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On the Principal Axes of Diffusion in Difference Schemes for 2D Transport Problems*

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Via Taylor series, we associate with a difference stencil L^h approximating $Lu := au_x + bu_y$ its modified equation: $L^h u = Lu + (h/2)\{Au_{xx} + 2Bu_{xy} + Cu_{yy}\} + O(h^2)$. By rotating axes to eliminate the $2Bu_{xy}$ term, the principle axes through which the diffusion in L^h acts is calculated. Interestingly, for many schemes proposed for 2D transport problems these axes have little to do with the "streamline" and "crosswind" directions of the continuous problem. Several examples are considered from this point of view. © 1990 Academic Press, Inc.

1. INTRODUCTION

The behavior of numerical methods in the solution of convection–diffusion problems and conservation laws is quite well understood in one space dimension (e.g., [1, 4, 5, 10, 13, 18, 19]). However, it is a continuing challenge to find the correct method for using these insights when designing schemes for *multi*-dimensional transport and slightly diffusive transport problems. Many possible extensions of 1D methods have been proposed. The goal of this report is to show that the leading order diffusive effects in these methods can be compared by means of a few simple calculations from the theory of *modified equations* [6, 20]. In particular, given a criteria one wishes in a method, one can frequently design a method with this criteria in mind, compare existing methods w.r.t. this criteria, or use the analysis to optimize the selection of undetermined parameters in a given method.

As an application in Section 2, we define and study the *principal axes of diffusion* which give the directions of the leading order diffusive effects in difference schemes for 2D transport problems and compare these in known schemes with the streamline and crosswind directions.

It is desirable that these axes are aligned with the streamline and crosswind directions for several reasons. The first reason is alignment of these axes with respect to the streamline and crosswind directions helps control the leading order grid orientation effects, which can cause major difficulties in complex transport problems,

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Ewing [23]. Also, it is well documented that excessive smearing of fronts which are skew to the mesh is associated with some types of artificial diffusion, see e.g., Brooks and Hughes [21, Figs. 3.6, p. 218; 3.7, p. 219; 3.1, p. 208], Leonard [22], and Masenge [24, Chap. 4]. Thus, it is desirable to have a clear description of the magnitude and action of the artificial diffusion which is implicit in various methods. Ideally, one wishes to restrict its magnitude as well as control its principal axes.

Section 3 compares these axes with the streamline and cross-wind directions for a number of schemes proposed for 2D transport problems. This comparison was expedited by the work of Roos [16] who collected and compared a number of such schemes with respect to sufficient conditions for uniform-in-ε convergence for 2D convection–diffusion equations.

2. Principal Axes of Diffusion

Given the transport operator $Lu = au_x + bu_y$, we consider a 9-point box type finite difference operator L^h which can be represented as the following 3×3 matrix

$$L^h \approx h^{-1} \begin{bmatrix} -a_{nw} & -a_n & -a_{ne} \\ -a_w & a_p & -a_e \\ -a_{sw} & -a_s & -a_{se} \end{bmatrix}.$$

Note that this is scaled so that $a_n a_s$, etc. are $O(1)$. Assume that L^h is consistent with L: for smooth functions $u(x, y)$

$$L^h u(x, y) = Lu(x, y) + O(h). \tag{2.1}$$

Equation (2.1) places the following restrictions on the coefficients:

$$\begin{aligned} a_p &= a_n + a_s + a_e + a_w + a_{ne} + a_{sw} + a_{se} + a_{nw} \\ a_e - a_w + a_{ne} + a_{se} - a_{sw} - a_{nw} &= -a \\ a_n - a_s + a_{ne} - a_{se} - a_{sw} + a_{nw} &= -b, \end{aligned} \tag{2.2}$$

where h is the mesh spacing, which is assumed here to be uniform. Indeed, by carrying out the Taylor series to one more term we obtain

