A High-Order and High-Resolution Nonlinear Weighted Compact Scheme for Compressible Flows involving Shocks and Turbulence

Akshay Subramaniam*† and Man Long Wong*†

Department of Aeronautics & Astronautics, Stanford University, Stanford, CA 94305, USA

Sanjiva K. Lele‡

Department of Aeronautics & Astronautics and Department of Mechanical Engineering, Stanford University, Stanford, CA 94305, USA

We present a new high-order weighted compact high resolution (WCHR) scheme based on the idea of weighted compact nonlinear schemes (WCNS's) for shock capturing in compressible flows that has improved resolution properties compared to previous WCNS's. This is achieved by using a compact (or spatially implicit) form instead of the explicit form used in WCNS's for the interpolation in conjunction with a compact finite difference scheme. Since compact interpolation and derivative schemes tend to have better resolution properties compared to standard finite difference schemes, this new scheme has the ability to resolve more fine scale features while still providing sufficient dissipation to capture shocks and discontinuities robustly. Approximate dispersion relation characteristics of this scheme shows the superior resolution properties of the scheme compared to other WCNS's of similar orders of accuracy. Different test cases demonstrate the ability of this scheme to capture discontinuities in a robust and stable manner while also localizing the required numerical dissipation to regions with discontinuities and high wavenumber features and hence preserving smooth flow features better in comparison to WCNS's.

I. Introduction

Simulations of compressible flows that involve shock waves, contact discontinuities and turbulence have conflicting requirements. While capturing discontinuities like shock waves, contact surfaces and slip lines require numerical dissipation for numerical stabilization, the fine scales of turbulence are severely affected by numerical dissipation. Hence, an adaptive method that can surgically switch between a low dissipation formulation near regions of smooth flows to a formulation that adds sufficient dissipation at discontinuities is of paramount importance. In the past, weighted essentially non-oscillatory[1–6] (WENO) schemes and their variants, weighted compact nonlinear schemes[7–11] (WCNS's) have been proposed as a method to provide this adaptation. These schemes capture shocks well and improvements like the WENO6-CU-M2[6] and WCNS6-LD[11] schemes localize the numerical dissipation to regions around discontinuities. However, their resolution properties are limited by the underlying explicit reconstruction and interpolation schemes. Lele[12] developed compact finite difference and interpolation schemes that are high order accurate and have spectral-like resolution properties. Although these schemes are well-suited for problems involving turbulence, they cannot be directly used for problems that contain sharp gradients like in shocks unless certain numerical regularization is used. One kind of numerical regularization for compact finite difference schemes is to add numerical dissipation explicitly[13–16] in solutions to capture shocks and material interfaces using the localized artificial diffusivity (LAD) method which was first proposed by Cook.[13] These regularization methods

*Graduate Research Assistant, Department of Aeronautics & Astronautics, Stanford University, and AIAA Student Member

†These authors contributed equally to the work in deriving the new scheme

‡Professor, Department of Aeronautics & Astronautics and Department of Mechanical Engineering, Stanford University, and AIAA Associate Fellow

preserve the resolution properties of compact schemes, but are still prone to some mild spurious oscillations near shocks or discontinuities. They also introduce additional time step limitations due to the extra artificial dissipation terms. In addition to adding dissipation terms, solutions also need to be filtered at every time step for de-aliasing. This precludes these schemes from being Galilean invariant.

As an alternative to adding artificial dissipation explicitly, Deng et al.[7] used a compact finite difference scheme with WENO interpolation in the context of WCNS. The process in obtaining flux at midpoints using nonlinear interpolations can be interpreted as a nonlinear filtering process to prevent spurious oscillations near discontinuities. However, the fact that WENO interpolation is explicit limits the effective resolution of the overall scheme even though compact finite difference scheme is used. Ghosh et al.[17] developed an upwind-biased compact reconstruction WENO scheme called CRWENO. This method is purely compact, but the scheme is upwind-biased and excessively damps the fine scales of turbulence.

In this paper, we develop a new scheme based on the WCNS formalism that uses a compact form for both the finite difference and the interpolation scheme. As shown in this paper, this new scheme has better resolution properties. The localized dissipation nonlinear weights of Wong et al.[11] are used to provide more localized dissipation compared to upwind-biased nonlinear weights in traditional WCNS's and WENO schemes.

II. Numerical method

In this section, a scalar conservation law of the following form is considered in a one-dimensional domain of size $x \in [x_a, x_b]$ for simplicity:

$$\frac{\partial u}{\partial t} + \frac{\partial F(u)}{\partial x} = 0 \tag{1}$$

where u is the conserved scalar quantity and $F(u)$ is a flux function of u. The equation above is discretized on a uniform grid with N cells and the solution u on the cell node at position $x_j = x_a + (1/2 + j)\Delta x$ is denoted by u_j, $\forall j \in \{0,\ 1,\ \cdots,\ N-1\}$, where $\Delta x = (x_b - x_a)/N$. The cell midpoints are indexed by half integer values $x_{j+\frac{1}{2}}$, $\forall j \in \{-1/2,\ 1/2,\ 3/2,\ \cdots,\ N-1/2\}$.

II.A. Compact and explicit finite difference schemes

Over the years, various forms of finite difference schemes have been used in WCNS's to obtain the flux derivative in Equation (1). Deng et al.[7] first used the sixth order midpoint-to-node compact finite difference (CMD) scheme by Lele[12] in following form:

$$\frac{9}{80}F'_{j-1} + \frac{31}{40}F'_j + \frac{9}{80}F'_{j+1} = \frac{1}{\Delta x}\left[\frac{63}{80}\left(\tilde{F}_{j+\frac{1}{2}} - \tilde{F}_{j-\frac{1}{2}}\right) + \frac{17}{240}\left(\tilde{F}_{j+\frac{3}{2}} - \tilde{F}_{j-\frac{3}{2}}\right)\right] \tag{2}$$

where F'_j are numerically approximated flux derivatives at cell nodes and $\tilde{F}_{j+\frac{1}{2}}$ are interpolated fluxes at cell midpoints. Nonomura et al.[18] suggested using a more efficient explicit sixth order midpoint-to-node finite difference (MD) scheme as the resolutions of WCNS's are mainly dominated by the nonlinear interpolations:

$$F'_j = \frac{1}{\Delta x}\left[\frac{75}{64}\left(\tilde{F}_{j+\frac{1}{2}} - \tilde{F}_{j-\frac{1}{2}}\right) - \frac{25}{384}\left(\tilde{F}_{j+\frac{3}{2}} - \tilde{F}_{j-\frac{3}{2}}\right) + \frac{3}{640}\left(\tilde{F}_{j+\frac{5}{2}} - \tilde{F}_{j-\frac{5}{2}}\right)\right] \tag{3}$$

Nonomura et al.[19] later also proposed a robust explicit sixth order midpoint-and-node-to-node finite difference (MND) scheme:

$$F'_j = \frac{1}{\Delta x}\left[\frac{3}{2}\left(\tilde{F}_{j+\frac{1}{2}} - \tilde{F}_{j-\frac{1}{2}}\right) - \frac{3}{10}\left(F_{j+1} - F_{j-1}\right) - \frac{25}{384}\left(\tilde{F}_{j+\frac{3}{2}} - \tilde{F}_{j-\frac{3}{2}}\right)\right] \tag{4}$$

where F_j are fluxes at cell nodes.

II.B. Weighted compact nonlinear schemes (WCNS's)

In WCNS's, the fluxes at the cell midpoints are obtained with aid of explicit nonlinear interpolations, which can also be interpreted as a nonlinear filtering process to avoid spurious oscillations near shocks and other discontinuities. For the scalar conservation equation Equation (1), the algorithm to obtain the flux derivative with WCNS's is given below:

1. Compute the left-biased and right-biased interpolated solution values $\tilde{u}_L$ and $\tilde{u}_R$ using explicit nonlinear interpolation.

2. Compute the flux at the cell midpoints using a flux difference splitting method $\tilde{F}_{j+\frac{1}{2}} = \mathrm{F}_{\mathrm{split}}(\tilde{u}_L, \tilde{u}_R)$ (typically a Riemann solver).

3. Compute the flux at the cell nodes $F_j = F(u_j)$ if the node values of flux are needed in the finite difference scheme e.g. MND scheme in Equation (4).

4. Using the flux(es) $\tilde{F}_{j+\frac{1}{2}}$ (and F_j) to compute the flux derivative F'_j with a compact or explicit finite difference scheme.

It should also be noted that flux vector splitting methods such as Lax Friedrichs flux splitting can also be used in WCNS's where the flux values are interpolated instead of the solution values.

Figure 1. Sub-stencils of WCNS's.

