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Performance of Five-Point Differencing Schemes for Two-Dimensional Fluid Transport Equations

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Sample exact solutions sweeping the Fourier spectrum of the steady-state, two-dimensional, constant coefficients, homogeneous linear equation for the convective and diffusive transport of a conserved property in fluid media are used as test cases for a comparative study of four numerical discretization schemes: central differencing, upwind scheme, and the exponential schemes due to Allen and Southwell and Dennis and Hudson. The generality provided by this method allows a discussion on the concept of numerical diffusion in multi-dimensional problems, which identifies the upwind and other schemes' errors with the angle between the flow and the grid. © 1992 Academic Press, Inc.

1. INTRODUCTION

A number of questions common to the numerical solution of a broad set of convective and diffusive fluid transport equations can be considered with recourse to one of the simplest forms: the steady-state, two-dimensional, constant coefficients, homogeneous linear equation,

$$u\frac{\partial\phi}{\partial x}+v\frac{\partial\phi}{\partial y}-\alpha\left(\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}\right)=0, \tag{1}$$

where u and v are, respectively, x- and y-direction velocity components, ϕ represents an intensive property such as temperature or concentration, and α is the appropriate diffusivity. Equation (1) can also be seen as a linearized homogeneous form of momentum or vorticity equations for viscous flows, considering ϕ as a velocity component or vorticity and α as the kinematic viscosity.

The discretization of both terms by the second-order central differencing leads to non-diagonally dominant matrices when one of the cell Peclet (or Reynolds) numbers is greater than 2 in absolute terms. If the system is solved iteratively the lack of diagonal dominance causes possible numerical instability, which can sometimes be avoided by using relaxation factors at the cost of slow convergence. For much higher cell Peclet numbers the matrix approaches a singular case, so that even direct solution methods are unstable or inaccurate.

Diagonally dominant matrices are obtained with the central differencing for the diffusive terms and the upwind scheme for the convective ones [1], introducing a first-order error often referred to as numerical diffusion for its proportionality to the second derivative. This is small in some cases (particularly boundary layer regions without strong adverse pressure gradients when one of the numerical axes is parallel to the main flow direction), but tends to increase in other situations (especially recirculating regions).

The performance of the upwind scheme in some standard test cases, such as the convective transport of a scalar with cross-flow step distribution, the solid-like rotating annular space, and the boundary layer transport of a scalar with Gaussian distribution, have led to the widespread view that, in the absence of strong transient or source terms, the upwind scheme's numerical diffusion is essentially associated with the angle between grid and flow, being negligible for flows parallel to the grid and maximum for flows inclined at 45° [2].

The limitations of classic central and upwind schemes in finite differencing, which are shared by most common finite element schemes, explain the need for investigating alternative procedures, here limited to 2 five-node exponential schemes, both second order and diagonally dominant.

The first was proposed by D. N. de G. Allen for solving the vorticity transport equation in a paper co-signed by R. S. Southwell [3]. The so-called Allen and Southwell scheme may be described on the basis of an exponential interpolating curve for each coordinate, say the x-direction, generated as a solution to the equation

$$u\frac{d\phi}{dx}-\alpha\frac{d^2\phi}{dx^2}=K, \tag{2}$$

which can be seen as a one-dimensional approximation to Eq. (1) if its y-derivatives are assumed locally constant. The

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exponential solution is fitted to the three x-direction nodes $(i-1, j)$, (i, j), and $(i+1, j)$.

The scheme was later extended to other equations [4]. Many reinventions and variations of the scheme appeared afterwards [5–7]. Despite its quadratic rate of spatial convergence, the Allen and Southwell scheme was said to present accuracy problems similar to those of the upwind [8].

The second exponential scheme is Dennis and Hudson's five-point scheme embodied in Eq. (13) of their paper [9]. It is based on an approximated one-dimensional form coinciding with (2) for the present case, although in general coefficients are allowed to vary. Variable ϕ is submitted to an exponential transformation, turning (2) into a Poisson-type equation. This is discretized by central differencing and then back transformed.

These authors also present a more accurate, fourth-order scheme obtained with a deferred correction term, which is not considered here, being a nine-node scheme.

Both exponential schemes will be compared to classic upwind and central differencings employing the exact solutions of Eq. (1) presented next.

2. EXACT SOLUTIONS OF THE TRANSPORT EQUATION

Coordinates x and y in Eq. (1) are rotationally transformed into s and n, respectively parallel and normal to the stream, as shown in Fig. 1. The new coordinates are non-dimensionalized by the square domain length, without notational changes. Finally, dividing by the diffusivity coefficient one obtains

$$\mathrm{Pe}\frac{\partial \phi}{Ss}-\frac{\partial^2 \phi}{\partial s^2}-\frac{\partial^2 \phi}{\partial n^2}=0, \qquad (3.1)$$

where Pe represents the global Peclet number,

$$\mathrm{Pe}=\frac{LV}{\alpha} \qquad (3.2)$$

$$V=(u^2+v^2)^{1/2}. \qquad (3.3)$$

Assuming for (3.1) solutions in the form

$$\phi(s, n)=S(s)\cdot N(n), \qquad (4.1)$$

one obtains, according to the method of separation of variables, the simultaneous ordinary equations