Lemma 2.1. *For smooth functions* $u(x, y)$

$$L^h u(x, y) = Lu(x, y) - \frac{h}{2} \{Au_{xx} + 2Bu_{xy} + Cu_{yy}\} + O(h^2), \tag{2.3}$$

where

$$\begin{aligned} A &= a_e + a_w + a_{ne} + a_{sw} + a_{se} + a_{nw}, \\ B &= a_{ne} + a_{sw} - a_{se} - a_{nw}, \\ C &= a_n + a_s + a_{ne} + a_{sw} + a_{se} + a_{nw}. \quad \blacksquare \end{aligned} \tag{2.4}$$

Thus, the leading order effects of diffusion in the scheme L^h are described through the operator:

$$Eu := Au_{xx} + 2Bu_{xy} + Cu_{yy}. \tag{2.5}$$

In the examples we consider E is (possibly degenerate) elliptic:

$$B^2 \leqslant AC. \tag{2.6}$$

In fact, for positive type schemes much more can be said. We quote one result:

PROPOSITION (Layton [14]). *Suppose L^h is a positive type, i.e., $a_p > 0$, and a_n, a_s, a_e, a_w, a_{ne}, a_{sw}, a_{nw}, a_s are all nonnegative (or $-L^h$ is of positive type). Then (2.6) holds, in fact, $B \leqslant \min\{A, C\}$.*

Schematically this is represented by Fig. 1

To analyze E we preform the obvious step of rotating axes to eliminate the $2Bu_{xy}$ term. Indeed, defining Θ^h via:

$$\tan(2\Theta^h) = \frac{2B}{A - C} = \frac{2(a_{ne} + a_{sw} - a_{se} - a_{nw})}{a_e + a_w - a_n - a_s}, \qquad 0 \leqslant \Theta^h < \pi/2,\ A \neq C. \tag{2.8}$$

We rotate axes through angle Θ^h, under which E reduces to $Eu = Au_{xx} + 2Bu_{xy} + Cu_{yy}$, $Eu = \tilde{A}u_{\tilde{x}\tilde{x}} + \tilde{C}u_{\tilde{y}\tilde{y}}$ (see Fig. 2).

DEFINITION 2.1. The $\tilde{x} - \tilde{y}$ axes are the *principal axes of diffusion* for L^h. If $\tilde{A} > \tilde{C}$ (resp. $<$) then $\tilde{x}$ (resp. $\tilde{y}$) is the *major axis of diffusion* (resp. $\tilde{x}$) is *minor axis of diffusion.*

One interest in the principal axes of diffusion lies in the fact that for some proposed schemes they *do not coincide* with the streamline and crosswind directions. This can be enforced in others through appropriate selection of parameters.

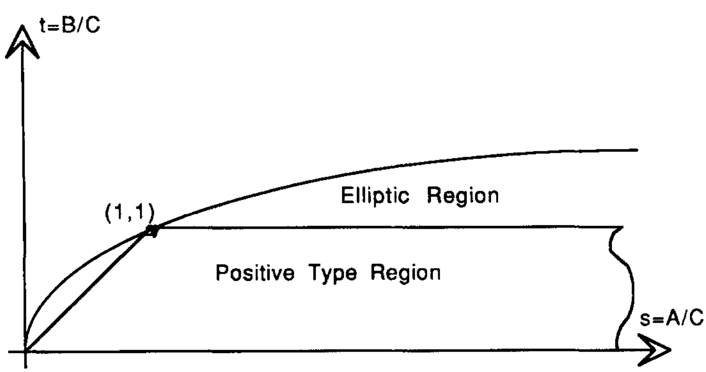

FIGURE 1

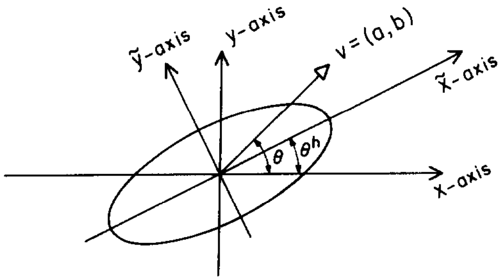

FIGURE 2. Analysis of quadratic form associated with operator E.

