

# AN EXACT $r$ -FACTOR TVD FORMULATION FOR UNSTRUCTURED GRIDS

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## ABSTRACT

The implementation of TVD schemes within a multi-dimensional structured grid environment is rather well understood. With the increasing importance of unstructured grid for CFD applications, a number of approaches have evolved for the implementation of these schemes within an unstructured grid finite volume method framework. Unfortunately none of these approaches has been comprehensive enough to permit the general implementation of TVD-based schemes in unstructured grids, and/or accurate enough to recover the exact TVD formulation in structured grids. In this paper we propose a simple method that allows the implementation of the full spectrum of TVD schemes in unstructured grids, while recovering their exact formulation on structured grids. Four schemes implemented using this approach, TVD-MINMOD, TVD-MUSCL, TVD-SUPERBEE, TVD-OSHER, are tested and compared to Bruner's TVD formulation [1], and to the Barth and Jespersen linear reconstruction scheme [2] by solving two problems involving advection of a step and a sinusoidal profile. Results indicate that the Bruner formulation yields, for the same original TVD scheme, overly diffusive results when compared to the current method. The BJ-MUSCL and TVD-MUSCL are shown to be comparable and more accurate than the OSHER scheme. The SUPERBEE performs best though showing tendency for stepping the modeled profile. In all tests the current method is found to retain the behavior of the structured grid TVD formulation.

## KEY WORDS

TVD schemes, unstructured grid, convection schemes.

## 1. Introduction

The last two decades have witnessed a sustained effort by the CFD community to develop robust high-resolution (HR) schemes [3-5] for the simulation of advection-dominated flows. Many of these schemes have been implemented on structured grids within the framework of finite volume methods. The main

ingredients common to all these schemes are a high order profile for the reconstruction of cell face values from cell averages, combined to a monotonicity criterion. The high order reconstruction is usually based on an upwind biased, sometimes symmetric, high order interpolation profile [6]. To satisfy monotonicity, a number of concepts have been proposed over the years [7], all within a structured grid framework. In the Flux Corrected Transport (FCT) approach of Boris and Book [8,9], a first order accurate monotone scheme is converted to a High Resolution scheme by adding limited amounts of anti-diffusive flux. In the monotonic upstream-centered scheme for conservation laws (MUSCL) of Van Leer [10], monotonicity is enforced through a limiter function applied to a piecewise polynomial flux reconstruction procedure. Harten [11] expressed monotonicity as a measure of discrete variation in the solution fields, hence the name Total Variational Diminishing (TVD). This criterion was then expressed as a flux limiter by Sweby using the  $r$ - $\psi$  diagram [12]. Leonard [4,13,14] presented his monotonicity criterion using a relation between a normalized face value,  $\tilde{\phi}_f$ , and a normalized upwind value,  $\tilde{\phi}_c$ . While on the conceptual level the above-mentioned monotonicity criteria can be shown to be related and sometimes equivalent, implementation-wise they are very different. However within the framework of structured grids these differences have not translated into increased difficulties in implementation.

For unstructured grids the situation is more complicated and high-resolution schemes are not as advanced as for structured grids [15]. This is specifically due to the difficulty in implementing and enforcing a monotonicity criterion that relies on logical or directional next-neighbor information, which is readily available in structured grids but missing in unstructured grids. To circumvent this difficulty a number of approaches have evolved, with varying degrees of success, based on different monotonicity criteria, such as the FCT [8,9], the flux difference splitting concepts [16], or the MUSCL approach [17]. The MUSCL-based technique developed by Barth and Jespersen (BJ) [2], by modifying the Spekreijse [18] definition of monotonicity to bound the

cell face values rather than the cell nodal value, is currently the most popular and successful approach for the implementation of high resolution schemes in unstructured grids [19], partly because of its simplicity. Unfortunately, most of the limiters developed for structured grids cannot be implemented using the BJ technique as it is restricted to schemes where the base high order profile uses a cell based gradient, which is basically equivalent to the FROMM scheme [10], whose bounded version is equivalent to the MUSCL scheme. In one dimension the BJ scheme can be shown to be equivalent to the TVD-MUSCL scheme [20]. Bruner [1,20] suggested a more general approach to bound convective schemes. In this approach he used the Sweby  $r$ - $\psi$  diagram with a modified  $r$  factor defined for unstructured grids. Unfortunately his modification did not recover the exact  $r$  factor on structured grids. In this paper we present a valid re-formulation of the  $r$  factor for unstructured grids that yields the exact TVD formulation on structured grids.

