Hybrid Compact-WENO Finite Difference Scheme For Detonation Waves Simulations

Yanpo Niu, Zhen Gao, Wai Sun Don, Shusen Xie, and Peng Li

Abstract The performance of a hybrid compact (Compact) finite difference scheme and characteristic-wise weighted essentially non-oscillatory (WENO) finite difference scheme (Hybrid) for the detonation waves simulations is investigated. The Hybrid scheme employs the nonlinear $5th$-order WENO-Z scheme to capture high gradients and discontinuities in an essentially non-oscillatory manner and the linear $6th$-order Compact scheme to resolve the fine scale structures in the smooth regions of the solution in an efficient and accurate manner. Numerical oscillations generated by the Compact scheme is mitigated by the high order filtering. The high order multi-resolution algorithm is employed to detect the smoothness of the solution. The Hybrid scheme allows a potential speedup up to a factor of three or more for certain classes of shocked problems. The simulations of one-dimensional shock-entropy wave interaction and classical stable detonation waves, and the two-dimensional detonation diffraction problem around a 90° corner show that the Hybrid scheme is more efficient, less dispersive and less dissipative than the WENO-Z scheme.

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1 Introduction

Detonation is a complex phenomenon that involves a shock front followed by a reaction zone. Accurate and efficient numerical simulations of a mathematical model of detonation waves provide a way to obtain insights in the physical problems and guide researchers to have a deeper understanding of the physics and to design better experiments.

Characteristic-wise WENO conservative finite difference schemes on an equidistant stencil as a class of high order/resolution nonlinear scheme for solutions of hyperbolic conservation laws in the presence of shocks and small scale structures was initially developed in [11] (for details and history of WENO scheme, see [14] and references contained therein). It has been shown that the WENO-Z scheme [1, 3] is less dissipative and has higher resolution power than the classical WENO-JS scheme [11] for a larger class of problems. High order compact finite difference (Compact) schemes are sufficiently accurate to resolve both small and large scale structures presented at direct numerical simulation of highly complex flows. However, when applied to simulate the propagation of detonation waves near the detonation front exhibiting high gradients and discontinuities, known as the Gibbs phenomenon, that causes loss of accuracy and numerical instability.

In this work, we aim at the conjugation of high order Compact scheme and the WENO-Z scheme (Hybrid) for numerical simulations of detonation waves. The $5th$-order characteristic-wise WENO-Z finite difference scheme and $6th$-order Compact finite difference scheme are employed to resolve solutions in the non-smooth parts and the smooth parts of the solution respectively. A high order multi-resolution analysis [9] is performed at every Runge-Kutta step to measure the degree of smoothness at a given grid point to maintain the high order/resolution nature of the Hybrid scheme.

The paper is organized as follows. In Sect. 2, a very brief introduction to the WENO-Z scheme, the Compact scheme and the Hybrid scheme for solving hyperbolic conservation laws on uniform cells are given. In Sect. 3, the one-dimensional shock-entropy wave interaction and classical stable detonation waves, and the two-dimensional detonation diffraction problem around a 90° corner are simulated by the Hybrid scheme and their results are discussed. Conclusions are given in Sect. 4.

2 Hybrid Compact-WENO Finite Difference Scheme

The nonlinear system of hyperbolic conservation laws can be written compactly as

$$\frac{\partial \mathbf{Q}}{\partial t} + \nabla \cdot \mathbf{F}(\mathbf{Q}) = \mathbf{S}, \tag{1}$$

where $\mathbf{Q}, \mathbf{F}$ and $\mathbf{S}$ are vectors of the conservative variables, flux and source term respectively.

Consider a uniformly spaced grid defined by the points $x_i = i\Delta x, i = 0, \ldots, N$, which are called cell centers, with cell boundaries given by $x_{i+\frac{1}{2}} = x_i + \frac{\Delta x}{2}$, where Δx is the uniform cell size. The semi-discretized form of (1) is transformed into the system of ordinary differential equations and solved by the method of lines

$$\frac{dQ_i(t)}{dt} = -\left.\frac{\partial f}{\partial x}\right|_{x=x_i}, \quad i = 0, \ldots, N, \tag{2}$$

where $Q_i(t)$ is a numerical approximation to the cell-averaged value $Q(x_i, t)$.

