1
      YG(J)=0.5*(YGN(J)+YGO(J))
  516 DYG(J)=YGN(J)-YGO(J)
C
      DO 517 J=2,NYP1
      DYGN(J)=YGN(J)-YGN(J-1)
      AY(J-1)=YG(J)-YG(J-1)
  517 RDYGN(J)=1.0/DYGN(J)
C
      GO TO 580
C
  520 CONTINUE
C
C     CYLINDRICAL R-Z COORDINATES
C
      IF(.NOT.XCHNG) GO TO 523
C
      DO 521 I=1,NXP1
      SQO(I)=0.5*(XGO(I)*XGO(I))
      SQN(I)=0.5*(XGN(I)*XGN(I))
      XG(I)=SQN(I)+SQO(I)
      DXG(I)=SQN(I)-SQO(I)
  521 SQ(I)=SQRT(XG(I))
C
```

```
      DO 522 I=2,NXP1
      DXGN(I)=SQN(I)-SQN(I-1)
      AX(I-1)=0.5*(XG(I)-XG(I-1))
  522 RDXGN(I)=1.0/DXGN(I)
C
  523 CONTINUE
      IF(.NOT.YCHNG) GO TO 580
C
      DO 526 J=1,NYP1
      YG(J)=0.5*(YGN(J)+YGO(J))
  526 DYG(J)=YGN(J)-YGO(J)
C
      DO 527 J=2,NYP1
      DYGN(J)=YGN(J)-YGN(J-1)
      AY(J-1)=YG(J)-YG(J-1)
  527 RDYGN(J)=1.0/DYGN(J)
C
      GO TO 580
C
  530 CONTINUE
C     CYLINDRICAL R-FYE COORDINATES
  540 CONTINUE
C     CYLINDRICAL Z-FYE COORDINATES
  550 CONTINUE
C     SPHERICAL R-THETA COORDINATES
  560 CONTINUE
C     SPHERICAL R-FYE COORDINATES
  570 CONTINUE
C     SPHERICAL THETA-FYE COORDINATES
C
      PRINT 70
      STOP
C
```

```
  580     CONTINUE
          IF(.NOT.XCHNG) GO TO 586
C
          DXGN(1)=DXGN(IL)
          DXGN(NXP2)=DXGN(IR)
          RDXGN(1)=RDXGN(IL)
          RDXGN(NXP2)=RDXGN(IR)
C
          DO 585 I=1,NXP1
          DXGNH(I)=0.5*(DXGN(I)+DXGN(I+1))
  585     RDXGNH(I)=0.5*(RDXGN(I)+RDXGN(I+1))
C
  586     CONTINUE
          IF(.NOT.YCHNG) RETURN
C
          DYGN(1)=DYGN(JB)
          DYGN(NYP2)=DYGN(JT)
          RDYGN(1)=RDYGN(JB)
          RDYGN(NYP2)=RDYGN(JT)
C
          DO 590 J=1,NYP1
          DYGNH(J)=0.5*(DYGN(J)+DYGN(J+1))
  590     RDYGNH(J)=0.5*(RDYGN(J)+RDYGN(J+1))
C
          RETURN
C
C
C
```

```
      ENTRY OGRID(XGN,YGN)
C     --------------------
C
C     RESET OLD GRID PARAMETERS, IN PREPARATION FOR A NEW TIME STEP
C
      IF(.NOT.XCHNG) GO TO 593
C
      DO 592 I=1,NXP2
  592 DXGO(I)=DXGN(I)
C
  593 CONTINUE
      IF(.NOT.YCHNG) GO TO 595
C
      DO 594 J=1,NYP2
  594 DYGO(J)=DYGN(J)
C
      GO TO 595
C
C
C
      ENTRY ORIGRD(XGN,YGN)
C     ---------------------
C
C     ORIGINATE THE GRID
C
C     SET DEFAULT : GRID IS MOVING
      XCHNG=.TRUE.
      YCHNG=.TRUE.
C
  595 CONTINUE
      IF(.NOT.XCHNG) GO TO 597
C
      DO 596 I=1,NXP1
  596 XGO(I)=XGN(I)
C
  597 CONTINUE
      IF(.NOT.YCHNG) RETURN
C
      DO 598 J=1,NYP1
  598 YGO(J)=YGN(J)
C
      RETURN
C
C
C
```

