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An improved r-factor algorithm for TVD schemes

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Abstract

An improved r-factor algorithm for TVD schemes on structured and unstructured grids within a finite volume method framework is proposed for numerical approximation to the convective term. The new algorithm is tested by a problem of pure convection with a double-step profile in an oblique uniform velocity field. The computational results are then compared with the results of Darwish's r-factor algorithm using Superbee and Osher limiters on both structured and unstructured grids. The numerical results show that the new algorithm can mitigate the oscillation behavior efficiently while still maintaining the boundedness of the solutions. When using a deferred correction technique to handle the non-linear term arising from the high resolution schemes, the proposed algorithm showed a smoother and faster convergence history on structured grids than Darwish' r-factor algorithm, while on unstructured grids the presented one is more accurate with a similar convergence history.

Keywords: Total variation diminishing scheme; Flux limiter; r-Factor; Unstructured grids; Deferred correction

1. Introduction

The convective term is seemly simple but hard to deal with in CFD [1]. The difficulties lie in false diffusion, non-conservative, overshoot/undershoot and phase error, etc. [2]. Central schemes work quite well in smooth regions but witness the undesirable severe oscillations around discontinuity. It would seem natural that a numerical scheme should be consistent with the velocity and direction with which information propagates throughout the flow field. Indeed, this is nothing more than obeying the physics of the flow. First-order schemes such as upwinding approach have the advantage that a monotone variation is achieved for the numerical flow-field properties in the vicinity of discontinuities; i.e., no oscillations appear in the numerical solutions around these discontinuities. However, they are diffusive and tend to smear out the flow-field variables, particularly in the vicinity of contact surfaces, which is often unacceptable [3,4]. To mitigate this diffusive effect, some high-order schemes such as second-order upwind schemes (SOU) are developed. Though they work well to diminish the diffusive character of the solution, oscillations which do not exist in the first-order schemes appears [5–7]. Then, to reduce or eliminate this undesirable property, while at the same time retaining the inherent advantages of an upwind scheme, some rather mathematically elegant algorithms have been developed over the past decades. These modern algorithms have introduced such terminology as total variation diminishing (TVD) schemes [8], flux splitting [9], flux limiters [10], Godunov schemes [11], and approximate Riemann solvers [12], etc. These ideas are all broadly classified as upwind schemes since they attempt to properly account for the propagation of information throughout the flow. This paper will discuss only the TVD schemes which are high resolution schemes.

A briefly description of present formulation of r-factor using in TVD schemes will be given firstly in the second section, then a new r-factor algorithm is proposed based on Darwish' r-factor, finally, a test example was illustrate and some conclusions concerning the improved r-factor was drawn in the end of the paper.

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Nomenclature

$\boldsymbol{d}$	distance vector
f	face of cell
r	r-factor
N	total number of cells
TV	total variation
x, y, z	components of Cartesian coordinate system
$\boldsymbol{V}$	velocity
Greek symbols	
ρ	density of fluid
Φ	independent variable
$\Psi(r)$	flux limiter
Subscripts	
i, $i+1$, $i+1/2$	index of cell or face
n, $n+1$	time step
U, C, D, $\mathrm{U_r}$	center of cell

2. The present formulations of r-factor in TVD schemes

Harten [7] introduced the following generalization of Godunov's monotonicity concept [11] in one dimension: if the solution of convection equation changes from time step n to $n+1$ such that

$$\left(\int\left|\frac{\partial\Phi}{\partial x}\right|\mathrm{d}x\right)^{n+1}\leqslant\left(\int\left|\frac{\partial\Phi}{\partial x}\right|\mathrm{d}x\right)^{n}\tag{1}$$

where $\mathrm{TV}=\left(\int\left|\frac{\partial\Phi}{\partial x}\right|\mathrm{d}x\right)$ was denoted as the total variation of Φ with x, then the scheme is said to be total variation diminishing (TVD).

Eq. (1) can be rewritten in discrete form,

$$\left(\sum_{i=1}^{N-1}|\Phi_{i+1}-\Phi_i|\right)^{n+1}\leqslant\left(\sum_{i=1}^{N-1}|\Phi_{i+1}-\Phi_i|\right)^{n}\tag{2}$$

where Φ_i and Φ_{i+1} denote the x component of the general dependent variable Φ estimated at point (i) and point ($i+1$), N is the number of total cells in computational domain. For a linear scheme, the TVD property is the same as monotonicity. For a non-linear scheme, however, one can maintain the TVD property while achieving higher order (at least in one dimension) by using non-linear functions called limiters to bound the solution variables such that Eq. (2) hold. Since these functions are intended to limit gradients by modifying the flux terms in the difference equations, they are called, quite naturally, flux limiters, which are quite widespread used in modern CFD algorithms [13–16].

