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Short note

Revision of the characteristics-based scheme for incompressible flows

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1. Introduction

The artificial compressibility method [1] is widely used mainly for solving the incompressible Navier–Stokes equations by introducing derivatives of the primitive values of velocity (u, v, w) and pressure (p) with respect to a pseudo-time variable τ. This enables the coupling between the continuity and momentum equations thus allowing time marching schemes developed for compressible flows to be used for incompressible flows in the sense that the pseudo-transient solution is marched to a steady state with respect to τ.

The present work is concerned with a variation of the schemes used in conjunction with the artificial compressibility method known as the characteristics-based (CB) scheme, which was first introduced for solving two-dimensional [2] and then three-dimensional flows [3] and developed further to incorporate multigrid techniques [4]. It has since been used in many flow-modelling studies e.g. [8–13], served as a basis for expanding the method for multi-species flows [5] and also for acceleration of the method for multigrid flow computations [7]. The CB scheme though exhibited substantial delays in terms of convergence in certain studies [12,13]. This led to a thorough investigation of the mathematical basis of the scheme in order to specify the cause of the aforementioned inefficiency. As a result of this investigation, the purpose of this study is to clearly indicate the necessary revisions in the construction of the scheme thus helping towards a solid mathematical establishment of the scheme.

2. Analysis

2.1. The characteristics based scheme

The characteristics based (CB) scheme is essentially an upwind scheme and is based on the formation of compatibility equations in characteristic directions as in the method of Riemann by splitting the Euler equations into one-dimensional equations.

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2.1.1. 2D Version

The analysis of the method for two dimensions [2] begins by expressing the Euler equations in curvilinear coordinates $\xi = \xi(x,y)$, $\eta = \eta(x,y)$ including the artificial compressibility term

$$\frac{\partial (JU)}{\partial \tau} + \frac{\partial \tilde{E}}{\partial \xi} + \frac{\partial \tilde{F}}{\partial \eta} = 0, \tag{1}$$

where

$$U = \begin{bmatrix} p/\beta \\ u \\ v \end{bmatrix}, \quad \tilde{E} = J\left(\xi_x \begin{bmatrix} u \\ u^2 + p \\ vu \end{bmatrix} + \xi_y \begin{bmatrix} v \\ uv \\ v^2 + p \end{bmatrix}\right), \quad \tilde{F} = J\left(\eta_x \begin{bmatrix} u \\ u^2 + p \\ vu \end{bmatrix} + \eta_y \begin{bmatrix} v \\ uv \\ v^2 + p \end{bmatrix}\right)$$

with $J = x_\xi y_\eta - y_\xi x_\eta$ the Jacobian of the transformation and β the artificial compressibility parameter the value of which plays an important role in determining the convergence rate. The Euler equations are then split into one-dimensional equations

$$\frac{\partial JU}{\partial \tau} + \frac{\partial \tilde{E}}{\partial \xi} = 0 \tag{2}$$

$$\frac{\partial JU}{\partial \tau} + \frac{\partial \tilde{F}}{\partial \eta} = 0, \tag{3}$$

and the analysis is carried out for Eq. (2) whereas similar procedure is supposed for (3). The non-conservative form of Eq. (2) is then given

$$\frac{1}{\beta} p_\tau + u_\xi \xi_x + v_\xi \xi_y = 0 \tag{4a}$$

$$u_\tau + u_\xi(u\xi_x + v\xi_y) + u(u_\xi \xi_x + v_\xi \xi_y) + p_\xi \xi_x = 0 \tag{4b}$$

$$v_\tau + v_\xi(u\xi_x + v\xi_y) + v(u_\xi \xi_x + v_\xi \xi_y) + p_\xi \xi_y = 0, \tag{4c}$$

where the Jacobian J in the pseudo-time derivatives in the corresponding equation in [2] should be neglected. In Eq. (4) the space derivatives are calculated using the known data at time step n. The updated values of vector U at time step $n+1$ can be defined by a linear Taylor series expansion around the previous time step (Fig. 1). A backward series expansion can be such that the vector U is to be defined as a function of the U_j value, which should lie between node i and an adjacent node ($i-1$ or $i+1$) in order to be inside the limits of stable integration. Therefore

$$U = U_j + U_\xi \cdot \Delta\xi' + U_\tau \cdot \Delta\tau \tag{5}$$

which is equal to

$$U_\tau = \frac{U - U_j}{\Delta\tau} - U_\xi \frac{\Delta\xi'}{\Delta\tau} \tag{6}$$