$$-\frac{d^2S}{ds^2}+\mathrm{Pe}\frac{dS}{ds}\pm\lambda^2 S=0 \qquad (4.2)$$

$$\frac{d^2N}{dn^2}\pm\lambda^2 N=0. \qquad (4.3)$$

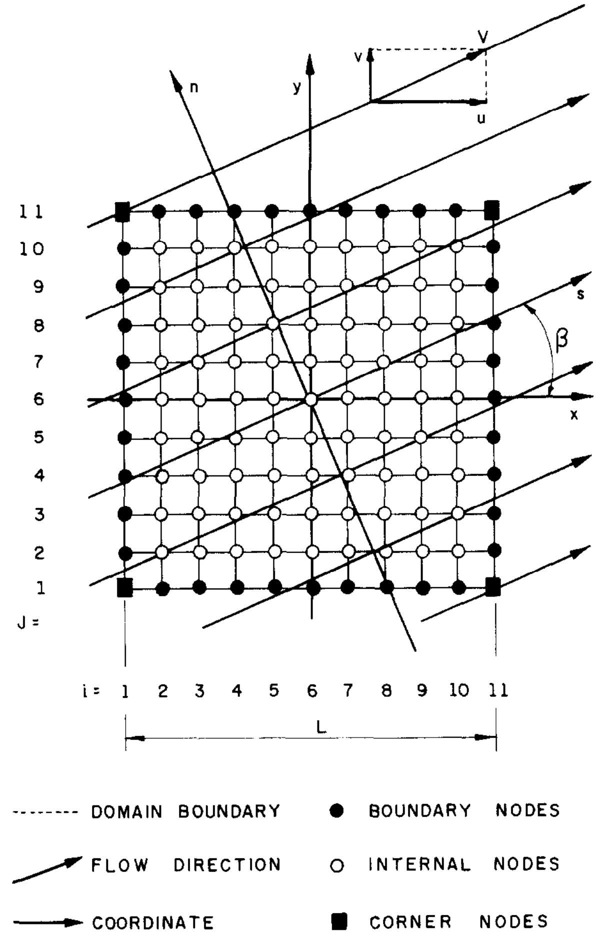

FIG. 1. Numerical and analytical coordinate systems and 10×10 spacing numerical grid.

If λ^2 is preceded by a positive sign the solution take the forms

$$\phi_A=\exp\{[\mathrm{Pe}-(\mathrm{Pe}^2+4\lambda^2)^{1/2}]\,s/2\}\cdot\sin(\lambda n) \qquad (5.1)$$

$$\phi_B=\exp\{[\mathrm{Pe}+(\mathrm{Pe}^2+4\lambda^2)^{1/2}]\,s/2\}\cdot\sin(\lambda n), \qquad (5.2)$$

together with solutions in $\cos(\lambda n)$, that differ from above types A and B only for a change of origin.

When λ^2 is preceded by a negative sign the real forms of solutions depend on the ratio λ/Pe. If this is below 0.5 there will be solutions of types

$$\phi_C=\exp\{[\mathrm{Pe}-(\mathrm{Pe}^2-4\lambda^2)^{1/2}]\,s/2\}\cdot\exp(\lambda n) \qquad (5.3)$$

$$\phi_D=\exp\{[\mathrm{Pe}+(\mathrm{Pe}^2-4\lambda^2)^{1/2}]\,s/2\}\cdot\exp(\lambda n). \qquad (5.4)$$

For $\lambda/\mathrm{Pe}>0.5$ solutions take the forms

$$\phi_{CD}=\exp\left(\frac{\mathrm{Pe}}{2}s\right)\cdot\sin[(\lambda^2-\mathrm{Pe}^2/4)^{1/2}\,s]\cdot\exp(\lambda n) \qquad (5.5)$$

$$\phi_{DC}=\exp\left(\frac{\mathrm{Pe}}{2}s\right)\cdot\cos[(\lambda^2-\mathrm{Pe}^2/4)^{1/2}\,s]\cdot\exp(\lambda n). \qquad (5.6)$$

At $\lambda/\text{Pe}=0.5$ all forms collapse to

$$\phi_{C/D}=\exp\left(\frac{\text{Pe}}{2}s\right)\cdot\exp\left(\frac{\text{Pe}}{2}n\right). \tag{5.7}$$

In both cases symmetric solutions in $\exp(-\lambda n)$ also appear.

For low λ/Pe ratios there are solutions on A, B, C, and D forms. A and C types are smoother in the flow direction than perpendicularly, representing situations of strong wross-wind diffusion, as for example in the hydrodynamic and the thermal thin boundary layers [10]. Note that strong cross-flow derivatives also characterize the test case functions upon which the angular concept of numerical diffusion is based.

On the other hand, B and D functions with low λ/Pe ratios present greater stream-direction diffusion, which is particularly strong in a boundary layer near the outlet of the domain.

The elementary solutions of all types with high λ/Pe ratios combine diffusion in both directions.

The discretization test cases employ all solution types. By varying Pe and λ the performance of the schemes will be studied for a wide domain of the general solution's Fourier spectrum.

3. THE NUMERICAL PROBLEM

Square grids of variable refinement are adopted for the square domain, as exemplified in Fig. (1) with a 10×10 spacing grid.

The well-known rotational transformation is used to obtain the s–n cordinates at each point, so that exact function values can be computed according to one of Eqs. (5). Internal values are stored for comparison of numerical solutions. The exact values at the boundary nodes are imposed as Dirichlet conditions for each scheme.

