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High-resolution finite volume computations using a novel weighted least-squares formulation

J. C. Mandal*,†, S. Rao and J. Subramanian

Department of Aerospace Engineering, Indian Institute of Technology Bombay, Mumbai 400076, India

SUMMARY

High-resolution finite volume schemes based on a novel reconstruction technique, SDWLS (solution-dependent weighted least squares) are considered. The SDWLS technique, originally developed for second-order variable reconstruction by Mandal and Subramanian (*Appl. Numer. Math.*, 2007; DOI: 10.1016/j.apnum.2007.02.003), is further extended to third-order reconstruction with compact stencils involving only the nearest neighbors. The new schemes are applied to solve a few numerical test examples, involving scalar conservation laws and the system of non-linear gas dynamics equations, in order to study their performance. Significant improvements in solution accuracy have been achieved with the second- and third-order SDWLS reconstruction techniques. Copyright © 2007 John Wiley & Sons, Ltd.

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1. INTRODUCTION

During the last few decades, there have been numerous efforts in constructing higher-order schemes for simulation of flows with discontinuities. The construction of higher-order schemes has been a challenge, as the classical higher-order schemes suffer from the problem of spurious oscillations around the discontinuities. After it was realized in the early 1980s that spurious oscillations can be avoided by bringing in non-linearity into the discretization process, mainly two distinct approaches have evolved since then. In the first approach, known as total variational diminishing method [1], the higher-order correction (anti-diffusive) terms are added after multiplying them with limiter functions. The limiters, being a function of solution, help in adding the higher-order correction terms in a non-linear manner. In the second approach, known as essentially non-oscillatory method [2], the

*Correspondence to: J. C. Mandal, Department of Aerospace Engineering, I.I.T. Bombay, Mumbai 400076, India.
†E-mail: mandal@aero.iitb.ac.in

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non-linearity is brought in with the use of variable stencils, depending on least oscillatory criterion. Although these two methods yield quite satisfactory results for structured grids, their extension to multidimensions on unstructured grids is not very straightforward and perfect. Therefore, a necessity is felt to look for an alternative approach.

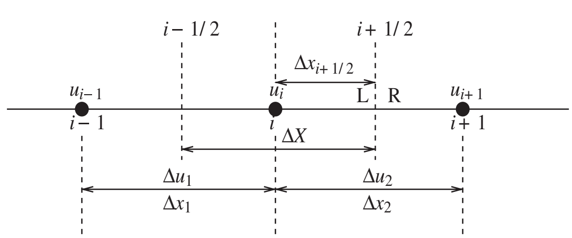
In this paper, a new approach is described to bring in non-linearity in the discretization procedure. Here, the gradient terms in the reconstruction steps are approximated with a novel weighted least-squares formulation (WLS), with the weights defined as functions of solution; thus, it is known as solution-dependent WLS (SDWLS) [3]. The primary motivating factor for considering least-squares formulation in this approach is its ability to handle arbitrary sets of data points arising in unstructured grid-based flow computations. Initial attempts at implementation of higher-order upwind schemes on unstructured grids focused on the extension of one-dimensional (1D) reconstruction procedure based on the MUSCL approach. Such an extension typically requires the use of one additional cell beyond the nearest neighbors. In the case of unstructured grids, consideration of additional neighbors to construct slopes for the higher-order part may introduce substantial complexity into the method and additional storage requirements [4]. In unstructured grid computations, the computational stencil is thus usually restricted to the nearest neighbors. Keeping this in mind, the least-squares approach for the estimation of the slopes within each control volume has been used to obtain higher-order accuracy without informal inquiries beyond the nearest neighbors. The SDWLS technique, originally developed for second-order variable reconstruction (in Mandal and Subramanian [3]), is further extended to third-order reconstruction with compact stencils involving only the nearest neighbors, so that it can be applied to unstructured grids. The second-order SDWLS method, which was found to perform well for scalar conservation laws (in [3]), is applied here to solve a system of non-linear gas dynamics equations. The third-order SDWLS is applied to both scalar and systems of conservation laws.