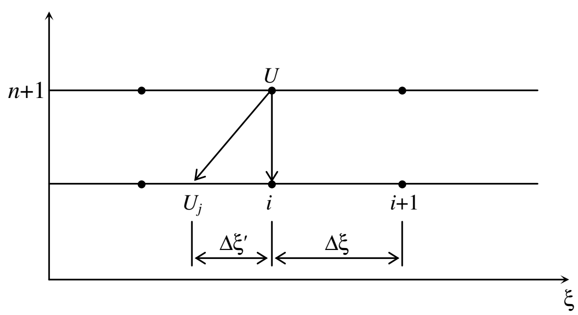

Fig. 1. Schematic representation of the characteristics-based scheme.

where $\Delta\xi'$ is defined by the introduction of a wave speed $\dot{\xi}$ such that

$$\Delta\xi' = \dot{\xi} \cdot \Delta\tau \tag{7}$$

and subsequently the line with slope $1/\dot{\xi}$ is the characteristic. By considering dimensional analysis it can be shown that $\dot{\xi}$ has dimensions of inverse time and therefore it is not a physical speed. In order for a wave speed with proper dimensions to be introduced, the wave speed λ is defined by

$$\dot{\xi} = \lambda\sqrt{\xi_x^2 + \xi_y^2}, \tag{8}$$

where the Jacobian J in the denominator of the corresponding equation in [2] should be neglected. A combination of Eqs. (6)–(8) yields

$$U_\tau = \frac{U - U_j}{\Delta\tau} - U_\xi \lambda \sqrt{\xi_x^2 + \xi_y^2}. \tag{9}$$

Substituting Eq. (9) into Eq. (4) leads to

$$\frac{1}{\beta}\frac{1}{\Delta\tau\sqrt{\xi_x^2 + \xi_y^2}}(p - p_j) - \frac{1}{\beta}p_\xi\lambda + u_\xi\tilde{x} + v_\xi\tilde{y} = 0 \tag{10a}$$

$$\frac{1}{\Delta\tau\sqrt{\xi_x^2 + \xi_y^2}}(u - u_j) + u_\xi(\lambda_0 - \lambda) + u(u_\xi\tilde{x} + v_\xi\tilde{y}) + p_\xi\tilde{x} = 0 \tag{10b}$$

$$\frac{1}{\Delta\tau\sqrt{\xi_x^2 + \xi_y^2}}(v - v_j) + v_\xi(\lambda_0 - \lambda) + v(u_\xi\tilde{x} + v_\xi\tilde{y}) + p_\xi\tilde{y} = 0, \tag{10c}$$

where

$$\lambda = u\tilde{x} + v\tilde{y}, \quad \tilde{x} = \frac{\xi_x}{\sqrt{\xi_x^2 + \xi_y^2}}, \quad \tilde{y} = \frac{\xi_y}{\sqrt{\xi_x^2 + \xi_y^2}}. \tag{11}$$

The spatial derivatives u_ξ, v_ξ, p_ξ, can be eliminated from Eq. (10) according to the following consideration. Because at each time step the system of equations is zero, every one of the three equations can be multiplied by an arbitrary coefficient for example, a, b, c, respectively, and after summation of the equations the resulting equation will also be zero. This is similar to the method of Riemann, according to which the purpose is to construct the solution in time following the characteristics corresponding to the values of λ as seen below, and along which the equations giving the value of the variable only as a function of the one at the previous time step and on the corresponding characteristic apply:

$$\frac{1}{\Delta\tau\sqrt{\xi_x^2 + \xi_y^2}}\left(\frac{a}{\beta}(p - p_j) + b(u - u_j) + c(v - v_j)\right) + p_\xi\left(-\frac{a}{\beta}\lambda + b\tilde{x} + c\tilde{y}\right)$$
$$+ u_\xi(a\tilde{x} + b(\lambda_0 - \lambda + u\tilde{x}) + cv\tilde{x}) + v_\xi(a\tilde{y} + bu\tilde{y} + c(\lambda_0 - \lambda + v\tilde{y})) = 0. \tag{12}$$