The five-point schemes result in systems of difference equations in the form

$$A_{i-1,j}\cdot\phi_{i-1,j}+A_{i+1,j}\cdot\phi_{i+1,j}+A_{i,j-1}\cdot\phi_{i,j-1} + A_{i,j+1}\cdot\phi_{i,j+1}+A_{i,j}\cdot\phi_{i,j}=0 \tag{6}$$

for each internal node (i, j).

Coefficients A are functions of the cell Peclet numbers

$$\Delta\,\text{Pe}_x=\frac{u\cdot\Delta x}{\alpha} \tag{7.1}$$

$$\Delta\,\text{Pe}_y=\frac{v\cdot\Delta y}{\alpha} \tag{7.2}$$

obeying the general relations

$$A_{i-1,j}=\pi(-\Delta\,\text{Pe}_x) \tag{8.1}$$

$$A_{i+1,j}=\pi(\Delta\,\text{Pe}_x) \tag{8.2}$$

$$A_{i,j-1}=\pi(-\Delta\,\text{Pe}_y) \tag{8.3}$$

$$A_{i,j+1}=\pi(\Delta\,\text{Pe}_y) \tag{8.4}$$

$$A_{i,j}=-(A_{i-1,j}+A_{i+1,j}+A_{i,j-1}+A_{i,j+1}). \tag{8.5}$$

The specific form of function $\pi(\Delta\,\text{Pe})$ depends on each discretization, as follows:

Central differencing,

$$\pi=1-\frac{\Delta\,\text{Pe}}{2}; \tag{9.1}$$

Upwind scheme,

$$\pi=\begin{cases}1 & \text{if } \Delta\,\text{Pe}\geqslant 0\\ 1-\Delta\,\text{Pe} & \text{if } \Delta\,\text{Pe}<0;\end{cases} \tag{9.2}$$

Allen and Southwell scheme,

$$\pi=\frac{\Delta\,\text{Pe}}{\exp(\Delta\,\text{Pe})-1}; \tag{9.3}$$

Dennis and Hudson scheme,

$$\pi=\exp\left(-\frac{\Delta\,\text{Pe}}{2}\right). \tag{9.4}$$

Numerical solutions were obtained by an iterative column-by-column procedure using the Tri-Diagonal Matrix Algorithm. The iterative process ended when variations of ϕ between successive iterations were below 10^{-9} times the difference between maximum and minimum values of the exact function. The iterative process required a relaxation factor for central differencing; the value used was the minimum factor that could turn the difference equation into a stepwise diagonally dominant form. Computations were performed on Digital PDP-10 and PDP-11 computer systems with single precision of 34 bits.

4. HIGH PECLET, LOW EIGENVALUE RESULTS

As widely recognized, the accuracy of all schemes becomes problematic for high Peclet number computations. The value $\text{Pe}=100$, whose exponential expressions are still within computer capabilities, was found sufficiently high to induce many questions of interest.

The normalization factor of the error is defined by the difference between maximum and minimum values of the discrete exact function, excluding corner nodes. Due to the well known maximum principle the extreme values are necessarily located on the boundary for linear homogeneous cases. The corner nodes are not involved in the numerical problem for five-point schemes, and their exclusion from the normalization factor was found relevant for steep functions, leading to more representative error evaluations [11].

Table I presents numerical solutions obtained by the second-order schemes, together with the exact solution, for the C type function considering $\lambda = 2.22$ and $\beta = 22.5°$. The solution obtained with a 10×10 spacing grid is represented by the value along columns $i = 2$, $i = 6$, and $i = 10$ only.

At point $(i, j) = (10, 10)$ the central differencing scheme shows a maximum error representing 0.6% of the normalization factor; the Allen and Southwell scheme error is 2.5%, and Dennis and Hudson's is 38%.

Table II considers the D function, maintaining Pe = 100, $\lambda = 2.22$, and $\beta = 22.5°$. At the same point (10, 10), the Allen and Southwell scheme's maximum error equals 0.6% of the local value, or only 0.00007% of the normalization factor of 7.40×10^{26}. The error of Dennis and Hudson's scheme rises to 6.6% of the local value. Central differencing presents unacceptable oscillatory results, often known as wiggles, with maximum error of about half the normalization factor.

Results for A and B functions, maintaining the quantitative parameters, are very similar to C and D, respectively [11]. Clearly central differencing is most effective in

TABLE I

Second-Order Schemes Solutions in Function C (Pe = 100, $\lambda = 2.22$, $\beta = 22.5°$) 10×10 Spacing

Node *i*	Node *j*	Solution: Exact	Central differencing	Allen and Southewell	Dennis and Hudson
	11		3.89		
	10	3.16	3.16	3.18	3.38
	9	2.57	2.57	2.58	2.75
	8	2.09	2.09	2.10	2.24
	7	1.70	1.70	1.71	1.82
2	6	1.38	1.38	1.39	1.48
	5	1.12	1.12	1.13	1.20
	4	0.912	0.911	0.917	0.976
	3	0.741	0.741	0.745	0.793
	2	0.602	0.602	0.605	0.643
	1		0.490		
	11		2.82		
	10	2.29	2.28	2.36	3.22
	9	1.86	1.86	1.92	2.62
	8	1.51	1.51	1.56	2.13
	7	1.23	1.23	1.27	1.73
6	6	1.00	1.00	1.03	1.41
	5	0.813	0.811	0.837	1.14
	4	0.661	0.659	0.679	0.930
	3	0.537	0.536	0.550	0.752
	2	0.437	0.436	0.443	0.588
	1		0.355		
	11		2.04		
	10	1.66	1.64	1.75	3.06
	9	1.35	1.34	1.43	2.50
	8	1.10	1.09	1.16	2.03
	7	0.892	0.885	0.941	1.65
10	6	0.725	0.720	0.764	1.34
	5	0.589	0.586	0.619	1.09
	4	0.479	0.476	0.500	0.884
	3	0.389	0.388	0.402	0.706
	2	0.317	0.316	0.322	0.521
	1		0.257		

