Numerical Dissipation and Wrong Propagation Speed of Discontinuities For Stiff Source Terms

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Abstract

In compressible turbulent combustion/nonequilibrium flows, the constructions of numerical schemes for (a) stable and accurate simulation of turbulence with strong shocks, and (b) obtaining correct propagation speed of discontinuities for stiff reacting terms on "coarse grids" share one important ingredient - minimization of numerical dissipation while maintaining numerical stability. Here "coarse grids" means standard mesh density requirement for accurate simulation of typical non-reacting flows. This dual requirement to achieve both numerical stability and accuracy with zero or minimal use of numerical dissipation is most often conflicting for existing schemes that were designed for non-reacting flows. The goal of this paper is to relate numerical dissipations that are inherited in a selected set of high order shock-capturing schemes with the onset of wrong propagation speed of discontinuities as a function of stiffness of the source term and the grid spacing.

Motivation and Results

To make accurate predictions in compressible turbulent combustion/nonequilibrium flows, one has to deal with the equations that describe time-dependent non-equilibrium effects, combustion, advanced thermodynamic models, and magnetic fields (MHD). Numerical simulation is challenging because of the conflicting requirements for numerical methods to be accurate enough to resolve the small scales of (magnetized) turbulence but robust enough to handle shock waves without generating spurious numerical noise. In addition, the different physics models have different time scales that, when underresolved, might interact numerically to produce erroneous results. Furthermore, the appearance of the source terms in modeling non-equilibrium flow problems containing finite-rate chemistry or combustion poses additional numerical difficulties beyond that for solving non-reacting turbulent flows. The so-called stiff source term problem [5] is a well-known example. For stiff reactions it is well known that the wrong propagation speed of discontinuities occurs due to the under-resolved numerical solutions in both space and time. Schemes to improve the wrong propagation speed of discontinuities for systems of stiff reacting flows remain a challenge for algorithm development [7].

In addition to the minimization of numerical dissipation while maintaining numerical stability in compressible turbulence with strong shocks, Yee & Sjögreen and Yee & Sweby [9, 10, 8] discussed a general framework for the design of such schemes. Yee & Sjögreen [12], Wang et al. [7] and references cited therein present their recent progress on the subject. In [13], a short overview of this recent progress is given. Two very important numerical challenges are "Stiffness and Nonlinearity of Source Terms".

The objective of the present paper is to a gain a deeper understanding on the behavior and performance of four high order shock-capturing schemes for two representative stiff detonation wave problems. The test cases consist of the Arrhenius 1D Chapman-Jouguet (C-J) detonation wave [4, 6] and a 2D Heaviside detonation wave [1]. These are the same two test cases considered in [7]. The considered four schemes are the fifth-order WENO, "WENO5", the [7] newly developed subcell resolution version of WENO5, "WENO5/SR", the Yee et al. nonlinear filter version of WENO5, "WENO5fi"

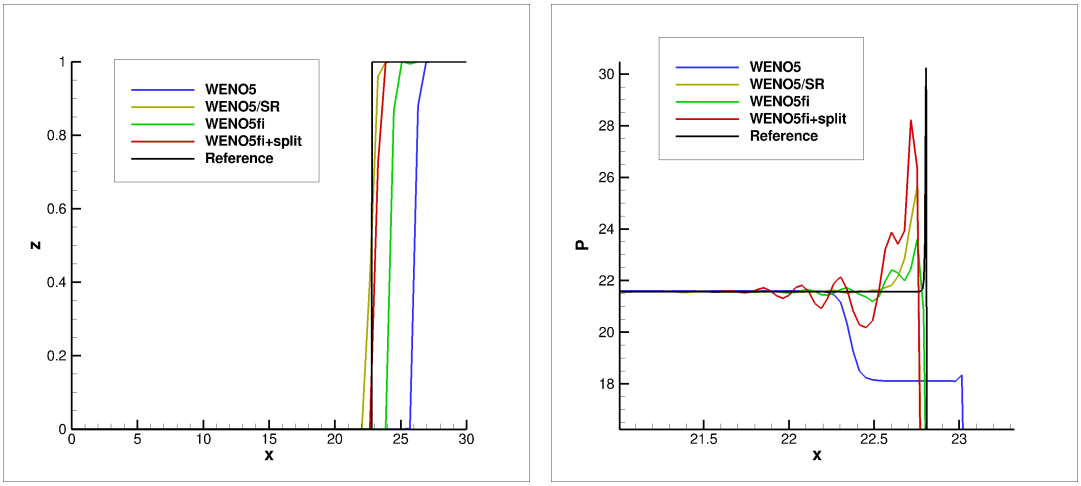


Figure 1: Density (mass fraction of the unburnt gas; 50 grid points) and pressure (800 grid points) comparison in the vicinity of the discontinuity among four high order shock-capturing methods for the C-J detonation problem, Arrhenius case at $t = 1.8$ using 50 and 800 uniform grid points.

and the Durcros split version of WENO5fi, "WENO5fi+split" [11, 12]. For the temporal discretization, the classical fourth-order Runge-Kutta method (RK4) is used. Although WENO5/SR, WENO5fi and WENO5fi+split use the same dissipative portion of WENO5 as the basic numerical dissipation model, the mechanism to further limit the inherited amount of WENO5 dissipation from one grid point to the next are different among the schemes. See the aforementioned references for the development of these schemes.