Despite of the robustness of interpolations using upwind-biased nonlinear weights in capturing shocks like those by Jiang and Shu[1] (JS) and that by Borges et al.[4] (Z), they are unavoidably dissipative in smooth regions. Wong et al.[11] therefore proposed a nonlinear localized dissipative (LD) interpolation that minimizes dissipation in smooth regions by including the downwind stencil, S_3 in Figure 1, in the nonlinear weighting process. The LD interpolation approximates the midpoint values by nonlinearly combining third order linear interpolated values from four different sub-stencils, S_0 - S_3, shown in Figure 1. The interpolated values at the midpoints $\tilde{u}_{j+\frac{1}{2}}$ from the four different explicit interpolations (EI_k) are given by:

$$EI_0: \quad \tilde{u}^{(0)}_{j+\frac{1}{2}} = \frac{1}{8}\left(3u_{j-2} - 10u_{j-1} + 15u_j\right) \tag{5}$$

$$EI_1: \quad \tilde{u}^{(1)}_{j+\frac{1}{2}} = \frac{1}{8}\left(-u_{j-1} + 6u_j + 3u_{j+1}\right) \tag{6}$$

$$EI_2: \quad \tilde{u}^{(2)}_{j+\frac{1}{2}} = \frac{1}{8}\left(3u_j + 6u_{j+1} - u_{j+2}\right) \tag{7}$$

$$EI_3: \quad \tilde{u}^{(3)}_{j+\frac{1}{2}} = \frac{1}{8}\left(15u_{j+1} - 10u_{j+2} + 3u_{j+3}\right) \tag{8}$$

The LD interpolation is formulated as a nonlinear combination of the four 3rd order interpolations in Equations (5)-(8) to yield a 6th order interpolation in smooth regions:

$$\tilde{u}_{j+\frac{1}{2}} = \sum_{k=0}^{3} \omega_k \tilde{u}^{(k)}_{j+\frac{1}{2}} \tag{9}$$

The nonlinear weights ω_k are given by:

$$\omega_k = \begin{cases} \sigma\omega_k^{\mathrm{upwind}} + (1-\sigma)\omega_k^{\mathrm{central}}, & \text{if } R_\tau > \alpha^\tau_{RL} \\ \omega_k^{\mathrm{central}}, & \text{otherwise} \end{cases}, \quad k = 0,1,2,3 \tag{10}$$

where ω_k^{upwind} are the Z nonlinear weights[4] given by:

$$\omega_k^{\text{upwind}} = \frac{\alpha_k^{\text{upwind}}}{\sum_{k=0}^{2} \alpha_k^{\text{upwind}}}, \quad \alpha_k^{\text{upwind}} = d_k^{\text{upwind}} \left(1 + \left(\frac{\tau_5}{\beta_k + \epsilon}\right)^p\right), \quad k = 0, 1, 2 \tag{11}$$

$$\omega_3^{\text{upwind}} = 0 \tag{12}$$

The smoothness indicators β_k are defined by

$$\beta_k = \sum_{l=1}^{2} \int_{x_{j-\frac{1}{2}}}^{x_{j+\frac{1}{2}}} \Delta x^{2l-1} \left(\frac{\partial^l}{\partial x^l} \tilde{u}^{(k)}(x)\right)^2 dx, \quad k = 0, 1, 2 \tag{13}$$

where $\tilde{u}^{(k)}(x)$ is the Lagrange interpolating polynomial from stencil S_k. The integrated forms of the smoothness indicators are given in Appendix V.A. $\tau_5 = |\beta_2 - \beta_0|$ is a reference smoothness indicator and $p = 2$ is used in this paper. The linear weights d_k^{upwind} of Equation (11) are given by:

$$d_0^{\text{upwind}} = \frac{1}{16}, \quad d_1^{\text{upwind}} = \frac{10}{16}, \quad d_2^{\text{upwind}} = \frac{5}{16} \tag{14}$$

$\omega_k^{\text{central}}$ is given by:

$$\omega_k^{\text{central}} = \frac{\alpha_k^{\text{central}}}{\sum_{k=0}^{3} \alpha_k^{\text{central}}}, \quad \alpha_k^{\text{central}} = d_k^{\text{central}} \left(C + \left(\frac{\tau_6}{\beta_k + \epsilon}\right)^q\right), \quad k = 0, 1, 2, 3 \tag{15}$$

where

$$\beta_3 = \sum_{l=1}^{5} \int_{x_{j-\frac{1}{2}}}^{x_{j+\frac{1}{2}}} \Delta x^{2l-1} \left(\frac{\partial^l}{\partial x^l} \tilde{u}^{(6)}(x)\right)^2 dx \tag{16}$$

where $\tilde{u}^{(6)}(x)$ is the Lagrange interpolating polynomials from stencil S_{central} in Figure 1. The integrated form of β_3 is given in Appendix V.A. The linear weights d_k^{central} of Equation (15) are given by:

$$d_0^{\text{central}} = \frac{1}{32}, \quad d_1^{\text{central}} = \frac{15}{32}, \quad d_2^{\text{central}} = \frac{15}{32}, \quad d_3^{\text{central}} = \frac{1}{32} \tag{17}$$

τ_6 is a reference smoothness indicator:

$$\tau_6 = |\beta_3 - \beta_{\text{avg}}| \tag{18}$$

where

$$\beta_{\text{avg}} = \frac{1}{8}\left(\beta_0 + 6\beta_1 + \beta_2\right) \tag{19}$$

R_τ is a relative sensor to distinguish smooth and non-smooth regions and is defined as

$$R_\tau = \frac{\tau_6}{\beta_{\text{avg}} + \epsilon} \tag{20}$$

α_{RL}^{τ} is a constant to determine the cut-off for the hybridization between upwind-biased and central nonlinear weights. $0 \leq \sigma \leq 1$ is a blending function that is close to one in regions near discontinuities and high wavenumber features. In this paper, the following form of σ is used:

$$\sigma_{j+\frac{1}{2}} = \max\left(\sigma_j, \sigma_{j+1}\right) \tag{21}$$

where σ_j is defined as

$$\sigma_j = \frac{\left|\Delta u_{j+\frac{1}{2}} - \Delta u_{j-\frac{1}{2}}\right|}{\left|\Delta u_{j+\frac{1}{2}}\right| + \left|\Delta u_{j-\frac{1}{2}}\right| + \epsilon} \tag{22}$$

$$\Delta u_{j+\frac{1}{2}} = u_{j+1} - u_j \tag{23}$$

$p = 2$, $q = 4$, $C = 1.0e9$ and $\alpha_{RL}^{\tau} = 35.0$ are chosen for WCNS with LD interpolation here. $\epsilon = 1.0e-40$ is a small constant to prevent division by zero. In smooth regions, ω_k approach d_k^{central} so the interpolated value approaches that given by a non-dissipative 6th order linear central interpolation from stencil S_{central}:

$$EI_{\text{central}} = \sum_{k=0}^{3} d_k^{\text{central}} EI_k \tag{24}$$

$$EI_{\text{central}}: \quad \tilde{u}_{j+\frac{1}{2}}^{\text{central}} = \frac{1}{256}\left(3u_{j-2} - 25u_{j-1} + 150u_j + 150u_{j+1} - 25u_{j+2} + 3u_{j+3}\right) \tag{25}$$

The CMD scheme (Equation (2)) with JS, Z and LD interpolations are called WCNS5-JS, WCNS5-Z and WCNS6-LD respectively. The MND scheme (Equation (4)) with the three different interpolations are called MND-WCNS5-JS, MND-WCNS5-Z and MND-WCNS6-LD. The numbers in the names indicate the formal orders of accuracy of the schemes. The difference between the three nonlinear interpolation methods is discussed in Wong et al.[11]

II.C. Weighted compact high resolution (WCHR) scheme

II.C.1. Explicit-compact interpolation (ECI)

WCNS's use explicit interpolations, which typically have more dissipative transfer functions in comparison to compact interpolations. In this sub-section, we propose a new nonlinear explicit-compact interpolation that minimizes the dispersion error by adaptively switching to linear compact interpolation in smooth regions.

Figure 2. Sub-stencils of the WCHR6 scheme. The solid circles represent points used in the right hand side of the compact interpolation stencil, while empty circles represent points used in the left hand side of the interpolation stencil.