The face value $\Phi_{i+1/2}$ of cell (i) in a TVD scheme, on the basis of Roe [17], can be written as the sum of a diffusive first-order upwind and an anti-diffusive term, shown as below:

$$\Phi_{i+1/2}=\Phi_i+\frac{1}{2}\Psi(r_{i+1/2})(\Phi_{i+1}-\Phi_i)\tag{3}$$

The anti-diffusive part is multiplied by the flux limiter function, $\Psi(r)$, which is often a non-linear function of r (also refer as to r-factor), the upwind ratio of consecutive differences of the solution, defined as [15] in structured grids (without loss of generality, assume the velocity at the face $v_{i+1/2}>0$):

$$r_{i+1/2}=\frac{\Phi_i-\Phi_{i-1}}{\Phi_{i+1}-\Phi_i}\tag{4}$$

For instance, the two limiters [10,18] used in this paper have the forms:

Osher limiter: $\Psi(r)=\max(0,\min(2,r))$.

Superbee limiter:

$$\Psi(r)=\max(0,\min(1,2r),\min(2,r))$$

However, it is not immediately obvious how to express r on an unstructured grid. Since the index-based notation used in structured grids is not suitable for unstructured grids, the more appropriate notation, shown in Fig. 1 as an example of two-dimensional unstructured grid is adopted. Nodes C and D are defined as the upwind and downwind nodes around face f of cell C, and the virtual node U is defined as the node of upwind of the node C.

Using this notation, Eq. (3) can be rewritten as

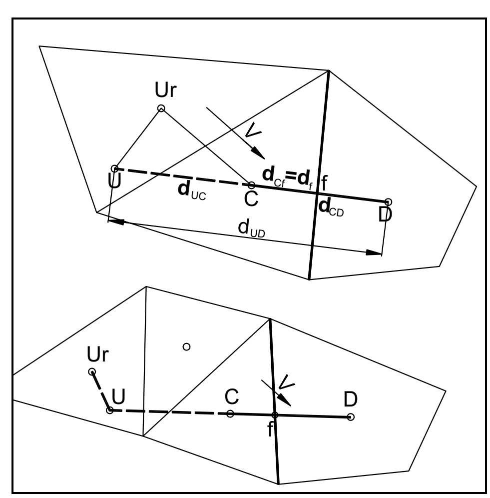

Fig. 1. Advection node stencil.

$$\Phi_f = \Phi_C + \frac{1}{2}\Psi(r_f)(\Phi_D - \Phi_C) \tag{5}$$

Eq. (5) has been used quite often as the TVD scheme for unstructured grids [15,19,20]. The r-factor in Eq. (5) becomes

$$r_f = \frac{\Phi_C - \Phi_U}{\Phi_D - \Phi_C} \tag{6}$$

where Φ_C, Φ_D and Φ_U represent the values of the nodes straddling the interface.

Since $\boldsymbol{d}_{UC} = 2\boldsymbol{d}_f$ ($\boldsymbol{d}_{UC}$ is the vector between the nodes U and C, $\boldsymbol{d}_f$ is the vector between the nodes C and face f) on a uniform one-dimensional grid, Bruner proposed the following r-factor [19]

$$r_{f,\text{Bruner}} \approx \frac{2\boldsymbol{d}_f \cdot (\nabla\Phi)_C}{\Phi_D - \Phi_C} \tag{7}$$

Note that the dependent variable estimated at the face f of cell C was denoted by

$$\Phi_f = \Phi_C + \boldsymbol{d}_f \cdot (\nabla\Phi)_C$$

where $(\nabla\Phi)_C$ represents the gradient of Φ at the center of cell C.

