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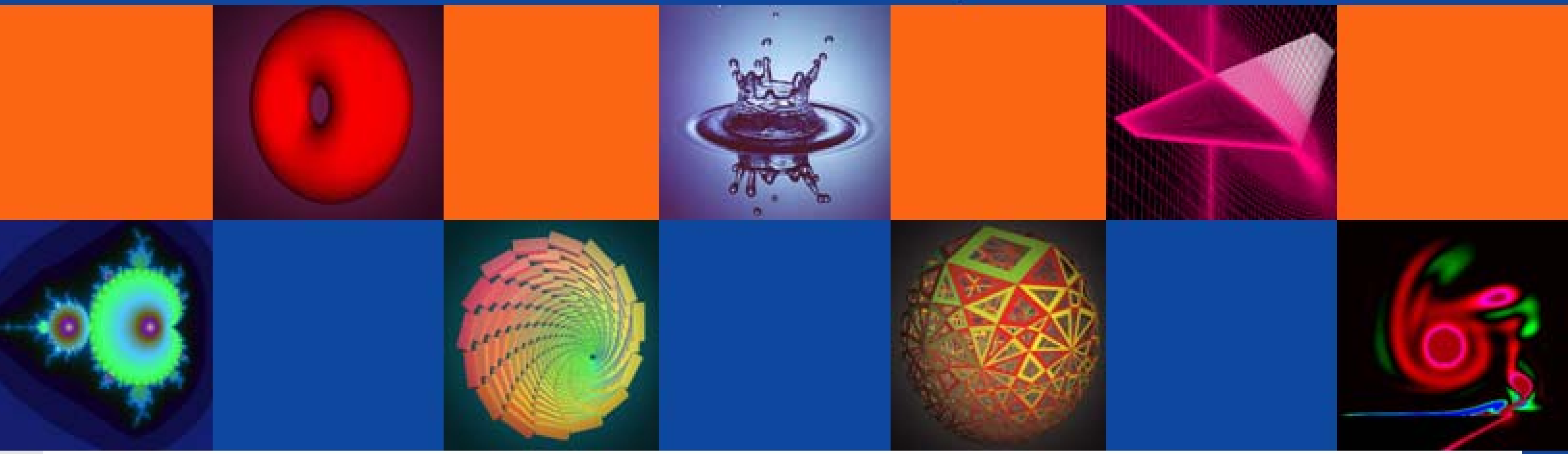

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Weighted Compact and Non-compact Scheme for Shock Tube and Shock Entropy Interaction

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[Abstract] In this paper, we introduce a new type of high order shock capturing schemes – uniform weighted compact and non-compact scheme (UWCNC) or simply XJL scheme developed by Xie, Jiang and Liu. This new scheme is based on the feature of discrete data sets instead of the physics. The fundamental task of CFD is to provide an accurate approximation of derivatives for a given discrete data set. The data are first normalized then measured by so called "smoothness". According to the smoothness, the set is divided into three regions: smooth, oscillatory, and non-differentiable (shock) regions. The strategy of this new scheme is to achieve spectral-like resolution and high order of accuracy by using central weighted compact scheme in smooth and oscillatory regions and use the non-compact scheme to cross the shock to capture shocks sharply without oscillation. In a 6th order one parameter family of the compact schemes (Lele, 1992), we turn the control parameter to 1/3, keeping the exact formulation of the 6th order weighted compact scheme and turn it to zero gradually when approaching the shock, which makes the scheme non-compact. Besides the WENO weights, there is only one additional control parameter, which we call smoothness function. In this new uniform weighted compact-non compact scheme, a sixth-order weighted compact scheme and a corresponding fourth-order weighted non-compact scheme are combined following this basic idea. Numerical tests show that the new scheme has captured the 1-D shock sharply without non-physical oscillation and obtained much higher resolution for 1-D shock-entropy interaction than the 5th order WENO scheme.

I. Introduction

1.1 A short overview on shock capturing schemes

The flow filed is in general governed by the Navier-Stokes system which is a system of time dependent partial differential equations. However, for external flows, the viscosity is important largely only in the boundary layers. The main flow can still be considered as inviscid and the governing system can be dominated by the time dependent Euler equations which are hyperbolic. The difficult problem with numerical solution is the shock capturing which can be considered as a discontinuity or mathematical singularity (no classical unique solution and no bounded derivatives). In the shock area, continuity and differentiability of the governing Euler equations are lost and only the weak solution in an integration form can be obtained. The shock can be developed in some cases because the Euler equation is non-linear and hyperbolic. On the other hand, the governing Navier-Stokes system presents parabolic type behavior in and is therefore dominated by viscosity or second order derivatives. One expects that the equation should be solved by high order central difference scheme, high order compact scheme is preferable, to get high order accuracy and high resolution. High order of accuracy is critical in resolving small length scales in flow transition and turbulence process. However, for the hyperbolic system, the analysis already shows the existence of characteristic lines and Riemann invariants. Apparently, the upwind finite difference scheme coincides with the physics for a hyperbolic system. History has shown the great success of upwind technologies. We should consider not only the eigenvalues and eigenvectors of the Jacobian system, but also non-linearity including the Rankine-Hugoniot shock relations. From the point of view of shocks, it makes no sense to use high order compact scheme for shock capturing which use all gird points on one grid line to calculate the derivative by solving a tri-diagonal or penta-diagonal linear system when shock does not have finite derivatives and downstream quantities cannot cross

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shock to affect the upstream points. From the point of view of the above statement, upwind scheme is appropriate for the hyperbolic system. Many upwind or bias upwind schemes have achieved great success in capturing the shocks sharply, such as Godunov (1959), Roe (1981), MUSCL (Van Leer, 1979), TVD (Harten, 1983), ENO (Harten et al, 1987; Shu et al, 1988, 1989) and WENO (Liu et al, 1994; Jiang et al, 1996). Roe's scheme may be better in capturing the shock sharply because it satisfies the Rankine-Hugoniot relation. Of course, Roe's method can also be considered as a method for flux difference splitting and any high order method such as ENO and WENO can use Roe's method as a splitting method. However, all these shock-capturing schemes are based on upwind or bias upwind technology, which is nice for hyperbolic system, but is not favorable to the N-S system which presents parabolic equation behavior. The small length scale is very important in the flow transition and turbulence process and thus very sensitive to any artificial numerical dissipation. High order compact scheme (Lele, 1992; Visbal, 2002) is more appropriate for simulation of flow transition and turbulence because it is central and non-dissipative with high order accuracy and high resolution.

Unfortunately, the shock-boundary layer interaction, which is important to high speed flow, is a mixed type problem which has shock (discontinuity), boundary layer (viscosity), separation, transition, expansion fans, fully developed turbulence, and reattachment. In order to capture the shock and keep high order accuracy and high resolution in the smooth area, we have developed the so called weighted compact scheme (WCS, Jiang et al, 2001) which works very well for 1-D convection equation, Burger's equation, but not so good for Euler's equation with shocks. Visible wiggles have been found near the shock. In the case of shock-boundary layer interaction, there are elliptic areas (separation, transition, turbulence) and hyperbolic areas (main flow, shocks, expansion fans), which makes the accurate numerical simulation extremely difficult if not impossible. We have to divide the computational domain to several parts: the elliptic, hyperbolic, and mixed. The division or detection can be performed by switch function automatically such as shock detector which simply sets for the shock area and for the rest. The switch function may give the best results for shock-boundary layer interaction, but it will have too many logical statements in the code which may slow down the computation. The switch function could also be case-related and very difficult to adjust. It would also slow down the convergence for steady problems. The use of "weights" will be naturally considered as a good candidate that succeeded for many schemes, WENO is a good example and our Weighted Compact Scheme is another example.

Traditional finite difference schemes use the idea of Lagrange interpolation. To obtain the n-th order of accuracy, a stencil covering n+1 grid points is needed. In other words, the derivative at a certain grid point depends upon the function values at these n+1 grid points and only these grid points. In contrast, standard compact schemes (Lele, 1992; Visbal, 2002) use the idea of Hermitian interpolation. By using derivatives as well as function values, a compact scheme achieves high order of accuracy without increasing the width of stencils. As discussed in Lele's paper, a compact scheme has not only high order of accuracy, but also high resolution. Fourier analysis indicates that, with the same order of accuracy, a compact scheme has better spectral resolution than a traditional, explicit finite difference scheme. For this reason, compact schemes are favorable in the simulation of turbulent flows where small-length-scale structures are important.

Due to the usage of derivatives, compact schemes usually give us a tri-diagonal or penta-diagonal system. Although the tri-diagonal matrix is sparse, the inverse of a tri-diagonal matrix is dense, which means the derivative at a certain grid point depends upon all the grid points along a grid line. The success of compact schemes indicates that the global dependency is very important for high resolution. However, the global dependency is good for resolution but not so applicable for shock capturing.

The basic idea proposed in ENO (Harten et al, 1987) and WENO (Jiang et al, 1996) schemes is to avoid the stencil containing a shock. ENO chooses the smoothest stencil from several candidates to calculate the derivatives. WENO controls the contributions of different stencils according to their smoothness. In this way, the derivative at a certain grid point, especially one near the shock, is dependent on a very limited number of grid points. The local dependency here is favorable for shock capturing and helps obtaining the non-oscillatory property. The success of ENO and WENO schemes indicates that the local dependency is critical for shock capturing.

The Weighted Compact Scheme (WCS) we developed (Jiang et al, 2001) is constructed by introducing the idea of WENO scheme to the standard compact schemes which uses weights for several candidates. The building block for each candidate is a Lagrange polynomial in WENO, but is Hermite in WCS. Therefore WCS achieves a higher accuracy with same stencil width. In shock regions, WCS controls the contributions of different candidate stencils to minimize the influence of the candidate which contains a shock. In smooth regions where shocks are not present, WCS recovers to the standard compact scheme to achieve high accuracy and resolution. The numerical tests indicate that original WCS works fine in some cases such as convection equation and Burger's equation, but not very well for Euler equation. As mentioned above, the usage of derivatives by compact schemes results in the global dependency. Although WCS tries to minimize the influence by reducing the weight, the stencil containing a shock is still used with smaller a weight leading to the global dependency.