Another interest in the principal axes of diffusion is that they describe the leading order diffusive effects in a very precise sense. Indeed, the solution of the continuous "modified equation" can be shown to be a higher order model of the approximate solution than is the solution of the continuous problem $u(x, y)$. (This result is similar in spirit to ones for modified equations used in other contexts see, e.g., Hedstrom [6] and Trefethen [20].) To be precise, let u, w be the solutions of, respectively,

$$L_\varepsilon u = f(x, y) \quad \text{in} \quad \Omega = [0, 1] \times [0, 1], \qquad u = g(x, y) \quad \text{on } \partial\Omega,$$

$$-\varepsilon\, \Delta w - \frac{h}{2}\{A w_{xx} + 2B w_{xy} + C w_{yy}\} + a w_x + b w_y = f(x, y) \quad \text{in } \Omega,$$

$$w = g \quad \text{on } \partial\Omega,$$

where A, B, C are constructed from the uniform mesh, consistent, 9-point box discretization L_ε^h of L_ε as described above. Then, one can prove, for example, by standard techniques.

PROPOSITION 2.1. (1) *Suppose f, g are continuous and, $B^2 < AC$ then w exists and is unique.* (2) *Suppose u and w exist, are sufficiently smooth, and L_ε^h is a positive type discretization of L_ε. Then,*

$$\max_{(x_i, y_j)} |u_{i,j} - u(x_i, y_j)| \leqslant C(u) h,$$

whereas

$$\max_{(x_i, y_j)} |u_{ij} - w(x_i, y_j)| \leqslant C(w) h^2.$$

(3) *If the discretization matrix arising from L_ε^h has inverse uniformly bounded in some operator norm, $\|\cdot\|$, and u and w are sufficiently smooth, then*

$$\|u_{ij} - u(x_i, y_j)\| \leqslant C(u) h,$$

whereas

$$\|u_{ij} - w(x_i, y_j)\| \leqslant C(w)h^2.$$

Before we consider examples, we enumerate three degenerate cases, which include *first-order upwind methods* and *streamline diffusion type methods.*

Case 1 (no preferred direction). $\tilde{A} = \tilde{C}$, or $B = 0$, $A = C$, in which case $Eu = \text{constant}^* \, \Delta u$ and the diffusion acts uniformly in all directions. One example is the usual first-order upwind method (Example 1).

Case 2 (pure streamline diffusion). $B^2 = AC$. In this case there is a $\mathbf{v}^h = (a^h, b^h)$ for which $Eu = \mathbf{v}^h \cdot \text{grad}[\mathbf{v}^h \cdot \text{grad}\, u]$. When $\mathbf{v}^h$ can be chosen to be (a, b) then this is a pure streamline diffusion method [8, 4] (i.e., when $\Theta^h = \Theta := \arctan(b/a)$).

Case 3. $E \equiv 0$. In this case L^h is at least formally second-order accurate and the third-order dispersive effects will predominate. The Taylor series analysis must be carried out to one or two extra terms. This is also the case of some accurate implementations of streamline diffusion methods.

3. Examples

We now survey a number of methods that have been proposed for the convection diffusion problem (we shall retain the choice of sign, plus or minus, multiplying ε of the original derivation of L^h_ε as this will not influence the subsequent analysis):

$$L_\varepsilon u := \pm \varepsilon \, \Delta u + a u_x + b u_y = f(x, y).$$

We set $\varepsilon = 0$ in these schemes and calculate Θ^h. Remarkably, for many schemes $\Theta^h \neq \Theta := \arctan(b/a))$ and, in fact, $\Theta^h - \Theta$ is bounded away from zero as $h \to 0$. For other schemes, it is, however, possible to adjust free parameters to have $\Theta^h \equiv \Theta$. We can check when $\Theta^h = \Theta$ directly from the stencil by noting (when $a \neq b$)

$$\tan(2\Theta) = \frac{2 \tan \Theta}{1 - \tan^2 \Theta} = \frac{2ab}{a^2 - b^2}. \tag{3.1}$$

