Hybrid Compact-WENO Scheme for Detonation Waves Simulations

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1. Introduction

We shall consider the reactive Euler equation

$$\mathbf{Q}_t + \nabla \cdot \mathbf{F} = \mathbf{S}, \tag{1}$$

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 $E = P/(\gamma-1) + \rho\mathbf{U}\cdot\mathbf{U}/2 + q_0\rho f_1$, $P = \rho R T$ and $\gamma = 1.2$.

We investigate the performance of a hybrid compact finite difference scheme and 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) 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 [1] and references contained therein for details.*).

2. Compact Difference Scheme

A compact finite difference scheme [2] approximates the derivative of a function on a uniformly spaced mesh can be written compactly as

$$Ag'_i = \frac{1}{\Delta x} B g_i, \tag{2}$$

where A and B are both *local*, one dimensional operators. The A and B are given by

- $4th$-order ($c_r = 4$)
$$(Av)_i = (v_{i-1} + 4v_i + v_{i+1})/6,$$
$$(Bv)_i = (v_{i+1} - v_{i-1})/2.$$
- $6th$-order ($c_r = 6$)
$$(Av)_i = (v_{i-1} + 3v_i + v_{i+1})/5,$$
$$(Bv)_i = (v_{i+2} + 28v_{i+1} - 28v_{i-1} - v_{i-2})/60.$$
- $8th$-order ($c_r = 8$)
$$(Av)_i = (3v_{i-1} + 8v_i + 3v_{i+1})/8,$$
$$(Bv)_i = (375v_{i+1} + 24v_{i+2} - v_{i+3} - 375v_{i-1} - 24v_{i-2} + v_{i-3})/480.$$

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 [3] of a given variable (usally density), a flag is specified by

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

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 $\text{Flag}_i = 1$.
- 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