If the coefficients of the spatial derivatives are set to be zero then

$$\frac{a}{\beta}(p - p_j) + b(u - u_j) + c(v - v_j) = 0, \tag{13}$$

provided that

$$-\frac{a}{\beta}\lambda + b\tilde{x} + c\tilde{y} = 0 \tag{14a}$$

$$a\tilde{x} + b(\lambda_0 - \lambda + u\tilde{x}) + cv\tilde{x} = 0 \tag{14b}$$

$$a\tilde{y} + bu\tilde{y} + c(\lambda_0 - \lambda + v\tilde{y}) = 0. \tag{14c}$$

A non-trivial solution for the coefficients a, b, c exists for the following values of λ, which are calculated when setting the determinant of Eq. (14) equal to zero:

$$\lambda_0 = u\tilde{x} + v\tilde{y} \tag{15a}$$

$$\lambda_1 = \lambda_0 + \sqrt{\lambda_0^2 + \beta} \tag{15b}$$

$$\lambda_2 = \lambda_0 - \sqrt{\lambda_0^2 + \beta}. \tag{15c}$$

For $\lambda = \lambda_0$ and from Eq. (14a) one obtains

$$a = \frac{b\tilde{x} + c\tilde{y}}{\lambda_0}\beta. \tag{16}$$

Substitution of a into (13) yields

$$b[\tilde{x}(p - p_0) - \lambda_0(u - u_0)] + c[\tilde{y}(p - p_0) - \lambda_0(v - v_0)] = 0, \tag{17}$$

where the subscript '0' denotes that this equation corresponds to $\lambda = \lambda_0$. According to the method, Eq. (17) must be satisfied regardless of the values b and c. Therefore the terms in brackets must be zero. Thus

$$(u - u_0)\tilde{y} - (v - v_0)\tilde{x} = 0. \tag{18}$$

Similarly for $\lambda = \lambda_1$, λ_2 the following equations are obtained:

$$(p - p_1) + \lambda_1[\tilde{x}(u - u_1) + \tilde{y}(v - v_1)] = 0 \tag{19}$$

$$(p - p_2) + \lambda_2[\tilde{x}(u - u_2) + \tilde{y}(v - v_2)] = 0. \tag{20}$$

The method presents Eqs. (18)–(20) as the compatibility equations, the solution of which gives the variables u, v and p as functions of their characteristic variables u_j, v_j, p_j with $j = 0, 1, 2$:

$$u = \tilde{x}R + \tilde{y}(u_0\tilde{y} - v_0\tilde{x}) \tag{21}$$

$$v = \tilde{y}R - \tilde{x}(u_0\tilde{y} - v_0\tilde{x}) \tag{22}$$

$$p = \frac{1}{2\sqrt{\lambda_0^2 + \beta}}(\lambda_1 k_2 - \lambda_2 k_1), \tag{23}$$

where

$$R = \frac{1}{2\sqrt{\lambda_0^2 + \beta}}((p_1 - p_2) + \tilde{x}(\lambda_1 u_1 - \lambda_2 u_2) + \tilde{y}(\lambda_1 v_1 - \lambda_2 v_2)) \tag{24a}$$

$$k_1 = p_1 + \lambda_1(u_1\tilde{x} + v_1\tilde{y}) \tag{24b}$$

$$k_2 = p_2 + \lambda_2(u_2\tilde{x} + v_2\tilde{y}). \tag{24c}$$

Using the finite volume method, Eq. (2) can be discretised as

$$\frac{\partial(JU)}{\partial\tau} + \tilde{E}_{i+1/2} - \tilde{E}_{i-1/2} = 0. \tag{25}$$