Thus, we calculate from (3.1), (2.8):

$$\tan(2\Theta^h) - \tan(2\Theta) = \frac{2(a_{ne} + a_{sw} - a_{se} - a_{nw})}{a_e + a_w - a_n - a_s} - \frac{2ab}{a^2 - b^2}. \tag{3.2}$$

Example 1. *Upwind finite difference methods.* L^h is represented by ($-1 \leqslant \alpha \leqslant +1$, $-1 \leqslant \beta \leqslant +1$, and the minus sign for ε)

$$\begin{bmatrix} \cdot & \frac{b}{2}(1+\beta)-\frac{\varepsilon}{h} & \cdot \\ (-1+\alpha)\frac{a}{2}-\frac{\varepsilon}{h} & -2\beta\frac{b}{2}-2\alpha\frac{a}{2}+4\frac{\varepsilon}{h} & \frac{a}{2}(1+\alpha)-\frac{\varepsilon}{h} \\ \cdot & \frac{b}{2}(-1+\beta)-\frac{\varepsilon}{h} & \cdot \end{bmatrix}, \tag{3.3}$$

where α, β are parameters, which are frequently chosen to make (3.3) exact on, e.g., exponentials, Kellogg [12], Roos [16], and to ensure that L^h is of positive (or negative) type.

We calculate directly that $B=0$ so that the principal axes of upwind methods are always the mesh-directions. When $\alpha=\beta=-1$ (pure upwind) it follows that $Eu=\text{const.}\cdot\Delta u$ so that, as is well known, the diffusion in pure upwind methods acts globally without preferred directions.

EXAMPLE 2. *A skew-upwind scheme* (proposed by Raithby [15]). Taking $a>0$, $b>0$, and the minus sign for ε, the stencil is given by

$$+\frac{\varepsilon}{h}\begin{bmatrix} \cdot & -1 & \cdot \\ -1 & 4 & -1 \\ \cdot & -1 & \cdot \end{bmatrix}+\frac{a}{2}\begin{bmatrix} \cdot & \cdot & \cdot \\ -1 & 1 & \cdot \\ -1 & +1 & \cdot \end{bmatrix}+\frac{b}{2}\begin{bmatrix} \cdot & \cdot & \cdot \\ 1 & 1 & \cdot \\ -1 & -1 & \cdot \end{bmatrix}. \tag{3.4}$$

We calculate from (3.4) and L^h that $\Theta^h-\Theta=0$ if and only if $(a+b)/(a-b)=2ab/(a^2-b^2)$. Hence, *scheme* (3.4) *has the correct principal axes of diffusion if and only if* $a=b\neq 0$, $a=0$, *or* $b=0$.

EXAMPLE 3. *A weighted Bubnov–Galerkin scheme* (proposed in Heinrich and Zienkiewicz [7]). With α, β free parameters, using linear shape functions and quadratic weights with an additive perturbation on a uniform mesh gives a stencil represented by (taking the plus sign for ε)