2.1 Weighted Essentially Non-Oscillatory Schemes

The $5th$-order WENO-Z scheme [1, 3] defines the nonlinear weights ω_k^Z as

$$\alpha_k^Z = \frac{d_k}{\beta_k^Z} = d_k\left(1 + \left(\frac{\tau_5}{\beta_k + \epsilon}\right)^p\right), \quad \omega_k^Z = \alpha_k^Z / \sum_{l=0}^{2} \alpha_l^Z, \quad k = 0, 1, 2, \tag{3}$$

where $\tau_5 = |\beta_0 - \beta_2|$, which has a leading truncation error of order $O(\Delta x^5)$. In contrary, the leading truncation error of β_k are of order $O(\Delta x^2)$ in an absence of critical points [5]. The sensitivity and power parameters are $\epsilon = 10^{-12}$ and $p = 2$, respectively. $\left\{d_0 = \frac{3}{10},\ d_1 = \frac{3}{5},\ d_2 = \frac{1}{10}\right\}$ are the ideal weights that, when the solution is sufficiently smooth, one has $\omega_k \approx d_k$ and the WENO-Z scheme becomes the optimal $5th$-order central upwind scheme.

2.2 Compact Finite Difference Schemes

A $6th$-order ($c_r = 6$) compact finite difference scheme [12] approximates the derivative of a function on a uniformly spaced grids can be written compactly as

$$\mathbf{A}\mathbf{g}' = \mathbf{B}\mathbf{g} + \mathbf{b}, \tag{4}$$

where **A** and **B** are the banded coefficient matrices,

$$\mathbf{A} = \begin{pmatrix} 1 & 1/3 & & & \\ 1/3 & 1 & 1/3 & & \\ & \ddots & \ddots & \ddots & \\ & & 1/3 & 1 & 1/3 \\ & & & 1/3 & 1 \end{pmatrix}, \quad \mathbf{B} = \frac{1}{36\Delta x} \begin{pmatrix} 0 & 28 & 1 & & & & \\ -28 & 0 & 28 & 1 & & & \\ -1 & -28 & 0 & 28 & 1 & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & & -1 & -28 & 0 & 28 \\ & & & & -1 & -28 & 0 \end{pmatrix}.$$

The vector **b** is

$$\mathbf{b} = \frac{1}{36\Delta x}\left(-g_{-1} - 28g_0, -g_0, 0, \cdots, 0, g_N, 28g_N + g_{N+1}\right)^{\mathrm{T}} - \frac{1}{3}\left(g'_0, 0, 0, \cdots, 0, 0, g'_N\right)^{\mathrm{T}},$$

where $g_{-1} = g(x_0 - \Delta x)$ and $g_{N+1} = g(x_N + \Delta x)$ are the ghost points. The derivatives at the two boundary points g'_0 and g'_N are computed by the WENO-Z scheme.

2.3 Hybrid Scheme

By performing a high order MR analysis [9, 10] of a given variable (usually density), a MR flag Flag is specified by

$$\text{Flag}_i = \begin{cases} 1, & |d_i| > \epsilon_{MR} \text{ Non-Smooth,} \\ 0, & \text{otherwise Smooth,} \end{cases} \tag{5}$$

where d_i is the MR coefficient at x_i which measures the error in approximating the function by a high degree polynomial ($8th$) and ϵ_{MR} is the MR tolerance parameter ($\epsilon_{MR} = 10^{-3}$ in this study.) Readers are referred to [4, 9] for details on the MR analysis. In the Hybrid scheme, a buffer zone is created around each cell that is flagged as non-smooth with $\text{Flag}_i = 1$ to allow a smooth transition between non-smooth and smooth stencils. Then, the PDEs (1) is solved by the WENO-Z and Compact schemes at non-smooth and smooth stencils respectively. In smooth stencils, the numerical fluxes on the non-smooth zones obtained by the WENO scheme are saved and automatically used as the internal boundary fluxes needed by the Compact scheme, and an $8th$-order finite difference filtering is applied to stabilize the Hybrid scheme ([15]).