For the calculation of the inviscid flux $\tilde{E}$ on the cell face of a control volume (Fig. 2) the values for pressure and velocities from Eqs. (21)–(23) are used. The characteristic variables u_j, v_j, p_j with $j = 0, 1, 2$ in (21)–(23) are calculated by upwind differences from the left or the right side of the cell face according to the sign of λ_j.

$$(U_j)_{i+1/2} = \frac{1}{2}[(1 + \mathrm{sign}(\lambda_j))U^-_{i+1/2} + (1 - \mathrm{sign}(\lambda_j))U^+_{i+1/2}], \tag{26}$$

where (U_j) is the vector of the characteristic variables for each $j = 0, 1, 2$ and sign (λ_j) equals +1 or −1 for positive or negative values of λ_j, respectively. The values of $U^+_{i+1/2}$ and $U^-_{i+1/2}$ can be calculated by high order interpolation formulas.

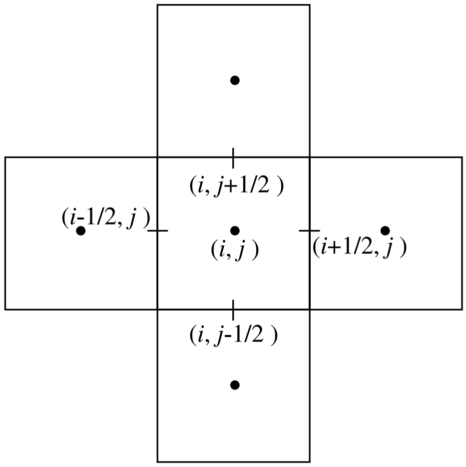

Fig. 2. A finite volume (i,j) with its cell faces.

2.1.2. 3D version

For the version of the scheme for three dimensions [3,4] the process follows the same rationale as in the 2D version splitting the Euler equation into one dimensional equations in the ξ, η and ζ directions and ultimately yielding for the ξ direction

$$\begin{aligned}&\frac{1}{\Delta\tau\sqrt{\xi_x^2+\xi_y^2+\xi_z^2}}\left(\frac{a}{\beta}(p-p_j)+b(u-u_j)+c(v-v_j)+d(w-w_j)\right)+p_\xi\left(-\frac{a}{\beta}\lambda+b\tilde{x}+c\tilde{y}+d\tilde{w}\right)\\&\quad+u_\xi(a\tilde{x}+b(\lambda_0-\lambda+u\tilde{x})+cv\tilde{x}+dw\tilde{x})+v_\xi(a\tilde{y}+bu\tilde{y}+c(\lambda_0-\lambda+v\tilde{y})+dw\tilde{y})\\&\quad+w_\xi(a\tilde{z}+bu\tilde{z}+cv\tilde{z}+d(\lambda_0-\lambda+w\tilde{z}))=0.\end{aligned}\tag{27}$$

similar to (12) and where the Jacobian J appearing in the corresponding equation in [3] should be neglected. If the coefficients of the spatial derivatives are set to be zero then

$$\frac{a}{\beta}(p-p_j)+b(u-u_j)+c(v-v_j)+d(w-w_j)=0,\tag{28}$$

provided that

$$-\frac{a}{\beta}\lambda+b\tilde{x}+c\tilde{y}+d\tilde{z}=0\tag{29a}$$

$$a\tilde{x}+b(\lambda_0-\lambda+u\tilde{x})+cv\tilde{x}+dw\tilde{x}=0\tag{29b}$$

$$a\tilde{y}+bu\tilde{y}+c(\lambda_0-\lambda+v\tilde{y})+dw\tilde{y}=0\tag{29c}$$

$$a\tilde{z}+bu\tilde{z}+cv\tilde{z}+d(\lambda_0-\lambda+w\tilde{z})=0,\tag{29d}$$

