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A finite-volume hybrid WENO/central-difference shock capturing approach with detailed state-to-state kinetics for high-enthalpy flows

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Abstract. This work shows novel space discretization capabilities of an innovative fluid dynamics solver able to deal with thermochemical non-equilibrium by using a detailed state-to-state model. The implementation of a WENO hybrid scheme is verified and thermochemical non-equilibrium effects are investigated by considering a high temperature shock tube test case. The work represents a first step to enable the solver to perform LES and DNS simulations of turbulent hypersonic flows.

Introduction

The investigation of high enthalpy flows is important in several fields, e.g., hypersonic flows in the context of entry objects (space capsules, reusable space vehicles, debris, meteoroids, etc.), laser applications (laser induced breakdown spectroscopy, etc.), high-enthalpy wind tunnels, rocket engines, etc. [1]. Such flows can involve different phenomena (e.g., strong shock waves, thermochemical non-equilibrium, turbulence, etc.) each of which requires a specific expertise and adequate modeling. In the last years, the authors have developed a finite-volume solver of the Navier-Stokes equations for the simulation of hypersonic flows in thermochemical non-equilibrium, see, e.g. [2,3]. From a numerical point of view the solver is based on conventional approaches that have demonstrated to be robust and affordable. A third order Runge-Kutta scheme and the flux vector splitting of Steger and Warming, with a second order MUSCL reconstruction, were employed for time and space discretization, respectively. On the other hand, to deal with thermochemical non-equilibrium an accurate state-to-state (StS) approach, in addition to the classical multi-temperature Park's model, makes the software a unique tool in the present scene. In order to extend code capabilities to problems that involve both shocks and turbulence, a hybrid WENO/central-difference scheme has been implemented. Indeed, this approach has shown to be among the most convincing when dealing with problems involving shocks and turbulence interacting dynamically [4]. In the present implementation, the popular fifth-order WENO scheme is coupled with a sixth-order central scheme with a shock sensor that limits the use of the shock capturing scheme to region of strong gradients, thus reducing numerical dissipation in smooth regions. To verify the algorithm implementation and to show code capabilities, the one dimensional Sod [5] and Shu–Osher [4] problems, and the two dimensional double Mach reflection (DMR) [5] have been analyzed. Finally, a high temperature shock tube has been investigated by using the hybrid scheme along with the StS approach.

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Governing Equations and Numerical Method

The system of Euler equations is solved for a calorically perfect gas ($\gamma = cp/cv = 1.4$) or, to consider high temperature effects, for a reacting mixture in thermochemical non-equilibrium.
A cell centered finite-volume (FV) approach is employed and the method of lines is used to separate space and time discretization. Upwind space discretization can be performed either by the Steger and Warming (SW) or by the Lax-Friedrichs (LF) Flux Vector Splitting (FVS). The accuracy of the upwind scheme is increased by a fifth order WENO reconstruction following a characteristic-wise FV method [6]. Then, to reduce numerical dissipation, the WENO scheme is hybridized with a numerical flux built from a sixth order central scheme (CD6). The hybrid approach switches from CD6 to WENO when a shock sensor (χ) [7] is larger than a threshold (χ_L). Time integration is performed by a third order explicit Runge-Kutta scheme [5]. In the case of reacting mixtures an operator splitting approach is applied to deal with stiff source terms [2,3]. Finally, thermochemical non-equilibrium is handled by a StS approach for a N_2-N mixture [2].

Results

Code verification has been performed by considering 1D and 2D test cases. All problems have been solved by using the SW-FVS except for the double Mach reflection for which the LF-FVS has been employed.

The first test is represented by Sod's shock tube [5]. In Fig. 1 (left) the exact solution is compared with the results obtained by the WENO scheme with three different resolutions: a very good agreement is obtained. Figure 1 (right) shows the results of the hybrid scheme with three different χ_L using 100 cells. Oscillations due to dispersive error increase with χ_L .

The Shu-Osher problem [4] is a benchmark for studying shock turbulence interactions being the propagation of a shock in a perturbed density field. A reference solution has been obtained by using the WENO scheme with mesh size $\Delta x = 6.25 \cdot 10^{-3}$ (1600 cells). Figure 2 shows that with the same resolution ($\Delta x = 5 \cdot 10^{-2}, 200$ cells) the hybrid scheme provides better results with respect to the WENO approach in terms of density profiles, whereas no difference emerges from velocity profiles.