2. FINITE VOLUME FORMULATION

For ease of explanation, the cell-centered finite volume discretization of a general form of a scalar conservation law in 1D, $u_t + f(u)_x = 0$, is considered, i.e.

$$u_i^{n+1} = u_i^n - \frac{\Delta t}{\Delta X}[f(u_{i+1/2}^n) - f(u_{i-1/2}^n)] \tag{1}$$

with $u_{i\pm 1/2} = u_{i\pm 1/2}^{\mathrm{L}}$ for $\mathrm{d}f/\mathrm{d}u > 0$ and $u_{i\pm 1/2} = u_{i\pm 1/2}^{\mathrm{R}}$ for $\mathrm{d}f/\mathrm{d}u < 0$, where superscript n is the time level, i is the cell index, Δt is the time step and ΔX is the length of the ith cell as shown in



$$\Delta u_1 = u_{i-1} - u_i$$
$$\Delta u_2 = u_{i+1} - u_i$$
$$\Delta x_1 = x_{i-1} - x_i$$
$$\Delta x_2 = x_{i+1} - x_i$$
$$\Delta X = x_{i+1/2} - x_{i-1/2}$$

Figure 1. 1D Stencil.

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Figure 1. $u^{L}_{i\pm 1/2}$ and $u^{R}_{i\pm 1/2}$ are the cell interface values at the left and right sides of the interfaces $i\pm\frac{1}{2}$ to be evaluated using higher-order reconstruction, as explained below.

3. HIGHER-ORDER RECONSTRUCTION

The reconstructed values at the cell interface $i+\frac{1}{2}$ (see Figure 1) using truncated Taylor series can be expressed as

$$u^{L}_{i+1/2}=u_i+\left(\frac{\mathrm{d}u}{\mathrm{d}x}\right)_i(x_{i+1/2}-x_i)+\frac{1}{2}\left(\frac{\mathrm{d}^2u}{\mathrm{d}x^2}\right)_i(x_{i+1/2}-x_i)^2+\cdots \tag{2a}$$

$$u^{R}_{i+1/2}=u_{i+1}+\left(\frac{\mathrm{d}u}{\mathrm{d}x}\right)_{i+1}(x_{i+1/2}-x_{i+1})+\frac{1}{2}\left(\frac{\mathrm{d}^2u}{\mathrm{d}x^2}\right)_{i+1}(x_{i+1/2}-x_{i+1})^2+\cdots \tag{2b}$$

where the order of accuracy of the scheme depends upon the number of terms kept on the right-hand side (RHS) of expression (2). For example, the first term alone leads to first-order scheme. Whereas, the first two terms lead to second-order scheme, which requires the evaluation of first-order derivatives of 'u' at cell centers i and $i+1$. The third-order scheme is obtained by keeping all the three terms, which requires evaluation of both first- and second-order derivatives of 'u' with respect to space variable at the cell centers i and $i+1$. Estimation of the above first- and second-order derivatives at the cell center i is described as follows.

4. ESTIMATION OF DERIVATIVES $(\mathrm{d}u/\mathrm{d}x)_i$ AND $(\mathrm{d}^2u/\mathrm{d}x^2)_i$ USING SDWLS

Traditionally, estimation of gradients at a point involves solution of a system of equations formed by the truncated Taylor series

$$u_j=u_i+\left(\frac{\mathrm{d}u}{\mathrm{d}x}\right)_i(x_j-x_i)+\frac{1}{2}\left(\frac{\mathrm{d}^2u}{\mathrm{d}x^2}\right)_i(x_j-x_i)^2+\cdots \tag{3}$$

where $j=i\pm 1$ (for a 3-point stencil as shown in Figure 1). The number of terms to be retained in the above expression (3) depends on the accuracy and the order of derivative to be evaluated. It may be noted that the derivatives in the other coordinate directions as well as cross-spatial derivatives need to be evaluated in case of higher dimensions.

4.1. *Estimation of* $(\mathrm{d}u/\mathrm{d}x)_i$ *for second-order scheme*

The system of equations obtained by applying the above expression (keeping only the first two terms in the RHS of (3)) to the points $j=i\pm 1$ in the stencil, shown in Figure 1, can be expressed as [3]

$$\mathbf{\Delta u}=\mathbf{S}\,\mathbf{du} \tag{4}$$

where $\mathbf{du}=[(\mathrm{d}u/\mathrm{d}x)_i]$, $\mathbf{\Delta u}=[\Delta u_1,\Delta u_2]^{\mathrm{T}}$ and $\mathbf{S}=[\Delta x_1,\Delta x_2]^{\mathrm{T}}$. The terms $\Delta u_1,\Delta u_2,\Delta x_1$ and Δx_2 are explained in Figure 1. The weighted (with diagonal weight matrix) least-squares approximation of the overdetermined system (4) can then be expressed as

$$\mathbf{du}=(\mathbf{S}^{\mathrm{T}}\mathbf{W}\mathbf{S})^{-1}\mathbf{S}^{\mathrm{T}}\mathbf{W}\mathbf{\Delta u} \tag{5}$$