where $\lambda_0=u\tilde{x}+v\tilde{y}+w\tilde{z}$. A non-trivial solution for the coefficients a, b, c, d exists for the following values of λ:

$$\lambda_0=u\tilde{x}+v\tilde{y}+w\tilde{z}\tag{30a}$$

$$\lambda_1=\lambda_0+\sqrt{\lambda_0^2+\beta}\tag{30b}$$

$$\lambda_2=\lambda_0-\sqrt{\lambda_0^2+\beta}.\tag{30c}$$

According to the method the compatibility equations for $\lambda=\lambda_0$ resulting from (28) are

$$(w-w_0)\tilde{x}-(u-u_0)\tilde{z}=0,\tag{31a}$$

$$(v-v_0)\tilde{x}-(u-u_0)\tilde{y}=0.\tag{31b}$$

For $\lambda = \lambda_1$ and $\lambda = \lambda_2$ the compatibility equations are

$$(p - p_1) + \lambda_1[\tilde{x}(u - u_1) + \tilde{y}(v - v_1) + \tilde{z}(w - w_1)] = 0 \quad (32)$$

$$(p - p_2) + \lambda_2[\tilde{x}(u - u_2) + \tilde{y}(v - v_2) + \tilde{z}(w - w_2)] = 0 \quad (33)$$

respectively. From the solution of the aforementioned equations the velocity components are defined:

$$u = \tilde{x}R + u_0(\tilde{y}^2 + \tilde{z}^2) - v_0\tilde{x}\tilde{y} - w_0\tilde{x}\tilde{z} \quad (34a)$$

$$v = \tilde{y}R + v_0(\tilde{x}^2 + \tilde{z}^2) - w_0\tilde{z}\tilde{y} - u_0\tilde{x}\tilde{y} \quad (34b)$$

$$w = \tilde{z}R + w_0(\tilde{y}^2 + \tilde{x}^2) - v_0\tilde{z}\tilde{y} - u_0\tilde{x}\tilde{z}, \quad (34c)$$

where

$$R = \frac{1}{2\sqrt{\lambda_0^2 + \beta}}((p_1 - p_2) + \tilde{x}(\lambda_1 u_1 - \lambda_2 u_2) + \tilde{y}(\lambda_1 v_1 - \lambda_2 v_2) + \tilde{z}(\lambda_1 w_1 - \lambda_2 w_2)). \quad (35)$$

Eq. (25) is again used for discretising the 1D equation in the ξ direction resulted from the splitting of the Euler equations. For the calculation of the inviscid flux the values of variables u, v, w, p are calculated from Eqs. (32), (33), (34) whereas the characteristic variables u_j, v_j, w_j, p_j with $j = 0, 1, 2$ in (34) and (35) are calculated by upwind differences from the left or the right side of the cell face according to the sign of λ_j by using (26).

2.2. Revision of the CB scheme

The mathematical inconsistencies within the scheme are spotted in the derivation of the compatibility equations for $\lambda = \lambda_0$ in both the 2D and 3D versions of the method.

2.2.1. 2D version

If (16) is substituted into (14b) then

$$b = -c\frac{\beta\tilde{y} + \lambda_0 v}{\beta\tilde{x} + \lambda_0 u}. \quad (36)$$

Substituting (36) into (16) yields

$$a = -c\beta\frac{u\tilde{y} - v\tilde{x}}{\beta\tilde{x} + \lambda_0 u}. \quad (37)$$

Then substituting (36) and (37) into (13) yields

$$(p - p_0)(u\tilde{y} - v\tilde{x}) - (u - u_0)(\beta\tilde{y} + \lambda_0 v) + (v - v_0)(\beta\tilde{x} + \lambda_0 u) = 0, \quad (38)$$

which is the compatibility equation for $\lambda = \lambda_0$.

However, in [2], Eq. (18) is reported as the compatibility equation for $\lambda = \lambda_0$ due to the following assumption: it is argued that (17) must be satisfied regardless of the values of b and c. This cannot be true since b and c are related as in (36), which is a condition in order for (13) to be true. In other words, there is only one degree of freedom, i.e. if an arbitrary value of c is chosen then a and b should satisfy (36) and (37), respectively, for (13) to be true.