Instead of using only explicit interpolations in sub-stencils, the interpolation methods in the central two sub-stencils in Figure 1 are replaced with compact interpolations. The interpolation methods (ECI_k) in the sub-stencils S_0 - S_3 of Figure 2 are given by:

$$ECI_0: \quad \tilde{u}_{j+\frac{1}{2}}^{(0)} = \frac{3}{8}u_{j-2} - \frac{5}{4}u_{j-1} + \frac{15}{8}u_j \tag{26}$$

$$ECI_1: \quad (1-\xi)\,\tilde{u}_{j-\frac{1}{2}}^{(1)} + \xi\tilde{u}_{j+\frac{1}{2}}^{(1)} = \left(-\frac{\xi}{2} + \frac{3}{8}\right)u_{j-1} + \frac{3}{4}u_j + \left(\frac{\xi}{2} - \frac{1}{8}\right)u_{j+1} \tag{27}$$

$$ECI_2: \quad \xi\tilde{u}_{j+\frac{1}{2}}^{(2)} + (1-\xi)\,\tilde{u}_{j+\frac{3}{2}}^{(2)} = \left(\frac{\xi}{2} - \frac{1}{8}\right)u_j + \frac{3}{4}u_{j+1} + \left(-\frac{\xi}{2} + \frac{3}{8}\right)u_{j+2} \tag{28}$$

$$ECI_3: \quad \tilde{u}_{j+\frac{1}{2}}^{(3)} = \frac{15}{8}u_{j+1} - \frac{5}{4}u_{j+2} + \frac{3}{8}u_{j+3} \tag{29}$$

where ξ is a free parameter that can be used to control the dispersion and dissipation characteristics of the scheme. When $\xi = 1$, the explicit-compact interpolations reduce to fully explicit interpolations. In general, S_1 and S_2 in Equations (27) - (28) are third order accurate except for $\xi = 5/8$ when they both become fourth order accurate.

The fifth order linear upwind-biased and sixth order linear central interpolations from S_{upwind} and S_{central}

in Figure 2 respectively can be obtained from linear combinations of the third order interpolations:

$$ECI_{\text{upwind}} = \sum_{k=0}^{2} d_k^{\text{upwind}} ECI_k \tag{30}$$

$$ECI_{\text{central}} = \sum_{k=0}^{3} d_k^{\text{central}} ECI_k \tag{31}$$

where the linear weights are given by:

$$d_0^{\text{upwind}} = \frac{8\xi - 5}{8(\xi+5)}, \quad d_1^{\text{upwind}} = \frac{5(13\xi - 7)}{8(\xi+5)(2\xi-1)}, \quad d_2^{\text{upwind}} = \frac{5(5\xi - 2)}{8(\xi+5)(2\xi-1)} \tag{32}$$

$$d_0^{\text{central}} = \frac{8\xi - 5}{16(\xi+5)}, \quad d_1^{\text{central}} = \frac{45}{16(\xi+5)}, \quad d_2^{\text{central}} = \frac{45}{16(\xi+5)}, \quad d_3^{\text{central}} = \frac{8\xi - 5}{16(\xi+5)} \tag{33}$$

The expanded form of the linear interpolations from S_{upwind} and S_{central} are given by:

$$\begin{aligned} ECI_{\text{upwind}}: \quad & \alpha^{\text{upwind}} \tilde{u}_{j-\frac{1}{2}}^{\text{upwind}} + \beta^{\text{upwind}} \tilde{u}_{j+\frac{1}{2}}^{\text{upwind}} + \gamma^{\text{upwind}} \tilde{u}_{j+\frac{3}{2}}^{\text{upwind}} = \\ & a^{\text{upwind}} u_{j-2} + b^{\text{upwind}} u_{j-1} + c^{\text{upwind}} u_j + d^{\text{upwind}} u_{j+1} + e^{\text{upwind}} u_{j+2} \end{aligned} \tag{34}$$

$$\begin{aligned} ECI_{\text{central}}: \quad & \alpha^{\text{central}} \tilde{u}_{j-\frac{1}{2}}^{\text{central}} + \beta^{\text{central}} \tilde{u}_{j+\frac{1}{2}}^{\text{central}} + \gamma^{\text{central}} \tilde{u}_{j+\frac{3}{2}}^{\text{central}} = \\ & a^{\text{central}} u_{j-2} + b^{\text{central}} u_{j-1} + c^{\text{central}} u_j + d^{\text{central}} u_{j+1} + e^{\text{central}} u_{j+2} + f^{\text{central}} u_{j+3} \end{aligned} \tag{35}$$

where

$$\begin{aligned} \alpha^{\text{upwind}} &= -\frac{5(\xi-1)(13\xi-7)}{8(\xi+5)(2\xi-1)}, & \beta^{\text{upwind}} &= \frac{53\xi - 5}{8(\xi+5)}, & \gamma^{\text{upwind}} &= -\frac{5(\xi-1)(5\xi-2)}{8(\xi+5)(2\xi-1)}, \\ a^{\text{upwind}} &= \frac{3(8\xi-5)}{64(\xi+5)}, & b^{\text{upwind}} &= -\frac{5\left(84\xi^2 - 103\xi + 31\right)}{64(\xi+5)(2\xi-1)}, & c^{\text{upwind}} &= \frac{5\left(68\xi^2 + 11\xi - 25\right)}{64(\xi+5)(2\xi-1)}, \\ d^{\text{upwind}} &= \frac{5\left(52\xi^2 - 11\xi - 5\right)}{64(\xi+5)(2\xi-1)}, & e^{\text{upwind}} &= -\frac{5(4\xi-3)(5\xi-2)}{64(\xi+5)(2\xi-1)} \end{aligned} \tag{36}$$

and

$$\begin{aligned} \alpha^{\text{central}} &= -\frac{45(\xi-1)}{16(\xi+5)}, & \beta^{\text{central}} &= \frac{53\xi - 5}{8(\xi+5)}, & \gamma^{\text{central}} &= -\frac{45(\xi-1)}{16(\xi+5)}, \\ a^{\text{central}} &= \frac{3(8\xi-5)}{128(\xi+5)}, & b^{\text{central}} &= -\frac{5(52\xi-37)}{128(\xi+5)}, & c^{\text{central}} &= \frac{75(2\xi+1)}{64(\xi+5)}, \\ d^{\text{central}} &= \frac{75(2\xi+1)}{64(\xi+5)}, & e^{\text{central}} &= -\frac{5(52\xi-37)}{128(\xi+5)}, & f^{\text{central}} &= \frac{3(8\xi-5)}{128(\xi+5)} \end{aligned} \tag{37}$$

Figure 3 shows the relations between the linear weights of the most upwind stencil S_0 in ECI_{upwind} and ECI_{central} and ξ. For both linear weights to be positive, ξ has to be larger than 5/8.

Even when used with a perfect derivative schemes, the interpolation transfer function creates dispersion and dissipation errors in a linear advection problem. Figures 4 and 5 show the modified wavenumber of ECI_{upwind} and ECI_{central} respectively when used with an analytical derivative scheme. It can be seen that when ξ is decreased from 1 to 5/8, the resolution increases in both ECI's and the dissipation of ECI_{upwind} decreases. It should be noted that the dissipation error of ECI_{central} is always zero independent of value of ξ and the dispersion errors of both ECI_{upwind} and ECI_{central} are the same when $\xi = 1$ or $\xi = 5/8$. We have chosen $\xi = 2/3$ in this paper in order to obtain high resolution but still have sufficient dissipation for stability.

Figure 3. Linear weight of sub-stencil S_0 of ECI_{upwind} and ECI_{central} against ξ. Red dashed line: ECI_{upwind}; blue solid line: ECI_{central}.

(a) Dispersion error

(b) Dissipative error

Figure 4. Modified reduced wavenumber Φ against reduced wavenumber ϕ of ECI_{upwind}. Black solid line with crosses: exact; green dotted line: $\xi = 1$; magenta dashed-dotted line: $\xi = 3/4$; blue solid line: $\xi = 2/3$; red dashed line: $\xi = 5/8$.

Figure 5. Real part of modified reduced wavenumber Φ against reduced wavenumber ϕ of ECI_{central} representing dispersion error. Black solid line with crosses: exact; green dotted line: $\xi = 1$; magenta dashed-dotted line: $\xi = 3/4$; blue solid line: $\xi = 2/3$; red dashed line: $\xi = 5/8$.

II.C.2. Weighted compact high resolution (WCHR) scheme

The finite difference schemes described in Section II.A are unstable near shocks or discontinuities with either ECI_{upwind} or ECI_{central}. Hence, we use a nonlinear combination of the sub-stencil interpolations with the LD nonlinear weights in Equation (10) at any midpoint:

$$ECI_{\text{nonlinear}} = \sum_{k=0}^{3} \omega_k ECI_k \tag{38}$$

The CMD scheme in Equation (2) with the nonlinear explicit-compact interpolation ($ECI_{\text{nonlinear}}$) is sixth order accurate in smooth regions and is called weighted compact high resolution scheme, WCHR6, in this paper due to its high resolution property compared to other WCNS's that is discussed in next section.