However, Darwish and Moukalled [20] pointed out that Bruner's r-factor is inconsistent and cannot recover TVD condition while being brought back into one dimension. In fact, in one-dimensional grid, Eq. (4) becomes

$$r_f \neq r_{f,\text{Bruner}} = \frac{\Phi_D - \Phi_U}{\Phi_D - \Phi_C} \tag{8}$$

Then the so-called exact r-factor formulation was proposed by Darwish and Moukalled [20]:

$$r_f = \frac{(\Phi_D - \Phi_U) - (\Phi_D - \Phi_C)}{\Phi_D - \Phi_C} \tag{9}$$

It was assumed by the authors that

$$(\Phi_D - \Phi_U) = 2(\nabla\Phi)_C \cdot \boldsymbol{d}_{CD} \tag{10}$$

where $\boldsymbol{d}_{CD}$ is the vector between the nodes C and D. Node U is chosen such that it lies along the line joining nodes D and C with C at the center of the UD segment.

Substituting Eq. (10) into Eq. (9), they gave the r-factor as below

$$r_f = \frac{2(\nabla\Phi)_C \cdot \boldsymbol{d}_{CD}}{\Phi_D - \Phi_C} - 1 \tag{11}$$

It is obvious that Φ_U in Darwish's r-factor is extrapolated by node 'D' and the nodal gradient at node C. So the key point in Darwish's r-factor is how reasonable it is to estimate Φ_U by Eq. (10). If the parabolic distribution of Φ along cell U, C and D in one-dimensional grid is assumed as shown in Fig. 2a, Φ_U can be estimated exactly by Eq. (10), otherwise, for instance, when exponential distribution is encountered (see Fig. 2b), which is true and encountered very common in case with discontinuity such as double-step convection to be illustrated in the next section, Eq. (10) will run into bad even erroneous estimation for Φ_U.

From the view point of deferred correction technique, which is quite often employed in high resolution schemes

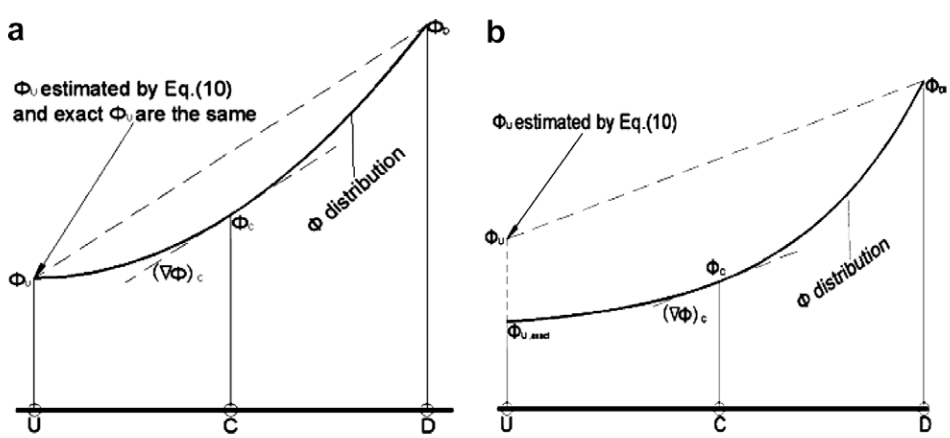

Fig. 2. Φ_U estimated by Eq. (10) under conditions of parabolic (a) and exponential (b) distributions along adjacent nodes in one dimension grid.

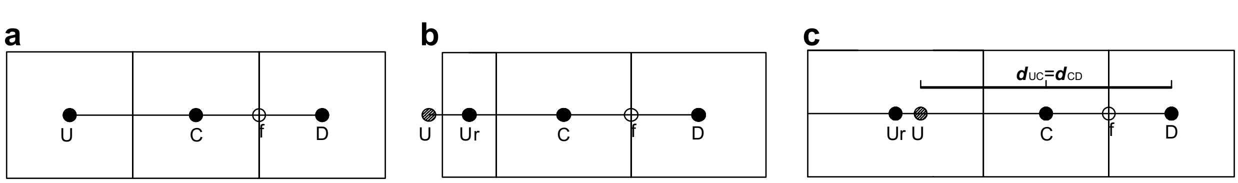

Fig. 3. U_r and U positions in: (a) uniform grids and (b, c) non-uniform grids.

to approximate convective problems and PDE with non-linear source/sink terms, the idea of using the real Φ_{U} directly in Eq. (6) instead of its approximation like Eq. (10) was proposed, since every nodal value has been given before the new iteration step was proceeded in the deferred correction method. The next section will show the derivation process of the new r-factor algorithm presented in this paper.

3. A new r-factor algorithm

The original form of r-factor in unstructured grids suggested by Bruner and Darwish can be expressed by Eq. (6).

