Computer methods in applied mechanics and engineering

ELSEVIER

Comput. Methods Appl. Mech. Engrg. 129 (1996) 221–233

A new approach for building bounded skew-upwind schemes

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Received 1 April 1994

Abstract

A new methodology for the construction of streamline bounded high resolution schemes is presented. The route followed in the development is to combine existing streamline schemes with the Normalized Variable Formulation (NVF) bounding approach. The procedure is applied to the Skew Upwind Differencing Scheme (SUDS) to yield a new composite high resolution bounded convective scheme (NVF SUDS). The increase in computational cost with NVF SUDS is very small as compared to the unbounded SUDS. The new scheme is tested and compared with the composite high resolution STOIC scheme, the upwind scheme, and the unbounded SUDS by solving for three pure convection test problems. Results generated, demonstrate the capability of the new upwind scheme in accurately resolving steep gradients (as accurate as the ones obtained with the third-order STOIC scheme) while retaining the solution bounded.

Nomenclature

a	Coefficients in the discretized equation
B	Volume integral of Q
b	Source term in the discretized equation
C	Convective flux coefficient
$f()$	Functional relationship
J	Total scalar flux across cell face
Q	Source term in the transport equation
S	Surface area of control volume face
RE	Residual error
u, v	Velocity components in x and y directions
ϕ	General dependent variable
Γ	Diffusion coefficient
ρ	Density
ε	Quantitative indicator of error

Superscripts

U	Upwind formulation
D	Diffusion contribution
C	Convection contribution
$\sim$	Refers to normalized variable

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SSDI 0045-7825(95)00881-0

Subscripts

e, w, n, s	Refer to control volume faces
E, W, N, S	Refer to neighbors of the P grid point
P	Main grid point
f	Refers to any of the control volume faces
U	Upstream grid point
D	Downstream grid point
C	Central grid point
nb	Refers to neighbors
dc	Deferred correction

1. Introduction

Two of the main sources of errors in numerical modeling of convection–diffusion transport problems are numerical diffusion and numerical dispersion. The term numerical diffusion refers to numerically induced smearing of the predicted profile while, numerical dispersion refers to non-physical spatial oscillations or over/under shoots produced in the solution. Numerical diffusion, a significant source of error in numerical solution of conservation equations, can be separated into two components namely cross-stream and streamwise numerical diffusion. The former occurs when gradients in a convected quantity exist perpendicular to the flow and the direction of flow is oblique to the grid lines, i.e. due to the multi-dimensional nature of the flow [1–3]. The latter happens when gradients in a convected quantity exist parallel to the flow [4] even in one-dimensional situations. Numerical dispersion, on the other hand, comes about when the convective scheme used is unstable [5] and large gradients are present.

Several approaches have been adopted to reduce these errors. To suppress numerical diffusion two routes have been followed: One way is to use higher-order schemes, which are basically derived as one-dimensional schemes and applied for multi-dimensional cases and help in reducing streamwise numerical diffusion. A variety of so-called higher-order schemes have been presented and evaluated over the years such as the QUICK scheme of Leonard [6], the third-order scheme of Agarwal [7] and the second-order upwind scheme of Fromm [8]. Another approach is to use skew upwind schemes, that reduce cross-stream numerical diffusion because of their multi-dimensional nature. A number of multi-dimensional schemes have been devised such as the SUDS and SUWDS schemes of Raithby [9], the VSUD scheme of Lilington [10], the DTUD of Sharif [11] and the SSUD scheme of Hassan et al. [12] to cite a few. Both higher-order and skew upwind schemes do yield more accurate results than the highly diffusive first-order upwind scheme, and are certainly more stable than the second-order central difference scheme, however, they suffer from a lack of boundedness, i.e. they tend to give rise to oscillations or under/over-shoots, especially in regions of strong gradients. These under/over-shoots can induce large errors and lead to unphysical results.

To suppress numerical dispersion, several procedures have also been developed. These procedures can be grouped along two lines. One approach is to follow a blending strategy where either a limited anti-diffusive flux is added to a first-order upwind scheme in such a way that the resulting scheme is capable of resolving sharp gradients without undue under/over-shoots, or on the contrary, some kind of smoothing diffusive agencies are introduced into an unbounded or a higher-order scheme to damp oscillations. The Flux-Corrected Transport (FCT) method of Zalesak [13] is an example of the first type of flux-blending technique, while examples of the second type are the Filtering Remedy and Methodology (FRAM) of Chapman [14], the Simple Blending (SB) methods of Peric [15] and Zhu and Leschziner [16]. Because of their multistep nature, flux-blending techniques tend to be very expensive computationally. A better way to remove unphysical oscillation is to use a composite flux limiter approach. In composite high resolution (HR) schemes, the numerical flux at the interface of the computational cell is modified by the use of a flux-limiter that enforces a monotonicity (boundedness) criteria. The family of *shock-capturing* schemes based on the Total Variational Diminishing flux-limiters (TVD) [17], widely used in compressible flow simulations, are well-known examples of composite schemes. A more recent formulation for high resolution flux-limiters has been developed by Leonard based on the normalized variable formulation (NVF) [18].