$$\begin{aligned} &-\frac{\varepsilon}{h}\left\{\frac{1}{3}\begin{bmatrix} -1 & -1 & -1 \\ -1 & 8 & -1 \\ -1 & -1 & -1 \end{bmatrix}-\frac{\alpha}{4}\begin{bmatrix} -1 & \cdot & +1 \\ 2 & \cdot & -2 \\ -1 & \cdot & 1 \end{bmatrix}-\frac{\beta}{4}\begin{bmatrix} +1 & -2 & 1 \\ \cdot & \cdot & \cdot \\ -1 & 2 & -1 \end{bmatrix}\right\} \\ &+a\left\{\frac{1}{12}\begin{bmatrix} -1 & \cdot & 1 \\ -4 & \cdot & 4 \\ -1 & \cdot & 1 \end{bmatrix}-\frac{\beta}{8}\begin{bmatrix} 1 & \cdot & -1 \\ \cdot & \cdot & \cdot \\ -1 & \cdot & 1 \end{bmatrix}-\frac{\alpha}{12}\begin{bmatrix} -1 & 2 & -1 \\ -4 & 8 & -4 \\ -1 & 2 & -1 \end{bmatrix}\right\} \\ &+b\left\{\frac{1}{12}\begin{bmatrix} 1 & 4 & 1 \\ \cdot & \cdot & \cdot \\ -1 & -4 & -1 \end{bmatrix}-\frac{\alpha}{8}\begin{bmatrix} 1 & \cdot & -1 \\ \cdot & \cdot & \cdot \\ -1 & \cdot & 1 \end{bmatrix}-\frac{\beta}{12}\begin{bmatrix} -1 & -4 & -1 \\ 2 & 8 & 2 \\ -1 & -4 & -1 \end{bmatrix}\right\}. \end{aligned} \tag{3.5}$$

We calculate (and simplify)

$$\tan(2\Theta^h)=\frac{a\beta+\alpha b}{a\alpha-b\beta}.$$

Thus, the scheme (3.5) *has the correct principal axes of diffusion provided* α, β *are chosen so that*

$$\frac{2ab}{a^2-b^2}=\frac{a\beta+\alpha b}{a\alpha-b\beta}$$

(alternately, with $t=a/b$, $\alpha=(2t/(t^2-1))(t-\beta)+t$). One obvious choice is $\alpha=a$, $\beta=b$.

EXAMPLE 4. *A realigned skew upwind scheme.* The skew upwind scheme can be modified to realign it with the streamlines, as follows. The discretization is represented by ($a\geqslant 0$, $b\geqslant 0$, and the minus sign for ε)

$$\begin{aligned}&-\frac{\varepsilon}{h}\begin{bmatrix}0 & -1 & 0\\ -1 & 4 & -1\\ 0 & -1 & 0\end{bmatrix}\\ &+a\begin{bmatrix}\cdot & \cdot & \cdot\\ -\alpha & \alpha & \cdot\\ -(1-\alpha) & (1-\alpha) & \cdot\end{bmatrix}+b\begin{bmatrix}\cdot & \cdot & \cdot\\ (1-\beta) & \beta & \cdot\\ -(1-\beta) & -\beta & \cdot\end{bmatrix}.\end{aligned} \tag{3.6}$$

Here α, β are chosen to realign the scheme by requiring $\Theta^h=\Theta$ as follows:

$$\tan(2\Theta^h)=2\,\frac{a(1-\alpha)+b(1-\beta)}{a-b}.$$

Requiring that $\Theta^h=\Theta$, restricts the parameters to

$$\beta=1-\frac{a}{a+b}+\frac{a}{b}(1-\alpha), \tag{3.7}$$

which realigns the skew upstream method. Interestingly, with this choice of parameters the realigned skew upwind scheme becomes a positive type scheme! Its stencil is represented by

$$-\frac{\varepsilon}{h}\begin{bmatrix}\cdot & -1 & \cdot\\ -1 & 4 & -1\\ \cdot & -1 & \cdot\end{bmatrix}+\begin{bmatrix}\cdot & \cdot & \cdot\\ \dfrac{-a^2}{a+b} & \dfrac{a^2+ab+b^2}{a+b} & \cdot\\ -\dfrac{ab}{a+b} & \dfrac{-b^2}{a+b} & \cdot\end{bmatrix}.$$