TABLE II

Second-Order Schemes Solutions in Function D (Pe = 100, $\lambda = 2.22$, $\beta = 22.5°$) 10×10 Spacings

Node *i*	Node *j*	Solution: Exact	Central differencing	Allen and Southwell	Dennis and Hudson
	11		7.20E − 8		
	10	1.28E − 9	−6.57E + 23	1.16E − 9	3.69E − 10
	9	2.28E − 11	9.65E + 23	1.62E − 11	1.35E − 12
	8	4.04E − 13	−5.50E + 23	2.04E − 13	4.10E − 15
	7	7.19E − 15	1.99E + 23	2.35E − 15	1.15E − 17
2	6	1.28E − 16	−5.39E + 22	2.53E − 17	3.94E − 20
	5	2.27E − 18	1.17E + 22	2.57E − 19	3.02E − 22
	4	4.03E − 20	−2.13E + 21	2.50E − 21	4.47E − 24
	3	7.17E − 22	3.33E + 20	2.35E − 23	8.65E − 26
	2	1.27E − 23	−5.02E + 19	3.79E − 25	5.45E − 26
	1		2.26E − 25		
	11		5.64E + 8		
	10	1.00E + 7	−2.01E + 25	1.02E + 7	7.52E + 6
	9	1.78E + 5	9.78E + 24	1.83E + 5	1.24E + 5
	8	3.17E + 3	−2.55E + 24	3.27E + 3	2.18E + 3
	7	5.63E + 1	4.81E + 23	5.84E + 1	3.87E + 1
6	6	1.00E0	−7.78E + 22	1.04E0	6.68E − 1
	5	1.78E − 2	1.29E + 22	1.85E − 2	1.22E − 2
	4	3.16E − 4	−2.47E + 21	3.30E − 4	2.17E − 4
	3	5.61E − 6	5.16E + 20	5.86E − 6	3.86E − 6
	2	9.97E − 8	−1.27E + 20	1.04E − 7	6.87E − 8
	1		1.77E − 9		
	11		4.42E + 24		
	10	7.85E + 22	−3.81E + 26	7.90E + 22	7.33E + 22
	9	1.40E + 21	2.85E + 25	1.41E + 21	1.30E + 21
	8	2.48E + 19	−1.83E + 24	2.50E + 19	2.30E + 19
	7	4.41E + 17	7.26E + 22	4.45E + 17	4.09E + 17
10	6	7.83E + 15	−9.98E + 21	7.90E + 15	7.27E + 15
	5	1.39E + 14	6.10E + 21	1.40E + 14	1.29E + 14
	4	2.47E + 12	−2.70E + 21	2.50E + 12	2.30E + 12
	3	4.40E + 10	8.90E + 20	4.43E + 10	4.08E + 10
	2	7.81E + 8	−3.17E + 20	7.88E + 8	7.25E + 8
	1		1.39E + 7		

Note. $E \pm n = 10^{\pm n}$.

cross-flow diffusion cases and Allen and Southwell's is the best when convection and diffusion are parallel.

The above results are now generalized for other angles and different refinement levels for $\mathrm{Pe} = 100$ and $\lambda = 2.22$ using the compact representation provided by the logarithmic scale error versus grid size curve. Errors are given by the root mean square norm divided by the normalization factor referred. The upwind scheme is here included.

Figure 2 shows the error for C type functions. In general the relative positions of the second order schemes are the same of Table I. The upwind scheme is close to Allen and Southwell's in rough grids, but the second-order scheme shows its superior accuracy with refinement. The errors of the Allen and Southwell scheme and the Dennis and Hudson scheme coincide for 45°. Actually, not only the errors but the solutions are coincident for any function because of the proportionality between the two schemes' difference equations when both coordinate direction cell Peclet numbers are equal.

Confirming the angular concept of numerical diffusion, both upwind and Allen and Southwell schemes follow closely central differencing at zero degrees but, for other angles their errors increase much more significantly.

Figure 3 represents the error in D type functions keeping Pe and λ unchanged. The general behaviour of the second-order schemes repeats that observed in Table II, except for the coincidence of Allen and Southwell and Dennis and Hudson schemes at 45°.

The upwind scheme has no similarity with Allen and Southwell's in this case. For refined grids it shows better accuracy at 45° than at 0°, investing the trend assumed by the angular concept of numerical diffusion. In contrast, the Allen and Southwell scheme is again favoured at 0°, where it exhibits only noise level round-off errors.