In order to overcome the drawback of the WCS scheme, we need to achieve local dependency in shock regions and recover the global dependency in smooth regions. This fundamental idea will naturally lead to a combination of compact and non-compact schemes, or, as we called, uniform weighted compact and non-compact scheme (UWCNC), or XJL scheme for simplicity.

1.2 Importance of high order scheme to DNS/LES

It should be pointed out that the order of accuracy of the finite difference scheme is absolutely not a trivial issue to CFD, especially to DNS and LES. There is a big difference in requirements of grid size by DNS/LES between low order schemes and high order schemes. Let us take a look at the local truncation error for 1-D problem. If one uses a second order scheme with a mesh size of Δx_2 and wants to have same truncation error as a sixth order scheme with a mesh size of Δx_6, one should have:

$$C_2(\Delta x_2)^2 = C_6(\Delta x_6)^6 \tag{1.1}$$

Assume $C_2 \approx C_6$ and $\Delta x_6 = 0.01$ (100 grid points in a normalized domain), we will get $(\Delta x_2)^2 = (10^{-2})^6$

$$\Delta x_2 = 10^{-6} \tag{1.2}$$

In other words, the second order scheme needs one million of grid points to beat the sixth order scheme with 100 grid points for same accuracy. This advantage of high order scheme will become more significant when one uses DNS for 3-D problems. We cannot use and do not want to use one million of grids in each direction for DNS, but prefer to use 100 grid points. Therefore high order scheme must be used. Of course, the global error does not only depend on the local truncation error and $C_2 \neq C_6$. The advantage of the sixth order scheme does not show 10 thousand times better than the second order scheme. However, it is now widely recognized that high order finite scheme is strongly encouraged to be used for DNS and LES which has much higher accuracy and higher resolution with same grid size than low order scheme has.

1.3 Comments on low order LES with low order subgrid models

Because the main purpose for this work is to find a high order shock capturing scheme for LES of shock-turbulence interaction, we would like to make some comments on low order LES. Most LES computations require use of a subgrid model trying to get the unresolved scales back which could be considered as truncation errors mathematically. Let us take a look at the famous Smagorinsky model:

$$\tau_{ij} = -\nu_t S_{ij} \quad \text{and}$$

$$\nu_t = (C_s\Delta)^2 \mid S \mid \tag{1.3}$$

Where τ_{ij}, S_{ij}, C_s, Δ are the unresolved stress tensor, resolved strain tensor, Smogorinsky constant, and filter width respectively Apparently, it is a second order model with Δ^2. Other models are similar. If we use sixth order compact scheme for LES without model (Implicit LES), we will get sixth order of accuracy. However, if we are asked to add the Smgorinsky subgrid model, our LES results will be degenerated to second order of accuracy, which is really bad. A carefully designed 6th order subgrid model may be needed for high order LES. Therefore, second order DNS, second order LES with second order subgrid models are not appropriate for DNS or LES.

Table 1 shows the orders obtained by different orders of schemes, which demonstrates the importance of high order numerical schemes for DNS/LES.

Table 1. Orders of DNS/LES approaches

Scheme	Truncation Errors	Comments
Second order DNS	$O(h^2)$	Bad
Second order LES +Second order subgrid model	$O(h^2)$ or up	Bad
Sixth order LES without subgrid model (ILES)	$O(h^6)$	Good
Sixth order LES with second order subgrid model	$O(h^2)$	Really bad
Sixth order LES with sixth order subgrid model	$O(h^6)$ or up	Best

1.4 New point of view on high order CFD

The 3-D time dependent Navier-Stokes equations in a general curvilinear coordinate can be written as

$$\frac{1}{J}\frac{\partial Q}{\partial t}+\frac{\partial(E-E_v)}{\partial \xi}+\frac{\partial(F-F_v)}{\partial \eta}+\frac{\partial(F-F_v)}{\partial \zeta}=0 \tag{1.4}$$

For 1-D conservation law, it will be:

$$\frac{\partial Q}{\partial t}+\frac{\partial E}{\partial \xi}=0 \tag{1.5}$$

The critical issue for high order CFD is to find a more accurate approximation of derivatives for a given discrete data set. The computer does not know any physical process but a discrete data set. The output is also a discrete data set. Therefore, the high order finite difference scheme should be based on the feature of the discrete data set, but not the physics, to find a good approximation for derivatives since the computer does not know the physics. We measure the data by slopes to determine it is smooth (slope is small), oscillatory (slope is large), and non-differentiable (slope is large on one side, but small on the other side), or, in other words, by a smoothness function, and then the appropriate numerical scheme is set up based on the feature of the discrete data set, but not the governing systems. This is the key issue of our new high order scheme and basic view point of our new scheme development.

People traditionally think to use high order compact scheme for smooth area and low order upwind scheme for shocks if they can detect the shock and think the difficulty is to detect shock for complex flow such as 3-D shock-boundary layer interaction. However, the answer is just the opposite. The easiest thing is to detect shock for complex flow by using our slope measurement and smoothness function. We never miss any shock because our scheme is based on the analysis of the discrete data set. For the smooth area, both low order and high order schemes can achieve satisfying results. We prefer to use high order of course, but it is not critical. The critical is to use high order compact scheme with high resolution for oscillatory waves and use the weighted high order central, non-dissipative scheme for shocks. The needed dissipation comes from weights, not from low order upwind scheme. The weights provide needed dissipation, but do not reduce the order of the scheme.

To make no confusion, we should address that the physical shock is a discontinuity with two solutions at the same grid point, but the best numerical method only can give the shock by two grid points. This tells us that the error for the finest grid and the best method is maximum first order. However, we believe we should use the fine grid solution as our reference solution which can never be the exact solution for shocks no matter how many grids to be used. However, it does not prohibit us from developing high order scheme for the shock-turbulence interaction and the high order of the local truncation error (not the global error) is critical to the simulation of flow transition and turbulence.

II. Numerical Scheme

2.1 ENO reconstruction function

For 1-D conservation laws:

$$u_t(x,t) + f_x(u(x,t)) = 0 \tag{2.1}$$

When a conservative approximation to the spatial derivative is applied, a semi-discrete conservative form of the equation (2.1) is described as follows:

$$\frac{du_j}{dt} = -\frac{1}{\Delta x}(\hat{f}_{j+(1/2)} - \hat{f}_{j-(1/2)}) \tag{2.2}$$

where $f_j = \frac{1}{\Delta x}\int_{x_j-\Delta x/2}^{x_j+\Delta x/2} \hat{f}(\xi)d\xi$ and then $(f_x)_j = -\frac{1}{\Delta x}(\hat{f}_{j+(1/2)} - \hat{f}_{j-(1/2)})$. Note that f is the original function, but $\hat{f}$ is the flux defined by the above integration which is an exact expression and is different from f.

Let H be the primitive function of $\hat{f}$ defined below:

$$H(x_{j+(1/2)}) = \int_{-\infty}^{x_j+\Delta x/2} \hat{f}(\xi)d\xi = \sum_{i=-\infty}^{i=j} \int_{x_i-\Delta x/2}^{x_i+\Delta x/2} \hat{f}(\xi)d\xi = \Delta x \sum_{i=-\infty}^{j} f_i \tag{2.3}$$

H is easy to be calculated, but is a discrete data set.

The numerical flux $\hat{f}$ at the cell interfaces is the derivative of its primitive function H. i.e.:

$$\hat{f}_{j+(1/2)} = H'_{j+(1/2)} \tag{2.4}$$

All formulae given above are exact without approximations. However, the primitive function H is a discrete data set or discrete function and we have to use numerical method to get the derivatives, which will introduce numerical errors, or, in other words, order of accuracy.

This procedure, $f \to H \to \hat{f} \to f_x'$, is called reconstruction introduced by Shu & Osher (1988, 1989). There is one and only one problem left for numerical methods, which is how to solve (2.4) or how to get accurate derivatives for a data set.

2.2 Data normalization and smoothness

2.2.1 Data normalization

In order to find universal formula, we need to normalize the data set, $u(i)$, i=1, n:

$$u_{diff} = | u_{\max} - u_{\min} | \tag{2.5}$$

$$\bar{u} = (u - u_{\min}) / u_{diff} \tag{2.6}$$

Here, $u_{\max}$ and $u_{\min}$ are the maximum and minimum values of u respectively and $\bar{u}$ is normalized. For simplicity, we throw out the hat of u and use $u(i)$ as the normalized data set.

2.2.2 Four measurements of smoothness

Similar to WENO, we define smoothness for each data point.