In what follows the formulation of TVD schemes is presented for structured grids following the  $r$ - $\psi$  diagram of Sweby. The modification of Bruner to the  $r$ -factor is then described before detailing the new  $r$ -formulation. Spekrijse's criterion is then presented and the BJ technique described. Finally, the new method is compared to the Bruner implementation and the BJ scheme. For that purpose, four TVD schemes (MINMOD [11], OSHER [21], TVD-MUSCL [10], and SUPERBEE [22]), implemented using the new formulation, are tested by solving a number of pure advection problems.

## 2. TVD Schemes

Following Roe [22], the face value  $\phi_{i+1/2}$  of a TVD scheme is written as the sum of a diffusive first order upwind term and an anti-diffusive one. The anti-diffusive part is multiplied by the flux limiter function,  $\psi(r)$ , which is a non-linear function of  $r$ , the upwind ratio of consecutive gradients of the solution, defined as (without loss of generality, we assume the velocity at the face  $v_{i+1/2} > 0$ ):

$$r_{i+1/2} = \frac{\phi_i - \phi_{i-1}}{\phi_{i+1} - \phi_i} \quad (1)$$

leading to the flux-limited scheme:

$$\phi_{i+1/2} = \phi_i + \frac{1}{2} \psi(r_{i+1/2}) (\phi_{i+1} - \phi_i) \quad (2)$$

Using a flux limiter,  $\psi(r)$ , which is simply a linear function of  $r$ , different high order schemes can be written in the form of equation (2). For example for,  $\psi$  equal to  $r$ , the second order upwind (SOU) scheme is obtained. Other schemes can be similarly formulated:

$$\begin{aligned} \text{DOWNWIND scheme} \quad \psi(r) &= 2 \\ \text{CD scheme} \quad \psi(r) &= 1 \\ \text{SOU scheme} \quad \psi(r) &= r \\ \text{FROMM scheme} \quad \psi(r) &= \frac{1+r}{2} \end{aligned} \quad (3)$$

Following Sweby [12], these schemes may be plotted along with the TVD monotonicity region on an  $r$ - $\psi$  diagram (see figure 1(a)). Using this diagram, it is simple to grasp the formulation of TVD schemes: any flux limiter function,  $\psi(r)$ , formulated to lie within the TVD monotonicity region yields a TVD scheme. Sweby has also shown that for second order schemes the flux limiter function,  $\psi(r)$ , has to pass through point (1,1). A number of TVD schemes are shown in figures 1(b)-1(e), and formulated as:

$$\begin{aligned} \text{SUPERBEE} \quad \psi(r) &= \max(0, \min(1, 2r), \min(2, r)) \\ \text{MINMOD} \quad \psi(r) &= \max(0, \min(1, r)) \\ \text{OSHER} \quad \psi(r) &= \max(0, \min(2, r)) \\ \text{MUSCL} \quad \psi(r) &= \frac{r + |r|}{1 + |r|} \end{aligned} \quad (4)$$

Since the index-based notation used above is not suitable for unstructured grids, the more appropriate notation, shown in figures 2(a), 2(b), is adopted. As shown in figure 2(b), nodes C and D are defined as the Upwind and Downwind nodes around face  $f$ , and the virtual U node is defined as the node upwind of the C node.

Using this notation equation (2) is rewritten as

$$\phi_f = \phi_C + \frac{1}{2} \psi(r_f) (\phi_D - \phi_C) \quad (5)$$

and the  $r$  ratio becomes

$$r_f = \frac{\phi_C - \phi_U}{\phi_D - \phi_C} \quad (6)$$

It is clear that the main difficulty in implementing TVD schemes in unstructured grids lies in the need for defining a 'virtual' U node.