If the gradient of node U, instead of node C, is used to estimate Φ_{U} in Eq. (6), a new scheme which includes more upwind information, can be developed:

$$\Phi_{\mathrm{U}} = \Phi_{\mathrm{U_r}} + \boldsymbol{d}_{\mathrm{UU_r}} \cdot (\nabla\Phi)_{\mathrm{U_r}} \tag{12}$$

Substituting Eq. (12) into Eq. (6), gives

$$r_{\mathrm{f}} = \frac{\Phi_{\mathrm{C}} - (\Phi_{\mathrm{U_r}} + \boldsymbol{d}_{\mathrm{UU_r}} \cdot (\nabla\Phi)_{\mathrm{U_r}})}{\Phi_{\mathrm{D}} - \Phi_{\mathrm{C}}} \tag{13}$$

It is just the new r-factor algorithm proposed in this paper, can be also written in the similar form to Eq. (11):

$$r_{\mathrm{f}} = -\frac{\boldsymbol{d}_{\mathrm{UU_r}} \cdot (\nabla\Phi)_{\mathrm{U_r}}}{\Phi_{\mathrm{D}} - \Phi_{\mathrm{C}}} + \frac{\Phi_{\mathrm{C}} - \Phi_{\mathrm{U_r}}}{\Phi_{\mathrm{D}} - \Phi_{\mathrm{C}}} \tag{14}$$

where $\mathrm{U_r}$ is the cell center which contains the virtual node U, $(\nabla\Phi)_{\mathrm{U_r}}$ represents the gradient of $\mathrm{U_r}$, $\boldsymbol{d}_{\mathrm{U_rU}}$ stands for the vector between nodes $\mathrm{U_r}$ and node U (see Fig. 1).

Normally, $\mathrm{U_r}$ does not always coincide with U (see Fig. 3b and c). This scheme causes that more upwind information are used. Eq. (13) will be reduced to Eq. (4) in a uniform grid system, in which U and $\mathrm{U_r}$ are the same point (see Fig. 3a).

On the other hand, as mentioned above, when the distribution of Φ_{U}, Φ_{C}, Φ_{f} and Φ_{D} does not fit in with parabolic curve (see Fig. 2b), Eq. (11) will not but Eq. (13) can work correctly.

Eqs. (11) and (13) have the similar structure as shown in Eq. (14) and both need to calculate a nodal gradient. But the latter has to do the work concerning the search of $\mathrm{U_r}$ given $\boldsymbol{d}_{\mathrm{UU_r}}$ (see Fig. 1) which is implemented easily but may cost a little extra time over Darwish's r-factor; this will be showed in the next section.

4. Numerical experiments

The test case is illustrated in Fig. 4, consisting of pure convection of a transverse double-step profile imposed at the inflow boundaries of a cubic domain $(1 \times 0.25 \times 1)$ with an oblique uniform velocity field $\mathbf{v} = (1, 1, 0)$.

The governing conservation equation and boundary conditions for the problem are given as:

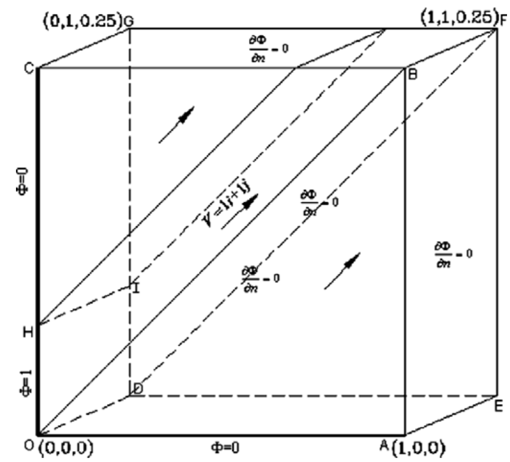

Fig. 4. Computational domain and boundary conditions.

$$\begin{cases} \nabla\cdot(\rho\mathbf{v}\Phi) = 0 \\ \Phi = \begin{cases} 1 & \text{at face: (1) } OHID(X = 0, 0 \leqslant Z \leqslant 0.3) \\ 0 & \text{at face: (1) } HCGI(X = 0, 0.3 \leqslant Z \leqslant 1); \\ & \qquad\quad\text{(2) } ODEA(Z = 0) \end{cases} \\ \frac{\partial\Phi}{\partial n} = 0 \quad \text{at face: } \begin{cases} \text{(1) } OABC(Y = 0); \\ \text{(2) } DGFE(Y = 0.25); \\ \text{(3) } AEFB(X = 1.0); \\ \text{(4) } CBFG(Z = 1) \end{cases} \end{cases}$$

where Φ is the dependent variable.