The parameters for computing the nonlinear weights in WCNS's and WCHR6 scheme are given in Table 1. For a discussion on choice of parameters in localized dissipative nonlinear weights, see Wong et al.[11] The parameters used here for WCHR6 provide stable results while preserving the high resolution property of the underlying compact interpolation scheme. They are also chosen so that numerical dissipation is only locally added to regions of discontinuity and have minimal effect on regions where the solution is smooth.

Numerical schemes	**Parameter values**				
	p	q	C	α^{τ}_{RL}	ξ
WCNS5-JS	2	–	–	–	–
WCNS5-Z	2	–	–	–	–
WCNS6-LD	2	4	$1.0e9$	35.0	–
WCHR6	2	4	$1.0e10$	55.0	2/3

Table 1. Parameters for different numerical schemes.

II.D. Approximate dispersion relation

For linear schemes, the dissipation and dispersion characteristics can be determined using a dispersion relation analysis discussed by Lele.[12] However, this analysis cannot be used for nonlinear schemes. Pirozzoli[20] therefore developed an approximate dispersion relation (ADR) technique to characterize the dispersion and dissipation characteristics of general nonlinear schemes. Results from ADR analysis are shown in Figure 6 for the WCHR6 scheme and three WCNS's using compact (CMD) and explicit (MND) derivatives. Figure 6(a) shows the dispersion characteristics. In the figure, we can see that the WCHR6 scheme outperforms other schemes in dispersion error. Explicit nonlinear interpolations with CMD in general have higher resolution than those with MND. Figure 7 shows the dispersion errors for WCHR6 and the WCNS's with explicit interpolations and compact derivatives (CMD) on a semi-log plot. Given a threshold ϵ_{res} for the maximum tolerable dispersion error, a resolving efficiency of the different schemes can be computed. The resolving efficiency is defined as the fraction of Nyquist wavenumber that the scheme can resolve within the given dispersion error tolerance ϵ_{res}. In Figure 7, the horizontal black dashed line represents $\epsilon_{\text{res}} = 0.01$ and the vertical colored dashed lines represent the maximum wavenumber that each scheme can resolve given this threshold. Table 2 shows the resolving efficiency for the four different schemes. From the plot, it can be seen that the WCHR6 has much higher resolution ability compared to other schemes of similar orders of accuracy ($\sim$ 46.3% more than the WCNS5-JS). All schemes considered here use CMD as the flux derivative. This shows the need for compact interpolation in order to achieve better resolution characteristics. Figure 6(b) shows the dissipation characteristics of the four schemes. In the plot, we can see that WCNS5-JS and WCNS5-Z have dissipation over a wide range of wavenumber while WCNS6-LD has much more localized dissipation only in high wavenumber range. Due the high resolution characteristic of WCHR6, we choose the parameters in the LD weights such that it has more localized dissipation than WCNS6-LD in the wavenumber space. The high resolution and localized dissipation characteristics of WCHR6 are especially important for problems involving turbulence where low resolution and excessive dissipation can curtail the range of scales in the problem.

(a) Dispersion characteristics

(b) Dissipation characteristics

Figure 6. Approximate dispersion relations (ADR) of different numerical schemes. Black solid line with crosses: spectral; dashed line with cyan circles: MND-WCNS5-JS; solid line with cyan circles: WCNS5-JS; dashed line with red squares: MND-WCNS5-Z; solid line with red squares: WCNS5-Z; dashed line with green diamonds: MND-WCNS6-LD; solid line with green diamonds: WCNS6-LD; solid line with blue triangles: WCHR6.

Figure 7. Approximate dispersion error (derivation of real part of modified reduced wavenumber from that of reduced wavenumber) for different numerical schemes. Solid line with cyan circles: WCNS5-JS; solid line with red squares: WCNS5-Z; solid line with green diamonds: WCNS6-LD; solid line with blue triangles: WCHR6.

Numerical schemes	Resolving efficiency	Improvement over WCNS5-JS
WCNS5-JS	0.291	–
WCNS5-Z	0.361	24.0%
WCNS6-LD	0.361	24.0%
WCHR6	0.426	46.3%

Table 2. Resolving efficiency of different schemes for $\epsilon_{\text{res}} = 0.01$.

II.E. Extension to Euler equations

The inviscid one-dimensional Euler equations are given by

$$\frac{\partial \boldsymbol{Q}}{\partial t} + \frac{\partial \boldsymbol{F}(\boldsymbol{Q})}{\partial x} = 0 \tag{39}$$

where

$$\boldsymbol{Q} = \begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix} \quad \text{and} \quad \boldsymbol{F}(\boldsymbol{Q}) = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ (E+p)\,u \end{pmatrix} \tag{40}$$

where ρ is the density, u is the velocity, E is the total energy and $p = (\gamma - 1)\left(E - \frac{1}{2}\rho u^2\right)$ is the pressure.

The WCNS's or WCHR6 scheme can be applied to the Euler equations in a similar fashion as the scalar conservation law. Equations (2), (3) and (4) can be used to get the flux derivative based on the flux at the nodes $\boldsymbol{F}_j$ and the flux at the midpoints $\tilde{\boldsymbol{F}}_{j+\frac{1}{2}} = \mathbf{F}_{\text{Riemann}}(\tilde{\boldsymbol{Q}}_L, \tilde{\boldsymbol{Q}}_R)$ where $\tilde{\boldsymbol{Q}}_L$ and $\tilde{\boldsymbol{Q}}_R$ are the left and right interpolated solution vectors at the midpoints and $\mathbf{F}_{\text{Riemann}}$ is the flux from a Riemann solver. In this work, we use the HLLC Riemann solver (see Appendix V.B for details on the Riemann solver). The interpolated solution vector at the edges can be computed by directly interpolating the conserved variables or interpolating the primitive variables (ρ, u, p) using the weighted compact interpolation. Although these methods work and provide stable results they are excessively dissipative. A more robust way to perform the interpolation is to interpolate the characteristic variables which exploits the fact that the equations are decoupled in the characteristic space. Interpolating the characteristic variables adds numerical dissipation much more locally around shocks. The characteristic decomposition and interpolation with the WCHR6 scheme is described in the section below.

II.E.1. Characteristic decomposition

For the one-dimensional Euler equation system in primitive form, the three characteristic variables at edge ξ^0, ξ^1 and ξ^2 are given by

$$\begin{pmatrix} \xi^0 \\ \xi^1 \\ \xi^2 \end{pmatrix} = \boldsymbol{A}^{RL} \cdot \begin{pmatrix} \rho \\ u \\ p \end{pmatrix} \tag{41}$$

where $\boldsymbol{A}^{RL}$ is the matrix of the left eigenvectors of the linearized Euler system given by

$$\boldsymbol{A}^{RL} = \begin{pmatrix} 0 & -\frac{\rho c}{2} & \frac{1}{2} \\ 1 & 0 & -\frac{1}{c^2} \\ 0 & \frac{\rho c}{2} & \frac{1}{2} \end{pmatrix} \tag{42}$$

where $c = \sqrt{\gamma p/\rho}$ is the speed of sound in the medium.

At a midpoint $j + 1/2$, the characteristic variables for the whole stencil are computed using the same left eigenvector matrix $\boldsymbol{A}^{RL}_{j+\frac{1}{2}}$ given by the Roe average of the matrix at node j and $j+1$ to maintain consistency between the transforms to and back from the characteristic space:

$$\alpha^l_{j+\frac{1}{2}}\tilde{\xi}^l_{j-\frac{1}{2}} + \beta^l_{j+\frac{1}{2}}\tilde{\xi}^l_{j+\frac{1}{2}} + \gamma^l_{j+\frac{1}{2}}\tilde{\xi}^l_{j+\frac{3}{2}} = a^l_{j+\frac{1}{2}}\xi^l_{j-2} + b^l_{j+\frac{1}{2}}\xi^l_{j-1} + c^l_{j+\frac{1}{2}}\xi^l_j$$
$$+d^l_{j+\frac{1}{2}}\xi^l_{j+1} + e^l_{j+\frac{1}{2}}\xi^l_{j+2} + f^l_{j+\frac{1}{2}}\xi^l_{j+3}, \quad l = 0, 1, 2 \tag{43}$$