## 3. Bruner $r$ Modification

Bruner [1] proposed the following modification to the definition of the  $r$ -factor for TVD schemes:

$$r_f = \frac{\phi_C - \phi_U}{\phi_D - \phi_C} \approx \frac{2(\phi_f - \phi_C)}{\phi_D - \phi_C} = \frac{2\Delta r^{\omega}(\nabla\phi)_C}{\phi_D - \phi_C} \quad (7)$$

This approximation is clearly inconsistent and when brought back into one dimension does not recover the TVD condition, as equation (6) becomes:

$$r_f = \frac{\phi_C - \phi_U}{\phi_D - \phi_C} \neq r_{f,bruner} = \frac{2\Delta r^{\omega}(\nabla\phi)_C}{\phi_D - \phi_C} = \frac{\phi_D - \phi_U}{\phi_D - \phi_C} \quad (8)$$

## 4. Exact $r$ Formulation

A better formulation for  $r$  in unstructured grids can still be derived. Returning to the definition of  $r$ , we can write:

$$\begin{aligned} r_f &= \frac{\phi_C - \phi_U}{\phi_D - \phi_C} = \frac{\phi_D + (\phi_C - \phi_U) - \phi_D}{\phi_D - \phi_C} \\ &= \frac{(\phi_D - \phi_U) - (\phi_D - \phi_C)}{\phi_D - \phi_C} \end{aligned} \quad (9)$$

Noting that values for  $\phi_D$  and  $\phi_C$  represent the values of the nodes straddling the interface and thus are readily available for unstructured grid. Therefore, the  $r$ -values

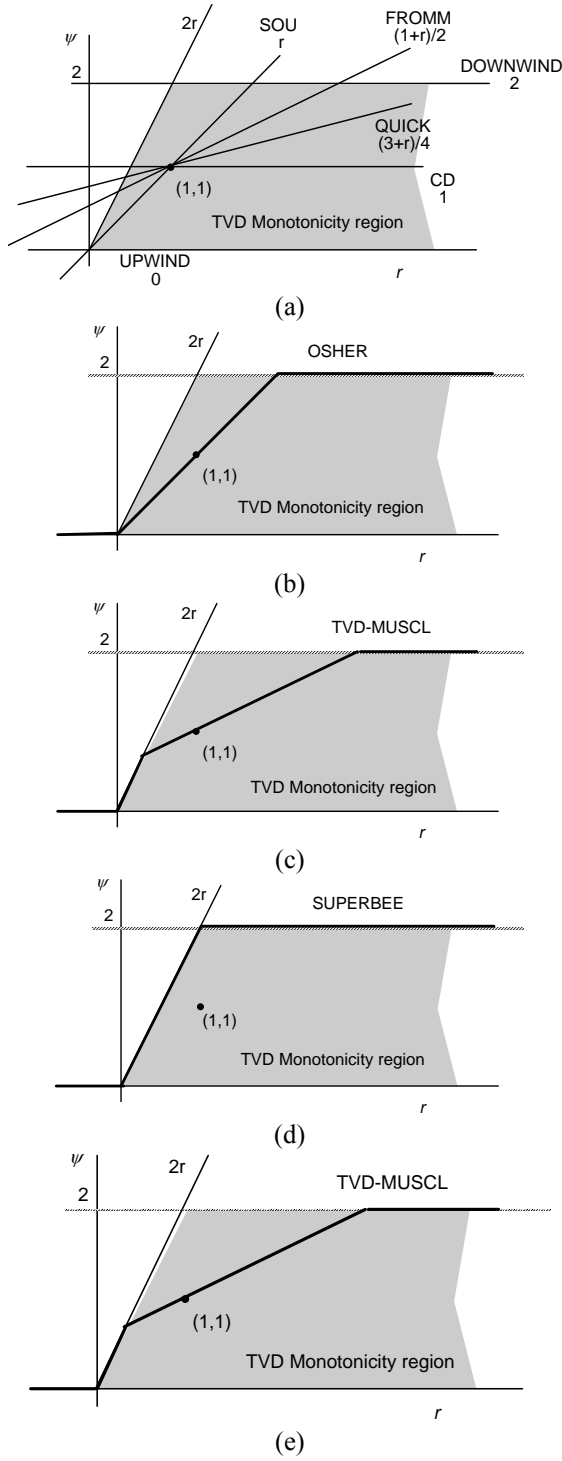


Figure 1 (a) High Order and TVD monotonicity region on Sweby's diagram, (b)-(e) TVD schemes in Sweby r- $\psi$  diagram.