While a number of bounded high-order schemes have been implemented to form a family of high-resolution schemes (HR) [18–21], few workers have implemented bounded skew upwind schemes. Sharif et al. have used the FRAM and the SB methods in combination with the SUDS [22,23] and the FCT in combination with the DTUD [11] schemes. All these bounding techniques, except for the SB method, are expensive computationally due to their multi-step nature. Results obtained with SB however, are over-diffusive. In this paper, the idea of bounding skew upwind schemes by enforcing the convective boundedness criteria is tested. This is done by combining the SUD scheme with the NVF bounding approach to yield a composite high resolution scheme with a light increase in computational cost in comparison with the unbounded SUD scheme.

The newly developed bounded skew upwind scheme (NVF SUDS) is tested and compared with the upwind scheme, the STOIC scheme [24], and the unbounded *SUD* scheme by solving for three problems (i) a two-dimensional pure convection of a scalar involving a step profile in an oblique velocity field, (ii) a two-dimensional pure convection of a scalar involving an elliptic profile in an oblique velocity field, (iii) and a two-dimensional pure convection of a scalar by a rotational velocity field (the Smith–Hutton problem). Results generated, demonstrate the capability of the bounded skew upwind scheme in resolving, with relatively little additional computational cost, steep gradients while retaining the solution bounded.

2. Numerical discretization of the transport equation

The transport equation governing two-dimensional incompressible steady flows may be expressed in the following general form

$$\frac{\partial}{\partial x}\left(\rho u\phi - \Gamma\frac{\partial \phi}{\partial x}\right) + \frac{\partial}{\partial y}\left(\rho v\phi - \Gamma\frac{\partial \phi}{\partial y}\right) = Q \tag{1}$$

where ϕ is any dependent variable, u and v are the x- and y-components of the velocity vector, and ρ, Γ and Q are the density, diffusivity and source terms respectively. Integrating the above equation over the control volume shown in Fig. 1, and applying the divergence theorem, the following discretized equation is obtained in Cartesian coordinates

$$J_e - J_w + J_n - J_s = B \tag{2}$$

where J_f represent the total flux of ϕ across cell face 'f' (f = e, w, n or s) and B is the volume integral of the source term Q. Each of the surface fluxes J_f contains a convective contribution, J_f^C, and a diffusive contribution, J_f^D, hence

$$J_f = J_f^C + J_f^D \tag{3}$$

For a purely convective scalar flow the diffusion flux, J_f^D, is zero, while the convective flux is given by

$$J_f^C = (\rho u.S)_f\phi_f = C_f\phi_f \tag{4}$$

where S_f is the surface of cell fact 'f', and C_f is the convective flux coefficient at cell face 'f'. As can be seen from Eq. (4), the accuracy of the control volume solution for the convective scalar flux depends on the proper estimation of the face value of ϕ_f as a function of the neighboring ϕ values. Using some assumed interpolation profile, ϕ_f can be explicitly formulated in terms of its node values by a functional relationship of the form

$$\phi_f = \mathrm{f}(\phi_{nb}) \tag{5}$$

where ϕ_{nb} denotes the neighboring node ϕ values (ϕ_E, ϕ_W, ϕ_N, ϕ_S, ϕ_{NE}, ϕ_{NW}, ϕ_{SE}, ϕ_{SW}). After substituting Eq. (5) into Eq. (4) for each cell face, Eq. (2) is transformed after some algebraic manipulations into the following discretized equation

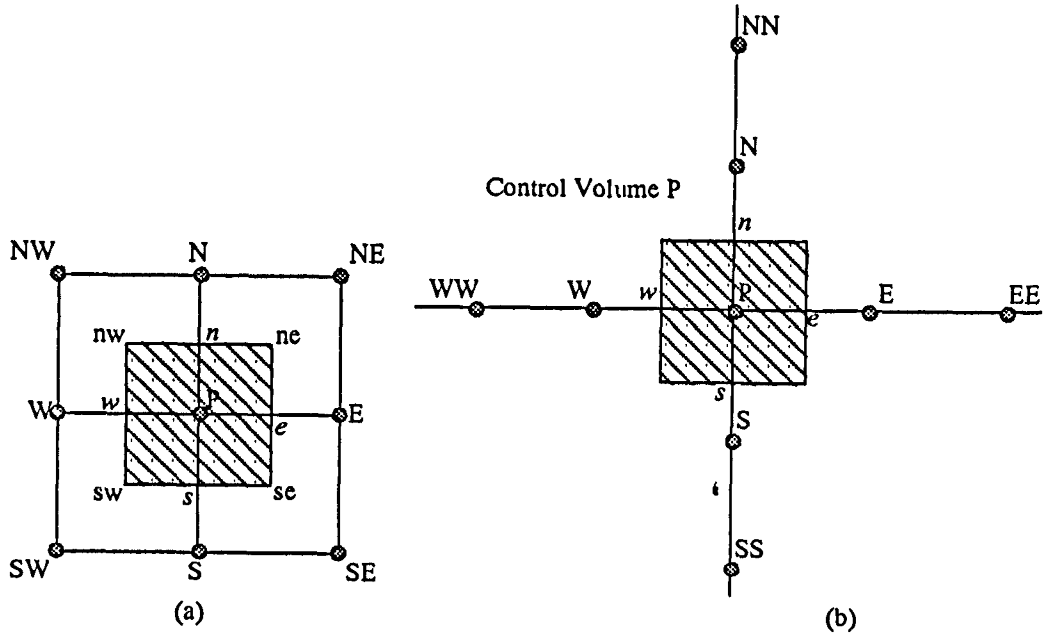


Fig. 1. Typical grid point cluster and control volume.