The resulting system of ordinary differentiation equations (ODEs) resulted from the spatial discretization is advanced in time via the third order TVD Runge-Kutta scheme [1]. The CFL condition is set to be CFL $= 0.4$ in this study. Readers are referred to [4, 6] for details. We would like to remark that, in implementation, the Hybrid Compact-WENO scheme is different from the Hybrid Central-WENO scheme [6] where the central scheme can first be applied at all grid points, and the solution in the non-smooth stencils are then updated by the WENO scheme.

3 Governing Equations and Numerical Results

For the one-dimensional unsteady reactive Euler equations with a perfect ideal gas coupled with one step irreversible chemical reaction, one has, from (1),

$$\mathbf{Q} = (\rho,\ \rho u,\ E,\ \rho f_1), \quad \mathbf{F} = (\rho u,\ (\rho u^2 + P),\ (E + P)u,\ \rho f_1 u), \quad \mathbf{S} = (0,\ 0,\ 0,\ \dot{\omega}), \tag{6}$$

where ρ is density, P is pressure, u is velocity, and $0 \le f_1 \le 1$ is the reactant mass fraction. The total specific energy, with an addition of energy $\rho f_1 q_0$ generated through the chemical reaction, is given by $E = \frac{P}{\gamma-1} + \frac{1}{2}\rho u^2 + \rho f_1 q_0$. The source term consists of the energy production term in the form of $\dot{\omega}(T, f_1) = -K\rho f_1 e^{-E_a/T}$ where γ is the ratio of specific-heat ($\gamma = 1.2$ is used in this study), q_0 is the heat-release parameter, E_a is the activation-energy parameter, and K is a pre-exponential factor that sets the spatial and temporal scales. The temperature $T = P/\rho R$, R is the specific gas constant ($R = 1$ in this study). Readers are referred to [7, 8] for details on the initial conditions and the boundary conditions.

3.1 Shock Interaction with Small Entropy Wave

To demonstrate the performance of the Hybrid scheme in terms of accuracy and efficiency, we solve the source-less Euler equations (6) in simulating a right moving Mach 3 shock interacting with a small amplitude sinusoidal perturbation of the entropy in the pre-shock region. The initial condition is

$$(\rho, u, P) = \begin{cases} \left(\frac{27}{7},\ \frac{4\sqrt{35}}{9},\ \frac{31}{3} \right), & x \le x_0, \\ \left(\exp(-\varepsilon \sin(k(x + x_0))),\ 0,\ 1 \right), & x > x_0, \end{cases}$$

where $x \in [-10, 10], \varepsilon = 0.01, x_0 = -9.5$ and $k = 13$. The final time is $t_f = 5$. Since there is no exact solution for this problem, the numerical solution computed by the WENO-JS9 scheme with $N = 10{,}240$ uniform cells is used as the reference solution.

The left figure of Fig. 1 shows that the MR analysis captures the location of the shock very well. In the middle and right figures of Fig. 1, it is clear from the evolution of the small amplitude high frequency entropy waves behind the main shock that the wave form computed by the Hybrid scheme has no discernible dissipation and dispersion errors over time at both lower and higher resolutions.

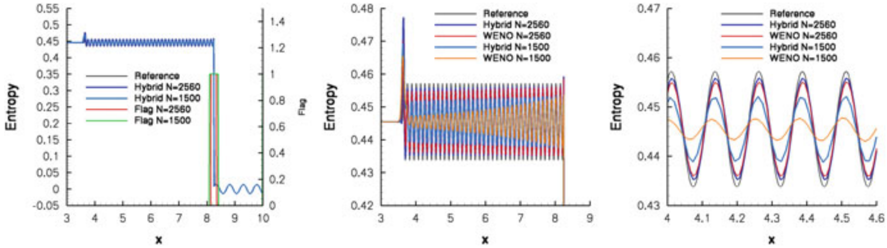

Fig. 1 (*Left*) The entropy and WENO flag (*red* and *green solid lines*) of the Hybrid scheme, (*Middle*) and (*Right*) close-up view of entropy as computed by the WENO-Z and Hybrid schemes with $N = 1500$ and $N = 2560$ at the final time $t_f = 5$