In both types C and D central differencing error versus grid size curves depart from straight lines in an oscillatory fashion for coarse, high cell Peclet number grids, which is attributed to an incomplete iterative process. Despite this fact, which can in principle be eliminated, central differencing curves are closer to straight lines than are those of any other scheme. Even the wiggly solution presented in

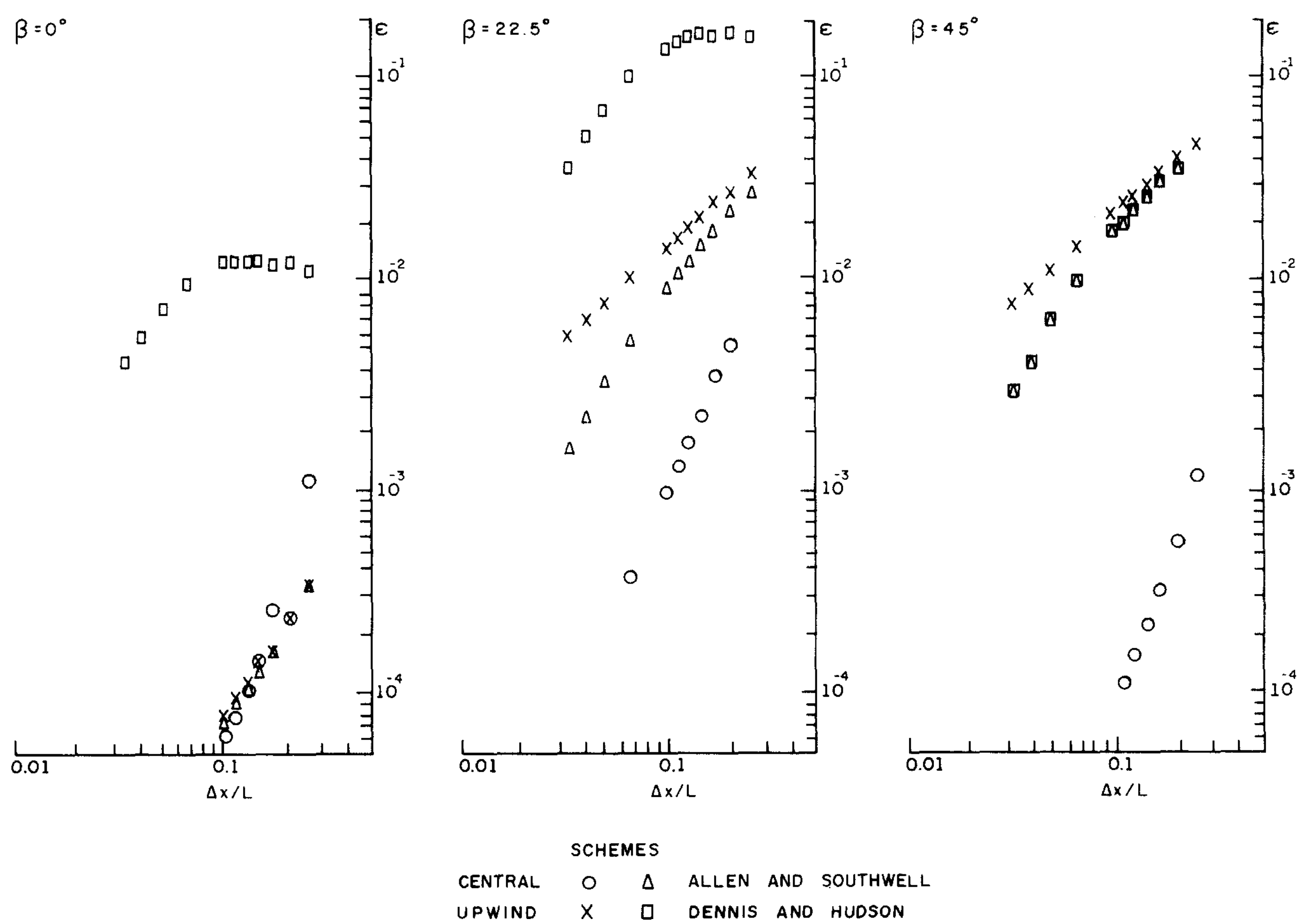

FIG. 2. Error versus grid size for five-node schemes in type C functions with different flow-to-grid inclinations. $\mathrm{Pe} = 100$, $\lambda = 2.22$.