$$a_P\phi_P = \sum_{\mathrm{nb}} (a_{\mathrm{nb}}\phi_{\mathrm{nb}}) + b_P \tag{6}$$

where the coefficients a_P and a_{nb} depend on the selected scheme and b_P is the source term of the discretized equation.

Since the functional derivative can involve a large number of neighboring grid points, especially when using higher-order streamline based schemes, the solution of Eq. (6) can become very expensive computationally, hence the use of a compacting procedure is most welcome. In the present work the deferred correction procedure of Rubin and Khosla [25] is used. In this procedure Eq. (2) is rewritten as

$$J_e^U - J_w^U + J_n^U - J_s^U = B + \underline{[C_e(\phi_e^U - \phi_e) - C_w(\phi_w^U - \phi_w) + C_n(\phi_n^U - \phi_n) - C_s(\phi_s^U - \phi_s)]} \tag{7}$$

where ϕ_f^U is the face value, J_f^U the total flux of ϕ, both calculated using the first-order upwind scheme, ϕ_f the cell face value calculated using the chosen streamline based or higher-order scheme, and the underlined terms represent the extra source term due to the deferred correction. Substituting the value of the cell flux obtained from the functional relationship of the upwind and high-resolution scheme at hand, the deferred correction results in an equation similar in form to Eq. (6), but where the coefficient matrix is pentadiagonal (for 2D) and always diagonally dominant since it is formed using the first-order upwind scheme. The discretized equation, Eq. (6), becomes

$$a_P\phi_P = \sum_{\mathrm{nb}} (a_{\mathrm{nb}}\phi_{\mathrm{nb}}) + b_P + b_{\mathrm{dc}} \tag{8}$$

where now the coefficients a_P and a_{nb} are obtained from a first-order upwind discretization, nb = (E, W, S, N) and b_{dc} is the extra deferred correction source term. This compacting procedure is simple to implement and effective when using higher-order or streamline based schemes.

3. The skew upwind differencing scheme (SUDS)

This scheme was first proposed by Raithby [9, 26] and was subsequently used by a number of investigators in treating high Reynolds number or convection-dominated flows. However, the skew

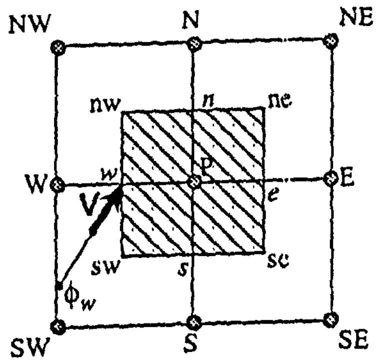


Fig. 2. SUDS Interpolation.

upwind scheme does suffer from unphysical oscillations as demonstrated by the results in the literature [1, 27].

In the SUDS, the advected values of ϕ at the cell faces are approximated by considering the direction of the velocity vector at the cell face and interpolating between the values at the two appropriate nodes among the nodes surrounding the cell face. The two appropriate nodes are selected by going upstream along the direction of the velocity vector at the cell face all the way back to the line joining the centers of the adjacent cells as shown in Fig. 2. The local profile for ϕ_w, for example, may be obtained (see the ϕ control volume) as follows

$$\phi_w \approx f(\phi_W, \phi_{SW}) = m_1\phi_W + m_2\phi_{SW} \quad \text{with} \begin{cases} \phi_w = \phi_W & \text{if } v_w = 0 \\ \phi_w = \phi_{SW} & \text{if } v_w/u_w = 2 \end{cases} \tag{9}$$

where $m1$ and $m2$ are weighing factors for ϕ_W and ϕ_{SW}, respectively, and depend on the stream direction.

4. The normalized variable formulation

4.1. The normalized variable

The proposed scheme is bounded on the basis of the normalized variable proposed by Leonard [18]. Considering face 'f' of a control volume (see Fig. 3), defining ϕ_U, ϕ_D, ϕ_C, and ϕ_f as the Upstream (U), downstream (D), central nodal values (C) and face value (f) for each cell face (see Fig. 3), the normalized variable is defined as

$$\tilde{\phi} = \frac{\phi - \phi_U}{\phi_D - \phi_U} \tag{10}$$

Note that with this normalization $\tilde{\phi}_D = 1$ and $\tilde{\phi}_U = 0$. The use of the normalized variable simplifies the definition of the functional relationships of HR schemes and is helpful in defining the conditions that the functional relationships should satisfy in order to be bounded and numerically stable.