where $\alpha^l_{j+\frac{1}{2}}$, $\beta^l_{j+\frac{1}{2}}$, $\gamma^l_{j+\frac{1}{2}}$, $a^l_{j+\frac{1}{2}}$, $b^l_{j+\frac{1}{2}}$, $c^l_{j+\frac{1}{2}}$, $d^l_{j+\frac{1}{2}}$, $e^l_{j+\frac{1}{2}}$ and $f^l_{j+\frac{1}{2}}$ are the coefficients obtained from the nonlinear explicit-compact interpolation method described in Equation (38). However, the above equation cannot be solved in the form presented since the interpolated characteristic variables are coupled across grid points due to the compact nature of the interpolation and solving it in this form would introduce a consistency error since each stencil uses a different characteristic matrix for the decomposition. A solution is to write the above equation in terms of the primitive variables at the cell nodes $\boldsymbol{V} = (\rho, u, p)^T$ and the midpoint interpolated primitive variables $\tilde{\boldsymbol{V}} = (\tilde{\rho}, \tilde{u}, \tilde{p})^T$ as

$$\boldsymbol{\alpha}_{j+\frac{1}{2}}\boldsymbol{A}^{RL}_{j+\frac{1}{2}} \cdot \tilde{\boldsymbol{V}}_{j-\frac{1}{2}} + \boldsymbol{\beta}_{j+\frac{1}{2}}\boldsymbol{A}^{RL}_{j+\frac{1}{2}} \cdot \tilde{\boldsymbol{V}}_{j+\frac{1}{2}} + \boldsymbol{\gamma}_{j+\frac{1}{2}}\boldsymbol{A}^{RL}_{j+\frac{1}{2}} \cdot \tilde{\boldsymbol{V}}_{j+\frac{3}{2}} = \boldsymbol{a}_{j+\frac{1}{2}}\boldsymbol{A}^{RL}_{j+\frac{1}{2}} \cdot \boldsymbol{V}_{j-2} + \boldsymbol{b}_{j+\frac{1}{2}}\boldsymbol{A}^{RL}_{j+\frac{1}{2}} \cdot \boldsymbol{V}_{j-1}$$
$$+\boldsymbol{c}_{j+\frac{1}{2}}\boldsymbol{A}^{RL}_{j+\frac{1}{2}} \cdot \boldsymbol{V}_j + \boldsymbol{d}_{j+\frac{1}{2}}\boldsymbol{A}^{RL}_{j+\frac{1}{2}} \cdot \boldsymbol{V}_{j+1} + \boldsymbol{e}_{j+\frac{1}{2}}\boldsymbol{A}^{RL}_{j+\frac{1}{2}} \cdot \boldsymbol{V}_{j+2} + \boldsymbol{f}_{j+\frac{1}{2}}\boldsymbol{A}^{RL}_{j+\frac{1}{2}} \cdot \boldsymbol{V}_{j+3} \tag{44}$$

where $\boldsymbol{\alpha}_{j+\frac{1}{2}}$, $\boldsymbol{\beta}_{j+\frac{1}{2}}$, $\boldsymbol{\gamma}_{j+\frac{1}{2}}$, $\boldsymbol{a}_{j+\frac{1}{2}}$, $\boldsymbol{b}_{j+\frac{1}{2}}$, $\boldsymbol{c}_{j+\frac{1}{2}}$, $\boldsymbol{d}_{j+\frac{1}{2}}$, $\boldsymbol{e}_{j+\frac{1}{2}}$ and $\boldsymbol{f}_{j+\frac{1}{2}}$ are diagonal matrices with the diagonal entries representing the coefficents obtained using the non-linear weighting procedure for the corresponding characteristic variable. With the characteristic decomposition, the interpolation reduces to one block tri-diagonal system of equations instead of three tri-diagonal systems of equations if only the primitive variables are interpolated.

Figure 8 shows the matrix structure for the left biased characteristic based weighted compact interpolation for the initial conditions of the Shu-Osher problem (Section III.D) with 80 points in the domain. Since the matrix is a block tri-diagonal system, the size of the matrix is 240×240 and the full matrix structure is shown in Figure 8(a). Figure 8(b) shows the first 50×50 portion of the interpolation matrix. Here, we see that across the shock at index ~ 24, the matrix decouples. This means that the interpolation stencil never crosses the shock. Additionally, the point closest to the shock has just one block in it's row indicating that the non-linear weighting procedure picked solely the most upwind stencil at the shock which is purely explicit. Figure 9 shows the left and right interpolated density, velocity and pressure. Since the interpolation stencil never crosses the shock, the interpolation is virtually perfect and no spurious oscillations are observed.

(a) Full (b) Top 50×50 portion

Figure 8. Block tri-diagonal matrix structure for the characteristic decomposition in left-biased interpolation for initial condition of the Shu-Osher problem with 80 points. The top portion of the matrix shows that the interpolation is decoupled across the shock.

The method can be easily extended from one spatial dimension to multi-dimensional problems by applying the algorithm along each spatial dimension to get the flux derivatives in that direction. For the three dimensional Euler equations

$$\frac{\partial \boldsymbol{Q}}{\partial t} + \frac{\partial \boldsymbol{F}(\boldsymbol{Q})}{\partial x} + \frac{\partial \boldsymbol{G}(\boldsymbol{Q})}{\partial y} + \frac{\partial \boldsymbol{H}(\boldsymbol{Q})}{\partial z} = 0 \tag{45}$$

(a) Density (b) Velocity (c) Pressure

Figure 9. Interpolated values of primitive variables from initial conditions of the Shu-Osher problem with 80 points. Black circles: node values; blue upper triangles: left interpolated midpoint values; red lower triangles: right interpolated midpoint values

the flux derivatives $\frac{\partial \boldsymbol{F}(\boldsymbol{Q})}{\partial x}$ are obtained using the algorithm outlined above in the x direction and similarly for the flux derivatives $\frac{\partial \boldsymbol{G}(\boldsymbol{Q})}{\partial y}$ and $\frac{\partial \boldsymbol{H}(\boldsymbol{Q})}{\partial z}$ in the other directions.

II.F. Discretization of viscous and diffusive fluxes for Navier-Stokes equations

The compressible Navier-Stokes equations are given by:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0$$
$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}\boldsymbol{u} + p\boldsymbol{\delta} - \boldsymbol{\tau}) = 0$$
$$\frac{\partial E}{\partial t} + \nabla \cdot [(E+p)\,\boldsymbol{u}] - \nabla \cdot (\boldsymbol{\tau} \cdot \boldsymbol{u} - \boldsymbol{q_c}) = 0$$

where $\boldsymbol{u} = (u, v, w)^T$ is the velocity vector. $\boldsymbol{\tau}$ and $\boldsymbol{q_c}$ are viscous stress tensor and conductive heat flux respectively. $\boldsymbol{\delta}$ is an identity matrix.
The viscous stress tensor $\boldsymbol{\tau}$ for a Newtonian fluid is

$$\tau = 2\mu \boldsymbol{S} + \left(\mu_v - \frac{2}{3}\mu\right) \boldsymbol{\delta}\,(\nabla \cdot \boldsymbol{u})$$

where μ, μ_v and $\boldsymbol{S}$ are the shear viscosity, bulk viscosity and strain-rate tensor respectively.
The conductive flux is given by:

$$\boldsymbol{q_c} = -\kappa \nabla T$$

where κ is the thermal conductivity.

The sixth order node-to-node compact finite difference scheme by Lele[12] in following form is used to compute viscous and diffusive fluxes:

$$\frac{1}{5}F'_{j-1} + \frac{3}{5}F'_j + \frac{1}{5}F'_{j+1} = \frac{1}{\Delta x}\left[\frac{7}{15}\left(F_{j+1} - F_{j-1}\right) + \frac{1}{60}\left(F_{j+2} - F_{j-2}\right)\right] \tag{46}$$

F_j at cell nodes contain first-order derivative and are computed using the same compact finite difference scheme.

III. Numerical Results

In this section, we present results using WCNS5-JS, WCNS5-Z, WCNS6-LD and WCHR6 schemes in different test problems. All tests are inviscid except the compressible homogeneous isotropic turbulence case where the compressible Navier-Stokes equations are used. In all the one-dimensional problems, the equations are integrated in time using a five-stage fourth order strong stability preserving Runge-Kutta scheme (SSP-RK54).[21] All other results in multi-dimensional spatial domains are obtained using the low-storage five-stage fourth order Runge-Kutta time integrator[22] to save memory cost.

III.A. Convergence test

The first problem is the advection of a sinusoidal entropy wave in a one-dimensional periodic domain $x \in [-1, 1)$. The initial conditions are given by

$$(\rho, u, p) = (1 + 0.5 \sin(\pi x), 1, 1)$$

Since the velocity and pressure are constant and only an entropic disturbance is present, the problem reduces to a linear advection of the entropy wave. Therefore, the exact solution is given by

$$(\rho, u, p) = (1 + 0.5 \sin(\pi (x - t)), 1, 1)$$

The ratio of specific heats γ is 1.4. The simulations using different schemes are conducted up to $t = 2$ with mesh refinements from $N = 4$ to $N = 128$. All simulations are run with very small constant time steps in order to observe the spatial order of accuracy of different numerical schemes. $\Delta t/\Delta x = 0.02$ is chosen for all simulations.