would be computable if the term involving  $\phi_U$  could be replaced by a known term. In this case

$$\begin{aligned} (\phi_D - \phi_U) &= \nabla \phi_C \cdot \mathbf{r}_{UD} \\ &= (2\nabla \phi_C \cdot \mathbf{r}_{CD}) \end{aligned} \quad (10)$$

and the formulation of  $r$  becomes

$$r_f = \frac{(2\nabla \phi_C \cdot \mathbf{r}_{CD}) - (\phi_D - \phi_C)}{\phi_D - \phi_C} = \frac{(2\nabla \phi_C \cdot \mathbf{r}_{CD})}{\phi_D - \phi_C} - 1 \quad (11)$$

which can be easily computed for unstructured grids.

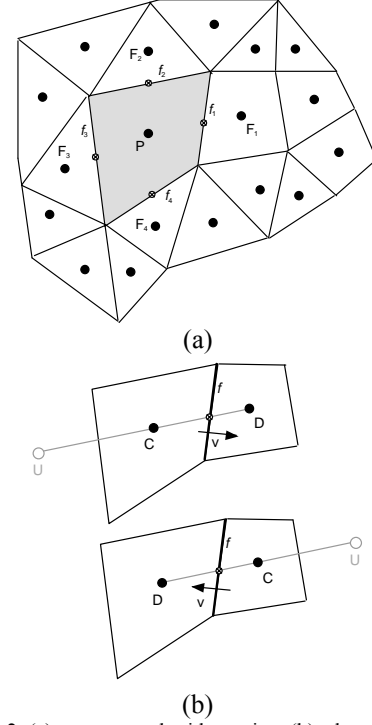


Figure 2: (a) unstructured grid notation, (b) advection node notation.

## 5. Barth and Jespersen Scheme

Barth and Jespersen [2] followed a different approach in enforcing the monotonicity criterion. In their approach the Speikreijse monotonicity criterion [18] was modified to apply it for the reconstruction of  $\phi$  within the control volume, i.e. the condition was changed to state that the values of the reconstructed polynomial within the control volume should not exceed the maximum and minimum values at the neighbors of the control volume.

Using the notation of figure 2(a) the Speikreijse criterion written as:

$$\min(\phi_N) \leq \phi_P \leq \max(\phi_N) \quad \forall N \in \text{Neighbors}(P) \quad (12)$$

was modified to:

$$\begin{aligned} \min(\phi_N, \phi_P) \leq R_P(\mathbf{r}_j) \leq \\ \max(\phi_N, \phi_P) \quad \forall N \in \text{Neighbors}(P) \end{aligned} \quad (13)$$

where  $j$  is some point within the control volume  $P$ , and  $R$  is the reconstruction operator given by:

$$R_P(\mathbf{r}_j) = \phi_P + \psi_j \nabla \phi_P \cdot (\mathbf{r}_j - \mathbf{r}_P) \quad (14)$$

where  $\psi$  is the flux limiter, and  $r$  the position vector. Instead of enforcing the condition of equation (2) over the control volume, it is enforced at the cell faces integration points, thus changing equation (13) into:

$$\begin{aligned} \min(\phi_N, \phi_P) \leq R_P(\mathbf{r}_f) \leq \\ \max(\phi_N, \phi_P) \quad \forall N \in \text{Neighbors}(P) \end{aligned} \quad (15)$$

where  $f$  is a cell face centroid. The computation of the value of the limiter  $\psi$  is performed in two steps as follows.