```
      ENTRY VOLFLX(U,V,DT)
C     --------------------
C
C     EVALUATE X AND Y VOLUMETRIC FLUX THROUGH INTERFACES
C
C
      DT2=0.5*DT
C
C
      DO 602 J=1,NY
      DO 602 I=1,NXP1
  602 ADUDT(I,J)=U(I,J+1)+U(I+1,J+1)
C
      DO 604 J=1,NYP1
      DO 604 I=1,NX
  604 ADVDT(I,J)=V(I+1,J)+V(I+1,J+1)
C
      GO TO (610,620,630,640,650,660,670) GEOM
C
C
  610 CONTINUE
C
C     CARTESIAN COORDINATES
C
      DO 611 J=1,NY
      DO 611 I=1,NXP1
      ADUDT(I,J)=ADUDT(I,J)*DT2
      ADUDT(I,J)=ADUDT(I,J)-DXG(I)
  611 ADUDT(I,J)=ADUDT(I,J)*AY(J)
C
      DO 612 J=1,NYP1
      DO 612 I=1,NX
      ADVDT(I,J)=ADVDT(I,J)*DT2
      ADVDT(I,J)=ADVDT(I,J)-DYG(J)
  612 ADVDT(I,J)=ADVDT(I,J)*AX(I)
C
      RETURN
C
  620 CONTINUE
C
C     CYLINDRICAL R-Z COORDINATES
C
      DO 621 J=1,NY
      DO 621 I=1,NXP1
      ADUDT(I,J)=ADUDT(I,J)*SQ(I)*DT2
      ADUDT(I,J)=ADUDT(I,J)-DXG(I)
  621 ADUDT(I,J)=ADUDT(I,J)*AY(J)
C
      DO 622 J=1,NYP1
      DO 622 I=1,NX
      ADVDT(I,J)=ADVDT(I,J)*DT2
      ADVDT(I,J)=ADVDT(I,J)-DYG(J)
  622 ADVDT(I,J)=ADVDT(I,J)*AX(I)
C
      RETURN
C
```

```
  630     CONTINUE
C     CYLINDRICAL R-FYE COORDINATES
  640     CONTINUE
C     CYLINDRICAL Z-FYE COORDINATES
  650     CONTINUE
C     SPHERICAL R-THETA COORDINATES
  660     CONTINUE
C     SPHERICAL R-FYE COORDINATES
  670     CONTINUE
C     SPHERICAL THETA-FYE COORDINATES
C
          PRINT 70
          STOP
C
C
C
```

```
      ENTRY SORCES(SRCTYP,SORCE,DT)
C     ------------------------------
C
C     MANAGEMENT OF SOURCE TERM EVALUATION
C
C
      IF(SRCTYP.EQ.BDF) GO TO 750
C
      IF(SRCTYP.EQ.XGRD) GO TO (760,800,999,999,999,999,999) GEOM
      IF(SRCTYP.EQ.YGRD) GO TO (780,780,999,999,999,999,999) GEOM
C
      IF(SRCTYP.EQ.DIV) GO TO (760,950,999,999,999,999,999) GEOM
C
      TEXT(6)=TEXT(18)
      TEXT(7)=TEXT(19)
      TEXT(8)=TEXT(20)
      PRINT 10, (TEXT(I),I=1,11)
C
      STOP
C
C
C
      ENTRY CLRSRC
C     ------------
C
C     CLEAR SOURCE TERM
      LSRC=.FALSE.
      DO 710 J=1,NY
      DO 710 I=1,NX
  710 SOURCE(I,J)=0.
C
      RETURN
C
C
C
      ENTRY BODY(SORCE,DT)
C     --------------------
C
C     EVALUATE  BODY FORCE TYPE SOURCE TERMS
  750 CONTINUE
      LSRC=.TRUE.
C
      DO 755 J=1,NY
      DO 755 I=1,NX
      TEMP3(I,J)=AX(I)*AY(J)
      TEMP4(I,J)=SORCE(I+1,J+1)*DT
      TEMP5(I,J)=TEMP3(I,J)*TEMP4(I,J)
  755 SOURCE(I,J)=SOURCE(I,J)+TEMP5(I,J)
C
      RETURN
C
C
C
```