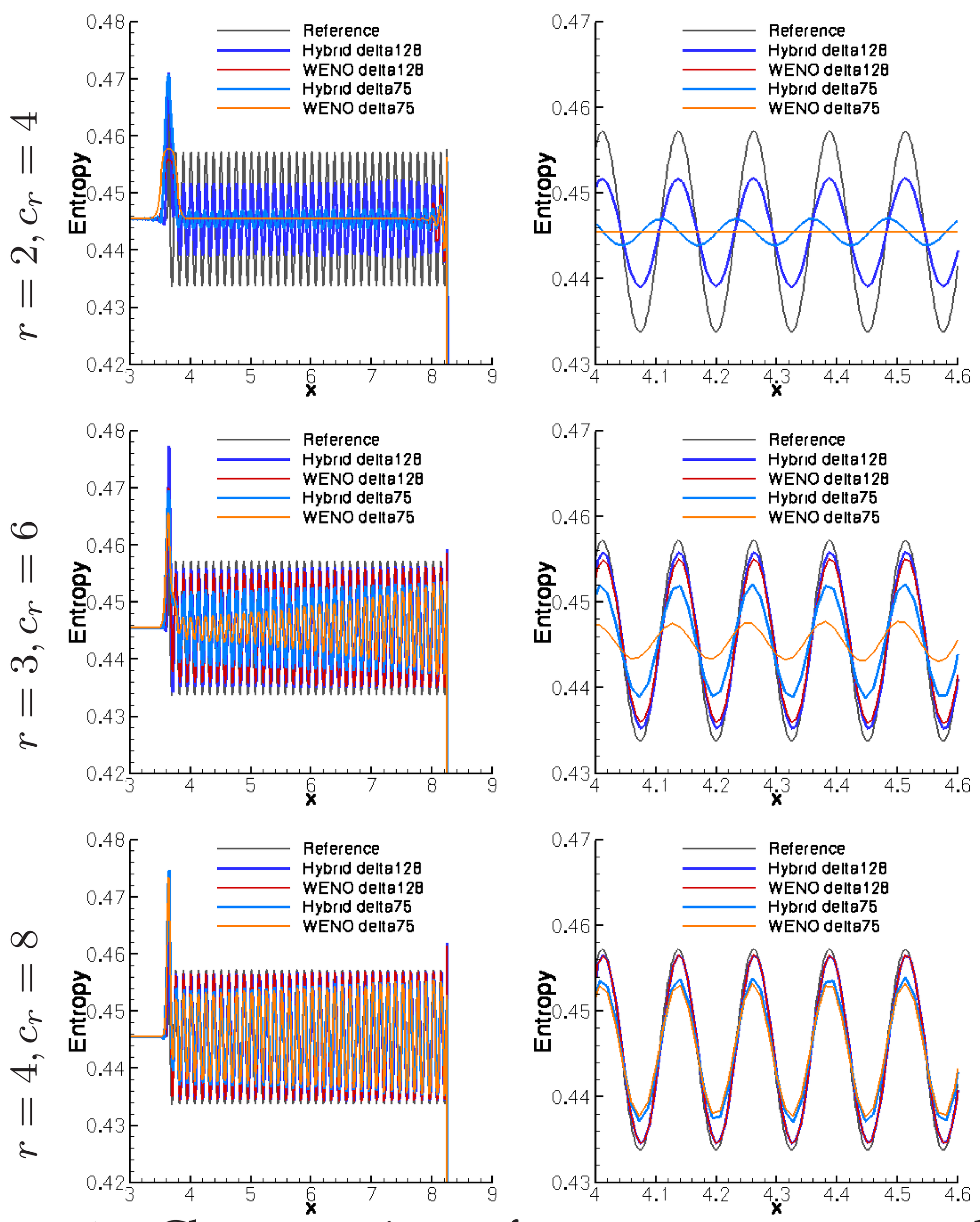

Figure 1: Close-up view of entropy as computed by the WENO-Z scheme and the Hybrid scheme for shock-entropy wave interaction problem at time t = 5.

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.

4.1. Shock small entropy wave

The Hybrid scheme is at least 2 times faster than the WENO-Z scheme.

Table 1: CPU timing results for the shock entropy wave.

r	c_r	δ	WENO-Z	Hybrid	Speedup
2	4	75	5.40×10^0	2.26×10^0	2.4
		128	1.49×10^1	0.553×10^1	2.7
3	6	75	7.28×10^0	2.48×10^0	2.9
		128	2.05×10^1	0.594×10^1	3.5
4	8	75	9.64×10^0	2.69×10^0	3.6
		128	2.71×10^1	0.645×10^1	4.2

4.2. 1D detonation wave

Table 2: CPU timing results for 1D detonation wave.

r	c_r	δ	WENO-Z	Hybrid	Speedup
2	4	30	2.41×10^2	0.780×10^2	3.1
		50	6.07×10^2	1.92×10^2	3.2
3	6	30	2.95×10^2	0.769×10^2	3.8
		50	8.15×10^2	2.05×10^2	4.0
4	8	30	3.92×10^2	0.918×10^2	4.3
		50	1.10×10^3	0.241×10^3	4.6