4.2. The convective boundedness criteria (CBC)

Based on the normalized variable analysis, Gaskell and Lau [28] formulated a convection boundedness criterion (CBC) for implicit steady-state flow calculation, which states that for a scheme to have the boundedness property its functional relationship should be continuous, should be bounded from below by $\tilde{\phi}_f = \tilde{\phi}_C$, and from above by unity, and should pass through the points (0,0) and (1,1), in the

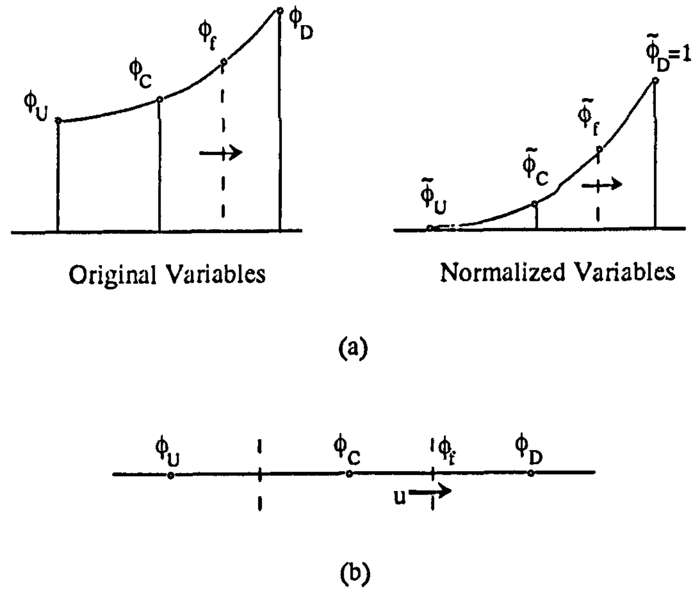
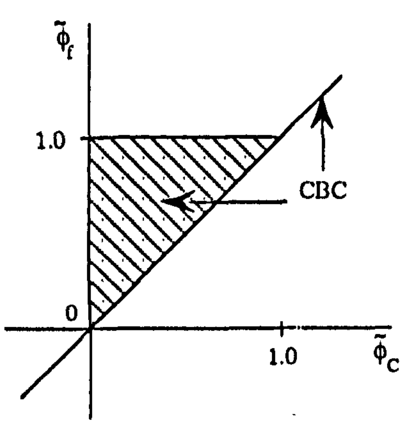


Fig. 3. (a) Original and normalized variables and profiles. (b) The interpolation points used in calculating ϕ_f.

monotonic range $(0<\tilde{\phi}_C<1)$, and for $1<\tilde{\phi}_C$ or $\tilde{\phi}_C<0$, the functional relationship $f(\tilde{\phi}_C)$ should equal $\tilde{\phi}_C$. The above conditions illustrated in Fig. 4, can be formulated as

$$\begin{cases} f(\tilde{\phi}_C) \text{ is continuous} & \\ f(\tilde{\phi}_C)=0 & \text{for } \tilde{\phi}_C=0 \\ f(\tilde{\phi}_C)=1 & \text{for } \tilde{\phi}_C=1 \\ f(\tilde{\phi}_C)<1 \text{ and } f(\tilde{\phi}_C)>\tilde{\phi}_C & \text{for } 0<\tilde{\phi}_C<1 \\ f(\tilde{\phi}_C)=\tilde{\phi}_C & \text{for } \tilde{\phi}_C<0 \text{ or } \tilde{\phi}_C>1 \end{cases} \tag{11}$$



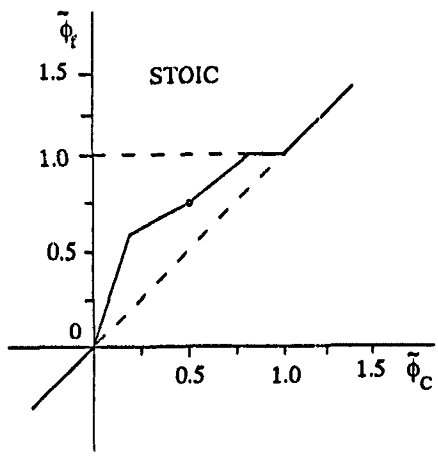


Fig. 4. Convective Boundedness Criterion (CBC).

Fig. 5. NVD plot for the STOIC High Resolution Scheme.

5. The NVF SKEW UPWIND scheme

After the calculation of ϕ_f using the SKEW UPWIND scheme, the cell face value is normalized to yield $\tilde{\phi}_f$ and the CBC criterion is enforced in the event when it is not satisfied. It is clear that this modification to the original skew upwind scheme is not difficult to implement and is not expensive computationally.