Step 1: The reconstruction polynomial is evaluated at each cell face integration point in order to determine the value of  $\psi_f$  that satisfies the relation:

$$\min(\phi_N, \phi_P) \leq R_P(\mathbf{r}_f) = \phi_P + \psi \nabla \phi_P \cdot (\mathbf{r}_f - \mathbf{r}_P) \leq \max(\phi_N, \phi_P) \quad (16)$$

which can be rewritten as

$$\psi_f = \begin{cases} \Phi \left( \frac{\max(\phi_N, \phi_P) - \phi_P}{\nabla \phi_P \cdot (\mathbf{r}_f - \mathbf{r}_P)} \right) & \phi_f > \phi_P \\ \Phi \left( \frac{\phi_P - \min(\phi_N, \phi_P)}{\nabla \phi_P \cdot (\mathbf{r}_f - \mathbf{r}_P)} \right) & \phi_f < \phi_P \\ 1 & \phi_f = \phi_P \end{cases} \quad (17)$$

where

$$\Phi(x) = \min(x, 1) \quad (18)$$

Step 2: The value of the limiter is computed as the minimal value of  $\psi$  over all cell faces, i.e.:

$$\psi_P = \min(\psi_f) \quad (19)$$

## 6. Test Problems

The validity of the newly proposed r-factor formulation in unstructured grids is demonstrated in this section. For that purpose four TVD schemes are implemented using the Bruner and the new formulations. The schemes are then used in solving two pure convection test problems: advection of a step profile and advection of a sinusoidal profile. Results obtained using the schemes are compared against those obtained using the BJ linear reconstruction scheme and the first order upwind scheme.

### 6.1. Advection of a Step Profile

Figure 3(a) shows the well known benchmark test problem consisting of a pure advection of a transverse step profile imposed at the inflow boundaries of a square computational domain. Two unstructured mesh systems consisting of 862 and 2094 cells (illustrated in Figure 3(b)) were used. The governing conservation equation for the problem is simply:

$$\nabla \cdot (\rho \mathbf{v} \phi) = 0 \quad (20)$$

where  $\phi$  is the dependent variable and  $\mathbf{v} = 1\mathbf{i} + 1\mathbf{j}$  is the Cartesian velocity vector. The computed values of  $\phi$  using the upwind scheme, the OSHER, the MINMOD, the MUSCL and the SUPERBEE schemes in addition to the BJ scheme are shown in Fig. 3(c) and 3(d) for the coarse and fine grids respectively. As is the case for structured grids [4] the MINMOD is the most diffusive, the BJ-MUSCL and TVD-MUSCL schemes yield comparable results that are better than the OSHER scheme. The performance of the upwind scheme is worse in unstructured grids than for structured grids because no flow can be aligned with the grid lines. As expected the SUPERBEE yields the best results because it is a highly compressive scheme. All results are devoid of over/undershoots. Performance-wise the TVD and BJ implementations required about the same computational

cost per iteration, TVD schemes generally did not experience any flattening of the convergence rate below a residual of  $10^{-6}$  except for the SUPERBEE scheme, while the BJ scheme experienced oscillations of the residual around  $10^{-6}$ . This was inconsequential with respect to the results.