Table 1 Comparative CPU timing and speedup for the shock-entropy wave interaction

$2r-1$	c_r	N	WENO-Z	Hybrid	*Speedup*
5	6	1500	7.3	2.5	2.9
		2560	20.5	5.9	3.5

In contrary, those computed by the WENO-Z scheme are severely dampened at a lower resolution and increasingly less so at the higher resolution. Table 1 gives the comparative CPU timing and speedup of both schemes. We observe that the Hybrid scheme is at least *three* times faster than the WENO-Z scheme.

3.2 One-Dimensional Detonation Waves

Here we evaluate the performance of the Hybrid scheme by simulating the one-dimensional stable detonation waves with the parameters $f = 1.8,\ q_0 = 50,\ E_a = 50,\ K = 145.69$ and the final time $t_f = 100$. The physical domain is set to be $x = [120, 180]$ with PML layer $x = [120, 130]$ and the location of the initial detonation front at $x_d = 160$. Readers are referred to [6] for details. The numerical solution computed by the WENO-Z scheme with $N = 4800$ uniform cells serves as the reference solution.

The left figure of Fig. 2 gives the density spatial profiles showing that the MR analysis captures the location of the detonation front very accurately. The peak pressure temporal histories $P_m(t)$ computed by the Hybrid and WENO-Z schemes with several resolutions at the time $t_f = 100$ are shown in the right figure of Fig. 2, which agree well with those given in [2, 13]. At the lower resolution $N = 1800$, the temporal history of the peak pressure of both schemes is oscillatory and does not seem to reach a steady state. As one increases the resolution to $N = 3000$, both schemes reach the constant steady state solution with a value slightly lower than the reference solution. Table 2 gives the comparative CPU timing and speedup, which shows that the Hybrid scheme is at least *three* times faster than the WENO-Z scheme.

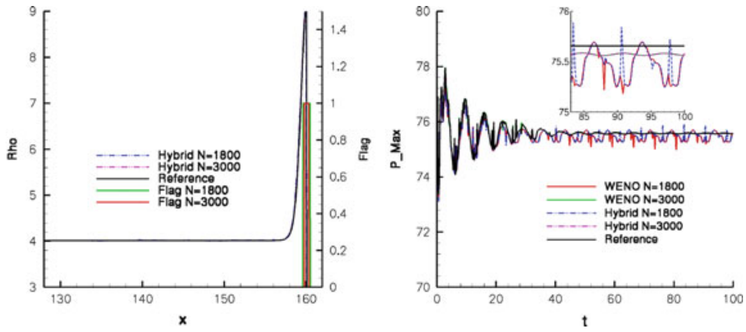

Fig. 2 (*Left*) The density and WENO flag (*green* and *red solid lines*) of the Hybrid scheme and (*Right*) the peak pressure temporal histories $P_m(t)$ of detonation waves with the overdrive factor $f = 1.8$ at the final time $t_f = 100$

Table 2 Comparative CPU timing and speedup for the one-dimensional detonation waves

$2r-1$	c_r	N	WENO-Z	Hybrid	*Speedup*
5	6	1800	295	77	3.8
		3000	815	205	4.0

3.3 Two-Dimensional Detonation Diffraction problem

In this section, we consider the detonation diffraction problem. It is numerically challenging especially for the high order schemes because the pressure and density may drop very close to zero when the shock wave is diffracted around an obstacle making an 90^o angle turn (see Fig. 4). The initial condition is

$$(\rho, u, v, E, f_1) = \begin{cases} (\ 11,\ 6.18,\ 0,\ 970,\ 1), & x < 0.5, \\ (\ \ 1,\quad\ 0,\ 0,\ \ 55,\ 1), & \text{otherwise}, \end{cases}.$$

The physical domain is set to be $(x, y) = [0, 5] \times [0, 5]$. The boundary conditions are reflective except that at $x = 0$, $(\rho, u, v, E, f_1) = (11, 6.18, 0, 970, 1)$. The uniform cells used are $N_x \times N_y = 400 \times 400$ and $N_x \times N_y = 1000 \times 1000$. The final time is $t_f = 0.6$.