For a given point j, three candidate stencils containing this point are defined as follows (Figure2.1):

$$S_0 = (x_{j-2}, x_{j-1}, x_j),\ S_1 = (x_{j-1}, x_j, x_{j+1}),\ S_2 = (x_j, x_{j+1}, x_{j+2}) \tag{2.7}$$

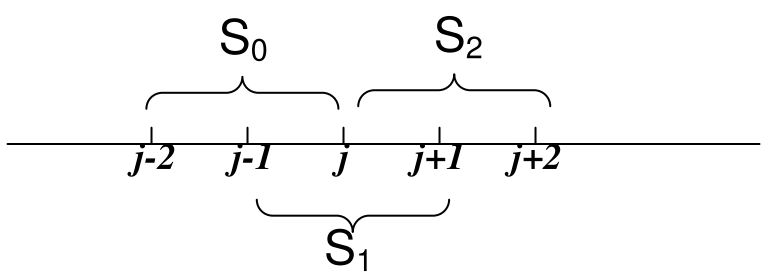


Figure 2.1 Candidate stencils for an interior point j

The smoothness of each point is described by four measurements:

$$IS_0 = \frac{13}{12}(f_{j-2} - 2f_{j-1} + f_j)^2 + \frac{1}{4}(f_j - f_{j-2})^2$$

$$IS_1 = \frac{13}{12}(f_{j-1} - 2f_j + f_{j+1})^2 + \frac{1}{4}(f_{j-1} - f_{j+1})^2 \tag{2.8}$$

$$IS_2 = \frac{13}{12}(f_j - 2f_{j+1} + f_{j+2})^2 + \frac{1}{4}(f_{j+2} - f_j)^2$$

$$IS_{ave} = (IS_0 + IS_1 + IS_2)/3$$

The first three are similar to WENO smoothness with some modifications. The modification is made to the first one and third one by using a second order central difference to replace the second order one side finite difference for the first order derivatives. The first three smoothness measurements are really a combination of first order derivatives and second order derivatives, or slope and curvature in other words, for the left hand side, central, and right hand side. These measurements will be used to construct XJL weights. We add the fourth measurement called the average smoothness, which could be used to distinguish the smooth (low frequency) waves and oscillatory (high frequency) waves. Note that WENO uses weights to detect shocks which has large derivative on one side but small derivative on the other side, but has no tools to differ the high frequency and low frequency waves as well as strong and weak shocks. We add the fourth measurement to achieve the above purpose to distinguish the high and low frequency waves as well as strong and weak shocks.

2.2.3 Three regions of data set

A data set is a group of numbers like grid function in CFD. A data set can be divided to three subset or three regions: smooth, oscillatory, and non-differentiable. A smooth subset could be described as low frequency waves, $Sin(kx), k = 0, K_{\max}/2$. An oscillatory subset could be maximum frequency of the resolved waves. The third subset can be distinguished by high smoothness on one side and low smoothness on the other side, or recognized by weights.

For the low frequency waves, any second order or higher order finite difference schemes are applausive. Of course, we prefer to use high order compact scheme. For the high frequency waves, the use of non-dissipative scheme is critical. Therefore, use of non-dissipative, high order, high resolution compact scheme is critical to the success of numerical methods. The 5th order WENO scheme has 5th order dissipation and will give a significant damp to the high frequency waves which is the reason why some people complain WENO is too dissipative to shock-turbulence interaction. Instead, we use weighted scheme, which is compact for smooth and oscillatory regions and non compact cross the shock or discontinuous regions. The approach looks like complicated, but is really very simple. The scheme has a uniform form which automatically switched by one control function, α. It is critical to use non-dissipative scheme everywhere, the weighted non-compact cross shock and weighted compact anywhere else. The dissipation is only introduced by weights.

2.3 Weighted compact scheme

2.3.1 High-order compact schemes

A Pade-type compact scheme could be constructed based on the Hermite interpolation where both function and derivatives at grid points are involved, e.g. a fourth order finite difference scheme can be constructed if both the function and first order derivative are used at three grid points. For a function f we may write a compact scheme by using five grid points (Lele, 1992):

$$\beta_- f'_{j-2} + \alpha_- f'_{j-1} + f'_j + \alpha_+ f'_{j+1} + \beta_+ f'_{j+2} = (b_- f_{j-2} + a_- f_{j-1} + c f_j + a_+ f_{j+1} + b_+ f_{j+2}) / \Delta\xi \qquad (2.9)$$

We can get 8th order of accuracy by using the above formula based on Taylor series.

Here, we use a symmetric and tri-diagonal system, by setting $\beta_- = \beta_+ = 0$, to get a one parameter family of compact scheme (Lele, 1992):

$$\alpha f'_{i-1} + f'_i + \alpha f'_{i+1} = \left[-\frac{1}{12}(4\alpha - 1) f_{i-2} - \frac{1}{3}(\alpha + 2) f_{j-1} + \frac{1}{3}(\alpha + 2) f_{j+1} + \frac{1}{12}(4\alpha - 1) f_{i+2} \right] / h \qquad (2.10)$$

If $\alpha = \frac{1}{3}$, we will get a standard sixth order compact scheme. But if $\alpha = 0$, we will get a fourth order non-compact central scheme. Note that both schemes are non-dissipative. The dissipative is added by weights.

When a compact scheme is used to differentiate a discontinuous or shock function, the computed derivative has grid to grid oscillations. In our previous work (Jiang et al, 2001) we proposed a new class of finite difference scheme - weighted compact scheme (WCS).

2.3.2 Basic formulations of weighted compact scheme

For a given point j, three candidate stencils containing this point are defined as follows (Figure2.2): $S_0 = (x_{j-2}, x_{j-1}, x_j)$, $S_1 = (x_{j-1}, x_j, x_{j+1})$, $S_2 = (x_j, x_{j+1}, x_{j+2})$

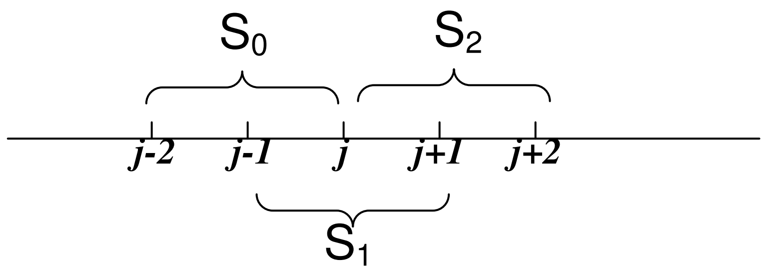


Figure 2.2 Candidate stencils for an interior point j

The schemes for the three candidate stencils are obtained by applying equation (2.9) to each of these stencils and are given by equation (2.11).

$$\begin{aligned} &S_0: \quad F_0 \qquad 2f'_{j-1} + f'_j = \frac{1}{h}\left(-\frac{1}{2} f_{j-2} - 2 f_{j-1} + \frac{5}{2} f_j \right) \\ &S_1: \quad F_1 \qquad \frac{1}{4} f'_{j-1} + f'_j + \frac{1}{4} f'_{j+1} = \frac{1}{h}\left(-\frac{3}{4} f_{j-1} + \frac{3}{4} f_{j+1} \right) \\ &S_2: \quad F_2 \qquad 2f'_{j+1} + f'_j = \frac{1}{h}\left(-\frac{5}{2} f_j + 2 f_{j+1} + \frac{1}{2} f_{j+2} \right) \end{aligned} \tag{2.11}$$

where h is the mesh size. The schemes corresponding to stencils S0 and S2 are third order one-sided finite difference schemes, and the scheme corresponding to S1 is a fourth order centered scheme. These three equations are denoted by F0, F1 and F2. Then a specific weight is assigned to each equation, and a new scheme is obtained by a summation of the equations.

$$F = C_0 F_0 + C_1 F_1 + C_2 F_2 \tag{2.12}$$

where C_0, C_1 and C_2 are weights and satisfy $C_0 + C_1 + C_2 = 1$. If the coefficients are chosen as

$$C_0 = C_2 = \frac{1}{18}, \; C_1 = \frac{8}{9} \tag{2.13}$$

The new scheme is a sixth order centered compact scheme and is given by:

$$\frac{1}{3} f'_{j-1} + f'_j + \frac{1}{3} f'_{j+1} = \frac{1}{h}\left(-\frac{1}{36} f_{j-2} - \frac{7}{9} f_{j-1} + \frac{7}{9} f_{j+1} + \frac{1}{36} f_{j+2}\right) \tag{2.14}$$

The procedure described above implies that a sixth order centered compact scheme can be constructed by a combination of three lower order schemes. In order to achieve the non-oscillatory property, the WENO weights (Jiang et al., 1996) are introduced to determine new weights for each stencil. The weights are determined according to the smoothness of the function on each stencil. Following the WENO method, the new weights are defined as

$$\omega_k = \frac{\gamma_k}{\sum_{i=0}^{2}\gamma_i} \qquad \gamma_k = \frac{C_k}{(\varepsilon + IS_k)^p} \tag{2.15}$$

where ε is a small positive number which is used to prevent the denominator becoming zero and p is a parameter to control the weighting. Actually, p is very sensitive to affect the weights. We set p as a function of smoothness instead of constant. When p=0, the 6th order standard compact scheme is recovered. IS_k is a smoothness measurement which is defined in 2.2.2.

Through the Taylor expansion, it can be easily proved that in smooth regions the new weights ω_k satisfy:

$$\omega_k = C_k + O(h^2) \text{ and}$$

$$\omega_2 - \omega_0 = O(h^3) \tag{2.16}$$

The new scheme is formed using these new weights:

$$F = \omega_0 F_0 + \omega_1 F_1 + \omega_2 F_2 \tag{2.17}$$

The leading error of F is a combination of the leading errors of the original schemes, which is:

$$(\frac{1}{12}\omega_0 - \frac{1}{12}\omega_2) f^{(4)} h^3 + (-\frac{1}{15}\omega_0 + \frac{1}{120}\omega_1 - \frac{1}{15}\omega_2) f^{(5)} h^4 \tag{2.18}$$

When equation (2.16) is satisfied, the leading error of the new scheme can be written as $O(h^6)$ and the new scheme still keeps its 6th order.