WENO5/SR [7] is a newly developed modified fractional step method which solves the convection step and reaction step separately. In the convection step any high order shock-capturing method can be used. In the reaction step an ODE solver is applied, but with the computed flow variables in the shock region modified by the Harten subcell resolution idea [3].

WENO5fi is the filter version of WENO5. On the first stage a full time step by RK4 is performed. For this stage the sixth-order central spatial base scheme is used. On the second stage the solution is filtered by the dissipative portion of WENO5 in conjunction with a wavelet flow sensor. The wavelet flow sensor indicates the locations where shock-capturing dissipations are needed and leaves the remaining region free of numerical dissipation contamination. WENO5fi+split is WENO5fi applied to the Ducros et al. split form of the governing equation [2] before the application of WENO5fi. The Ducros et al. split form is a preprocessing step to condition the governing equation(s) before the application of high order central schemes. This preprocessing step improves numerical stability and is widely used in numerical modeling and simulation of turbulent flows.

The comparison of the performance of the four schemes is largely based on the degree that each method captures the correct location and jump size of the stiff reaction front for coarse grids. It is remarked that, in order to resolve the sharp stiff reaction zone, sufficiently many grid points in this zone are still needed. The behavior of these schemes in the vicinity of a sharp reaction zone with several levels of grid refinement will be briefly touched upon. Figures 1 and 2 show the comparison among WENO5, WENO5/SR, WENO5fi and WENO5fi+split for the the Arrhenius 1D Chapman-Jouguet (C-J) detonation wave [4, 6] and a 2D Heaviside detonation wave [1]. The reference solution for the 1D stiff detonation wave case is computed by the regular WENO5 scheme with $10,000$ uniform grid points. The initial values consist of totally burnt gas on the left-hand side and totally unburnt gas on the right-hand side. The reference solution for the 2D stiff detonation wave case is computed by standard WENO5 with 2000×400 grid points. The chemical reaction for this 2D problem is modeled by the Heaviside form.

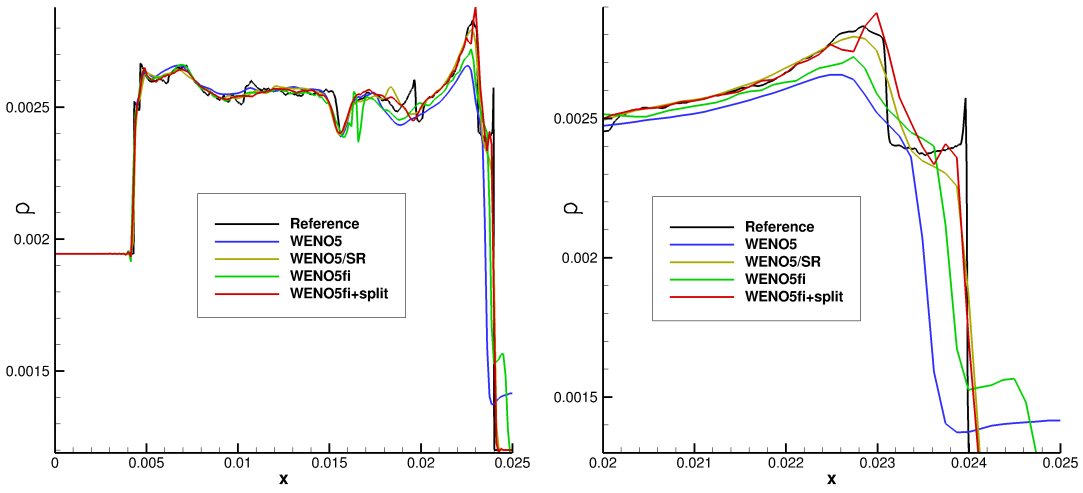


Figure 2: 1D cross-section of density at $t = 1.7 \times 10^{-7}$ by four high order shock-capturing methods for the 2D detonation problem using 200×40 uniform grid points with left figure in the vicinity of the discontinuity.

The grid density for all computed solutions is considered to be very coarse for the subject combustion test cases. From the result, WENO5/SR and WENO5fi+split are able to obtain the correct shock speed with similar accuracy whereas this is not the case for WENO5 WENO5fi using the same coarse grids. Using its original form [12] without further modification, the accuracy of WENO5fi+split is nearly as good as the newly developed high-order finite difference schemes with subcell resolution. The results indicate the influence of numerical dissipation on the behavior of the computed solution around the stiff reaction front. In the final paper, we will examine the subcell resolution version of WENO5fi and WENO5fi+split and their seventh-order counterparts.

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