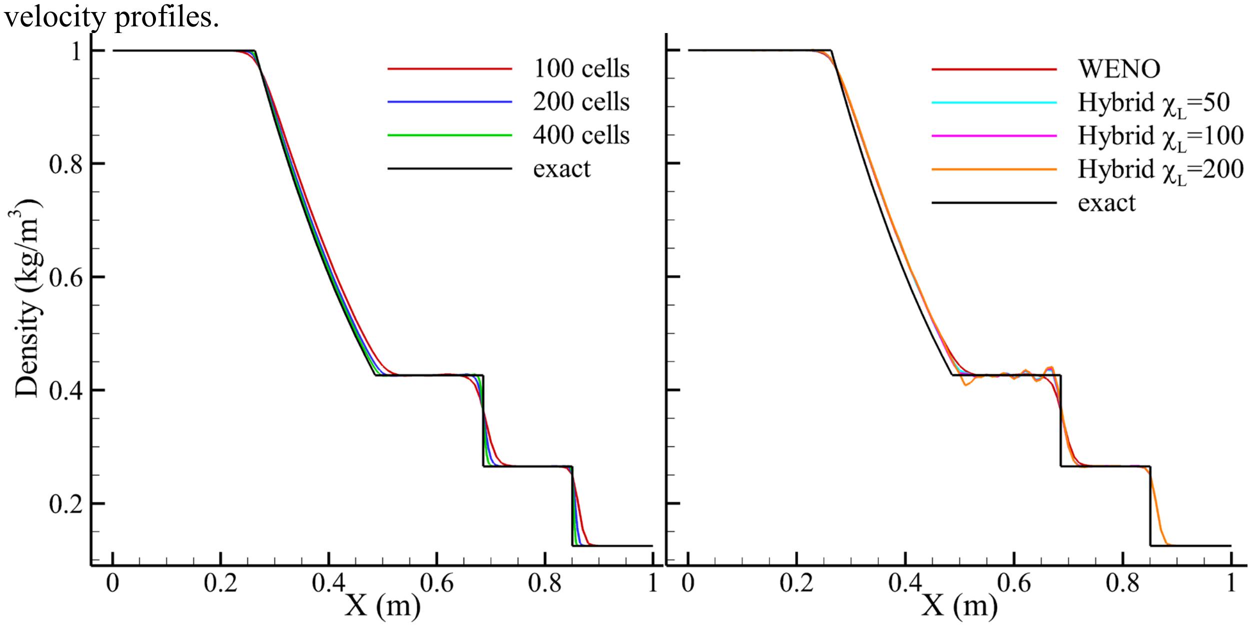

Fig. 1 Sod's shock tube at t=0.2: (left) WENO scheme; (right) WENO/CD6 hybrid scheme.

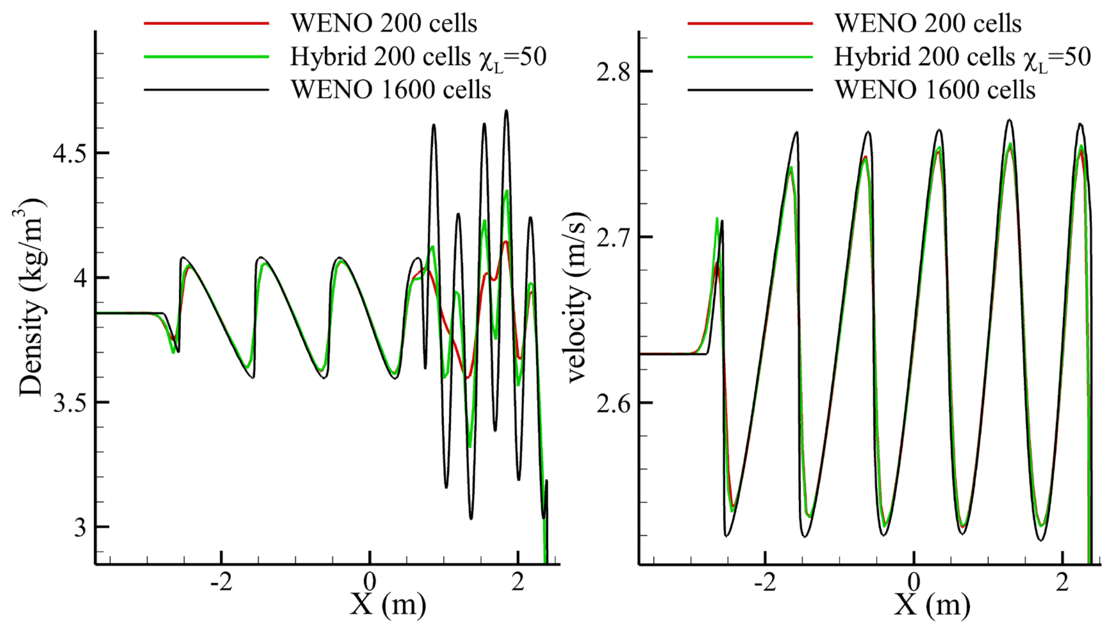

Fig. 2 Shu-Osher problem: (left) density profiles; (right) velocity profiles.