6. The STOIC scheme

The STOIC scheme (Second- and Third-Order Interpolation for Convection) is a high-resolution scheme developed and implemented in the context of the NVF methodology. Its development is based on the premise that the normalized variable at the cell face, $\tilde{\phi}_f$ can be related to the normalized variable at the center, $\tilde{\phi}_C$ by a combination of linear functions. In the monotonic range, the second-order central difference scheme and the third-order QUICK scheme are combined in the manner shown in Fig. 5, to form a Second- and Third-Order Interpolation for Convection (STOIC) scheme. An ad-hoc linear function is used in the [0–0.2] segment of the NVD diagram to enforce the CBC condition $f(0) = 0$. The functional relationship of the STOIC scheme passes through the points (0,0) and (1,1) and satisfy the rest of the CBC conditions. This functional relationship of the STOIC scheme, illustrated in Fig. 5, is given by

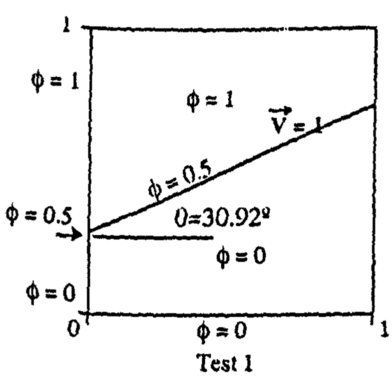
$$\tilde{\phi}_f = f(\tilde{\phi}_C) = \begin{cases} \tilde{\phi}_f = 3\tilde{\phi}_C & \text{for } 0 < \tilde{\phi}_C < 0.2 \\ \tilde{\phi}_f = \frac{1}{2}(1 + \tilde{\phi}_C) & \text{for } 0.2 < \tilde{\phi}_C < 0.5 \\ \tilde{\phi}_f = \frac{3}{8} + \frac{3}{4}\tilde{\phi}_C & \text{for } 0.5 < \tilde{\phi}_C < 5/6 \\ \tilde{\phi}_f = 1 & \text{for } 5/6 < \tilde{\phi}_C < 1 \\ \tilde{\phi}_f = \tilde{\phi}_C & \text{elsewhere} \end{cases} \tag{12}$$

7. Applications

In what follows, the results of calculations for three test situations (Figs. 6–8) involving purely convective transport of scalars containing discontinuities or large gradients, are presented.

In all three tests, the computational results were considered 'converged' when the residual error given by Eq. (13) became smaller than 0.08%.

$$\mathrm{RE} = \sum \left| a_P\phi_P - \left[\sum_{\mathrm{nb}} a_{nb}\phi_{nb} + b_P + b_{dc} \right] \right| \tag{13}$$



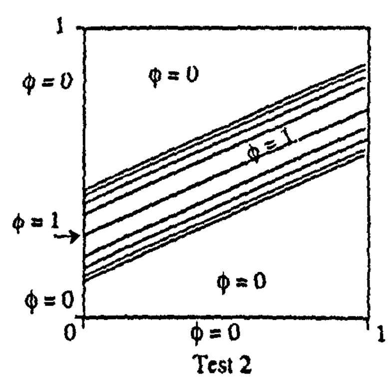


Fig. 6. Pure convection of a scalar discontinuity (test 1).

Fig. 7. Pure convection of an elliptic profile by a uniform velocity field (test 2).

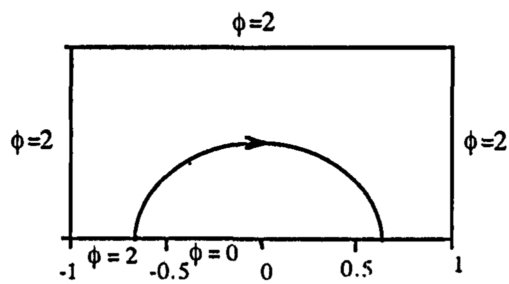


Fig. 8. Pure convection of a scalar by a rotational velocity field (test 3).

and the quantitative indication of the error was calculated using the following relation

$$\varepsilon = \sum |\phi_{\text{computed}} - \phi_{\text{exact}}| \tag{14}$$

summed over all computed grid points.

Test 1: Convection of a step profile in an oblique velocity field

Fig. 6 shows the well known benchmark test problem consisting of a pure convection of a transverse step profile imposed at the inflow boundaries of a square computational domain. A 25×25 mesh was used giving in this case $\Delta x = \Delta y = 1/25$. The location of the boundary step is chosen so that the exact convected step passes through the midpoint of the grid. The angle θ was chosen to be 30.92° and $|V| = 1$, so as to have the analytical profile coincide with grid nodes in the last grid column. The governing conservation equation of the problem is

$$\frac{\partial(u\phi)}{\partial x} + \frac{\partial(v\phi)}{\partial y} = 0 \tag{15}$$

where ϕ is the dependent variable and u and v are the cartesian components of the uniform velocity vector V. The computed values of ϕ using the upwind scheme, the SUDS the NVF SUDS, and the STOIC scheme along with the exact analytical solution to the problem are shown in Fig. 9. The results presented are very clear and self explanatory. The worst performance is for the upwind scheme and the best results obtained are for the NVF SUDS and the STOIC scheme. The maximum error for the NVF SUDS is slightly lower than the error obtained with the high-resolution STOIC scheme. The maximum error associated with the unbounded SUDS is more than twice the error of the NVF SUDS, but what is worse than that, are the oscillations in the solution obtained with SUDS. These oscillations are the result of the SUDS not satisfying the CBC criterion. The results of the new NVF SUDS are very smooth and oscillations free since the CBC criterion is enforced. Furthermore, the performance of the new scheme, even though developed based on a first-order upwind scheme, is as good as the performance of the high-order STOIC scheme due to a large reduction in the cross-stream numerical diffusion.