The simulations by using Darwish's and new r-factors are carried out with the same deferred correction technique. Two 3D mesh systems were used. One is structured consisting of 2000 cells, and the other is unstructured consisting of 7318 cells, illustrated in Figs. 5a and 7a, respectively. Both algorithms need to compute a nodal gradient, so the same method to approximate the nodal gradient, i.e. the least square method, was adopted in this paper.

On the structured grid, the results obtained from upwind, TVD schemes using Superbee and Osher limiters estimated r-factor by Eqs. (11) and (13) are shown in Figs. 5–7.

It is clear that on structured grids the result of upwinding is seriously diffusive (Fig. 5b). When a TVD scheme was used, which is implemented by the deferred correction technique, the false diffusion was controlled in much degree (Fig. 5c and d) compared with upwinding. Superbee and Osher schemes using the new r-factor algorithm yield better results than using that of Eq. (11), because the latter suffers an oscillation-like pattern near the discontinuous regions (see the regions labeled A∼D of Fig. 5c), which can be further manifested in Figs. 6 and 7. Besides, the former has a smoother and faster convergence pattern than the latter as shown in Fig. 8.

The computed results on unstructured grids using the upwind and Superbee schemes implemented using Eqs. (11) and (13) are depicted in Fig. 9. From the figures, they are shown similar to those in structured grids. However,