```
          ENTRY XGRAD(SORCE,DT)
C         ---------------------
C
C     EVALUATE  CARTESIAN X GRADIENT COMPONENT
          SRCTYP=XGRD
  760     CONTINUE
          LSRC=.TRUE.
          DT2=0.5*DT
C
          DO 765 J=1,NY
          DO 765 I=1,NXP1
  765     TEMP3(I,J)=SORCE(I,J+1)+SORCE(I+1,J+1)
C
          DO 770 J=1,NY
          DO 770 I=1,NX
          TEMP4(I,J)=TEMP3(I+1,J)-TEMP3(I,J)
          TEMP5(I,J)=TEMP4(I,J)*AY(J)*DT2
  770     SOURCE(I,J)=SOURCE(I,J)+TEMP5(I,J)
C
          IF(SRCTYP.EQ.DIV) GO TO 780
C
          RETURN
C
C
C
          ENTRY YGRAD(SORCE,DT)
C         ---------------------
C
C     EVALUATE  CARTESIAN Y GRADIENT COMPONENT
  780     CONTINUE
          LSRC=.TRUE.
          DT2=0.5*DT
C
          DO 785 J=1,NYP1
          DO 785 I=1,NX
  785     TEMP3(I,J)=SORCE(I+1,J)+SORCE(I+1,J+1)
C
          DO 790 J=1,NY
          DO 790 I=1,NX
          TEMP4(I,J)=TEMP3(I,J+1)-TEMP3(I,J)
          TEMP5(I,J)=TEMP4(I,J)*AX(I)*DT2
  790     SOURCE(I,J)=SOURCE(I,J)+TEMP5(I,J)
C
          RETURN
C
C
C
```

```
      ENTRY RCGRAD(SORCE,DT)
C     ----------------------
C
C  EVALUATE  CYLINDRICAL R GRADIENT COMPONENT
  800 CONTINUE
      LSRC=.TRUE.
C
      DO 805 J=1,NY
      DO 805 I=1,NXP1
      TEMP3(I,J)=SORCE(I,J+1)+SORCE(I+1,J+1)
      TEMP4(I,J)=SQ(I)*AY(J)*DT
  805 TEMP3(I,J)=0.5*TEMP3(I,J)
C
      DO 810 J=1,NY
      DO 810 I=1,NX
      TEMP3(I,J)=TEMP3(I,J)*TEMP4(I+1,J)
  810 TEMP5(I,J)=TEMP4(I+1,J)-TEMP4(I,J)
C
      DO 815 J=1,NY
      DO 815 I=1,NX
      TEMP4(I,J)=TEMP3(I+1,J)-TEMP3(I,J)
      TEMP5(I,J)=TEMP5(I,J)*SORCE(I+1,J+1)
      SOURCE(I,J)=SOURCE(I,J)+TEMP4(I,J)
  815 SOURCE(I,J)=SOURCE(I,J)+TEMP5(I,J)
C
      RETURN
C
C
C
      ENTRY RCDIV(SORCE,DT)
C     ---------------------
C
C  EVALUATE  CYLINDRICAL DIVERGENCE
  950 CONTINUE
      LSRC=.TRUE.
      DT2=0.5*DT
C
      DO 955 J=1,NY
      DO 955 I=1,NXP1
      TEMP3(I,J)=SORCE(I,J+1)+SORCE(I+1,J+1)
  955 TEMP4(I,J)=SQ(I)*AY(J)*DT2
C
      DO 960 J=1,NY
      DO 960 I=1,NX
      TEMP5(I,J)=TEMP3(I+1,J)-TEMP3(I,J)
      TEMP3(I,J)=TEMP5(I,J)*TEMP4(I+1,J)
  960 SOURCE(I,J)=SOURCE(I,J)+TEMP3(I,J)
C
      GO TO 780
C
      RETURN
C
  999 PRINT 70
      STOP
C
C
C
```