EXAMPLE 5. *Upwind finite element scheme* (due to Tabata [17]). Let $\bar{\Omega} = [0, 1] \times [0, 1]$ is divided into uniform rectangles and then subdivided into triangles by lines with slope 1. Using C^0 piecewise linear shape functions and the centroids of the triangles to produce the "dual" domain in Tabata's procedure yields a stencil of the form (when $a \geqslant 2b > 0$ and the plus sign for ε)

$$-\frac{\varepsilon}{h}\begin{bmatrix} \cdot & -1 & \cdot \\ -1 & 4 & -1 \\ \cdot & -1 & \cdot \end{bmatrix} + \frac{1}{3}\begin{bmatrix} \cdot & a-2b & a+b \\ \cdot & 3(b-a) & \cdot \\ \cdot & a-2b & \cdot \end{bmatrix}, \qquad (a \geqslant 2b).$$

We compute

$$\tan(2\Theta^h) = \frac{a+b}{2b-a}.$$

In this case $\Theta^h = \Theta$ if and only if $t = a/b$;

$$P(t) := t^3 + 8t^2 - 5t - 1 = 0.$$

It is straightforward to check that $\Theta^h = \Theta$ *for only one value of* Θ *in the interval* $0 \leqslant a \leqslant 2b$. *For all other choices of* (a, b), $\Theta^h \neq \Theta$. *Thus, this scheme is not aligned with the streamline directions in general.*

EXAMPLE 6. *Upwind Bubnov–Galerkin F.E.M.* Using triangular elements, linear shape functions, and quadratic weights, the upwind F.E.M. of Huyakorn [9] gives a stencil of the form (taking the plus sign for ε)

$$\begin{aligned}
-\frac{\varepsilon}{h}&\left\{\begin{bmatrix} \cdot & -1 & \cdot \\ -1 & 4 & -1 \\ \cdot & -1 & \cdot \end{bmatrix} + \frac{1}{2}(\alpha_1+\alpha_2+2\alpha_3)\begin{bmatrix} \cdot & -1 & 1 \\ 1 & \cdot & -1 \\ -1 & 1 & \cdot \end{bmatrix}\right\} \\
&+ a\left\{\frac{1}{6}\begin{bmatrix} \cdot & -1 & 1 \\ -2 & \cdot & 2 \\ -1 & 1 & \cdot \end{bmatrix} + \frac{\alpha_1}{4}\begin{bmatrix} \cdot & \cdot & \cdot \\ -1 & 2 & -1 \\ \cdot & \cdot & \cdot \end{bmatrix} + \frac{\alpha_2}{8}\begin{bmatrix} \cdot & 1 & -1 \\ -1 & 2 & -1 \\ -1 & 1 & \cdot \end{bmatrix}\right. \\
&\left. + \frac{\alpha_3}{8}\begin{bmatrix} \cdot & -1 & 1 \\ 1 & -2 & 1 \\ 1 & -1 & \cdot \end{bmatrix}\right\} + b\left\{\frac{1}{6}\begin{bmatrix} \cdot & 2 & +1 \\ 1 & \cdot & -1 \\ -1 & -2 & \cdot \end{bmatrix}\right. \\
&\left. + \frac{\alpha_1}{8}\begin{bmatrix} \cdot & 1 & -1 \\ 1 & -2 & 1 \\ -1 & 1 & \cdot \end{bmatrix} + \frac{\alpha_2}{4}\begin{bmatrix} \cdot & -1 & \cdot \\ \cdot & 2 & \cdot \\ \cdot & -1 & \cdot \end{bmatrix} + \frac{\alpha_3}{8}\begin{bmatrix} \cdot & 1 & 1 \\ -1 & -2 & -1 \\ 1 & 1 & \cdot \end{bmatrix}\right\}.
\end{aligned} \tag{3.8}$$

Thus, after a calculation, we conclude:

$$\tan(2\Theta^h) = \frac{a\alpha_2 - a\alpha_3 + b\alpha_1 - b\alpha_3}{a\alpha_2 - a\alpha_3 - b\alpha_2 + b\alpha_3 + a\alpha_1}.$$