2.3.3 Weighted compact and non-compact schemes

Now, we try to use one parameter α -family of the compact scheme. On each stencil, a compact difference scheme is derived as follows by matching the coefficients in Taylor series to obtain corresponding orders.

$$S_0 : F_0 \qquad \alpha_0^- f'_{i-1} + f'_i = \frac{1}{h}\left[b_0^- f_{i-2} + a_0^- f_{i-1} + c_0 f_i\right]$$

$$S_1 : F_1 \qquad \alpha_1^- f'_{i-1} + f'_i + \alpha_1^+ f'_{i+1} = \frac{1}{h}\left[a_1^- f_{i-1} + c_1 f_i + a_1^+ f_{i+1}\right]$$

$$S_2 : F_2 \qquad f'_i + \alpha_2^+ f'_{i+1} = \frac{1}{h}\left[c_2 f_i + a_2^+ f_{i+1} + b_2^+ f_{i+2}\right]$$

The linear weight for each stencil is C0, C1, C2, respectively. Then we have 16 unknowns,

$$\begin{array}{llllll} C_0, & \alpha_0^-, & b_0^-, & a_0^-, & c_0, & \\ C_1, & \alpha_1^-, & \alpha_1^+, & a_1^-, & a_1^+, & c_1, \\ C_2, & \alpha_2^+, & a_2^+, & b_2^+, & c_2, & \end{array}$$

For each stencil, a compact scheme of lower order is established. By matching the coefficients in Taylor's series, we have the following conditions:

$$c_0 = \frac{3+\alpha_0^-}{2},\quad c_1 = 0,\quad c_2 = -\frac{3+\alpha_0^-}{2},\quad a_2^+ = 2,\quad a_0^- = -2,\quad b_0^- = \frac{1-\alpha_0^-}{2},\quad b_2^+ = -\frac{1-\alpha_0^-}{2},$$
$$a_1^- = \frac{\alpha_1^+ - 3\alpha_1^- - 1}{2},\quad a_1^+ = -\frac{\alpha_1^+ - 3\alpha_1^- - 1}{2} \tag{2.20}$$

In order to reassemble the standard compact scheme in equation (2.10), we have the following conditions:

$$C_0\alpha_0^- + C_1\alpha_1^- = \alpha,\ C_0 + C_1 + C_2 = 1,\ C_1\alpha_1^+ + C_2\alpha_2^+ = \alpha,\ C_0 b_0^- = -\frac{1}{12}(4\alpha - 1),$$
$$C_0 a_0^- + C_1 a_1^- = -\frac{1}{3}(\alpha+2),\ C_0 c_0 + C_1 c_1 + C_2 c_2 = 0,\ C_1 a_1^+ + C_2 a_2^+ = \frac{1}{3}(\alpha+2),\ C_2 b_2^- = \frac{1}{12}(4\alpha-1) \tag{2.21}$$

where α is treated as a parameter.

All these nonlinear equations above are not independent of each other. Therefore, the system is not closed for 16 unknowns. We can add an artificial condition to close the system. Note that this is a non-linear system. Let us try to use $\alpha_1^+ = \frac{3\alpha}{4}$ artificially. We have a closed system with the following solution listed in Table 1.

Table 1. Coefficients for the compact scheme on each stencil S0, S1, S2 ($\alpha_1^+ = \frac{3\alpha}{4}$)

	C	α_-	α_+	b_-	a_-	c	a_+	b_+
S_0	$\frac{5\alpha-2}{6(3\alpha-2)}$	$\frac{6\alpha(2\alpha-1)}{5\alpha-2}$		$\frac{1}{2}-\frac{3\alpha(2\alpha-1)}{5\alpha-2}$	-2	$\frac{3}{2}+\frac{3\alpha(2\alpha-1)}{5\alpha-2}$		
S_1	$\frac{4(\alpha-1)}{3(3\alpha-2)}$	$\frac{3\alpha}{4}$	$\frac{3\alpha}{4}$		$-\frac{3\alpha}{4}-\frac{1}{2}$	0	$\frac{3\alpha}{4}+\frac{1}{2}$	
S_2	$\frac{5\alpha-2}{6(3\alpha-2)}$		$\frac{6\alpha(2\alpha-1)}{5\alpha-2}$			$-\frac{3}{2}-\frac{3\alpha(2\alpha-1)}{5\alpha-2}$	2	$-\frac{1}{2}+\frac{3\alpha(2\alpha-1)}{5\alpha-2}$

where every coefficient varies smoothly and monotonically when α varies from 0 to 1/3. Therefore, the scheme is formulated as follows,

$$S_0 : F_0 \qquad \frac{6\alpha(2\alpha-1)}{5\alpha-2} f'_{j-1} + f'_j = \frac{1}{h}\left[\left(\frac{1}{2} - \frac{3\alpha(2\alpha-1)}{5\alpha-2}\right) f_{j-2} - 2 f_{j-1} + \left(\frac{3}{2} + \frac{3\alpha(2\alpha-1)}{5\alpha-2}\right) f_j\right]$$

$$S_1 : F_1 \qquad \frac{3\alpha}{4} f'_{j-1} + f'_j + \frac{3\alpha}{4} f'_{j+1} = \frac{1}{h}\left[-\left(\frac{3\alpha}{4} + \frac{1}{2}\right) f_{j-1} + \left(\frac{3\alpha}{4} + \frac{1}{2}\right) f_{j+1}\right] \tag{2.22}$$

$$S_2 : F_2 \qquad f'_j + \frac{6\alpha(2\alpha-1)}{5\alpha-2} f'_{j+1} = \frac{1}{h}\left[-\left(\frac{3}{2} + \frac{3\alpha(2\alpha-1)}{5\alpha-2}\right) f_j + 2 f_{j+1} - \left(\frac{1}{2} - \frac{3\alpha(2\alpha-1)}{5\alpha-2}\right) f_{j+2}\right]$$

For candidates S_0 and S_2, the function values at three grid points and first derivative at one grid point are used to calculate f'_j. Thus the scheme is at least second-order accurate (third-order if α = 1/3) and one sided. For candidate S_1, the function values at two grid points and first derivative at two grid points are used to calculate f'_j. Thus the scheme is at least second-order accurate (fourth-order if $\alpha = 1/3$) and centered. Then a specific weight is assigned to each equation, and a new scheme is obtained by a summation of the equations.

$$F = C_0 F_0 + C_1 F_1 + C_2 F_2 \tag{2.23}$$

where $C_0 + C_1 + C_2 = 1$. By choosing the weights in table 1, the scheme reproduces the standard compact scheme:

$$\alpha f'_{i-1} + f'_i + \alpha f'_{i+1} = \left(-\frac{1}{12}(4\alpha - 1) f_{i-2} - \frac{1}{3}(\alpha + 2) f_{i-1} + \frac{1}{3}(\alpha + 2) f_{i+1} + \frac{1}{12}(4\alpha - 1) f_{i+2} \right) / h + \tau_i \tag{2.24}$$

which has sixth-order of accuracy if we pick $\alpha = 1/3$, but fourth-order if we pick $\alpha \neq 1/3$.

As we discussed in section 2.3.2, we use WENO weights, $\omega_0, \omega_1, \omega_2$ instead of C_0, C_1, C_2.

Following the WENO method, the weights are defined as:

$$\omega_k = \frac{\gamma_k}{\sum_{i=0}^{2} \gamma_i}, \quad \gamma_k = \frac{C_k}{(\varepsilon + IS_k)^p},$$

$$C_0 = \frac{5\alpha - 2}{6(3\alpha - 2)}, C_1 = \frac{4(\alpha - 1)}{3(3\alpha - 2)}, C_2 = \frac{5\alpha - 2}{6(3\alpha - 2)},$$

where ε is a small number to prevent the denominator becoming zero. p is an important parameter to control weights. IS_k is the smoothness measurements which are defined in section 2.2.2.

The final scheme is $F = \omega_0 F_0 + \omega_1 F_1 + \omega_2 F_2$:

$$\begin{aligned}
&[\omega_0 \frac{6\alpha(2\alpha - 1)}{5\alpha - 2} + \omega_1 \frac{3\alpha}{4}] f'_{j-1} + f'_j + [\omega_1 \frac{3\alpha}{4} + \omega_2 \frac{6\alpha(2\alpha - 1)}{5\alpha - 2}] f'_{j+1} = \\
&\{\omega_0 [\frac{1}{2} - \frac{3\alpha(2\alpha - 1)}{5\alpha - 2}] f_{j-2} - [2\omega_0 + \omega_1 (\frac{3\alpha}{4} + \frac{1}{2})] f_{j-1} + (\omega_0 - \omega_2)[\frac{3}{2} + \frac{3\alpha(2\alpha - 1)}{5\alpha - 2}] f_j \\
&+ [2\omega_2 + \omega_1 (\frac{3\alpha}{4} + \frac{1}{2})] f_{j+1} - \omega_2 [\frac{1}{2} - \frac{3\alpha(2\alpha - 1)}{5\alpha - 2}] f_{j+2}\} / h
\end{aligned} \tag{2.25}$$

Note that there is only one parameter α which has not been determined yet.

2.3.4 Determination of parameter α

Apparently, determination of α becomes the central stage of our research. Instead of using fixed α, we determine the value of α according to the smoothness of the function. All the other coefficients become the functions of α. In this work, we first define α as

$$\alpha = \frac{1}{3} - \left[\left(\overline{IS_0} - \frac{1}{3} \right)^2 + \left(\overline{IS_1} - \frac{1}{3} \right)^2 + \left(\overline{IS_2} - \frac{1}{3} \right)^2 \right]^{\frac{1}{2}} / 2 \tag{2.26}$$

where $\overline{IS_k} = \dfrac{IS_k + \varepsilon}{\sum_{i=0}^{2}(IS_k + \varepsilon)}$,

ε is a small positive number. In smooth regions, the three normalized smoothness are nearly equal, namely, $\overline{IS_0} = \overline{IS_1} = \overline{IS_2} = \dfrac{1}{3}$. Then α equals to 1/3 and the 6th order standard compact scheme recovered. We achieve global dependency and the best resolution. In shock regions, for instance, the worst case gives us dramatically different weights. After normalization we have $\overline{IS_0} = 1, \overline{IS_1} = \overline{IS_2} = 0$. Then $\alpha = 0$ and we achieve the local dependency and non-oscillatory property from the weighting procedure.