From Table 3 and Figure 10, we can see that all schemes can achieve their formal orders of accuracy when the number of points is large enough. Although both WCNS6-LD and WCHR6 are sixth order accurate, the latter scheme is more accurate than the former with errors that are $\sim 4 - 5$ times smaller.

Number	WCNS5-JS		WCNS5-Z		WCNS6-LD		WCHR6	
of points	error	order	error	order	error	order	error	order
4	4.1289e-1		3.5192e-1		1.6424e-1		6.2582e-2	
8	4.2324e-2	3.29	1.1778e-2	4.90	3.4076e-3	5.59	8.9641e-4	6.13
16	2.7638e-3	3.94	3.4688e-4	5.09	5.6967e-5	5.90	1.3666e-5	6.04
32	8.9388e-5	4.95	1.0718e-5	5.02	9.0502e-7	5.98	2.1216e-7	6.01
64	2.6945e-6	5.05	3.3540e-7	5.00	1.4193e-8	5.99	3.3085e-9	6.00
128	8.2260e-8	5.03	1.0488e-8	5.00	2.2203e-10	6.00	5.2279e-11	5.98

Table 3. L_2 **error and order of convergence from difference schemes for the density at** $t = 2$**.**

Figure 10. L_2 **error against number of points** (N) **in convergence test of different schemes. Cyan circles: WCNS5-JS; red squares: WCNS5-Z; green diamonds: WCNS6-LD; blue triangles: WCHR6; dashed-dotted line: fifth-order; dashed line: sixth-order**

III.B. Advection of broadband disturbances

This problem is similar to the earlier one but with the density field of a uniform flow being disturbed by a broadband signal instead of a single mode. The initial conditions are given by

$$\begin{pmatrix} \rho \\ u \\ p \end{pmatrix} = \begin{pmatrix} 1 + \delta \sum_{k=1}^{N/2} \left(E_\rho(k)\right)^{1/2} sin\left(2\pi k \left(x + \psi_k\right)\right) \\ 1 \\ 1 \end{pmatrix}$$

where ψ_k is a random number between 0 and 1 with uniform distribution, $\delta = 1.0e-2$ and the ratio of specific heats γ is 1.4. The density spectrum $E_\rho(k)$ is given by

$$E_\rho(k) = \left(\frac{k}{k_0}\right)^4 \exp(-2\left(\frac{k}{k_0}\right)^2)$$

We have chosen $k_0 = 12$. The computational domain is periodic with size $x \in [0, 1)$. The simulations are run with $N = 128$ and $\Delta t = 0.002$ until $t = 1$.

(a) Global density profile

(b) Spectrum of density disturbances

Figure 11. Advection of density disturbances problem at $t = 1.0$ using different schemes. Black solid line: exact; cyan circles: WCNS5-JS; red squares: WCNS5-Z; green diamonds: WCNS6-LD; blue triangles: WCHR6.

The density solutions from various schemes after one period are shown in Figure 11(a). Figure 11(b) compares the spectra of the density disturbance from different schemes. We see that both WCNS5-JS and WCNS5-Z are too dissipative to preserve the initial spectrum due to their upwind nature. WCNS6-LD preserves the initial spectrum better, but still has some deviations from the prescribed spectrum. WCHR6 preserves the initial spectrum virtually perfectly. Unlike the WCNS's almost no errors due to the nonlinear nature of the scheme are seen. This is attributed to its higher resolution characteristics.

III.C. Sod shock tube problem

This is a one-dimensional shock tube problem introduced by Sod.[23] The problem consists of the propagation of a shock wave, a contact discontinuity and an expansion fan. The initial conditions are

$$(\rho, u, p) = \begin{cases} (1, 0, 1)\,, & x < 0 \\ (0.125, 0, 0.1)\,, & x \geq 0 \end{cases}$$

The ratio of specific heats γ is 1.4. The computational domain has size $x \in [-0.5, 0.5]$. Simulations are performed with constant time steps $\Delta t = 0.002$ on a uniform grid composed of 100 grid points where $\Delta x = 0.01$.

Comparison between the exact solution and the numerical solution for the density at $t = 0.2$ is shown in Figure 12. It can be seen that all of the schemes can capture the shock well. WCHR6 and WCNS6-LD have sharper profiles at the shock in comparison to WCNS5-JS and WCNS5-Z.

III.D. Shu-Osher problem

This one-dimensional problem first proposed by Shu and Osher[24] involves the interaction of a Mach 3 shock wave with an entropy wave. The interaction creates a high wavenumber entropy wave and a nonlinear acoustic wave that steepens and forms a shock train. This problem can hence assess the ability of a scheme to capture discontinuities well, while also retaining the smooth features of the solution. The initial conditions

(a) Global density profile

(b) Local density profile

Figure 12. Sod shock tube problem at $t = 0.2$ using different schemes. Black solid line: exact; cyan circles: WCNS5-JS; red squares: WCNS5-Z; green diamonds: WCNS6-LD; blue triangles: WCHR6.

are given by

$$(\rho, u, p) = \begin{cases} (3.857143, 2.62936, 10.33339)\,, & x < -4 \\ (1 + 0.2\sin(5x), 0, 1)\,, & x \geq -4 \end{cases}$$

The ratio of specific heats γ is 1.4. The spatial domain of the problem is $x \in [-5, 5]$. Simulations are conducted with constant time steps $\Delta t = 0.005$ on a uniform grid with 150 grid points and also with constant time steps $\Delta t = 0.004$ on a uniform grid with 200 grid points. A reference solution is computed using the WCNS6-LD scheme with 2000 points and time step of $\Delta t = 0.0002$. All results shown here are at time $t = 1.8$.

Figures 13 and 14 show the density profile at $t = 1.8$ obtained using various schemes compared to the reference solution with the two different grid resolutions. Both WCNS5-JS and WCNS5-Z dissipate the high wavenumber entropy wave significantly which is not seen in the results from the WCNS6-LD and WCHR6 schemes. Figure 13(b) shows that WCHR6 has less dispersion error around the region where the entropy wave and weak shock interacts from the results with 150 points due to the higher resolution characteristics of WCHR6.

(a) Global density profile

(b) Local density profile

Figure 13. Shu-Osher problem at $t = 0.2$ using different schemes with $\Delta x = 1/15$. Black solid line: reference; cyan circles: WCNS5-JS; red squares: WCNS5-Z; green diamonds: WCNS6-LD; blue triangles: WCHR6.

(a) Global density profile

(b) Local density profile

Figure 14. Shu-Osher problem at $t = 0.2$ using different schemes with $\Delta x = 0.05$. Black solid line: reference; cyan circles: WCNS5-JS; red squares: WCNS5-Z; green diamonds: WCNS6-LD; blue triangles: WCHR6.

III.E. Two-dimensional shock-vortex interaction

This two-dimensional shock-vortex interaction problem was studied previously in several papers.[25–27] The inviscid version of this problem is studied here which consists of a stationary Mach 1.2 shock and a strong vortex characterized by the vortex Mach number M_v initially in the pre-shock region. The initial configuration and computation domain are shown in Figure 15. The shock is at $x = 0$ and the vortex is located upstream of the shock at $(x_v, y_v) = (4, 0)$ initially. The initial conditions of the vortex are given by

$$\begin{pmatrix} \rho \\ p \\ \delta u \\ \delta v \end{pmatrix} = \begin{pmatrix} \left(1 - \frac{1}{2}(\gamma - 1) M_v^2 e^{1-(r/R)^2}\right)^{\frac{1}{\gamma-1}} \\ \frac{1}{\gamma}\left(1 - \frac{1}{2}(\gamma - 1) M_v^2 e^{1-(r/R)^2}\right)^{\frac{\gamma}{\gamma-1}} \\ -M_v e^{\frac{1}{2}(1-(r/R)^2)}(y - y_v) \\ M_v e^{\frac{1}{2}(1-(r/R)^2)}(x - x_v) \end{pmatrix}$$

$M_v = 1.0$ and vortex radius $R = 1.0$ are chosen in this paper. The ratio of specific heats $\gamma = 1.4$ is used. The problem domain is chosen to be $[-D, D) \times [-D/2, D/2)$, where $D = 40$. The shock is initialized at $x = 0$ and an expansion wave of equal strength is initialized at $x = 40$ so that periodic boundary conditions can be used in both x and y directions. For the times considered here, the expansion does not interact with any of the flow features investigated. A 2D grid with 1024×512 points is used for all the schemes. All cases in this section are run with CFL $= 0.5$.