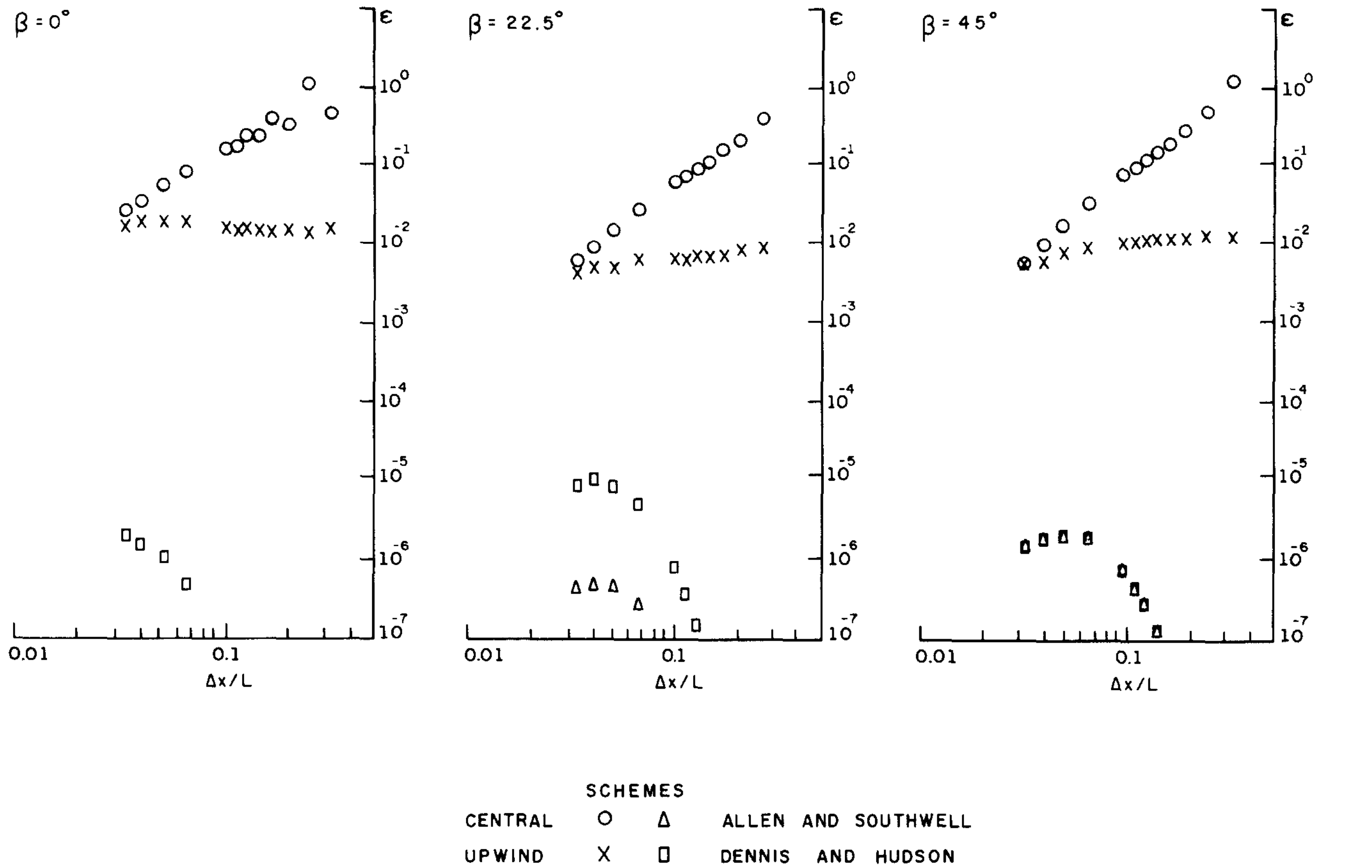

Fig. 3. Error versus grid size for five-node schemes in type D functions with different flow-to-grid inclinations. Pe = 100, $\lambda = 2.22$.

Table II corresponds in Fig. 3 to a point on the straight line, whose error is therefore dominated by the second-order term of the series expansion.

All other schemes, which are diagonally dominant and whose solutions and errors are bounded in the homogeneous case, show concave error versus grid size curves, indicating that the error is generally smaller than the extrapolated asymptotic value.

The behaviour of all schemes in A and B functions at the same Pe and λ is very close to their performance in C and D, respectively, except for functions B at 45°, where the errors of all schemes are reduced by three orders of magnitude compared with D, due to the anti-symmetry of the function about the s-axis [11].

HIGH λ/Pe RESULTS

Figure 4 presents the performance of the second-order schemes in A and B functions for Pe = 10 and $\beta = 22.5°$ with variable λ. For the smaller eigenvalue ($\lambda = 2$) the relative positions of the schemes are analogous to the previously considered C and D cases, respectively, although the curves show a less concave aspect at such smaller Pe. For $\lambda = 10$ all discretization errors are greater and relatively closer to each other.

The evolution of the schemes' performance with frequency is more complex in C and D types. A significant test case provided by the situation where $\lambda/\mathrm{Pe} = 0.5$ (function C/D) is exemplified in Fig. 5, showing the error versus grid size curves for $\mathrm{Pe} = 2\lambda = 4.44$ with different angles.

The errors of the Dennis and Hudson scheme are always of round-off noise level and are not reproduced. Clearly this scheme has greater accuracy for increasing λ in a region of C and D functions up to $\lambda/\mathrm{Pe} = 0.5$.

The central and the Allen and Southwell schemes have coincident asymptotic errors at 0° and 22.5°, but Allen and Southwell's has nodally exact values at 45°, where it coincides with Dennis and Hudson's.

Greater λ/Pe values, yielding functions CD and DC, are considered in Fig. 6, representing the case Pe = 10, $\beta = 22.5°$, and variable λ. Central differencing is favoured for $\lambda = 6$ in both cases, despite Dennis and Hudson's optimality at $\lambda = 5$ for this Pe. For $\lambda = 10$ the errors of all schemes increase and tend to become close, analogous to A and B cases.