However, these kinds of WENO weights based on differences of left hand side, central, right hand side smoothness would not distinguish the low and high frequency waves and will give same α for both low frequency and high frequency waves. It may mislead to give $\alpha = 1/3$ for center point of the shock if we capture the shock with more than three grid points. Apparently, we need to consider the fourth measurement of the smoothness, IS_{ave} which is high for high frequency and low for low frequency. In this work, we define α in the following way:

$$\alpha_{final} = \min\{\alpha(1 - a_1 * IS_{ave}) * a_2, \frac{1}{3}\} \tag{2.27}$$

We also define a function called smoothness which will control the compact and non-compact switch and everything:

Smoothness=1.0-3.0*α or α =(1.0-smoothness)/3.0

When smoothness=1.0 where is non-differentiable, α =0.0 and non-compact scheme will be used. When smoothness=0.0, α =1/3 and the standard 6th order compact scheme will be recovered.

2.4 Recovery to 8th order in smooth areas

In smooth area, the scheme will become a standard 6th order compact scheme and keep 6th order in accuracy:

$$\frac{1}{3}f'_{j-1} + f'_j + \frac{1}{3}f'_{j+1} = \frac{1}{h}\left(-\frac{1}{36}f_{j-2} - \frac{7}{9}f_{j-1} + \frac{7}{9}f_{j+1} + \frac{1}{36}f_{j+2}\right) \tag{2.28}$$

Using 5 grid points, we can also get an 8th order scheme by following scheme:

$$\frac{1}{36}f'_{j-2} + \frac{4}{9}f'_{j-1} + f'_j + \frac{4}{9}f'_{j+1} + \frac{1}{36}f'_{j+2} = \frac{1}{h}\left(-\frac{25}{216}f_{j-2} - \frac{40}{54}f_{j-1} + \frac{40}{54}f_{j+1} + \frac{25}{216}f_{j+2}\right) \tag{2.29}$$

Subtracting (2.29) by (2.28), we get the residual:

$$F_3 : \frac{1}{36}f'_{j-2} + \frac{1}{9}f'_{j-1} + \frac{1}{9}f'_{j+1} + \frac{1}{36}f'_{j+2} = \frac{1}{h}\left(-\frac{19}{216}f_{j-2} + \frac{1}{27}f_{j-1} - \frac{1}{27}f_{j+1} + \frac{19}{216}f_{j+2}\right) \tag{2.30}$$

The final finite difference scheme can be written as

$$F = \omega_0 F_0 + \omega_1 F_1 + \omega_2 F_2 + \omega_3 F_3 \tag{2.31}$$

Where

$$\omega_3 = 3.0 * \alpha = 1.0 - Smoothness \tag{2.32}$$

which is 1 in the smooth area and becomes zero near the shock or other discontinuities. In this way, the accuracy will be recovered to 8th order by 5-point stencil in the smooth area. Of course, a penta-diagonal system has to be solved on each grid line.

The above derivation is based on the six order compact scheme:

$$F_6 = \omega_0 F_0 + \omega_1 F_1 + \omega_2 F_2 + O(h^6) \tag{2.33}$$

In order to get 8th order accuracy in the smooth area, we can use:

$$F = (1-\omega_3)[\omega_0 F_0 + \omega_1 F_1 + \omega_2 F_2] + \omega_3 F_8 + (1-\omega_3)k_6 h^6 + \omega_3 k_8 h^8 \tag{2.34}$$

where F_8 is a standard 8th order compact scheme with 5 grid points. In the smooth area, $\omega_3 = 1.0$, we obtain 8th order of accuracy.

Here, we use the 6th order WCS as our base scheme. However, this method is universal and we can use for any base scheme. For example, we can use 5th order WENO as our base scheme or use the uniform compact and non-compact scheme (UCNC) as our base scheme. The basic idea is to get 8th order of accuracy recovered in the smooth area, but bias near the shock to avoid numerical oscillations.

The remained question is how to detect shock correctly and accurately and then chose a right switch function or sharply weighted function, ω_3 , based on the smoothness, which has been discussed much by above sections.

2.5 Comments on the new scheme:

It is very natural for one to have an idea to use high order compact scheme for smooth area and low order upwind scheme for shocks. However, it is not true. For the smooth area, both low order and high order schemes can achieve satisfying results. We prefer to use high order of course, but it is not critical. The critical is to use high order compact scheme with high resolution for oscillatory waves and use the weighted high order central, non-dissipative scheme for shocks. The needed dissipation comes from weights, not from low order upwind scheme. The weights provide needed dissipation, but do not reduce the order of the scheme.

There is only one major problem for numerical methods: how to get the derivative more accurately for a discrete data set which could be partially smooth (derivative is small), partially oscillatory (derivative is large), and partially non-differentiable (finite difference on left hand side, central, right hand side, or δ^+, δ, δ^- , are quite different).

The new scheme tries to give a right and accurate approximation of derivative for a data set by using compact scheme in the smooth area, weighted compact scheme in the oscillatory area, and weighted non-compact scheme cross the shock. All controlled by the so called "smoothness"

The new scheme is a subroutine which can be used in any finite difference CFD code to find right derivatives.

The new scheme is applicable to 2-D or 3-D problems by calling a subroutine for twice or three times. However, there is a boundary condition issue for 2-D and 3-D problems.

III. Numerical Test and Analysis

Throughout this report the 3-tep, 3rd order TVD Runge-Kutta method is applied for time discretization.

3.1 Order of Accuracy

The scheme is tested by solving a linear wave equation with a smooth initial function:

$$u_t + u_x = 0, \; u(x,0) = \sin(2\pi x) \text{ where } 0 \le x \le 1 \tag{3.1}$$

The calculation stops at $t = 0.3$ and the errors are listed in table 2. The computation shows the 6the order accuracy is achieved.

Table 2. Errors and Order of Accuracy

N	L_1 Error	L_1 Order	L_2 Error	L_2 Order	L_∞ Error	L_∞ Order
8	1.06E-02	-	3.67E-03	-	2.05E-02	-
16	8.66E-05	6.93	2.46E-05	7.22	2.00E-04	6.68
32	1.37E-06	5.98	2.94E-07	6.39	4.37E-06	5.51
64	2.23E-08	5.93	3.74E-09	6.30	1.11E-07	5.30
128	3.45E-10	6.01	4.95E-11	6.24	2.86E-09	5.27
256	4.49E-12	6.26	5.73E-13	6.43	5.98E-11	5.58

3.2 Comparison of dissipation for 1-D linear wave equation

The same governing equation is solved and high frequency initial condition is applied in order to test the numerical dissipation of different schemes.

$$u_t + u_x = 0, \; u(x,0) = \sin(20\pi x) \text{ where } 0 \le x \le 1 \tag{3.2}$$

The solutions at t=1.0 are put together in figure 3.1. The results show that standard 6th order compact scheme has the least numerical dissipation which should be zero theoretically. UWCNC scheme also has very small dissipation while WENO-5 scheme has dramatically smeared the high frequency solution.

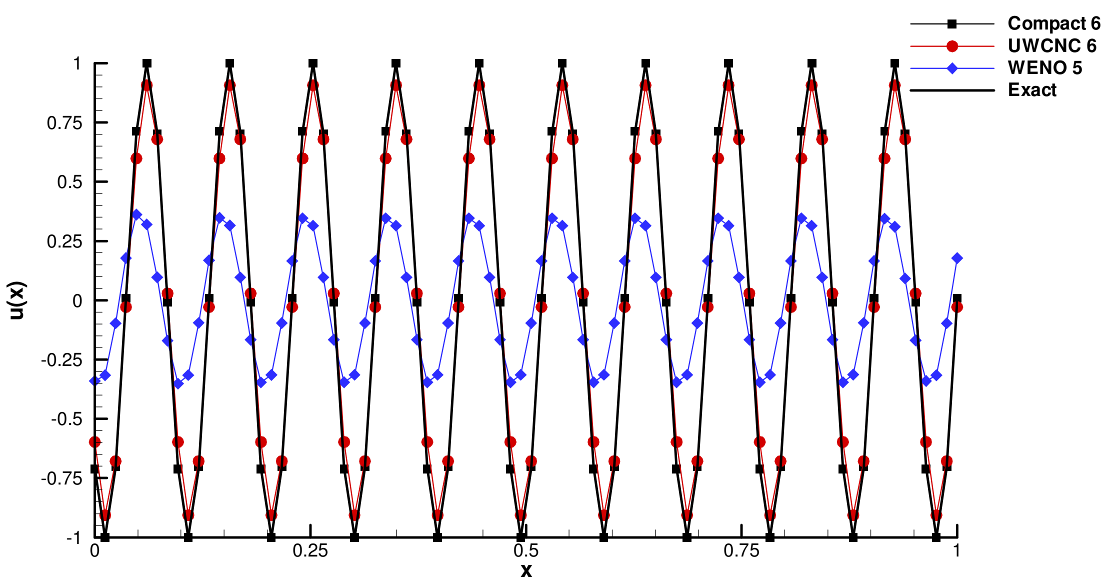


Figure 3.1 Numerical test over linear wave equation.

3.3 1-D linear wave equation with jump initial function

The same governing equation is used but the initial condition is discontinuous:

$$u_t + u_x = 0\,,\quad u(x,0) = \begin{cases} 1.0 & if \quad 0.1 \le x \le 0.4 \\ 0.5 & \quad otherwise \end{cases} \tag{3.3}$$

The calculation stops at $t = 0.3$ and the solutions are illustrated in figure 3.2. The results indicate that standard compact scheme doesn't work for shocks while both XJL (with variable α) presented in this report and WENO scheme work. Furthermore, XJL-6 has less dissipation than WENO-5 near shocks which means a sharper transition is obtained.