Figure 15. Schematic diagram of initial flow field and computational domain of 2D shock-vortex interaction problem.

Figure 16 shows the pressure contours at $t = 6$ for the four different schemes. At this time instant,

(a) WCNS5-JS

(b) WCNS5-Z

(c) WCNS6-LD

(d) WCHR6

Figure 16. Contours of pressure in the shock-vortex interaction problem on a 1024×512 grid at $t = 6$.

the vortex has passed through the nominal shock plane, but its interaction with the shock leads to several curved and highly deformed shock structures. WCNS5-JS and WCNS5-Z are dissipative but yield essentially non-oscillatory solutions. WCNS6-LD and WCHR6 are less dissipative and have sharper features. However, they both have some mild oscillations at the radial shock front.

(a) WCNS5-JS

(b) WCNS5-Z

(c) WCNS6-LD

(d) WCHR6

Figure 17. Contours of sound pressure defined by $(p - p_\infty) / (\rho_\infty c_\infty^2)$ in a problem with a $M_s = 1.2$ shock interacting with a strong vortex with vortex Mach number $M_v = 1$ on a 1024×512 grid at $t = 16$. The black dashed line in (a) shows the line used to get the radial sound pressure profile plotted in Figure 18.

Figure 17 shows the sound pressure contours defined as $(p - p_\infty) / (\rho_\infty c_\infty^2)$ at $t = 16$ for the four different schemes. Here, the $(\cdot)_\infty$ quantities are all taken to be the post-shock values. The vortex, having passed through the shock gets deformed and as a result we see a quadrupole sound signature. However, since the vortex strength is very high, many weak shock waves are generated and propagate radially outward. Again, from Figure 17, we see that WCNS5-JS and WCNS5-Z are more dissipative and damp the fine scale structures of the sound field. WCNS6-LD and WCHR6 are less dissipative and have more fine-scale features. Figure 18 shows the sound pressure on a radial line from the center of the vortex with an angle of $\phi = -45°$ (see Figure 15) for the four schemes considered here and a reference solution obtained using the WCNS5-Z on a grid with eight times the number of points in each direction. Figure 18(a) plots a global view of the radial sound pressure profile and all schemes seem to overlap with the reference solution at this scale. Figure 18(b) shows a local view of the outgoing shock front at $r \approx 14.5$. Here we see that WCHR6 and WCNS6-LD overshoot the peak sound pressure while the WCNS5-JS and WCNS5-Z under-predict the peak sound pressure level. Figure 18(c) shows a local view of the radial sound pressure profile around $r = 7.5$. Here, the local peak of the sound pressure profile in the reference solution is not captured by any of the

WCNS's while the WCHR6 scheme is able to capture the peak owing to its higher resolution property.

(a) (b) (c)

Figure 18. Sound pressure defined by $(p - p_\infty) / (\rho_\infty c_\infty^2)$ for the shock vortex interaction problem at $t = 16$ on a radial line centered at the vortex core with $\theta = -45^\circ$ as indicated by the black dashed line in Figure 17(a). Black solid line: reference; cyan circles: WCNS5-JS; red squares: WCNS5-Z; green diamonds: WCNS6-LD; blue triangles: WCHR6.

III.F. Taylor-Green vortex

The three-dimensional inviscid Taylor-Green vortex problem is a popular test case used to compare the numerical dissipation of different schemes and has been used widely in previous literature.[6,28] The initial conditions of the problem are given by

$$\begin{pmatrix} \rho \\ u \\ v \\ w \\ p \end{pmatrix} = \begin{pmatrix} 1 \\ \sin x \cos y \cos z \\ -\cos x \sin y \cos z \\ 0 \\ 100 + \frac{(\cos(2z)+2)(\cos(2x)+\cos(2y))-2}{16} \end{pmatrix}$$

The ratio of specific heats of the gas is $\gamma = 5/3$. The domain is periodic with size $[0, 2\pi)^3$. The problem is solved with the four schemes considered here on a 32^3 and a 64^3 grid. Simulations are conducted until $t = 10$ with a constant CFL $= 0.6$.

As the mean pressure is chosen to be very large compared to the dynamic pressure, the flow problem is essentially incompressible. Thus, the kinetic energy of the flow is conserved in the inviscid limit and the problem can be used as a test to examine the dissipative property of different schemes. As time evolves, the initial flow gets stretched and energy is transferred from larger to finer scales.

Figure 19 plots the mean kinetic energy ($\frac{1}{2}\langle \rho u_i u_i \rangle$) and enstrophy ($\langle \omega_i \omega_i \rangle$) normalized by their respective initial values on a 32^3 grid. The $\langle \cdot \rangle$ operator indicates averaging in space. Here, we see that WCHR6 is the least dissipative and retains the largest amount of the kinetic energy at $t = 10$. Both upwind biased schemes (WCNS5-JS and WCNS5-Z) are more dissipative than the hybrid central-upwind schemes (WCHR6 and WCNS6-LD). Similar trends can also been seen in the enstrophy plot. WCHR6 captures significantly larger amount of enstrophy compared to WCNS6-LD while the upwind biased schemes are very dissipative and deviate from the semi-analytical solution of Brachet et. al.[29] much earlier than the hybrid central-upwind schemes. Figure 20 plots the kinetic energy and enstrophy for the four schemes on a 64^3 grid and show the same trends as in Figure 19 with WCHR6 being the least dissipative and capturing significantly more enstrophy than the WCNS's. It can be noted that with the increased resolution the schemes WCHR6 and WCNS6-LD results are close to the semi-analytical result over a larger time interval.

Figure 21 compares the velocity and vorticity spectra of various schemes on a 64^3 grid. The velocity spectrum is much more revealing than the mean kinetic energy plot. WCHR6 is the least dissipative since it is able to preserve more high wavenumber features while the other schemes dissipate the high wavenumber content more aggressively. WCHR6 and WCNS6-LD agree well until $k \approx 8$. For $k > 8$, WCNS6-LD starts becoming more dissipative. WCNS5-JS and WCNS5-Z start adding dissipation from $k \approx 4$. The vorticity spectrum highlights the high wavenumber content more. From the vorticity spectrum, we again see that WCHR6 has much more energy in the high wavenumber region compared to the WCNS's.

(a) Kinetic energy

(b) Enstrophy

Figure 19. Time evolution of statistical quantities for Taylor-Green vortex problem on a 32^3 grid. Black dashed line : exact; Black crosses: semi-analytical result; cyan circles: WCNS5-JS; red squares: WCNS5-Z; green diamonds: WCNS6-LD; blue triangles: WCHR6.

(a) Kinetic energy

(b) Enstrophy

Figure 20. Time evolution of statistical quantities for Taylor-Green vortex problem on a 64^3 grid. Black dashed line : exact; Black crosses: semi-analytical result; cyan circles: WCNS5-JS; red squares: WCNS5-Z; green diamonds: WCNS6-LD; blue triangles: WCHR6.

(a) Velocity energy spectrum

(b) Vorticity energy spectrum

Figure 21. Spectra at $t = 8$ for Taylor-Green vortex problem on a 64^3 grid. Cyan circles: WCNS5-JS; red squares: WCNS5-Z; green diamonds: WCNS6-LD; blue triangles: WCHR6.

III.G. Compressible homogeneous isotropic turbulence

A more realistic and suitable test case for shock-capturing schemes than the Taylor-Green vortex problem is the decaying compressible homogeneous isotropic turbulence problem.[28,30] This is a viscous test case with the initial RMS velocity fluctuation being large enough to create eddy shocklets[30] that serves as a good problem to test the ability of numerical methods to capture shocks while also examine their dissipation characteristics for turbulence.

The initial velocity profile is a random solenoidal field that has an energy spectrum

$$E(k) \propto k^4 \exp\left(-2\left(\frac{k}{k_0}\right)^2\right)$$

where k_0 is the most energetic wavenumber and the RMS velocity fluctuation $u_{\text{rms}} = \frac{\langle u_i u_i \rangle}{3} = \frac{2}{3}\int_0^\infty E(k)\mathrm{d}k$. This gives an initial Taylor scale $\lambda_0 = 2/k_0$. Details in obtaining the initial velocity profiles can be found in Johnsen et. al.[28]

The two important parameters in this problem are the turbulent Mach number $M_t = \frac{\sqrt{3}u_{\text{rms}}}{\langle c \rangle}$ and the Taylor scale Reynolds number $\text{Re}_\lambda = \frac{\langle \rho \rangle u_{\text{rms}} \lambda}{\langle \mu \rangle}$. In this section, we consider the problem with $M_t = 0.6$, $\text{Re}_\lambda = 100$ and $k_0 = 4$. The density and pressure fields are taken to be constant initially.