Test 2: Convection of an elliptic profile in an oblique velocity field

An elliptic profile was also used for the same geometric situation. This second problem, illustrated in Fig. 7, was used in order to test the resolution of the different schemes for a profile involving a gradually decreasing gradient. The elliptic profile is generated using the following equation

$$\phi = \sqrt[2]{1 - \frac{[j + (1/5)]^2}{(9/25)^2}} \quad \text{for } 2 \leq j \leq 12 \tag{16}$$

The same mesh as for test 1 was used. Moreover, the governing conservation equation and the variables of the problem, are the same as in the previous problem. The numerical results of the various

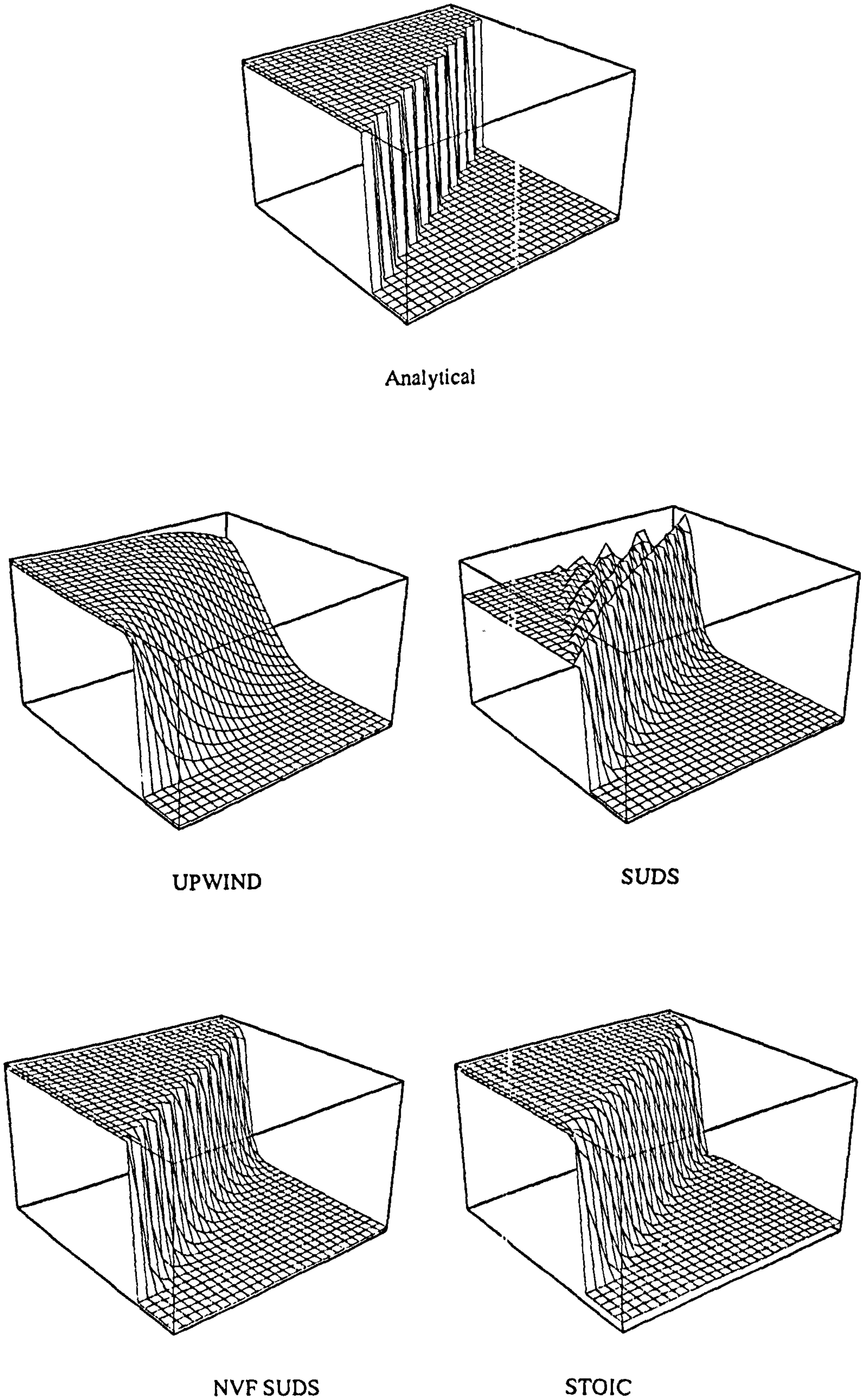


Fig. 9. Projections of ϕ field for test 1.

convective schemes along with the exact analytical solution to the problem are shown in Fig. 10. The trend of results is similar to that of test 1 with substantial improvement obtained with the NVF SUDS over the SUDS. In addition, the results of the NVF SUDS are as accurate as the ones obtained with the composite high-resolution STOIC scheme. As in the previous problem, the worst performance is for the upwind scheme.