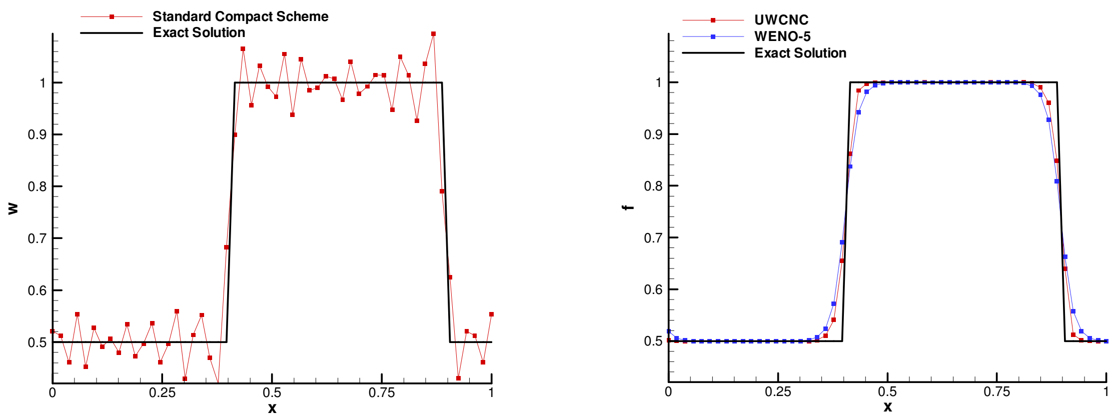


Figure 3.2 Numerical test over linear wave equation.

3.4 1-D Shock Tube Problem

To test the capability of the new scheme in shock capturing, we applied it to the 1-D shock tube problem. The governing equations are 1D Euler equations:

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = 0 \tag{3.4}$$

$$U = (\rho,\, \rho u,\, E)^T\,;\;\; F = (\rho,\, \rho u + p,\, u(E+p))^T$$

The initial conditions are given as follows:

$$(\rho,\, u,\, p) \;= \begin{cases} (1,0,1), & x < 0; \\ (0.125,0,0.1) & x \ge 0. \end{cases} \tag{3.5}$$

To solve the Euler equations, Steger-Warming flux vector splitting is used and the derivatives of splitting flux F^+, F^- are calculated using our new scheme. In this case, α is defined as in Equation 2.27. The distributions of velocity u and pressure are shown in figure3.3. Comparisons are also made with the solutions obtained using 5th order WENO scheme. From figure 3.3, it can be found the XJL scheme captured the shock sharper and smeared the expansion wave and shock less then the 5th order WENO. Figure 3.4 shows a locally enlarged comparison between XJL, WENO, and WENO with 1600 grid points which we consider as an exact solution. Figure 3.4 show the smoothness measured by our definition which is the only parameter to control the compact and non-compact scheme switch. The figure shows the shock is well captured with smoothness=1.0 ($\alpha = 0$) and the smoothness measured on the coarser grid (N=100) and finer grid (N=200) are pretty consistent.

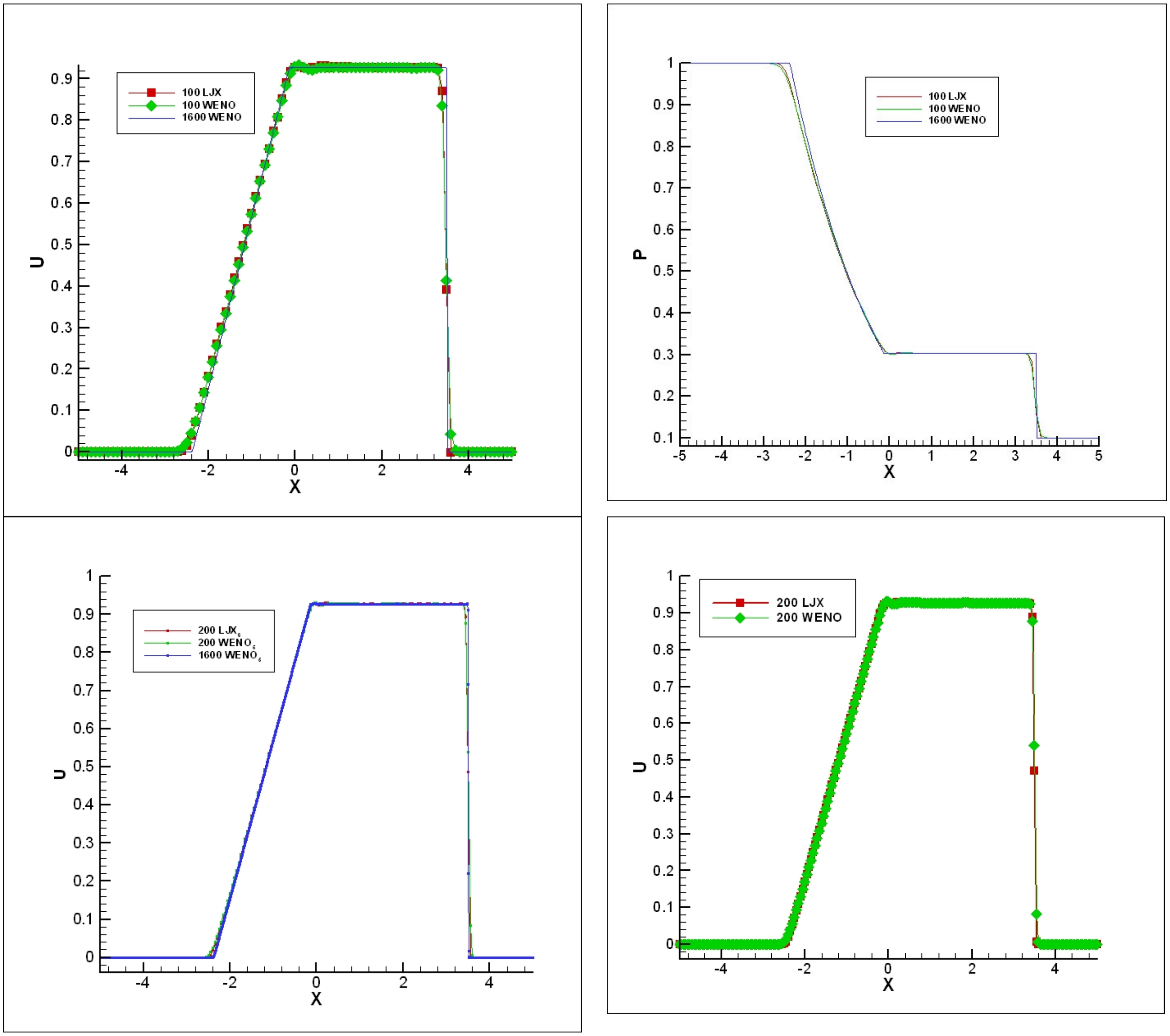
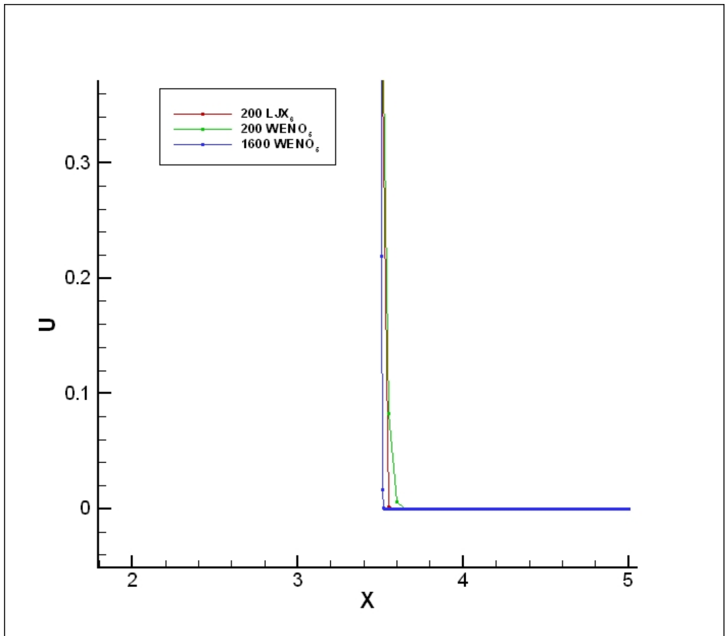