For $\lambda = \lambda_1$ and $\lambda = \lambda_2$, the compatibility equations are (19) and (20), respectively, and are obtained following a procedure similarly as for the derivation of (38) and not (18). Therefore, it is (38) and not (18) that together with (19) and (20) are the compatibility equations, the solution of which gives the primitive values p, u and v as functions of their characteristic values. Consequently, the values of p, u and v given in Eqs. (21)–(23) of the method are meaningless.

2.2.2. 3D version

For a non-trivial solution of Eq. (29), the determinant of the system should be zero, yielding the values of λ as in (30), where $\lambda = \lambda_0$ is a double root. Substitution of $\lambda = \lambda_0$ in (29a) yields

$$a = \frac{\beta}{\lambda_0}(b\tilde{x} + c\tilde{y} + d\tilde{z}), \tag{39}$$

whereas Eqs. (29b)–(29d) are reduced to

$$a = -(bu + cv + dw). \tag{40}$$

This implies two degrees of freedom i.e. two linearly independent vectors $\boldsymbol{L}$, where $\boldsymbol{L} = [a,b,c,d]^{\mathrm{T}}$, can be obtained as non-trivial solutions of (39) and (40). All other solutions would stem from a linear combination of these two vectors. For the derivation of the first vector $\boldsymbol{L}^1$ one can set $c = q$ and $d = 0$. Substitution of these values into (39) and (40) and rearranging yields

$$b = -q\frac{\beta\tilde{y} + \lambda_0 v}{\beta\tilde{x} + \lambda_0 u}, \tag{41}$$

$$a = -q\beta\frac{u\tilde{y} - v\tilde{x}}{\beta\tilde{x} + \lambda_0 u}. \tag{42}$$

Substituting these relations into (28) yields

$$(p - p_0)(u\tilde{y} - v\tilde{x}) - (u - u_0)(\beta\tilde{y} + \lambda_0 v) + (v - v_0)(\beta\tilde{x} + \lambda_0 u) = 0, \tag{43}$$

which is the same as (38). Eq. (43) is the first compatibility equation corresponding to $\lambda = \lambda_0$. For the derivation of the second vector $\boldsymbol{L}^2$ one can set $c = 0$ and $d = q$. Substitution of these values into (39) and (40) and rearranging yields

$$b = -q\frac{\beta\tilde{z} + \lambda_0 w}{\beta\tilde{x} + \lambda_0 u}, \tag{44}$$

$$a = -q\beta\frac{u\tilde{z} - w\tilde{x}}{\beta\tilde{x} + \lambda_0 u}. \tag{45}$$

Substituting these relations into (28) yields

$$(p - p_0)(u\tilde{z} - w\tilde{x}) - (u - u_0)(\beta\tilde{z} + \lambda_0 w) + (w - w_0)(\beta\tilde{x} + \lambda_0 u) = 0. \tag{46}$$

Eq. (46) is the second compatibility equation corresponding to $\lambda = \lambda_0$.

However in the description of the method [3,4], Eqs. (31a) and (31b) are reported as the compatibility equations for $\lambda = \lambda_0$. This outcome also appears in the derivation of the scheme in [5] referred to therein as transport formulation. In a more detailed description of the derivation of the scheme [6], it appears that this outcome is based on a similar argument as in the 2D version, namely that when (39) is substituted into (28) the resulting equation is satisfied regardless of the values of the coefficients b, c and d thus yielding Eq. (31). However this cannot be true because, as also explained in the revision of the 2D version, the coefficients b, c and d are related as in (40) for (28) to be true. For $\lambda = \lambda_1$ and $\lambda = \lambda_2$, the compatibility equations are (32) and (33), respectively, and are obtained following a procedure similarly as for the derivation of (43) and (46) and not (31).

Therefore, it is (43) and (46) and not (31) that together with (32) and (33) are the compatibility equations, the solution of which gives the primitive values p, u, v and w as functions of their characteristic values. Consequently and similarly as for the 2D version, the values of u, v and w given in Eq. (34) of the method are meaningless.