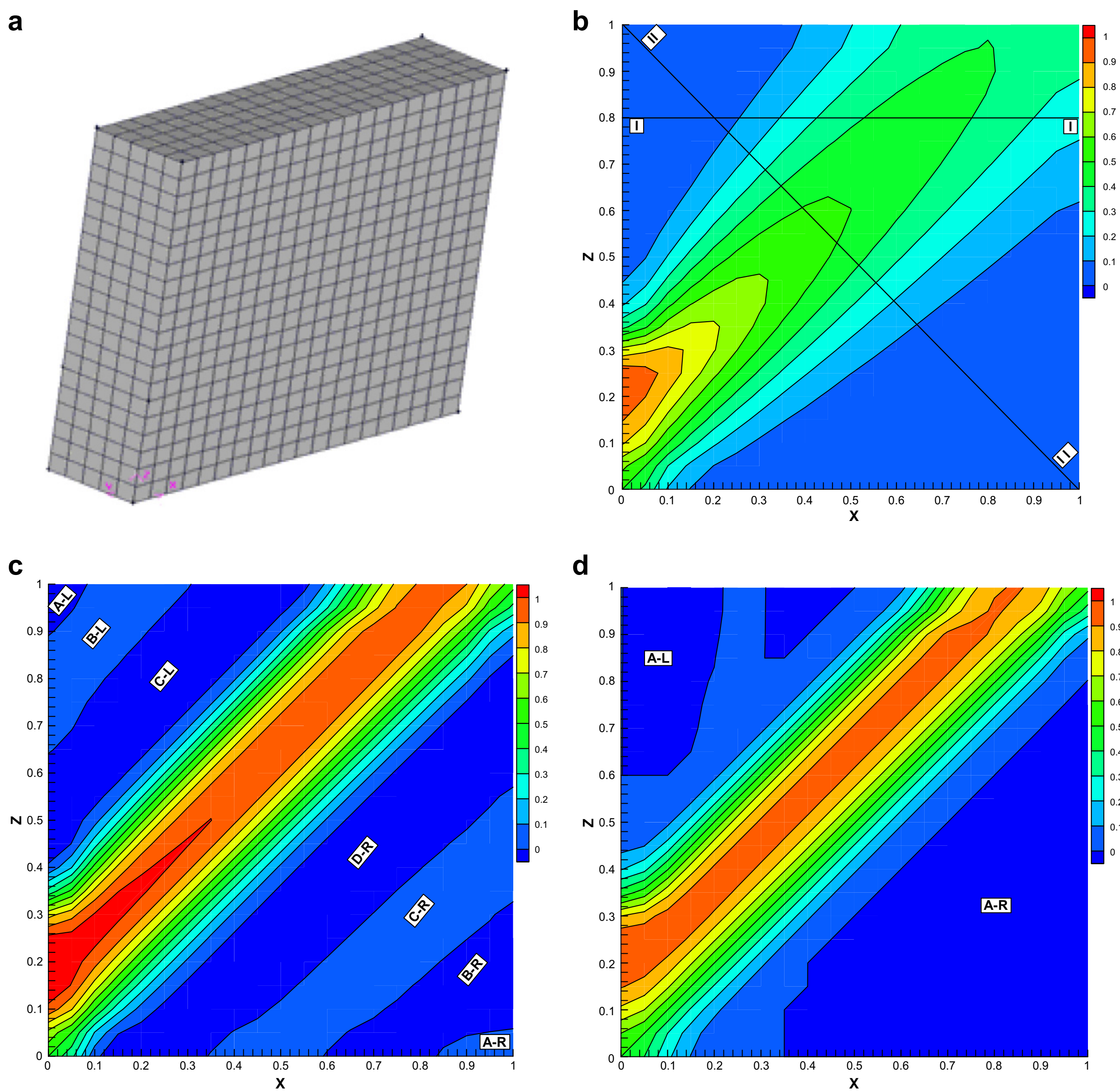

Fig. 5. Comparisons of Φ colour maps at $y = 0.125$ via different r-factors implemented on structured grids: (a) grid used, (b) upwinding, (c) Superbee scheme using Eq. (11) and (d) Superbee scheme using Eq. (13). (For interpretation of the references in colour in this figure legend, the reader is referred to the web version of this article.)

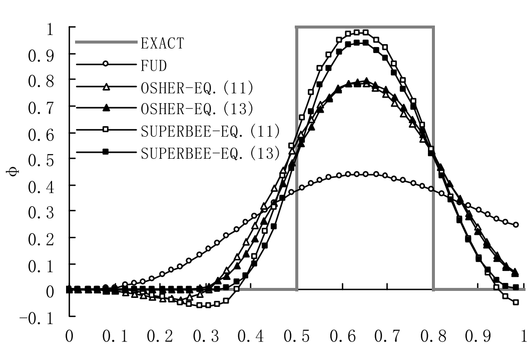

Fig. 6. Comparison of Φ profiles at $z = 0.8$, $y = 0.25$ via different r-factors implemented on structured grids (section I-I).

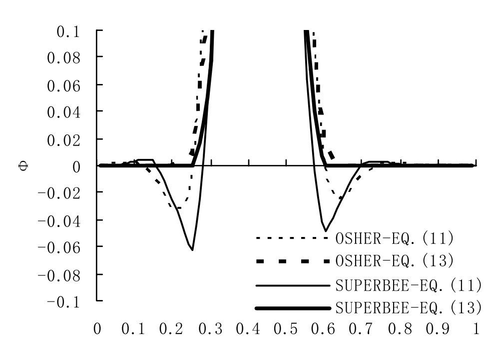

Fig. 7. Comparison of oscillation-like undershoot via different r-factors implemented on structured grids (section II-II).

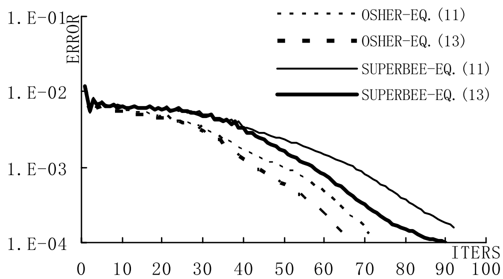

Fig. 8. Comparison of iteration history via different r-factors implemented on structured grids.

both the two r-factor algorithms gave rise to undershoot around the discontinuity, yet the proposed one produced less which can be seen in the regions labeled A∼C of Figs. 9c and d either using Superbee or Osher scheme. It can be seen from Figs. 9b and 5b that dissipation of upwinding has been reduced somewhat due to the grid was refined. In fact, when the grid becomes denser and denser, the differences between the two algorithms are less and less. Their convergence processes when applying the deferred correction technique are shown in Fig. 10. From that, it is evident that both r-factor algorithms give almost the same convergence behavior.