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In the case of 1D mesh with 3-point stencil (Figure 1), Equation (5) can be used to obtain an explicit formula for the required gradient as

$$\left(\frac{\mathrm{d}u}{\mathrm{d}x}\right)_i = \frac{w_1\Delta x_1\Delta u_1 + w_2\Delta x_2\Delta u_2}{(w_1\Delta x_1^2 + w_2\Delta x_2^2)} \tag{6}$$

with weights, derived in [3], as $w_\alpha = \sum_{m=1}^{N} a_\alpha^m/[|\Delta u_1|^{\gamma_{\alpha,1}^m}|\Delta u_2|^{\gamma_{\alpha,2}^m}]$ where $\alpha = 1$ and 2 (corresponding to $i-1$ and $i+1$ grid points, respectively) for the 3-point stencil. Many expressions for w_α are possible that will produce non-oscillatory solutions (depending on various choices of the parameters N, $\gamma_{\alpha,1}^m$, $\gamma_{\alpha,2}^m$ [3]). Two examples of such weights are $w_\alpha = 1/(\Delta u_\alpha + \varepsilon)$ or $1/(\Delta u_\alpha^2 + \varepsilon)$ with $\alpha = 1$ and 2, and ε is a small number (10^{-12}) used to prevent division by zero. Derivative (6) is used in the case of linear reconstruction to obtain second-order accuracy.

4.2. *Estimation of* $(\mathrm{d}u/\mathrm{d}x)_i$ *for third-order scheme*

For third-order scheme, an improved estimate of first-order derivative $(\mathrm{d}u/\mathrm{d}x)_i$, to be used in (2), is evaluated by considering all the three terms in the RHS of Equation (3). The second derivative in this case is approximated, using the previously evaluated first-order derivatives in Section 4.1, as $(\mathrm{d}^2u/\mathrm{d}x^2)_i = [(\mathrm{d}u/\mathrm{d}x)_j - (\mathrm{d}u/\mathrm{d}x)_i]/(x_j - x_i)$ for $j = i \pm 1$. A system similar to (4) is solved using WLS for computing the first derivative, $(\mathrm{d}u/\mathrm{d}x)_i$ with a modified value of $\boldsymbol{\Delta}\mathbf{u} = [\widetilde{\Delta u_1}, \widetilde{\Delta u_2}]$, where $\widetilde{\Delta u_1} = \Delta u_1 - [(\mathrm{d}u/\mathrm{d}x)_{i-1} - (\mathrm{d}u/\mathrm{d}x)_i]\Delta x_1/2$ and $\widetilde{\Delta u_2} = \Delta u_2 - [(\mathrm{d}u/\mathrm{d}x)_{i+1} - (\mathrm{d}u/\mathrm{d}x)_i]\Delta x_2/2$. The weights are $w_\alpha = 1/(\widetilde{\Delta u_\alpha} + \varepsilon)$ or $1/(\widetilde{\Delta u_\alpha^2} + \varepsilon)$, where $\alpha = 1$ and 2 (corresponding to $i-1$ and $i+1$ grid points) for the 3-point stencil.

4.3. *Estimation of* $(\mathrm{d}^2u/\mathrm{d}x^2)_i$ *for third-order scheme*

A multiple-step approach is used while evaluating the second-order derivative $(\mathrm{d}^2u/\mathrm{d}x^2)_i$. That is, the second-order derivative is calculated based on the values of first derivatives $(\mathrm{d}u/\mathrm{d}x)_i$ evaluated in the previous step as described in Section 4.2. The motivation behind using the multiple step approach is as follows. First, it avoids the use of additional cells beyond the nearest neighbors, thereby keeping the stencil compact and usable for unstructured grid computations. Second, it helps to bring in the information implicitly from the further neighbors through the first derivatives derived *a priori*. Third, it also avoids inversion of matrix in 1D that would arise in usual case, when both first- and second-order derivatives in (3) are evaluated simultaneously. In the case of higher dimensions, the multiple-step approach helps in reducing the size of the matrix to be inverted.