Requiring $\Theta^h = \Theta$ gives the equation

$$\frac{a(\alpha_2 - \alpha_3) + b(\alpha_1 - \alpha_3)}{a(\alpha_1 + \alpha_2 - \alpha_3) - b(\alpha_2 - \alpha_3)} = \frac{2ab}{a^2 - b^2},$$

which yields the linear constraint on $\alpha_{1,2,3}$:

$$\alpha_1(a^2b - b^3 - 2a^2b) + \alpha_2(a^3 + ab^2 - 2a^2b) + \alpha_3(a^3 - 3ab^2 + a^2 + b^3) = 0. \quad (3.9)$$

Thus, provided the parameters $\alpha_{1,2,3}$ *are chosen so that* (3.9) *holds, the principal axes of diffusion of* (3.8) *are aligned with the streamlines.*

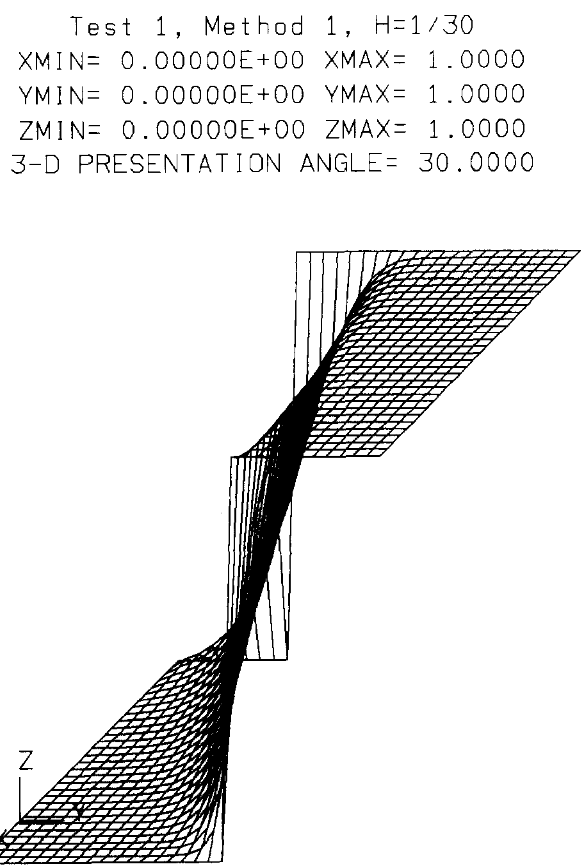

FIG. 3. First-order upwind outflow is at rear of figure.

4. An Illustration

We consider the slightly diffusive transport problem of Section 3 with $a = \cos(17.5°)$, $b = \sin(17.5°)$, and $f = 0$. The square is divided by a characteristic line through (0,0.3) with slope b/a. Boundary conditions are taken to be $u = 1$ above the line and $u = 0$ below the line so that the exact solution is a step function with a sharp transition layer along the distinguished characteristic. Figures 3, 4, and 5 are plots of the numerical solution of this B.V.P. with $h = \frac{1}{30}$, $\varepsilon = h^2$ using, respectively, first-order upwind, Raithby's skew upwind, and the realigned skew upwind scheme. In Fig. 3 we take the plus sign for ε and the minus sign in Figs. 4 and 5. Note that the "outflow" side of the step is the back (y-axis) in Fig. 3 and the front ($x = 1$, $0 \leqslant y \leqslant 1$) in Figs. 4 and 5.