Figure 3.3 Numerical test for 1D shock-tube problem, t=2, N=100 and 200



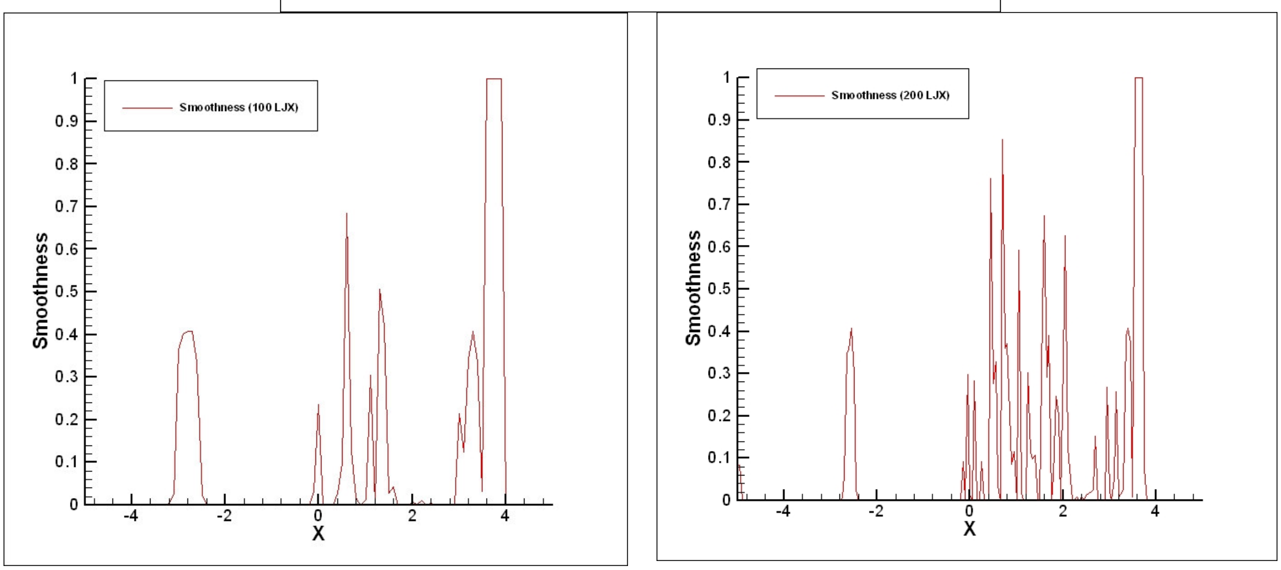


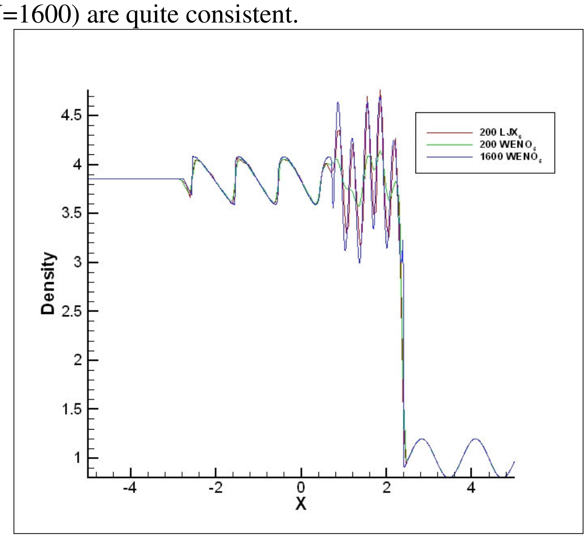
Figure 3.4 Smoothness for 1D shock-tube problem, t=2, N=100 and 200

3.5 1-D Shock/Entropy Wave Interaction

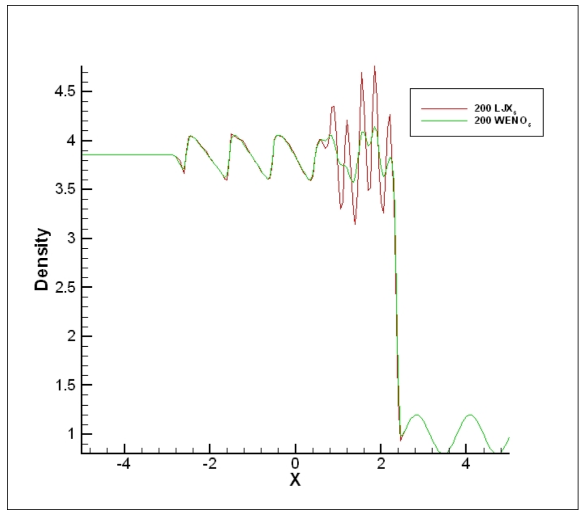
To test the capability of the new scheme in both shock capturing and resolution, we applied it to the 1-D problem of shock/entropy wave interaction. In this case, Euler equations (3.3) are solved with the following initial conditions:

$$(\rho, u, p)_0 = \begin{cases} (3.857143, 2.629369, 10.33333), & x < -4; \\ (1 + 0.2\sin(5x), 0, 1) & x \geq -4. \end{cases} \tag{3.6}$$

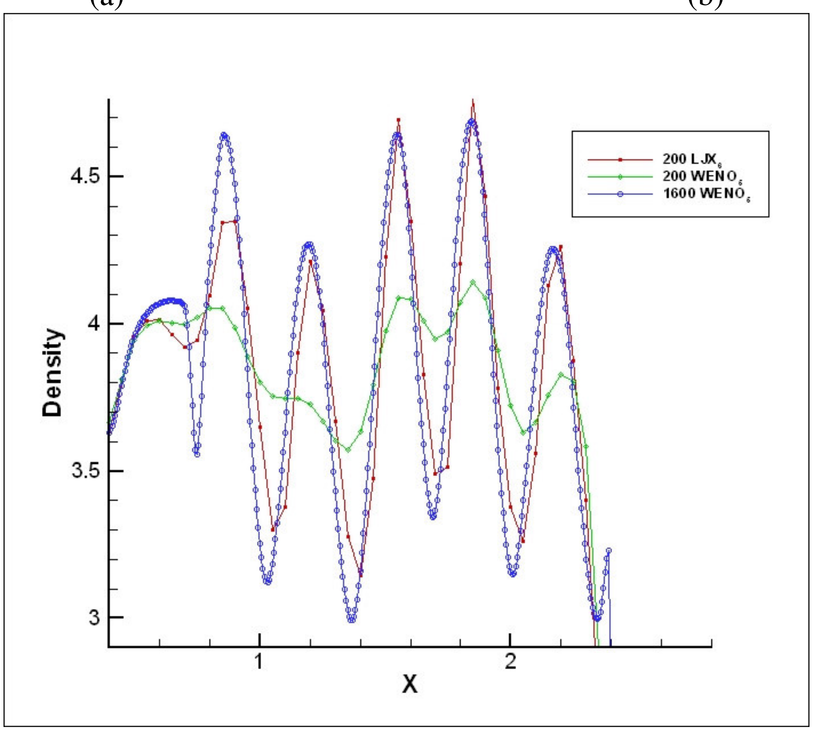
α is calculated using (2.27). Figure 3.5 and 3.6 depict the solutions of the density distribution on the coarser and finer grids respectively. On the coarser grid with grid number of N=200, our new scheme shows much better resolution for small length scales than the 5th order WENO (Figure 3.5 (a), (b), (c)). Apparently, there is an order difference in resolution between our 6th order XJL scheme and the 5th order scheme. This is because XJL uses central, non-dissipative, compact scheme with weights in the shock area and recovers high order compact away from the shock. The numerical results by our XJL scheme with 200 grid points are even comparable with the 5th order WENO scheme with 1600 grid points (Figure 3.5 (d) and (e)). On the finer grid (N=400), both the 6th order XJL and 5th order WENO schemes show a good resolution (Figure 3.6 (a), (b), and (c)). However, we can still find our 6th order XJL scheme has a much better resolution for the fifth wave left from the shock (Figure 3.6(d)). In addition, the XJL captures the shock in a much sharper way for all shocks. On the shocks developed by the sinuous waves, only one grid point was found on the shock (Figure 3.5 (d) and 3.6(a)). Again, Figure 3.7 shows the smoothness measured by our definition which is the only parameter to control the compact and non-compact scheme switch. The figure shows the main shock is well captured with smoothness=1.0 ($\alpha = 0$) and the shocks developed by the sine function are also well captured. The smoothness measured on the coarser grid (N=200 and 400) and finer grid (N=1600) are quite consistent.



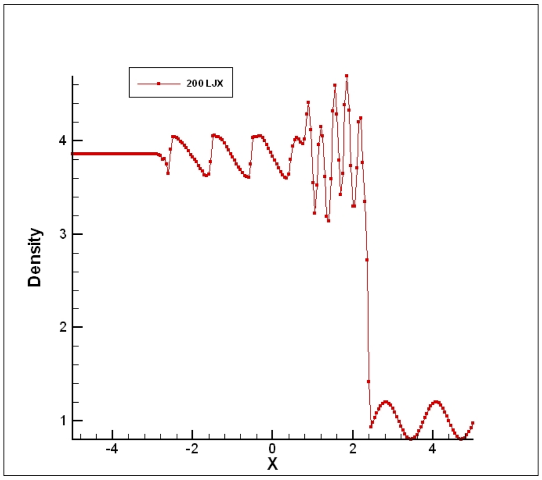
(a)



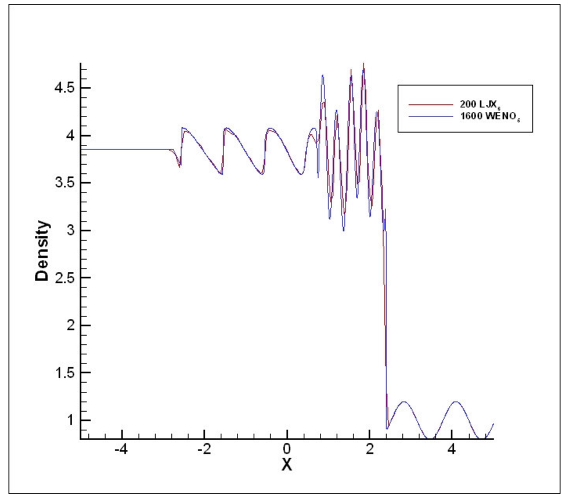
(b)



(c)

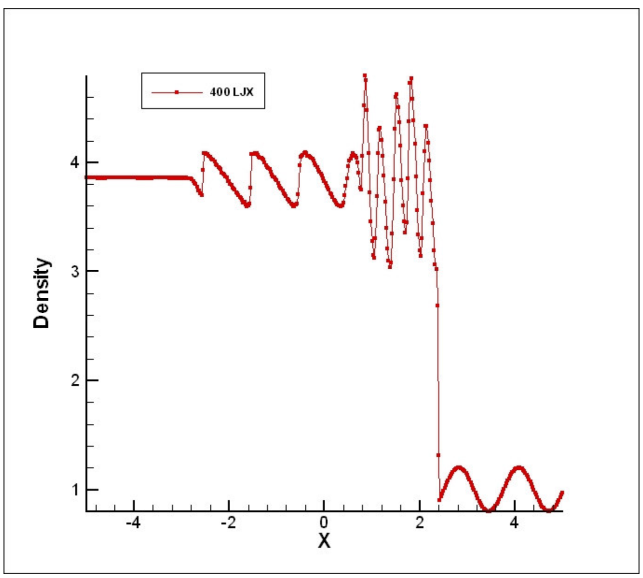


(d)