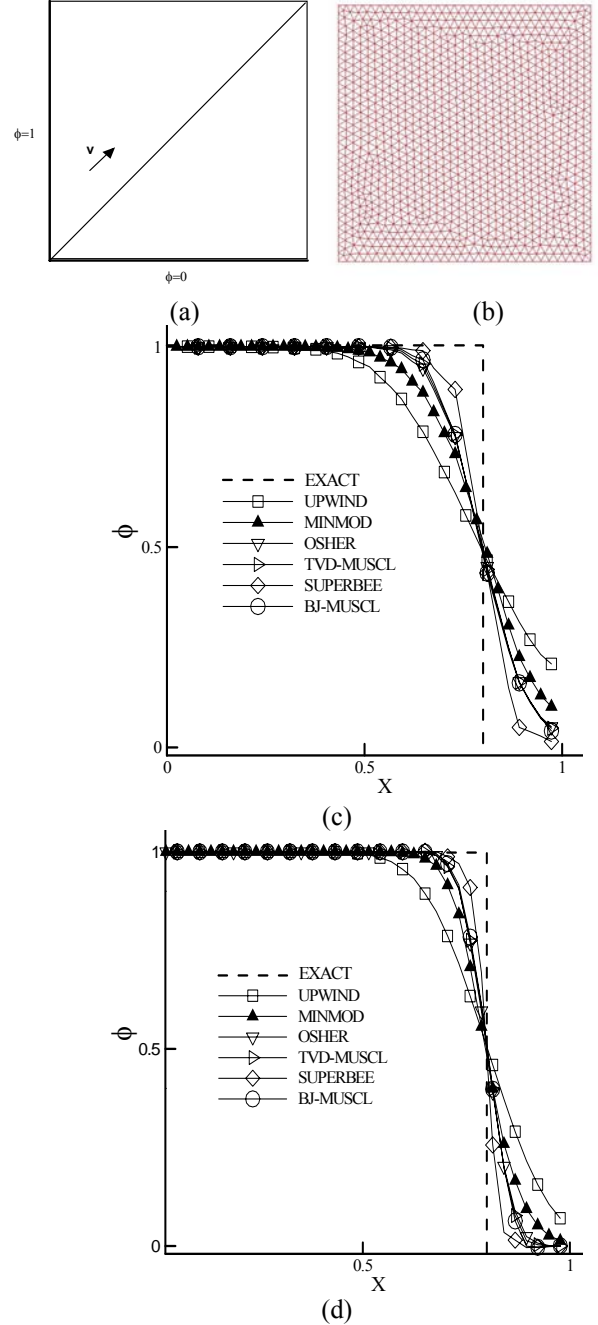


Figure 3: Convection of a step profile; (a) physical domain, (b) dense grid used, (c)  $\phi$  profile at  $y=0.8$  using coarse grid, (d)  $\phi$  profile at  $y=0.8$  using dense grid.

In Figure 4, the TVD-MUSCL scheme profiles generated using the current formulation are compared against profiles obtained following Bruner's formulation on both coarse (Figure 4(a)) and dense (Figure 4(b)) grid systems. As depicted, Bruner's scheme results are over diffusive due to the approximation introduced in the

formulation of r. The same trend was observed with all the other schemes and deemed unnecessary to be reported for compactness.

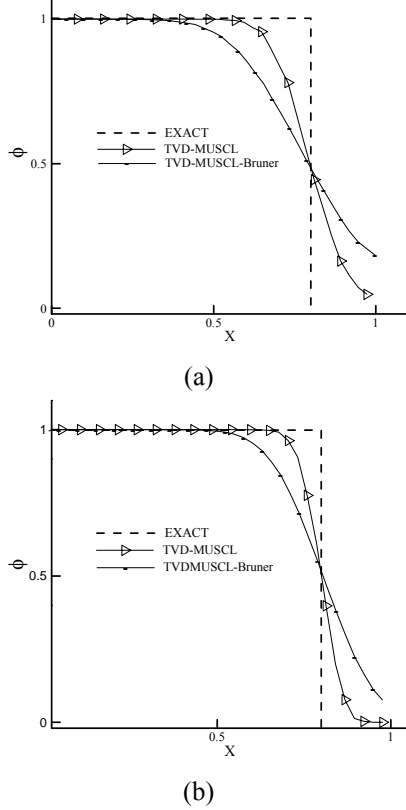


Figure 4: Comparison of  $\phi$  profiles at  $y=0.8$  using MUSCL implemented via the new TVD formulation against Bruner's formulation [1] over (a) coarse and (b) dense grid systems for the pure convection of a step profile problem.

