Hybrid Compact-WENO Scheme for Detonation Waves Simulations

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1. Introduction

We shall consider the reactive Euler equation

$$\mathbf{Q}_t + \nabla \cdot \mathbf{F} = \mathbf{S}, \qquad (1)$$

where $\mathbf{S}$ is the source $\omega(T, f_1) = -K\rho f_1 \exp -E_a/T$ on the total energy E due to chemical reaction of an reactive species f_1. The EOS is $E = P/(\gamma-1) + \rho\mathbf{U}\cdot\mathbf{U}/2 + q_0\rho f_1$, $P = \rho RT$ and $\gamma = 1.4$.

We investigate the performance of a hybrid $6th$-order compact finite difference scheme [5] and $5th$-order characteristic-wise weighted essentially non-oscillatory (WENO) finite difference scheme (Hybrid) for the numerical simulations of the detonation waves on a uniformly discretized Cartesian domain.

The smoothness of the solution is measured by the high order multi-resolution analysis (MR) [1] at each grid point. The Hybrid scheme conjugates a high order shock-capturing WENO-Z *nonlinear* scheme in non-smooth stencils with a non-dissipative compact *linear* scheme in smooth stencils, yielding a high fidelity and efficient scheme for applications containing both discontinuous and complex smooth structures. (*See [2] and references contained therein for details.*).

2. Compact Difference Scheme

A $6th$-order compact finite difference scheme approximates the derivative of a function on a uniformly spaced mesh can be written compactly as

$$\mathbf{A}\mathbf{g}' = \mathbf{B}\mathbf{g} + \mathbf{b}, \qquad (2)$$

where $\mathbf{A}$ and $\mathbf{B}$ are the banded coefficient matrices,

$$\mathbf{A} = \begin{pmatrix} 1 & 1/3 & & & & \\ 1/3 & 1 & 1/3 & & & \\ & \ddots & \ddots & \ddots & & \\ & & 1/3 & 1 & 1/3 & \\ & & & 1/3 & 1 & \end{pmatrix},$$

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

The vectors $\mathbf{g}, \mathbf{g}'$ and $\mathbf{b}$ are

$$\mathbf{g} = \left(g_1, g_2, \ldots, g_{N-1} \right)^{\mathrm{T}}, \mathbf{g}' = \left(g_1', g_2', \ldots, g_{N-1}' \right)^{\mathrm{T}},$$

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

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 scheme.

3. Hybrid Scheme

By performing a high order MR analysis of a given variable (usally density), a flag is specified by

$$\mathrm{Flag}_i = \begin{cases} 1, & |d_i| > \epsilon_{MR} \quad \text{Non-Smooth} \\ 0, & \text{otherwise} \quad \text{Smooth} \end{cases}, \qquad (3)$$

where ϵ_{MR} is the MR tolerance parameter and d_i is the MR coefficient at x_i.

- A buffer zone is created around each grid point that is flagged as non-smooth with $\mathrm{Flag}_i = 1$.
- The PDEs (1) is solved by the WENO and compact schemes at non-smooth and smooth stencils respectively.
- In smooth stencils, the fluxes on the non-smooth zones obtained by the WENO scheme are automatically used as the internal boundary fluxes for the compact scheme, and a weak $8th$-order filtering is applied in the smooth stencils to stabilize the Hybrid scheme.

4.1. Shock Small Entropy Wave

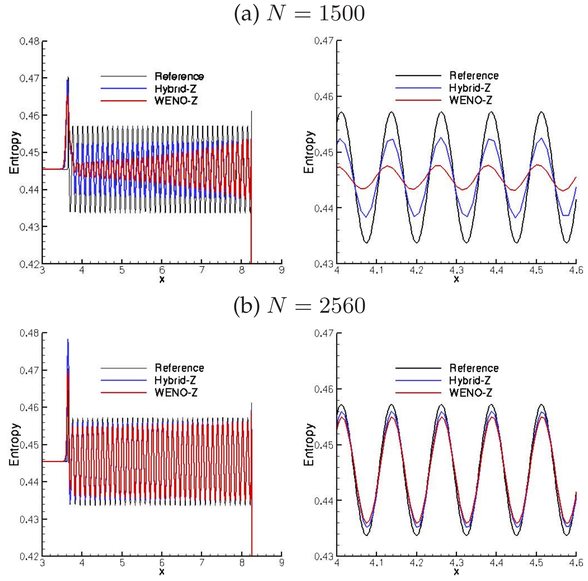

Figure 1: Close-up view of entropy as computed by the WENO-Z scheme and the Hybrid scheme with (a) $N = 1500$ and (b) $N = 2560$ for shock-entropy wave interaction problem ($t = 5$).