2.2.3. Interpolation formula

For the calculation of characteristic values from (26) for both the 2D and the 3D versions of the scheme the following upwind interpolation formulas are used for approximating the term U on the cell face $i + 1/2$ (Fig. 3)

$$U^-_{i+1/2} = \frac{1}{6}(5U_i - U_{i-1} + 2U_{i+1}) \tag{47a}$$

$$U^+_{i+1/2} = \frac{1}{6}(5U_{i+1} - U_{i+2} + 2U_i) \tag{47b}$$

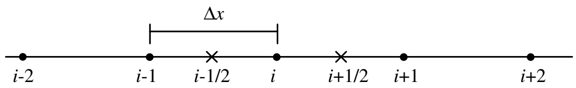

Fig. 3. Topology of a one-dimensional uniform grid.

depending on the side of upwinding. This interpolation formula is reported in the presentation of the CB scheme as of third order of accuracy for the term U on $i+1/2$ [2–5]. However, Eq. (47), referred to also as the CUI scheme [14] are not third but only second order accurate for the term U on $i+1/2$ (see Appendix). They give a third order accurate approximation when used in the term $(U_{i+1/2} - U_{i-1/2})/\Delta x$ or otherwise the discretised derivative $\partial U/\partial x$ at the cell centre i (or $\partial U/\partial y$, $\partial U/\partial z$ accordingly) either as:

$$\frac{\partial U}{\partial x} = \frac{U^+_{i+1/2} - U^+_{i-1/2}}{\Delta x} \tag{48a}$$

or

$$\frac{\partial U}{\partial x} = \frac{U^-_{i+1/2} - U^-_{i-1/2}}{\Delta x} \tag{48b}$$

depending on the side of upwinding. This is what the conclusion from the analysis in the Appendix of [5] should actually be and not that (47) are a 3rd order interpolation formula.

Finally, due the fact that they are derived assuming a uniform grid (see Appendix), (47) are not the optimum choice for interpolation formulas when the CB scheme is used in applications employing non-uniform or/and curvilinear grids as in [6,7,9,12,13].

3. Conclusions

The necessary revisions in the mathematical basis of the characteristics-based scheme for incompressible flows were presented. These revisions concern the compatibility equations and consequently the calculation of the primitive variables within the iterative process of the scheme for both the 2D and 3D versions. Since the iterative process is directly related to the convergence rate, the lacking of the scheme in terms of convergence compared to the hybrid/conservative schemes as reported in [5] may be explained together with the convergence delays encountered in the use of the scheme in several studies [12,13].

Finally, the interpolation formula approximating the values of the characteristic variables on the cell faces is used repeatedly in the method as of third order of accuracy whereas it is only of second order. If third order of accuracy for a three point interpolation formula for a variable on a cell face is needed, then the QUICK scheme [15] should be used (see also Appendix) in the latter form or, when required, in the form for non-uniform grids [16].

Appendix

A general form of an interpolation formula for the value of φ at a cell face is:

$$\varphi_{i+1/2} = \sum_{k=-k_L}^{k_R} b_k \varphi_{i+k} + \text{T.E.} \quad \text{with T.E.} = \sum_{m=n}^{\infty} c_m \Delta x^m \frac{\partial^m \varphi}{\partial x^m}, \tag{A.1}$$

where T.E. is the truncation error, k_L and k_R are two non-negative integers, b_k and c_m are real numbers and Δx is the distance between two adjacent grid nodes when uniform grid is assumed (Fig. 3). Similarly, a general form of an interpolation formula for the value of $\partial\varphi/\partial x$ at the cell face $i+1/2$ is similar to (A.1) and is

$$\left(\frac{\partial \varphi}{\partial x}\right)_{i+1/2} = \frac{\sum_{k=-k_L}^{k_R} b_k \varphi_{i+k}}{l \cdot \Delta x} + \text{T.E.} \quad \text{with T.E.} = \sum_{m=n}^{\infty} c_m \Delta x^m \frac{\partial^{m+1} \varphi}{\partial x^{m+1}}, \tag{A.2}$$

where l is an integer. The exponent n of Δx in the leading term of T.E. defines the order of accuracy of the formula in both (A.1) and (A.2).