## 6.2. Advection of a Sinusoidal Profile

This problem is similar to the previous one in geometry except that a sinusoidal profile is used. The sinusoidal profile involves steep and smooth regions, as well as an extremum point, making its simulation much more demanding than the simple step profile. The profile is given as

$$\phi = \begin{cases} \sin\left(\frac{\pi}{2} \max\left(1 - \frac{\text{abs}(y - 0.1707)}{0.1707}, 0\right)\right) & 0 \leq y \leq 0.3414 \\ 0 & \text{otherwise} \end{cases} \quad (20)$$

The problem is depicted in Figure 5(a), the same meshes as the step-profile problem were used. Results are shown in Figures 5(b) and 5(c) for the coarse and fine meshes respectively. As expected all the schemes suffer from a substantial decrease in the numerical extremum, with its value decreasing down to 0.48 for the UPWIND scheme. The SUPERBEE preserves on the coarse mesh more of the extremum value (0.83), and experience no loss in extremum on the fine mesh. The BJ-MUSCL, TVD-MUSCL and OSHER schemes results are much better than those of the UPWIND scheme and the MINMOD scheme, while still experiencing on the coarse

and fine meshes a decrease in the extrema down to 0.68 and 0.92 respectively.

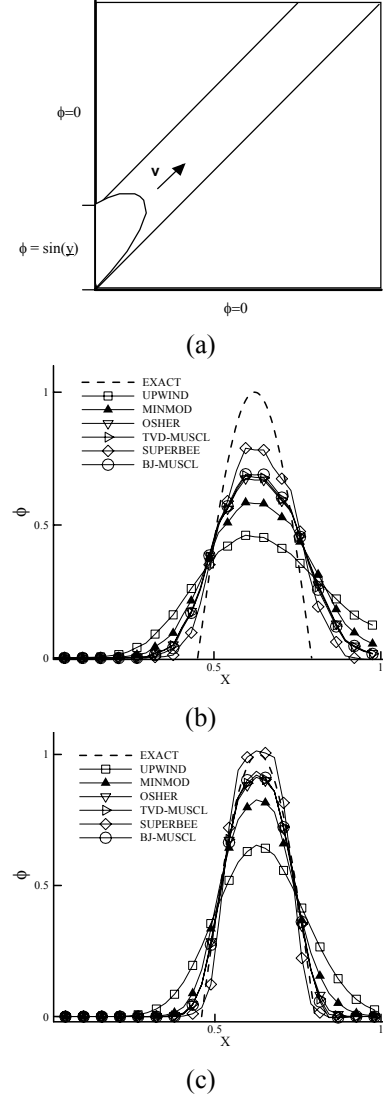


Figure 5: Convection of a sinusoidal profile; (a) physical domain, (b)  $\phi$  profile at  $y=0.8$  using coarse grid, (c)  $\phi$  profile at  $y=0.8$  using dense grid.

## 7. Conclusion

In this paper, a number of TVD schemes, namely the SUPERBEE, TVD-MUSCL, OSHER, and MINMOD schemes, in addition to the BJ-MUSCL scheme were implemented on unstructured grids. As expected, results for the BJ-MUSCL and TVD-MUSCL were found to be similar. The approach followed was proved to be general and consistent with the Sweby TVD formulation for structured grids. Results for the test problems presented showed that TVD monotonicity was properly enforced for all schemes resulting in oscillation free profiles. The benefit of such an approach are twofold: (i) a wide range of TVD schemes including compressive schemes such as the SUPERBEE scheme can be readily implemented; (ii) improvement to the standard TVD formulation such as extremum preserving algorithms [23] can now be used for unstructured grids.

## 7. Acknowledgement

The financial support provided by the University Research Board of the American University of Beirut through Grant No. 17988899702 is gratefully acknowledged.