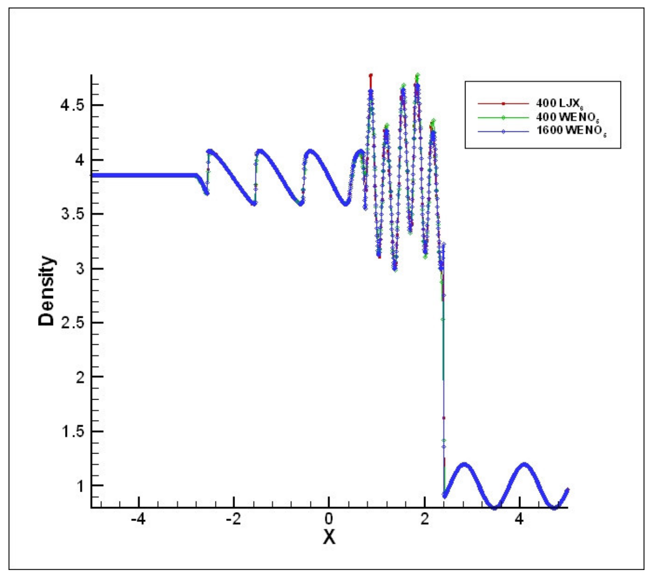


(e)

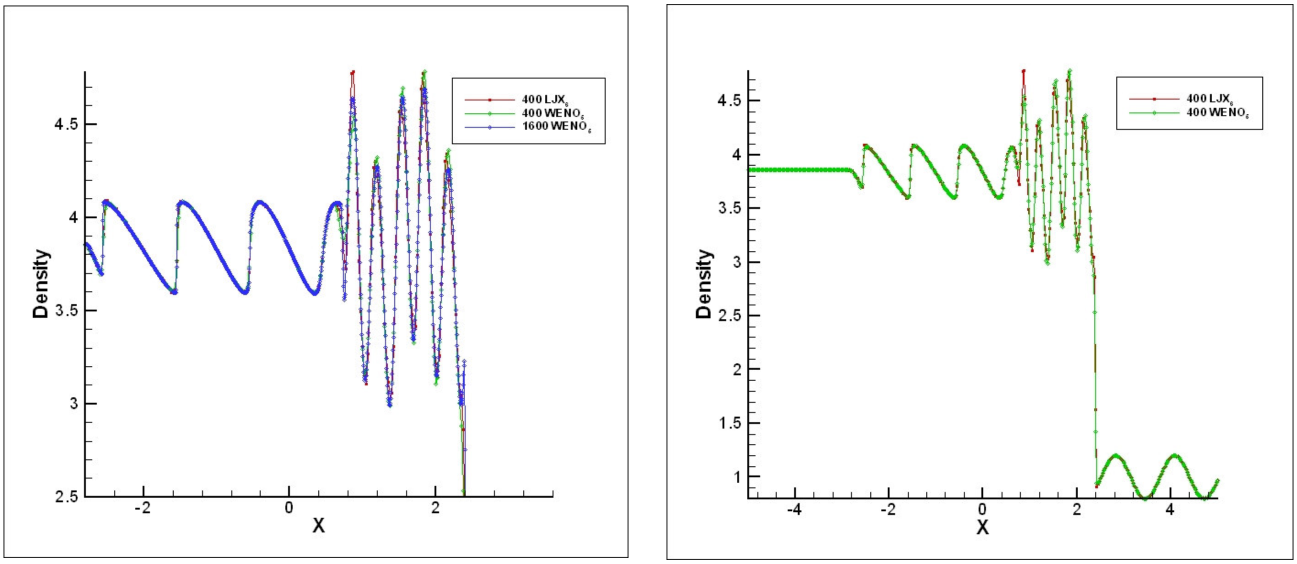
Figure 3.5 Numerical test for 1D shock-entropy wave interaction problem, t=1.8, N=200



(a)



(b)



(c) (d)

Figure 3.6 Numerical test for 1D shock-entropy wave interaction problem, t=1.8, N=400

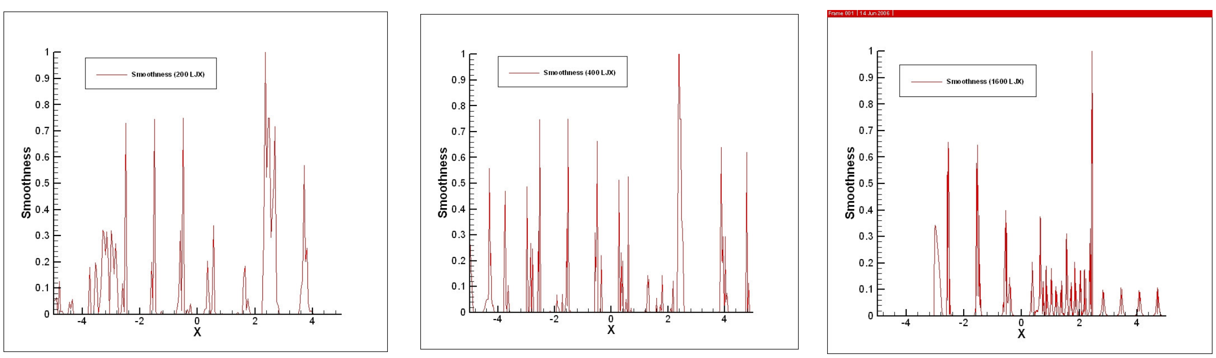


Figure 3.7 Smoothness for 1D shock-entropy problem, t=2, N=200, 400, 1600

IV. Questions and answers about the new work

In order to make the things more clear, we write flowing questions and answers:

Q: What is the most critical problem for CFD?

A: The critical problem is to give an accurate approximation of derivatives for a discrete data set which is partially smooth, partially oscillatory, and partially non-differentiable.

Q: How to measure?

A: Use slope. The smooth part has small slope, the oscillatory part has large slope, and the non-differentiable part has one large slope on one side, but small slope on the other side. They can be detected by our smoothness function α. We never missed them.

Q: What are you doing now?

A: We try to develop a new scheme which is super than other numerical scheme in capturing shock and resolving small high frequency length scales. Actually, it is a subroutine which has a discrete data set as input and gives an accurate derivative data set as output. This subroutine can be added to any finite difference code by AFRL researchers or other people.

Q: People think we can detect the shock and then use upwind scheme for shock and high order scheme for the smooth part. Is it right?

A: It looks like a good idea, but, unfortunately, it does not work. Both low order and high order schemes can provide satisfying results for the smooth problem. Although we prefer to use high order compact scheme for the smooth solution, it is not critical.

Q: What is critical?

A: The critical thing is to use high order compact scheme for the oscillatory part to get high order accuracy and high resolution. This is the key issue for the success of the numerical simulation.

Q: How about shock? Should we use low order upwind scheme to capture the shock?

A: No, we should use high order, central, non-dissipative scheme to capture the shock sharply.

Q: How to get dissipation to remove the wiggles near the shock ?

A: We use the weights. The weights can generate the dissipation.

Q: What is the difference between using weights and artificial dissipations?

A: The upwind scheme or artificial viscosity will reduce the order of the finite difference scheme, but the weights will keep the high order accuracy, but provide necessary dissipation for the non-differentiable part.

Q: Why does your weighted compact scheme has wiggles around the shock?

A: No matter how small the weights are for the downstream candidate, the matrix has global dependence.

Q: How to solve the problem?

A: We use the weighted central non-compact scheme, which will decouple the matrix and remove the global dependency.

Q: How to control?

A: We use the one parameter family of compact scheme. When $\alpha = 1/3$, we will have the standard 6th order weighted compact scheme. When $\alpha \neq 1/3$, the scheme will become 4th order. When $\alpha = 0$ the scheme will become a 4th order standard weighted non-compact scheme. The global dependency will be removed and no-oscillation will be generated around the shock.

Q: How to control?

A: This is a uniform scheme with one parameter only. α is a function of smoothness. It will be 1/3 in the smooth area and gradually becomes zero when approaching the shock.

Q: How good is the scheme?

A: The new scheme can capture the shock sharper than the 5th order WENO and the resolution for high frequencies is one order higher than the 5th order WENO for the shock-entropy interaction problem.

Q: Is it case related?

A: No, there are no case-related coefficients. It in general does not need any low order filter at all.

Q: Can the subroutine be used any finite difference CFD code?

A: Yes. Anyone and any code. We only give a right derivative for a given discrete data set.

Q: Can the scheme be used for 2-D and 3-D problems?

A: Yes, you can call the subroutine for each direction. However, we need to develop high order compatable scheme for boundary points and need more work on 2-D and 3-D problems.

V. Concluding remarks

The new uniform weighted compact and non-compact scheme (UWCNC), or XJL scheme for simplicity, introduced in this paper is applicable for the simulation of flows containing both shock waves and small structures which is particularly important for shock-turbulence interaction. The scheme is constructed according to the feature of the input discrete data set but not the physics and, therefore, can be used anywhere or any computation program as a subroutine to find right derivatives. The advantage is that the scheme keeps the form of standard central compact scheme in smooth regions, while degenerates to weighted non-compact scheme near a shock to preserve a sharp and almost monotonic transition. This goal is achieved by using the same formulation without switching to a different scheme or using a low order filter. The new scheme does not have any case-related coefficients either. The numerical test shows the new scheme captures the shock sharper (almost one grid point) than the 5th order WENO scheme and has much better capability to resolve the small length scales than the 5th order WENO scheme for the shock-entropy interaction. The further application of this scheme to the simulations of shock/vortex interaction or shock/turbulence interaction appears to be promising.

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