As shown in Fig. 3, the MR analysis captures the detonation front very accurately. In Fig. 4, the density and pressure computed by the Hybrid scheme at $t_f = 0.6$ are in a very good agreement with those in [16]. The solution computed by the WENO-Z scheme is omitted as they are very similar to the one computed by the Hybrid scheme. One can see that the density becomes very small when the flow expands around the corner and is well handled by the Hybrid scheme. In Table 3, the comparative CPU timing and speedup show that the Hybrid scheme is at least *two and half* times faster than the WENO-Z scheme.

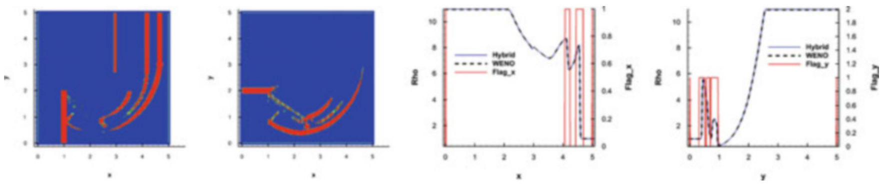

Fig. 3 The multi-resolution flags in the x- and y-directions of detonation diffraction around a 90° corner computed by the Hybrid scheme with the uniform cells $N_x \times N_y = 400 \times 400$

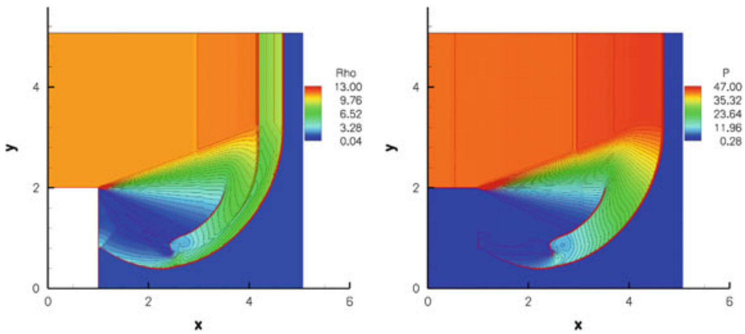

Fig. 4 The density and pressure of detonation diffraction around a 90° corner as computed by the Hybrid scheme with the uniform cells $N_x \times N_y = 400 \times 400$

Table 3 Comparative CPU timing and speedup for the two-dimensional detonation diffraction problem

$2r-1$	c_r	$N_x \times N_y$	WENO-Z	Hybrid	*Speedup*
5	6	400× 400	1697	691	2.5
		1000× 1000	27,980	8430	3.3

4 Conclusion

We studied the performance of the hybrid Compact-WENO finite difference scheme (Hybrid) in the simulations of detonation waves. The Hybrid scheme is used to keep the solutions parts displaying high gradients and discontinuities always captured by the WENO-Z scheme in an essentially non-oscillatory manner while the smooth parts are highly resolved by a more efficient and high resolution compact finite difference scheme and to speedup the computation of the overall scheme. Here, the 5*th*-order WENO-Z schemes and the 6*th*-order Compact scheme are conjugated in the discontinuous and smooth parts respectively. To detect the smooth and discontinuous parts of the solutions, a high order multi-resolution algorithm was used. The 8*th*-order finite difference filter was used to mitigate the numerical oscillations of the Compact scheme. We conducted several numerical comparisons between the WENO-Z and Hybrid schemes in the simulations of the one-dimensional shock-entropy wave interaction, stable detonation waves and two-dimensional detonation diffraction problem. The results showed that the Hybrid scheme can be *three* times faster than and as accurate as the WENO-Z scheme. The FORTRAN 95 program is written based on subroutines contained in the high performance software library HOPEpack.

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