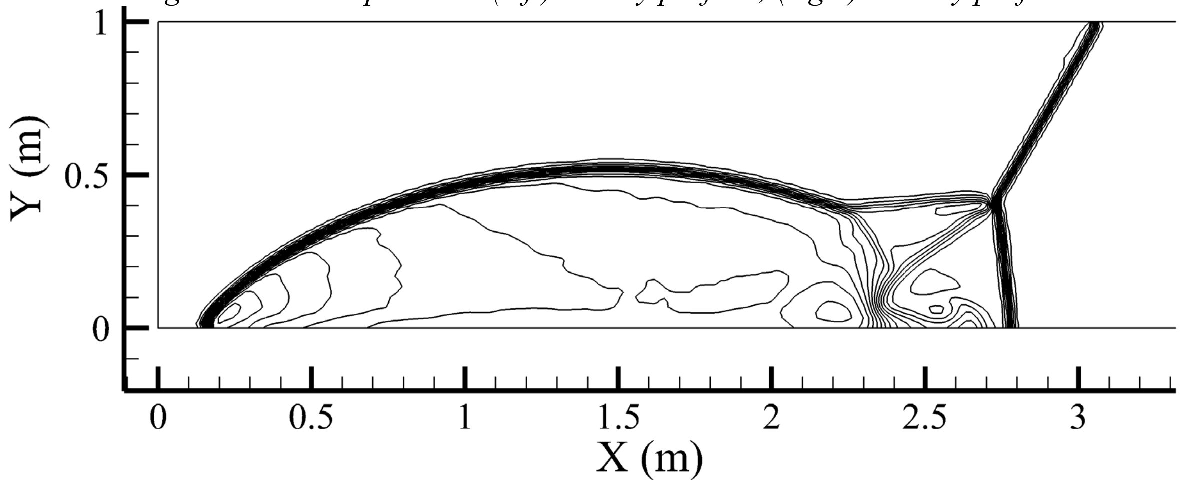

Fig. 3 DMR: 240x59 cells, t=0.2, CFL=0.6, 30 levels from 1.731 to 20.92, $\boldsymbol{\chi_L = 200}$.

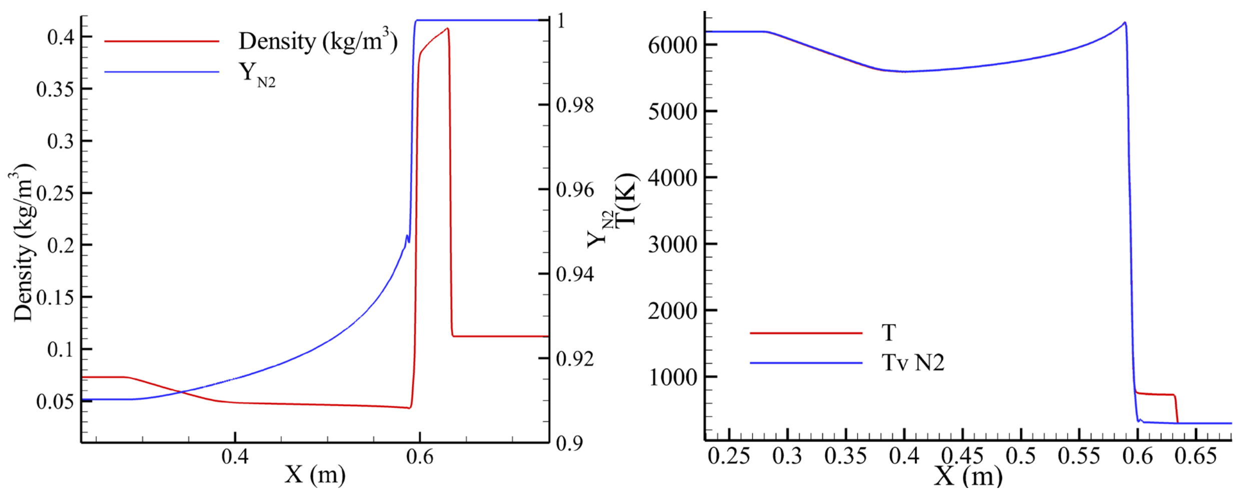

Fig. 4 High temperature shock tube at $t = 1.3 \cdot 10^{-4}$s*: (left) density and* Y_{N2}*; (right) T and* Tv_{N2}

Figure 3 shows the density isolines for the double Mach reflection problem (hybrid scheme). A very good agreement is obtained with Jiang and Shu [5]. Finally, a high temperature shock tube has been simulated by using the StS approach. The initial conditions are those given in Grossmann and Cinnella [8] except for the initial mixture composition that here is a pure N_2 mixture (mass fraction Y_{N2}=1). The hybrid scheme with χ_L=100 has been employed. Figure 4 shows an important N_2 dissociation which causes a temperature reduction in the upstream region. The translational (T) and the vibrational (Tv_{N2}) temperature differ in the region between the shock wave and the contact discontinuity thus showing a small thermal non-equilibrium.

Conclusions

In this work a WENO/CD6 hybrid scheme was implemented in a fluid dynamics solver able to deal with thermochemical non-equilibrium by using a StS approach. The solver was verified by considering benchmark test cases. Finally, a high temperature shock tube was analyzed showing the ability of the scheme to deal with high temperature gases in thermochemical non-equilibrium.

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