The realigned skew upwind scheme happens to be a positive type method so it is subject to the crosswind diffusion implicit in all positive type schemes (see Fig. 1)

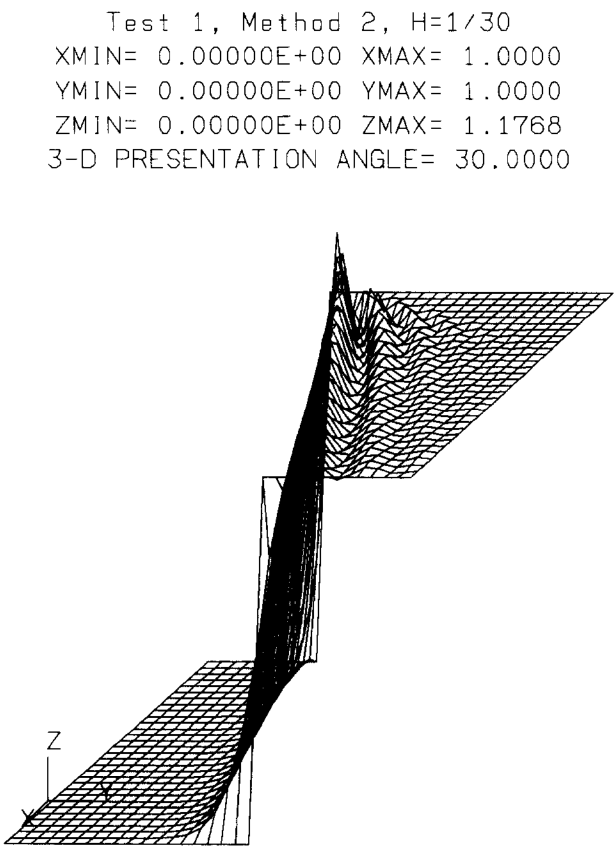

Fig. 4. Skew upwind scheme outflow is at front of figure.

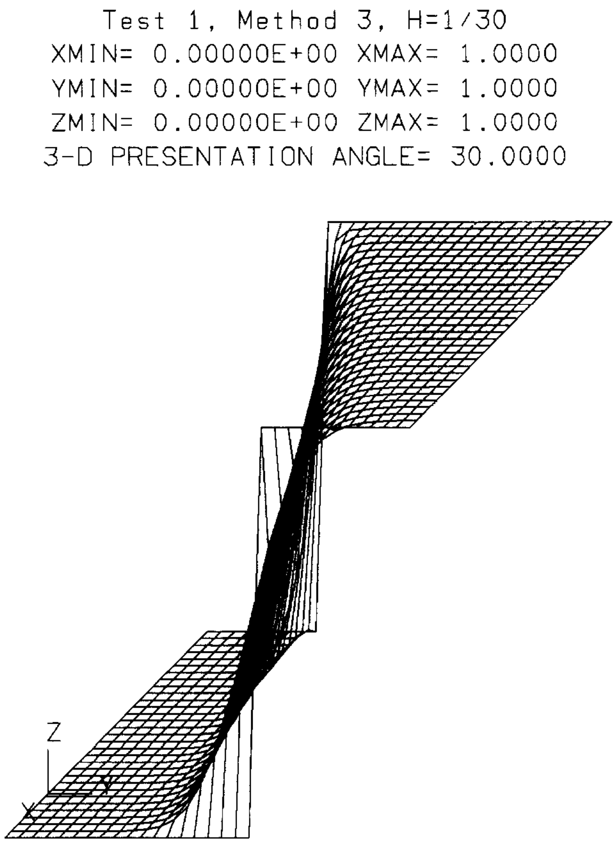

FIG. 5. Realigned skew upwind outflow is at front of figure.

Raithby's scheme (Fig. 4) is not of positive type, so it suffers oscillations near the transition region.

The realigned skew upwind scheme is, in some sense, intermediate between Raithby's scheme and first-order upwind. Namely, it does not smear the front nearly as much as first-order upwind—compare the outflow boundaries in Figs. 3 ($x = 0$) and 5 ($x = 1$). On the other hand, it is also a positive type scheme so its stability properties are better than Raithby's scheme.

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