```
      ENTRY SETGOM(GOMTRY,CRD1,CRD2,N1,N2)
C     ------------------------------------
C
C     SET AND CHECK REQUEST FOR A PARTICULAR GEOMETRY
C
C
      GEOM=0
C
      IF(GOMTRY.EQ.TGM(1)) GEOM=1
C
      IF(GOMTRY.NE.TGM(2)) GO TO 1210
      IF(CRD1.NE.TCRD(4)) GO TO 1205
      IF(CRD2.EQ.TCRD(3)) GEOM=2
      IF(CRD2.EQ.TCRD(6)) GEOM=3
 1205 CONTINUE
      IF(CRD1.EQ.TCRD(3).AND.CRD2.EQ.TCRD(6)) GEOM=4
C
 1210 CONTINUE
      IF(GOMTRY.NE.TGM(3)) GO TO 1220
      IF(CRD1.NE.TCRD(4)) GO TO 1215
      IF(CRD2.EQ.TCRD(5)) GEOM=5
      IF(CRD2.EQ.TCRD(6)) GEOM=6
 1215 CONTINUE
      IF(CRD1.EQ.TCRD(5).AND.CRD2.EQ.TCRD(6)) GEOM=7
C
 1220 CONTINUE
      IF(GEOM.GT.0) GO TO 1225
C
C     ISSUE AN ERROR MESSAGE UPON REQUEST OF AN UNRECOGNIZED GEOMETRY
C     AND STOP
      TEXT(6)=TEXT(12)
      TEXT(7)=TEXT(13)
      TEXT(8)=TEXT(14)
      PRINT 10, (TEXT(I),I=1,11)
C
      STOP
C
 1225 CONTINUE
C
C
      NX=N1
      NXP1=NX+1
      NXP2=NX+2
C
      NY=N2
      NYP1=NY+1
      NYP2=NY+2
C
      XPRDC=.FALSE.
      IL=2
      IR=NXP1
C
      YPRDC=.FALSE.
      JB=2
      JT=NYP1
C
      LSRC=.FALSE.
C
```

```
C      SET DEFAULT : ALL BOUNDARIES ASSUMED PERMEABLE
            DO 1226 I=1,NXP2
            PRMBLB(I)=1.0
 1226       PRMBLT(I)=1.0
C
            DO 1227 J=1,NYP2
            PRMBLL(J)=1.0
 1227       PRMBLR(J)=1.0
C
            PRINT 30
C
            RETURN
C
C
C
```

```
          ENTRY PRODIC(CRDNT,CRD)
C         -----------------------
C
C     IDENTIFY X OR Y COORDINATE AS PERIODIC
C
C
          IF(CRDNT.NE.1) GO TO 1230
C
          XPRDC=.TRUE.
          IR=2
          IL=NXP1
C
          PRINT 40, CRD
C
 1230     CONTINUE
          IF(CRDNT.NE.2) GO TO 1240
C
          YPRDC=.TRUE.
          JT=2
          JB=NYP1
C
          PRINT 40, CRD
C
 1240     CONTINUE
          IF(CRD.EQ.TCRD(4).OR.CRD.EQ.TCRD(5)) PRINT 20,CRD
C
          RETURN
C
C
C
```