On unstructured grids, note that both the two r-factor algorithms suffer oscillations near the discontinuous regions, though they are all minor (see Figs. 11 and 12). This may be attributed to the following reasons: (1) the

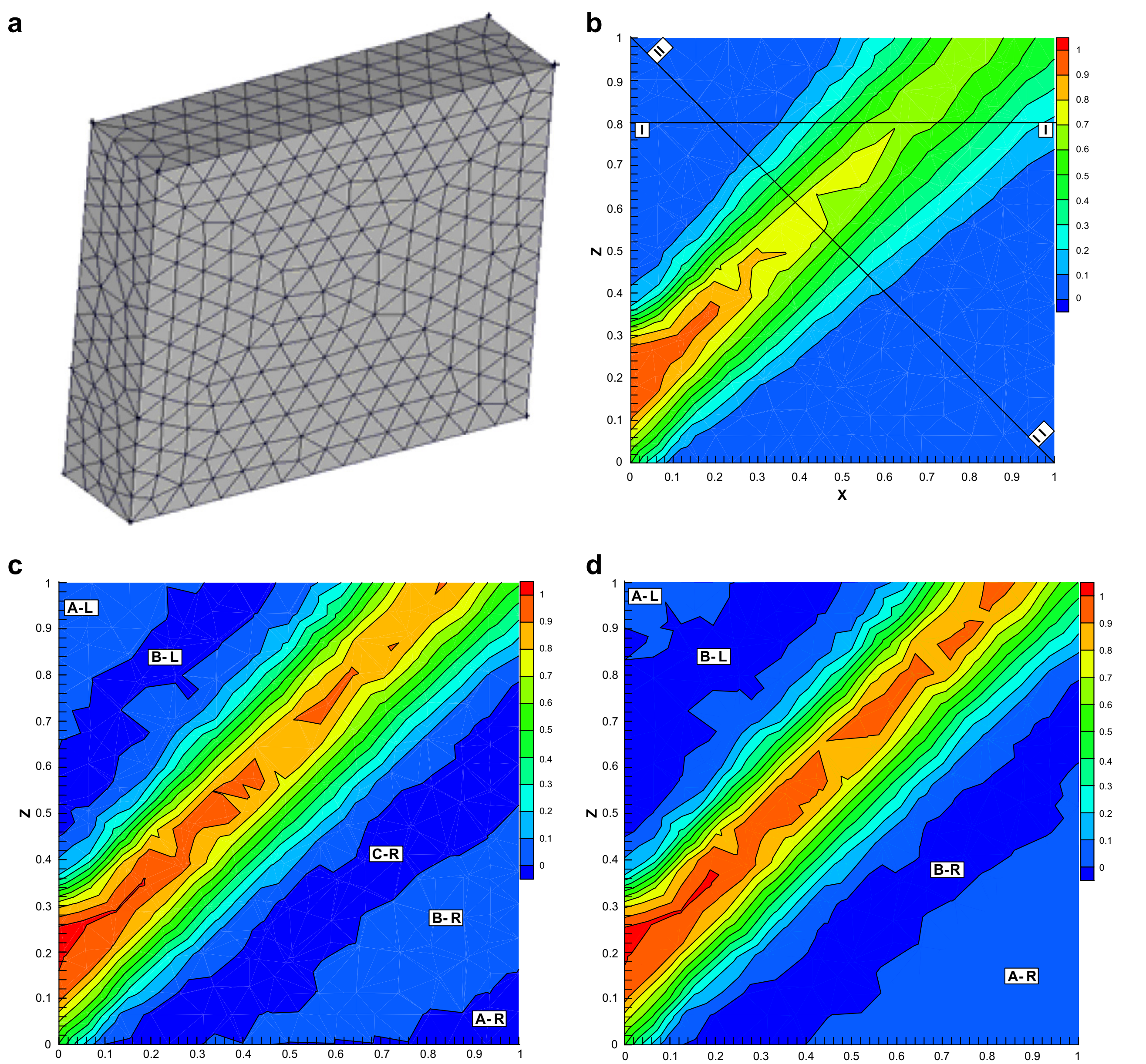

Fig. 9. Comparisons of Φ profiles at $y = 0.125$ via different r-factors implemented on unstructured grids: (a) grid used, (b) upwinding, (c) Superbee using Darwish's r-factor and (d) Superbee using the new r-factor.

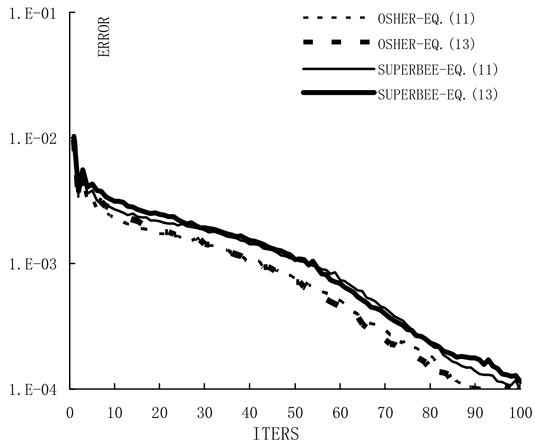

Fig. 10. Comparison of iteration history by using deferred correction technique via different r-factors implemented on unstructured grids.