The shear viscosity is assumed to follow a power law temperature dependence given by

$$\frac{\mu}{\mu_{\text{ref}}} = \left(\frac{T}{T_{\text{ref}}}\right)^{\frac{3}{4}}$$

and the bulk viscosity is assumed to be zero. Ratio of specific heats $\gamma = 1.4$ and a constant Prandtl number $\text{Pr} = 0.7$ are used. The domain is periodic with size $[0, 2\pi)^3$. The problem is solved on a 64^3 grid with the four schemes considered in this work. A reference solution obtained from a DNS dataset spectrally filtered to a 64^3 grid[28] is used for comparison. Simulations are run with a constant CFL $= 0.5$ until $t/\tau = 4$ where τ is the eddy turnover time given by $\tau = \lambda_0/u_{\text{rms},0}$.

Figure 22 shows the velocity variance, enstrophy and dilatation variance as a function of time for the four schemes and the filtered DNS solution.[28] Here, we see that WCHR6 is the least dissipative and is the closest to the filtered DNS profiles for all the three statistics plotted. The enstrophy profiles highlight the difference between the schemes. WCNS5-JS and WCNS5-Z are excessively dissipative and capture very little amount of the enstrophy. WCHR6 agrees the best with the filtered DNS solution and shows that it is minimally dissipative even in the presence of eddy shocklets. Similar trends are seen in the plot of the dilatation variance. WCHR6 agrees very well with the filtered DNS solution while the other schemes dissipate dilatational motions more.

(a) Velocity variance

(b) Enstrophy

(c) Dilatation variance

Figure 22. Time evolution of statistical quantities for compressible homogeneous isotropic turbulence on a 64^3 grid with $M_t = 0.6$. Black circles : spectrally filtered DNS data of Johnsen et. al.;[28] cyan circles: WCNS5-JS; red squares: WCNS5-Z; green diamonds: WCNS6-LD; blue triangles: WCHR6.

(a) Velocity energy spectrum

(b) Vorticity energy spectrum

(c) Dilatation energy spectrum

(d) Density energy spectrum

Figure 23. Spectra at $t/\tau = 2$ for compressible homogeneous isotropic turbulence on a 64^3 grid with $M_t = 0.6$. Cyan circles: WCNS5-JS; red squares: WCNS5-Z; green diamonds: WCNS6-LD; blue triangles: WCHR6.

(a) Isotropic velocity spectrum

(b) Isotropic vorticity spectrum

(c) Isotropic dilatation spectrum

(d) Isotropic density spectrum

Figure 24. Spectra at $t/\tau = 4$ for compressible homogeneous isotropic turbulence on a 64^3 grid with $M_t = 0.6$. Cyan circles: WCNS5-JS; red squares: WCNS5-Z; green diamonds: WCNS6-LD; blue triangles: WCHR6.

Figures 23 and 24 show the velocity, vorticity, dilatation and density spectra for the four different schemes. Similar to the Taylor-Green vortex case, it can be seen that WCHR6 is the best at capturing the fine scale features in both vorticity and dilatation while the upwind biased schemes are more dissipative.

IV. Conclusions

In summary, we have developed a new sixth order accurate weighted compact high resolution (WCHR6) scheme that has higher resolution and more localized dissipation than WCNS's in previous literature. The scheme is presented for use with conservation equations such as the Euler equations and compressible Navier-Stokes equations in one, two and three dimensions. The block tri-diagonal characteristic decomposition method is shown to be effective at interpolating primitive variables across shocks. Approximate dispersion relation (ADR) analysis of the scheme shows the superior resolution ability of the scheme compared to other WCNS's of similar orders of accuracy. Sixth order of accuracy of the scheme was demonstrated for the advection of an entropy wave. For all the test problems, the WCHR6 scheme was compared with WCNS's that utilized the same compact finite difference scheme but different interpolation methods to highlight the benefit of the new compact non-linear interpolation method. The advection of a broadband entropy wave showed that the WCHR6 scheme was better than the WCNS's at preserving the spectral features of the solution. The 1D Sod shock tube problem and Shu-Osher problem showed the ability of the method to capture shocks robustly while localizing the dissipation to regions near shocks. The WCHR6 scheme was shown to have much better dispersion and dissipation characteristics compared to the other schemes considered. The 2D shock interaction with a strong vortex showed the ability of the scheme to capture shocks with complex structures and large pressure variations. The 3D Taylor-Green problem highlighted the minimal dissipation characteristic of the scheme for a 3D problem with a large range of scales. Finally, the compressible homogeneous isotropic turbulence test case showed that the WCHR6 scheme was capable of capturing eddy shocklets randomly distributed in the turbulent field while still being minimally dissipative for both the solenoidal and dilatational motions. Appropriate boundary closures and efficient algorithms for the characteristic interpolation will be the focus of future work.

V. Appendices

V.A. Integrated forms of smoothness indicators

The integrated forms of the smoothness indicators are given by Liu et al.:[10]

$$\beta_0 = \frac{1}{3}\left[u_{j-2}\left(4u_{j-2} - 19u_{j-1} + 11u_j\right) + u_{j-1}\left(25u_{j-1} - 31u_j\right) + 10u_j^2\right], \tag{47}$$

$$\beta_1 = \frac{1}{3}\left[u_{j-1}\left(4u_{j-1} - 13u_j + 5u_{j+1}\right) + 13u_j\left(u_j - u_{j+1}\right) + 4u_{j+1}^2\right], \tag{48}$$

$$\beta_2 = \frac{1}{3}\left[u_j\left(10u_j - 31u_{j+1} + 11u_{j+2}\right) + u_{j+1}\left(25u_{j+1} - 19u_{j+2}\right) + 4u_{j+2}^2\right] \tag{49}$$

$$\begin{aligned}\beta_3 = \frac{1}{232243200}\big[&u_{j-2}\left(525910327u_{j-2} - 4562164630u_{j-1} + 7799501420u_j\right.\\ &\left.-6610694540u_{j+1} + 2794296070u_{j+2} - 472758974u_{j+3}\right)\\ &+5u_{j-1}\left(2146987907u_{j-1} - 7722406988u_j + 6763559276u_{j+1} - 2926461814u_{j+2} + 503766638u_{j+3}\right)\\ &+20u_j\left(1833221603u_j - 3358664662u_{j+1} + 1495974539u_{j+2} - 263126407u_{j+3}\right)\\ &+20u_{j+1}\left(1607794163u_{j+1} - 1486026707u_{j+2} + 268747951u_{j+3}\right)\\ &+5u_{j+2}\left(1432381427u_{j+2} - 536951582u_{j+3}\right) + 263126407u_{j+3}^2\big]\end{aligned} \tag{50}$$

V.B. HLLC Riemann solver

The flux from HLLC Riemann solver $\mathbf{F}_{\text{HLLC}}$ is used as the midpoint flux $\tilde{\boldsymbol{F}}$.

$$\mathbf{F}_{\text{HLLC}} = \frac{1+\text{sign}(s_*)}{2}\left[\mathbf{F}(\tilde{\boldsymbol{Q}}_L) + s_-\left(\mathbf{Q}_{*L} - \tilde{\boldsymbol{Q}}_L\right)\right] + \frac{1-\text{sign}(s_*)}{2}\left[\mathbf{F}(\tilde{\boldsymbol{Q}}_R) + s_+\left(\mathbf{Q}_{*R} - \tilde{\boldsymbol{Q}}_R\right)\right] \tag{51}$$

where L, R are the left and right states respectively. With $K = L$ or R, the star state is defined as

$$\mathbf{Q}_{*K} = \chi_{*K} \begin{bmatrix} \rho_K \\ \rho_K s_* \\ E_k + (s_* - u_K)\left(\rho_K s_* + \frac{p_K}{s_K - u_K}\right) \end{bmatrix} \tag{52}$$

where

$$\chi_{*K} = \frac{s_K - u_K}{s_K - s_*} \tag{53}$$

We use the waves speeds suggested by Einfeldt et al.:[31]

$$s_- = \min(0, s_L), \quad s_+ = \max(0, s_R) \tag{54}$$

and

$$s_L = \min(\bar{u} - \bar{c}, u_L - c_L), \quad s_R = \max(\bar{u} + \bar{c}, u_R + c_R) \tag{55}$$

where $\bar{u}$ and $\bar{c}$ are the averages from the left and right states. Roe averages are used in this paper. Following Batten et al.,[32] the wave speed for the star state is:

$$s_* = \frac{p_R - p_L + \rho_L u_L (s_L - u_L) - \rho_R u_R (s_R - u_R)}{\rho_L (s_L - u_L) - \rho_R (s_R - u_R)} \tag{56}$$

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