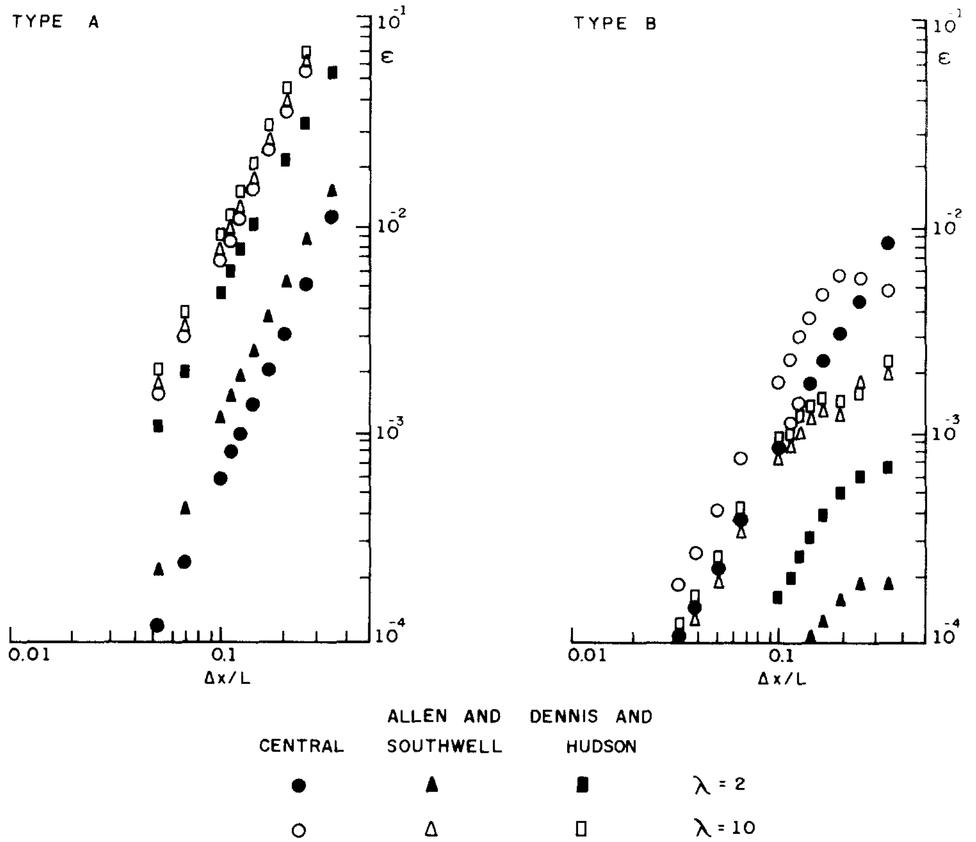

Fig. 4. Error versus grid size for second order schemes in type A and type B functions with different λ. Pe $= 10$, $\beta = 22.5°$.

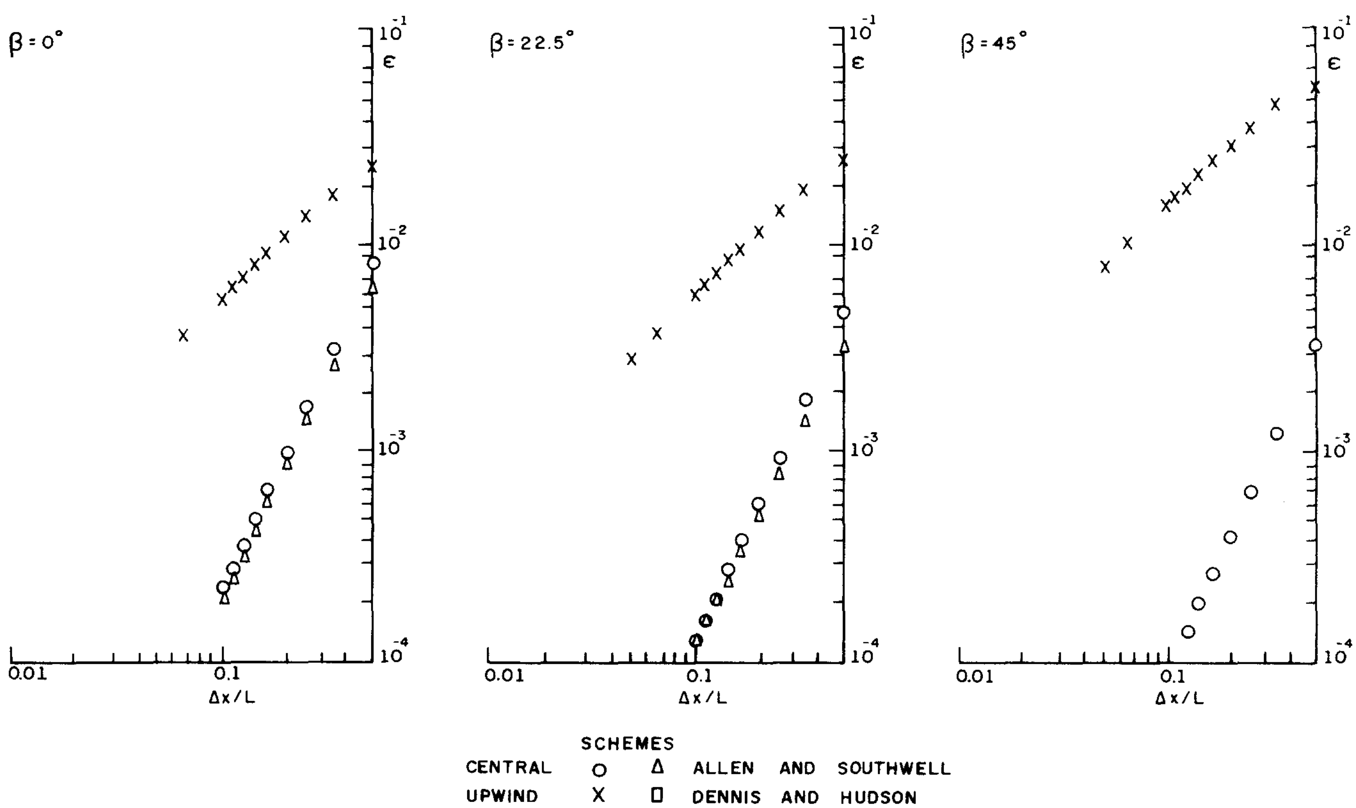

FIG. 5. Error versus grid size for five-node schemes in type C/D functions (Pe $= 2\lambda = 4.44$) with different flow-to-grid inclinations.