In this case, the system of equations is formed by using the truncated Taylor series expansion (3) (keeping the first three terms in RHS) at $j = i \pm 1$ for the 3-point stencil shown in Figure 1. The system of equations used here is given by

$$\boldsymbol{\Delta}^2\mathbf{u} = \mathbf{S}'\mathbf{d}^2\mathbf{u} \tag{7}$$

where $\mathbf{d}^2\mathbf{u} = [(\mathrm{d}^2u/\mathrm{d}x^2)_i]$, $\boldsymbol{\Delta}^2\mathbf{u} = [\Delta^2 u_1, \Delta^2 u_2] = [\Delta u_1 - (\mathrm{d}u/\mathrm{d}x)_i\Delta x_1, \Delta u_2 - (\mathrm{d}u/\mathrm{d}x)_i\Delta x_2]^{\mathrm{T}}$ and $\mathbf{S}' = [\Delta x_1^2/2, \Delta x_2^2/2]^{\mathrm{T}}$. The WLS approximation of the overdetermined system (7) can then be expressed as

$$\mathbf{d}^2\mathbf{u} = (\mathbf{S}'^{\mathrm{T}}\mathbf{W}'\mathbf{S}')^{-1}\mathbf{S}'^{\mathrm{T}}\mathbf{W}'\Delta^2\mathbf{u} = 2\frac{w_1'(\Delta x_1)^2\Delta^2 u_1 + w_2'(\Delta x_2)^2\Delta^2 u_2}{(w_1'\Delta x_1^4 + w_2'\Delta x_2^4)}$$

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with weights as $w'_\alpha = 1/(\Delta^2 u_\alpha + \varepsilon)$ or $w'_\alpha = 1/[(\Delta^2 u_\alpha)^2 + \varepsilon]$ with $\alpha = 1, 2$. The third-order accurate scheme is obtained by using quadratic reconstruction (2) with the first-order derivative $(\mathrm{d}u/\mathrm{d}x)_i$ evaluated in Section 4.2 and the second-order derivative $(\mathrm{d}^2u/\mathrm{d}x^2)_i$ above.

5. RESULTS AND DISCUSSIONS

Two 1D and two two-dimensional (2D) test problems [3, 5, 6] involving linear advection equations and Euler equations are considered for validating the present formulation. Figure 2 shows the result of 1D linear advection equation [3]. Figure 3 shows density distribution obtained from solving 1D Euler equations along shock tube at $t = 0.0075$ units [5]. Figure 4 shows the results for 2D linear advection equation [3]. Figure 5 shows density contours for a shock reflection problem

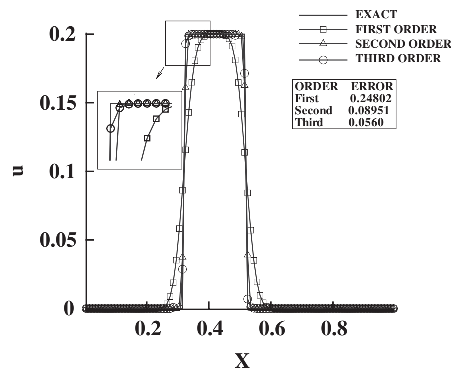

Figure 2. Linear advection equation.

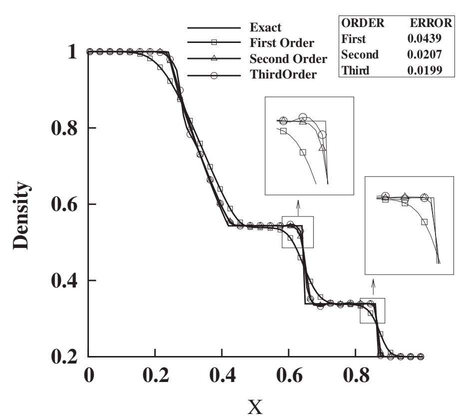

Figure 3. Shocktube problem.