Test 3: Smith–Hutton Problem

In the third test problem shown schematically in Fig. 8, a step discontinuity at $x = -0.5$ is convected clockwise from the inlet plane ($x < 0$, $y = 0$) to the outlet plane ($x > 0$, $y = 0$) by a rotational velocity field given by

$$u = 2y(1 - x^2) \tag{17}$$

$$v = -2x(1 - y^2) \tag{18}$$

The solution to this test, which was devised for evaluating a number of numerical convection schemes [29], is given by

$$\phi = \begin{cases} 0 & \text{for } -0.5 < x < 0 \quad y = 0 \\ 2 & \text{for } -1 < x < -0.5 \quad y = 0 \\ 2 & \text{for } -1 < x < 1 \quad y = 1 \\ 2 & \text{for } x = -1 \quad 0 < y < 1 \\ 2 & \text{for } x = 1 \quad 0 < y < 1 \end{cases}$$

In this test, no physical diffusion was considered and the same mesh as for the previous two tests was employed. Moreover, the conservation equation and variables of the problem, are the same as in the previous ones. The computed results of the various convective schemes are displayed in Fig. 11. Again, numerical results obtained with the NVF SUDS are substantially better than those achieved with SUDS which show unboundedness. Furthermore, the results of the NVF SUDS are as accurate as the ones obtained using the STOIC scheme while the most diffusive results are those generated by the upwind scheme.

The maximum errors in all three problems for the various convective schemes used are presented in Table 1. From this table, it can be inferred once more than the worst results are for the upwind scheme and the best ones are for the NVF SDS and the STOIC scheme. Since the employment of the NVF bounding methodology with the SUDS is easy to implement and is not expensive computationally, its use is recommended in CFD applications.

8. Concluding remarks

A new bounded skew upwind scheme was presented. The newly developed high resolution convective scheme was formulated by combining the skew upwind scheme with the NVF bounding technique. The results of three test problems demonstrated the capability of the new scheme in eliminating oscillations from the solution and in generating results as accurate as the ones obtained with the composite high-resolution STOIC scheme. Moreover, the paper has shown quantitatively the importance of minimizing cross stream false diffusion when solving numerically advection problems. Furthermore, it has revealed the gain that could be achieved by implementing skew high resolution schemes, in which case, both cross stream and streamwise diffusion would be greatly reduced. Finally, the implementation of the new scheme in CFD codes is straightforward and is associated with a light increase in computational cost as compared to the unbounded skew upwind differencing scheme.

Acknowledgments

The financial support provided by the University Research Board of the American University of Beirut through grants No. 48820 and 48816 is gratefully acknowledged.