In Fig. 1, the temporal and spatial evolution of the small amplitude high frequency entropy waves behind the main shock computed by the Hybrid scheme is well captured with least dissipation and dispersion errors. The WENO-Z nonlinear solver yields a highly dissipated result when the solution is under-resolved.

4.2. 1D Detonation Waves

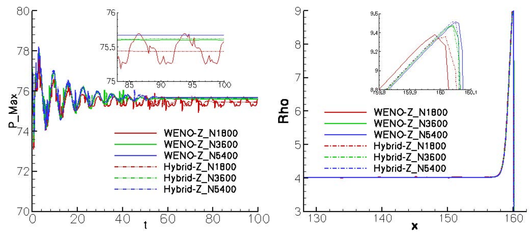

Figure 2: (Left) The peak pressure temporal histories and (Right) the density spatial profiles with overdrive factor $f = 1.8$ and $N = 1800, 3600, 5400$ grid points.

As shown in Fig. 2, both the WENO-Z and Hybrid schemes converge to the peak pressure of steady state solution for $t > 50$. However, the Hybrid scheme is at least 4 times faster than the WENO-Z scheme.

N_x	WENO-Z	Hybrid	Speedup
1800	2.7×10^2	0.7×10^2	3.9
3600	11×10^2	2.3×10^2	4.8
5400	26×10^2	5.8×10^2	4.5

Table 1: CPU timing results for 1D detonation waves.

4.3. 2D Detonation Waves

Fig. 3 shows the pressure, temperature, vorticity and M-R Flag computed by the Hybrid scheme with 20 grid points per half reaction zone and they agree well with the WENO-Z scheme. The Hybrid scheme is about 2 times faster than the WENO-Z scheme.

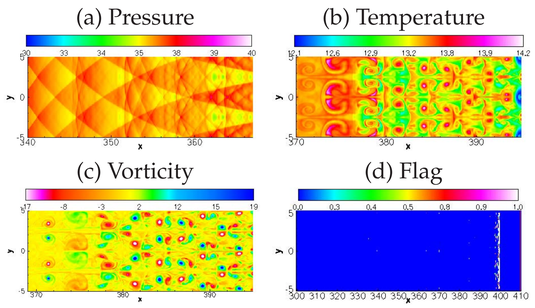

Figure 3: $(H_{50}, E_{10}, f_{1.2})$ pressure, temperature, vorticity, and MR Flag for 2D detonation waves with a sinusoidal perturbation waves $\sin(2y)$ within the reaction zone.

$N_x \times N_y$	WENO-Z	Hybrid	Speedup
1101×101	1.9×10^3	1.1×10^3	1.7
2201×201	15×10^3	6.6×10^3	2.3
4401×401	12×10^4	4.2×10^4	2.9

Table 2: CPU timing results for 2D detonation waves.

4.4. Detonation Waves with Obstacles in Duct

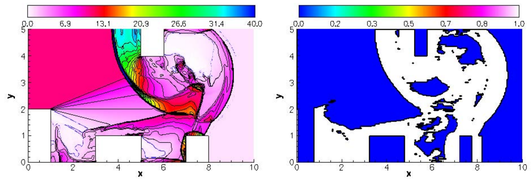

Figure 4: (Left) the density and (Right) the MR Flag for the detonation waves interacting with rectangular shaped obstacles as computed by the Hybrid scheme.

In Fig. 4, the detonation wave interacting with rectangular shaped obstacles in the duct is simulated. One of the challenges in this problem is that the negative density or pressure may appear during the time evolution and causes numerical instability.

The Hybrid scheme is well behaved. It captures the large scale shock structures and resolves small scales smooth structures resulted from the complex shock interactions with shocks and structures.

References

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Future Work

We plan to construct a (CPU/GPU) parallel high order/resolution Hybrid scheme for solving the multi-dimensional multi-species compressible detonation waves equations in a single- and multi-domain frameworks. Numerical experiments in detonation, compressible turbulence, and shock-particle laden flows will be performed in our future research to validate advantages of using the Hybrid scheme.

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