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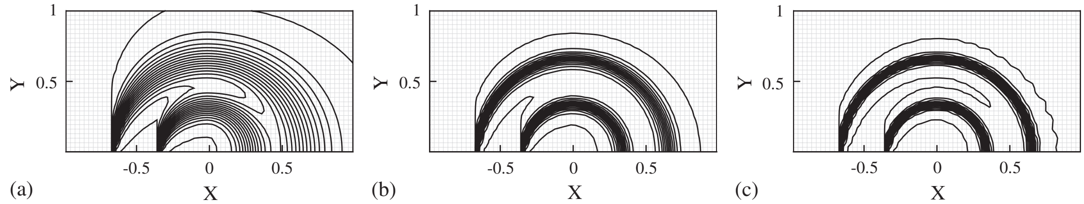

Figure 4. Contours from 0 to 1 with an interval of 0.07 for 2D linear advection equation: (a) first order (error = 0.398481); (b) second order (error = 0.247517); and (c) third order (error = 0.193361).

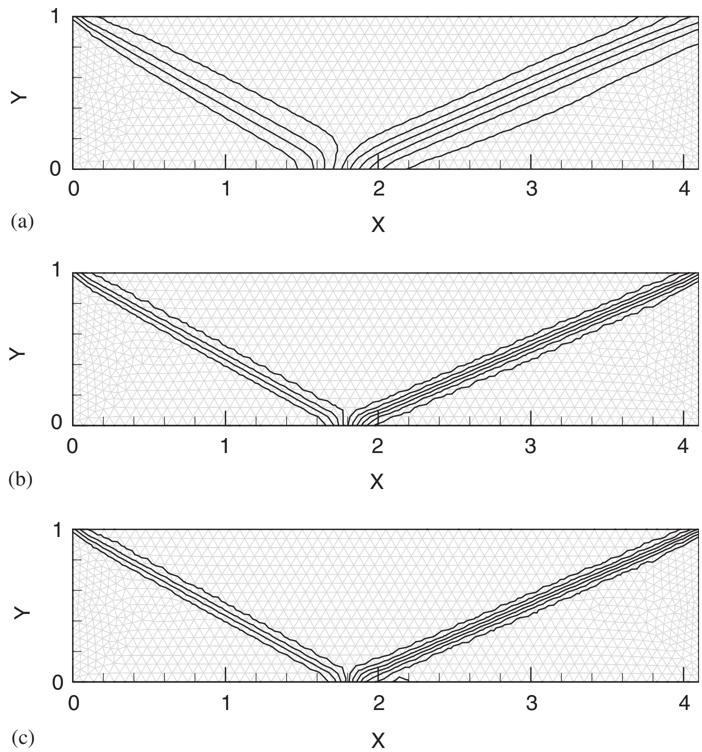

Figure 5. Density contours from 0.2 to 3.2 with an interval of 0.2 for shock reflection problem: (a) first order (error = 0.070623); (b) second order (error = 0.04228); and (c) third order (error = 0.04155).

obtained by solving 2D Euler equations, where an oblique shock with an upstream Mach number of 2.9 and an angle of incidence of 29° entering the computational domain in the top left corner is reflected by a flat plate placed at the bottom [6]. In the case of unstructured grid, edge-based data structure [7] for cell-centered finite volume method has been used. The unstructured grid with 1192 vertices, 2222 cells and 3413 edges is used for the shock reflection problem. All the test cases are solved using Harten Lax and van Leer with Contact solver and with solution-dependent weights of the type $w_\alpha = 1/(\Delta u_\alpha + \varepsilon)$. The error norms for the first-, second- and third-order SDWLS

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reconstruction schemes are reported on the above-mentioned figures. The $L2$ error norm of the computation is defined as

$$\text{error} = \sqrt{\sum_i (u_{\text{ex}_i} - u_{\text{cp}_i})^2 / u_{\text{ex}_i}^2}$$

where u_{ex_i} and u_{cp_i} are, respectively, exact and computed solutions at grid point i. The computed results demonstrate that the accuracy of the present method increases with the increase in the order of accuracy of the SDWLS scheme.

6. CONCLUDING REMARKS

The SDWLS approach provides an alternative means in achieving higher-order accuracy for finite volume formulation. Since the present approach can handle arbitrary set of data points and uses compact stencils involving only the nearest neighbors, it is ideally suitable for unstructured grids computations. Another notable feature of the present approach is its ability to incorporate cross-derivatives appearing in higher-order reconstruction for higher dimensions, which helps in improving the accuracy further.

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