For deriving interpolation formulas for the value of φ at the cell face $i+1/2$ (Fig. 3), $\varphi_{i+1/2}$ can be written in the following right upwind-biased form

$$\varphi^{+}_{i+1/2} = a\varphi_i + b\varphi_{i+1} + c\varphi_{i+2} \tag{A.3}$$

Expanding the values of φ at the RHS around $x_{i+1/2}$ yields

$$\begin{aligned}(\varphi^{+}_{i+1/2})^D = {} & a\left[\varphi_{i+1/2} - \left(\frac{\Delta x}{2}\right)\cdot\left(\frac{\partial\varphi}{\partial x}\right)_{i+1/2} + \frac{1}{2!}\left(\frac{\Delta x}{2}\right)^2\cdot\left(\frac{\partial^2\varphi}{\partial x^2}\right)_{i+1/2} - \frac{1}{3!}\left(\frac{\Delta x}{2}\right)^3\cdot\left(\frac{\partial^3\varphi}{\partial x^3}\right)_{i+1/2} + \dots\right] \\ & + b\left[\varphi_{i+1/2} + \left(\frac{\Delta x}{2}\right)\cdot\left(\frac{\partial\varphi}{\partial x}\right)_{i+1/2} + \frac{1}{2!}\left(\frac{\Delta x}{2}\right)^2\cdot\left(\frac{\partial^2\varphi}{\partial x^2}\right)_{i+1/2} + \frac{1}{3!}\left(\frac{\Delta x}{2}\right)^3\cdot\left(\frac{\partial^3\varphi}{\partial x^3}\right)_{i+1/2} + \dots\right] \\ & + c\left[\varphi_{i+1/2} + \left(\frac{3\Delta x}{2}\right)\cdot\left(\frac{\partial\varphi}{\partial x}\right)_{i+1/2} + \frac{1}{2!}\left(\frac{3\Delta x}{2}\right)^2\cdot\left(\frac{\partial^2\varphi}{\partial x^2}\right)_{i+1/2} + \frac{1}{3!}\left(\frac{3\Delta x}{2}\right)^3\cdot\left(\frac{\partial^3\varphi}{\partial x^3}\right)_{i+1/2} + \dots\right]\end{aligned} \tag{A.4}$$

and therefore

$$\begin{aligned}(\varphi^{+}_{i+1/2})^D = {} & (a+b+c)\varphi_{i+1/2} + (b-a+3c)\left(\frac{\Delta x}{2}\right)\cdot\left(\frac{\partial\varphi}{\partial x}\right)_{i+1/2} + (a+b+9c)\frac{1}{2!}\left(\frac{\Delta x}{2}\right)^2\cdot\left(\frac{\partial^2\varphi}{\partial x^2}\right)_{i+1/2} \\ & + (b-a+27c)\frac{1}{3!}\left(\frac{\Delta x}{2}\right)^3\cdot\left(\frac{\partial^3\varphi}{\partial x^3}\right)_{i+1/2} + \dots\end{aligned} \tag{A.5}$$

where superscript D denotes interpolated term so as to distinguish from the exact term in the RHS.

For deriving a second order interpolation formula for $\varphi_{i+1/2}$ in (A.3), the term containing Δx in (A.5) should vanish thus

$$a+b+c=1,$$
$$b-a+3c=0.$$

The above system has one degree of freedom therefore the values of one of the unknowns can be chosen arbitrarily, leading to variety of 2nd order interpolation formulas, one of which is (47b) when $c=-1/6$. A third order interpolation formula of $\varphi_{i+1/2}$ in (A.3) is derived when the aforementioned system containing an additional equation from eliminating the term containing Δx^2 in (A.5) is solved leading to the QUICK [15] scheme.

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