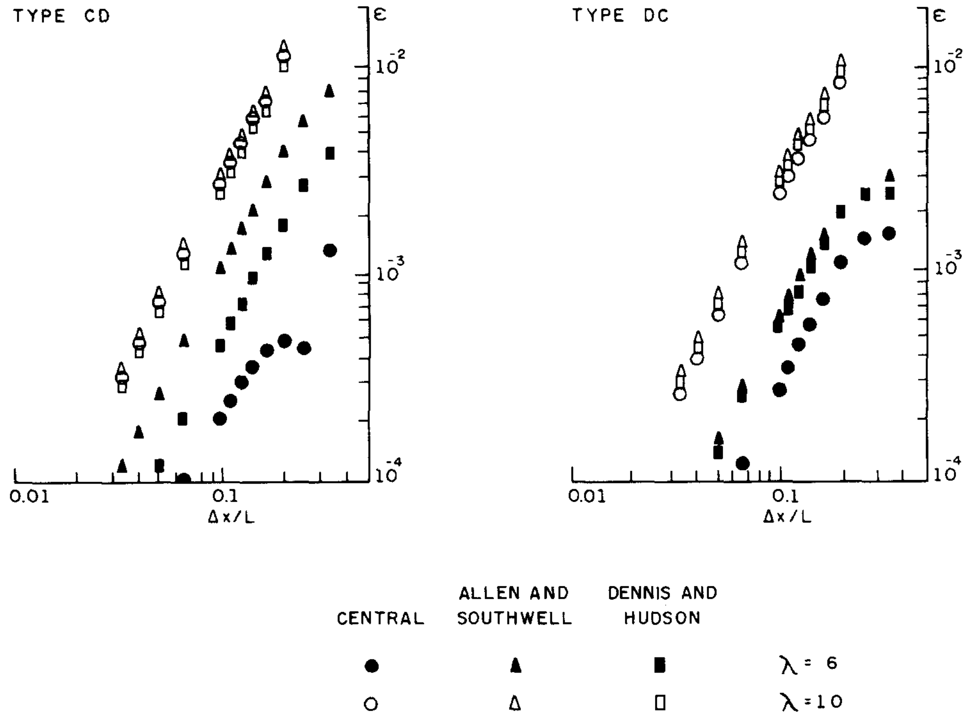

FIG. 6. Error versus grid size for second-order schemes in type CD and type DC functions with different λ. $Pe = 10$, $\beta = 22.5°$.

6. CONCLUSIONS

Clearly the performance of all schemes depends on the particular solution of the transport equation. The Allen and Southwell scheme is favoured in cases with strong flow-direction diffusion, associated with B and D functions with low λ/Pe. Central differencing, disregarding its instability problems, is favoured in cross-flow diffusion cases given by A and C functions with low λ/Pe. Dennis and Hudson's method is the best for the C/D case with $\lambda/Pe = 0.5$. For λ/Pe around or above unity, the errors of all schemes are high and close among themselves, whatever kind of function is considered.

Although second-order schemes are necessarily more accurate than first-order ones for sufficiently refined grids, both the central and Dennis and Hudson schemes were worse than the upwind in some moderately refined cases. In this sense Allen and Southwell's scheme is preferable as the scheme which proved to be almost always better than the upwind, even at rough or moderately refined grids, in a wide set of tests [11].

It has been shown that the angular concept of numerical diffusion is restricted to subsets of the possible solutions of the transport equation, particularly to low λ/Pe A and C types. When a numerical coordinate is parallel to the flow all errors associated with the solution of convection terms, in particular the upwind errors, are necessarily on the streamline direction coordinate. In the normal direction all schemes, the upwind included, coincide with the second-order central differencing. Since A and C functions with low λ/Pe present low streamline derivatives, the convection errors are negligible. If the flow is inclined with respect to the grid there are convection terms and high derivatives in both numerical coordinates, so the error becomes considerable. However, the performance of the upwind scheme in other function types has shown that such a specific circumstance cannot be taken as basis for a general theory on numerical error analysis.

Although based on experiments with five-node schemes, the above conclusion is relevant for schemes such as the skew- or fector-upwind [12, 13] and the skew-exponential [14, 15], which are up to nine-point schemes. These schemes, inspired by the angular concept of numerical diffusion, avoid the flow-to-grid angle effect by using upwind or exponential interpolation in the stream-oriented coordinate only.

The skewing procedure with upwind operates very well in the case of low λ/Pe A and C function types, since it reduces the error to the level of upwind error at 0°. But the procedure fails to improve the accuracy in B and D function types where the upwind error at 0° is greater that at 45°, for instance. Also, the skew-exponential is not always more accurate than the exponential, at least with the exception found at C/D function with $\lambda/Pe = 0.5$.

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