```
      ENTRY SETLMT(LMTR1,LMTR2)
C     -------------------------
C
C     SET AND CHECK REQUEST FOR A PARTICULAR FLUX LIMITER
C
C
      DO 1255 I=1,4
C
      DO 1251 J=1,2
      IF(LMTR1(J).NE.TLM1(J,I)) GO TO 1255
 1251 CONTINUE
C
      DO 1252 J=1,2
      IF(LMTR2(J).NE.TLM2(J,I)) GO TO 1255
 1252 CONTINUE
C
      GO TO 1260
C
 1255 CONTINUE
C
C     ISSUE AN ERROR MESSAGE UPON REQUEST OF AN UNRECOGNIZED FLUX
C     LIMITER AND STOP
      TEXT(6)=TEXT(15)
      TEXT(7)=TEXT(16)
      TEXT(8)=TEXT(17)
      PRINT 10, (TEXT(I),I=1,11)
C
      STOP
C
 1260 CONTINUE
      ILMTR=I
C
      RETURN
C
C
C
```

```
      ENTRY FIXGRD(CRDNT,CRD)
C     -----------------------
C
C     LABEL X OR Y GRID AS FIXED
C
C
      IF(CRDNT.NE.1) GO TO 1265
C
      XCHNG=.FALSE.
      PRINT 50, CRD
C
 1265 CONTINUE
      IF(CRDNT.NE.2) GO TO 1270
C
      YCHNG=.FALSE.
      PRINT 50, CRD
C
 1270 CONTINUE
      RETURN
C
C
C
```

```
      ENTRY SOLDFY(BONDRY,KSTRT,KEND)
C     -------------------------------
C
C     CANCEL  THE DIFFUSION AND ANTI-DIFFUSION FLUXES THROUGH PATCHES
C     OF BOUNDARY INTERFACES
C
C
      IF(BONDRY.NE.TBND(1)) GO TO 1280
C
      DO 1275 J=KSTRT,KEND
 1275 PRMBLL(J)=0.
C
      PRINT 60, BONDRY,KSTRT,KEND
C
 1280 CONTINUE
      IF(BONDRY.NE.TBND(2)) GO TO 1290
C
      DO 1285 J=KSTRT,KEND
 1285 PRMBLR(J)=0.
C
      PRINT 60, BONDRY,KSTRT,KEND
C
 1290 CONTINUE
      IF(BONDRY.NE.TBND(3)) GO TO 1300
C
      DO 1295 I=KSTRT,KEND
 1295 PRMBLB(I)=0.
C
      PRINT 60, BONDRY,KSTRT,KEND
C
 1300 CONTINUE
      IF(BONDRY.NE.TBND(4)) GO TO 1310
C
      DO 1305 I=KSTRT,KEND
 1305 PRMBLT(I)=0.
C
      PRINT 60, BONDRY,KSTRT,KEND
C
 1310 CONTINUE
      RETURN
C
C
C
      END
```

```
      SUBROUTINE NUMU(NI,NJ,EPS,NUV,MUV)
C
C     EVALUATE  DIFFUSION AND ANTI-DIFFUSION COEFFICIENTS
C
      PARAMETER      NPX=100,NPY=100
      PARAMETER      NP1X=NPX+1,NP1Y=NPY+1
      PARAMETER      NP2X=NPX+2,NP2Y=NPY+2
C
      REAL      EPS(NP1X,NP1Y),NUV(NP2X,NP2Y),MUV(NP2X,NP2Y)
C
      DO 100 J=1,NJ
      DO 100 I=1,NI
      EPS(I,J)=EPS(I,J)*EPS(I,J)
      NUV(I,J)=0.333333*EPS(I,J)
      NUV(I,J)=0.166667+NUV(I,J)
  100 MUV(I,J)=NUV(I,J)-EPS(I,J)
C
      RETURN
      END
```