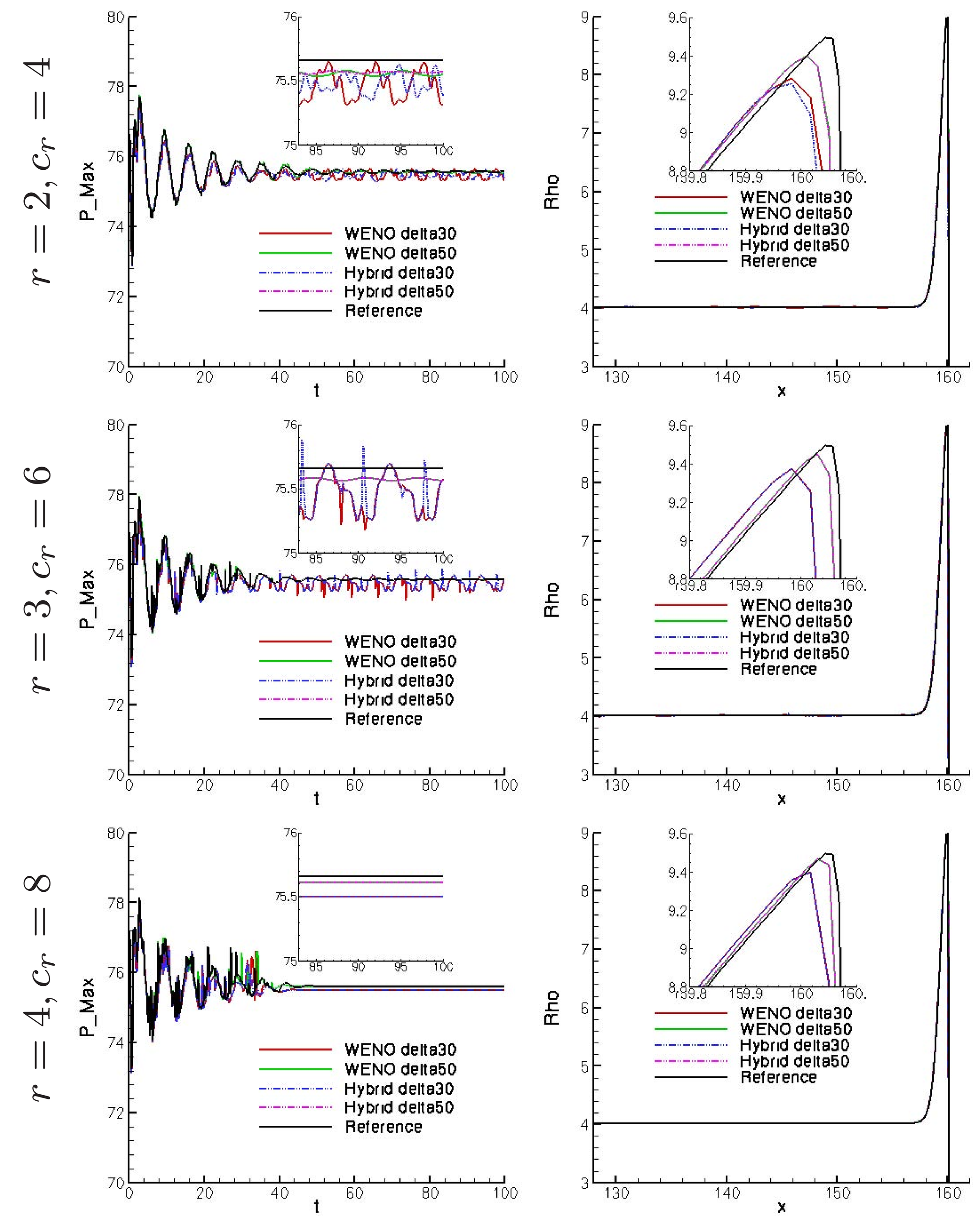

Figure 2: (Color online) (left) The peak pressure temporal histories and (right) the density spatial profiles with overdrive factor $f = 1.8$ at time $t = 100$.

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 3 times faster than the WENO-Z scheme.

4.3 2D detonation waves

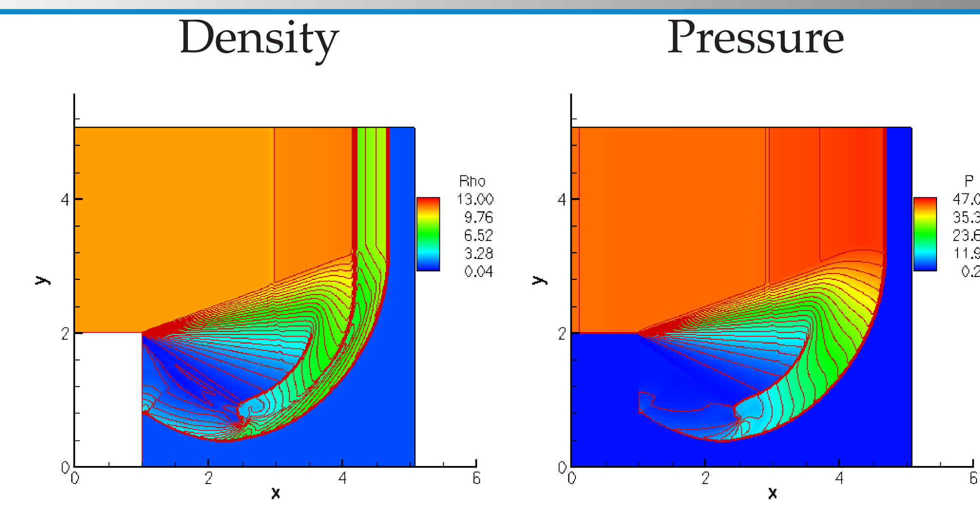

Figure 3: Detonation diffraction at a 90^o corner.

Fig. 3 shows the density and pressure computed by the Hybrid scheme and they agree well with those computed by the pure WENO-Z scheme. The density may become very small when the flow expands around the corner.

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.

References

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