## References

- [1] Bruner, C.W.S. "Parallelization of the Euler Equations on Unstructured Grids", AIAA paper 97-1894, 1997.
- [2] Barth, T., Jespersen, D.C., "The Design and Application of Upwind Schemes on Unstructured Meshes", AIAA paper 89-0366, 1989.
- [3] Leonard, B.P., "The ULTIMATE Conservative Difference Scheme Applied to Unsteady One-Dimensional Advection", *Comp. Methods Applied Mech. Eng.*, vol. 88, pp. 17-74, 1991.
- [4] Moukalled, F. and Darwish, M.S., "A New Bounded-Skew Central Difference Scheme- Part I: Formulation & Testing", *Num. Heat Transfer, Part B: Fundamentals*, vol. 31, pp. 91-110, 1996.
- [5] Deconinck, H., Roe, P.L., and Struijs, R., "A Multidimensional Generalization of Roe's Flux Difference Splitter for the Euler Equations", *Comp. and Fluids*, Vol. 22, No 23, pp 215-222, 1993.
- [6] Leonard, B.P., "A Stable and Accurate Convective Modeling Procedure Based on Quadratic Interpolation", *Comp. Methods Appl. Mech. & Eng.*, vol. 19, pp. 59-98, 1979.
- [7] Godunov, S.K., "A difference scheme for numerical computation of discontinuous solution of hydrodynamic equations", translated from the Russian by US joint Publ. Res. Service, 1969) *JPRS 7226*, 1959.
- [8] Zalesak, S., "Fully Multidimensional Flux Corrected Transport Algorithms for Fluids", *J. Comp. Phys.*, 31, pp 335-362, 1979.
- [9] Boris, J.P. and Book, D.L. "Flux Corrected Transport III, Minimal Error FCT Algorithms", *J. Comp. Phys.*, vol. 20, p.397-431, 1976.
- [10] Van Leer, B., "Towards the Ultimate Conservative Difference Scheme. V. A Second-Order Sequel to Godunov's Method", *J. Comp. Physics*, vol. 32, p. 101-136 1979.
- [11] Harten, A., "High Resolution Schemes for Hyperbolic Conservation Laws", *J. Comp. Phys.*, vol. 49, p. 357-393, 1983.
- [12] Sweby, P.K., "High Resolution Schemes Using Flux-Limiters for Hyperbolic Conservation Laws", *SIAM J. Num. Anal.*, vol. 21, pp. 995-1011, 1984.
- [13] Gaskell, P. H. and Lau, A. K. C., "Curvature Compensated Convective Transport: SMART, a new boundedness preserving transport Algorithm", *Int. J. Num. Meth. Fluids*, vol. 8, pp. 617-641, 1988.
- [14] Darwish, M.S. "A new high-resolution scheme based on the normalized variable formulation", *Num. Heat. Transfer part B.*, vol. 24, p. 353-371, 1993.
- [15] Aftomis, M. and Kroll, N., "A Quadrilateral-Based Second Order TVD Method for Unstructured Adaptive Meshes", AIAA Paper 91-0124, Jan 1991.
- [16] Löhner, R., Morgan, K., Peraire, J., and Vahdati M., "Finite Element Flux-Corrected Transport (FEM-FCT) For the Euler and Navier-Stokes Equations", *Int. J. Num. Methods Fluids.*, vol. 7, pp. 1093-1109, 1987.
- [17] Venkatakrishnan, V. and Barth, T.J. "Application of Direct Solvers to Unstructured Meshes", *J. Comput. Phys.* Vol. 105, pp.83-91, 1993.
- [18] Spekreijse, S., "Multigrid Solution of Monotone, Second Order Discretization of Hyperbolic Conservation Laws", *Math. Comp.*, vol 45, p. 15-21, 1987.
- [19] Barth, T.J., "Recent development in High Order k-Exact Reconstruction on Unstructured Meshes", AIAA paper 93-0668, Jan. 1993.
- [20] Bruner, S., "parallelization of the Euler Equations on unstructured grids", PhD thesis, Virginia Polytechnic Institute and State University, Department of Aerospace engineering, 1996.
- [21] Chakravarthy, S. R. and Osher, S., "High Resolution Applications of the OSHER Upwind Scheme for the Euler Equations," *AIAA Paper 83-1943*, 1983.
- [22] Roe, P.L., "Some Contributions to the Modelling of Discontinuous Flows", *Proc. AMS/SIAM Seminar*, San Diego, 1983.
- [23] Darwish, M.S. and Moukalled, F., "B-EXPRESS: A new Bounded EXtrema PREServing Strategy for Convective Schemes", *Num. Heat Trans., Part B.*, vol. 37, No. 2, pp. 227-246, 2000.