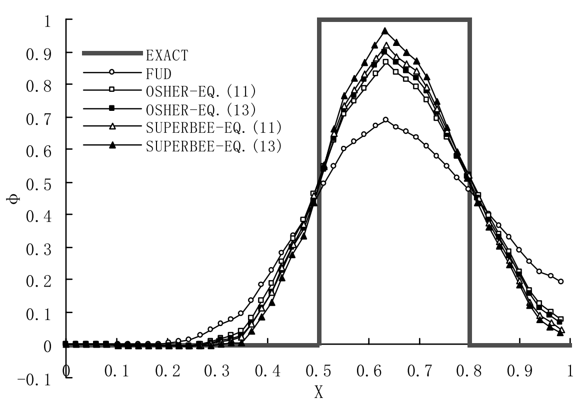

Fig. 11. Comparison of Φ profiles at $z = 0.8$, $y = 0$ via different r-factors implemented on unstructured grids (section I-I).

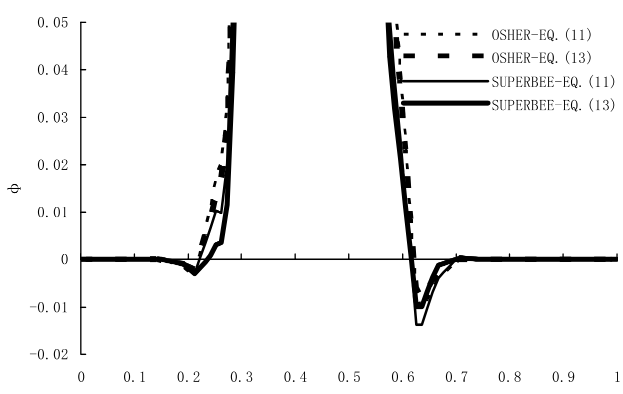

Fig. 12. Comparison of oscillation and undershoot via different r-factors on unstructured grids (section II-II).

TV definition cannot be directly extended to 3D dimensional unstructured gird and (2) the gradient formulation used above does not limit the oscillations. In fact, the limiter have great influence on the scheme and the relation between flux limiter and r-factor may not be always follow the Sweby's r–Ψ diagram, which has great influence on the schemes and simulation results [21]. The details, which are beyond the scope of the paper, can be found in Ref. [22]. Nevertheless, the same gradient formulation, same grid system and same deferred correction technique were adopted, in terms of the results, conclusion can be drawn that the new r-factor formulation presented in this paper is more reasonable and accurate than Eq. (11).

Table 1
Comparison of running time via different r-factors

Case	Grid system		Allowed error	CPU time (s)	
	Type	Cells		Eq. (11)	Eq. (13)
1	Structured	2000	10^{-6}	1861	2241
2	Unstructured	7318	10^{-6}	18,540	19,474

Besides, to confirm the efficiency of the new r-factor algorithm, comparison of the computational time of Darwish's and the new r-factor algorithms was conducted under the same condition with Superbee limiter. The results are listed in Table 1. It indicates that although the extra work concerning the search of U_r as mentioned above is required, the time consumed of the two algorithms is almost the same due to the faster convergence history of the new r-factor algorithm, and the latter is a little more than the former.

5. Conclusion

A new r-factor algorithm used in flux limiter function when TVD schemes are applied was proposed in this paper. The new algorithm has been proved that it shows better behavior over Darwish's r-factor formulation in terms of accuracy and convergence history: (1) On structured grids, the former has almost no while the latter has obvious oscillations at the sharp gradient position, and the former has a smoother and faster convergence history. (2) On unstructured grids, the former is more accurate than the latter and has a similar convergence history and CPU time to the latter. (3) Both in structured and unstructured grids, the new r-factor algorithm shows minor oscillations, even if the grids become denser. It is also pointed out in this paper that the original TVD definition in uniform and one-dimensional grids system may not directly be extended to multidimensional and unstructured one, though it works well in many problems. In light of the definition of TVD schemes, any numerical scheme that gives rise to oscillations does not satisfy the TVD conditions. So it is need future study on multidimensional and unstructured grids when intent to apply TVD schemes.

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