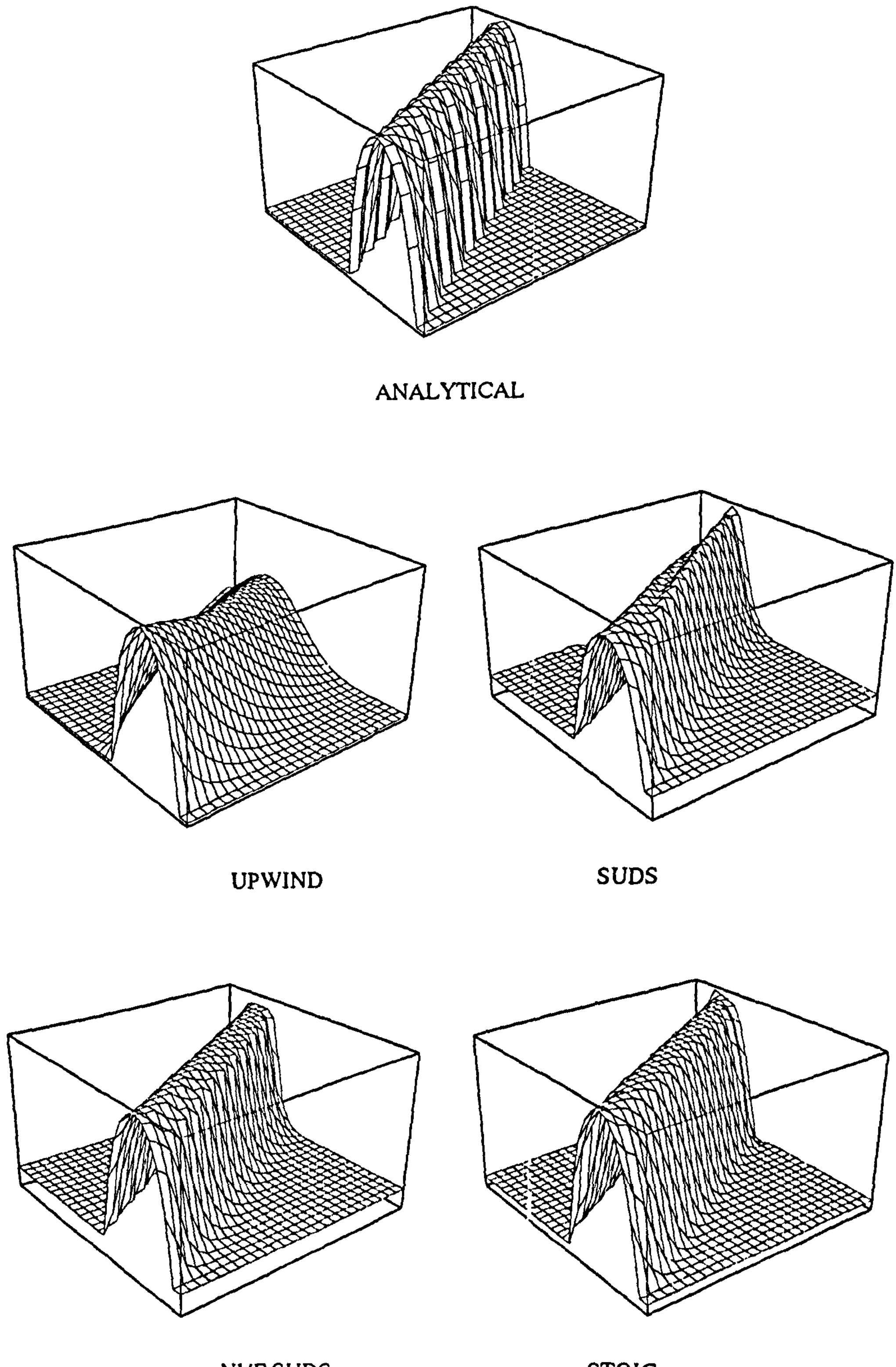


Fig. 10. Projections of ϕ field for test 2.

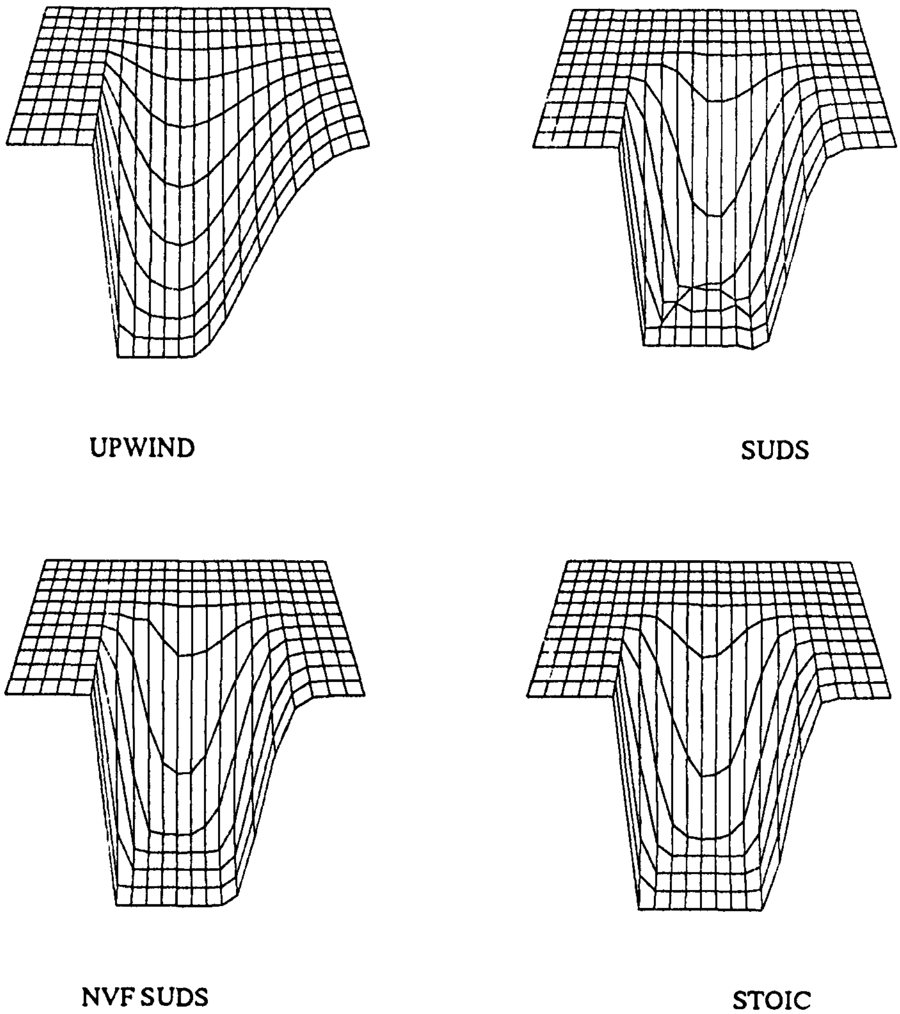


Fig. 11. Projections of ϕ field for test 3.

Table 1
Errors in tests 1, 2 and 3

Scheme	% Error for test 1	% Error for test 2	% Error for test 3
UPWIND	65.54	93.06	41.3
SUDS	36.57	27.16	20.8
NVF SUDS	15.36	16.87	16.8
STOIC	17.93	16.23	15.1

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