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An artificial nonlinear diffusivity method for supersonic reacting flows with shocks

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Abstract

A computational approach for modeling interactions between shocks waves, contact discontinuities and reactions zones with a high-order compact scheme is investigated. To prevent the formation of spurious oscillations around shocks, artificial nonlinear viscosity [A.W. Cook, W.H. Cabot, A high-wavenumber viscosity for high resolution numerical method, J. Comput. Phys. 195 (2004) 594–601] based on high-order derivative of the strain rate tensor is used. To capture temperature and species discontinuities a nonlinear diffusivity based on the entropy gradient is added. It is shown that the damping of 'wiggles' is controlled by the model constants and is largely independent of the mesh size and the shock strength. The same holds for the numerical shock thickness and allows a determination of the L2 error. In the shock tube problem, with fluids of different initial entropy separated by the diaphragm, an artificial diffusivity is required to accurately capture the contact surface. Finally, the method is applied to a shock wave propagating into a medium with non-uniform density/entropy and to a CJ detonation wave. Multi-dimensional formulation of the model is presented and is illustrated by a 2D oblique wave reflection from an inviscid wall, by a 2D supersonic blunt body flow and by a Mach reflection problem.

Keywords: High-order scheme; Shock capturing; Supersonic combustion; Nonlinear diffusivity

1. Introduction

Supersonic combustion involves complex interactions between turbulence, shock waves and combustion. Because of their capability to reproduce unsteady effects, Direct (DNS) or large-eddy numerical simulations (LES) are attractive to model such supersonic reactive flows. In order to capture the physically important turbulent and chemical scales, such simulations require the use of accurate numerical schemes. As they can reproduce a wide range of wavenumbers, compact schemes [2] are well adapted. Unfortunately, the use of high-order compact schemes to solve steep gradients like those in shock waves generates non-physical oscillations [3]. The objective of this article is to develop and to validate a numerical methodology adequate for resolving interactions between shocks, turbulence and combustion.

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Several approaches that modify or adapt high-order schemes to capture shock waves have been proposed in the literature. For shock–turbulence interaction problems, Adams and Shariff [4,5] proposed a high-order compact-ENO scheme and later Pirozzoli [6] introduced a conservative compact-WENO scheme. Deng and Zhang [7] developed high-order compact schemes based on the weighted technique. Rizzetta et al. [8] proposed a hybrid compact-Roe approach in order to simulate a supersonic compression-ramp flow. Visbal and Gaitonde [9] introduced an adaptive filter methodology to maintain the same high-order compact scheme in all of the numerical domain. An attractive alternative to these has been proposed by Cook and Cabot [1,10] who avoid the use of a shock detector by adding an artificial dissipation term. A nonlinear artificial viscosity, based on high-order derivatives of the strain rate tensor, is introduced. The capability of this approach to accurately treats shock–turbulence interaction was successfully demonstrated.

In the context of supersonic combustion, high temperature and species gradients are expected in addition to shock waves. In order to accurately predict the interactions between these phenomenon, the original methodology proposed by Cook and Cabot [1,10] is extended. In addition to the nonlinear viscosity, an artificial diffusivity based on high-order derivatives of the entropy is introduced. Detailed analysis of the errors associated with shock-capturing and contact-surface capturing was conducted for the new scheme. These have shown that new scheme is able to capture both weak and strong shocks without any degradation of performance. Both the numerical shock thickness, which is related to the number of points used to 'capture' the discontinuity, and the magnitude of the spurious wiggles are shown to be largely independent of the mesh size and the shock/contact surface strength. The original methodology and its extension are tested on the shock tube problem. It is observed that when the temperature from each side of the shock is initially different the original method by Cook and Cabot [1,10] is not sufficient. Introduction of an artificial diffusivity is required to accurately capture the contact surface. The Shu–Osher problem [11] which consists of a shock wave crossing sinusoidal density waves is then considered. This test case has been used by many authors [4,10,11] for one-dimensional shock turbulence interactions. The computation of a Chapman–Jouguet detonation wave demonstrates the capability of the model to reproduce interactions between shock wave and combustion. The formulation of the model in multiple dimensions is then proposed and is illustrated by the computations of a 2D oblique shock, a 2D blunt body flow and a Mach reflection problem.

2. Shock capturing model: 1D formulation

2.1. Governing equations

The governing equations of a one-dimensional compressible reactive flow are:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0, \tag{1}$$

$$\frac{\partial \rho u}{\partial t} + \frac{\partial}{\partial x}(\rho u u + p) = \frac{\partial}{\partial x}\left(\mu_l \frac{\partial u}{\partial x}\right), \tag{2}$$

$$\frac{\partial \rho E}{\partial t} + \frac{\partial}{\partial x}[(\rho E + p)u] = \frac{\partial}{\partial x}\left(\mu_l u \frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial x}\left(\lambda \frac{\partial T}{\partial x}\right), \tag{3}$$

$$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial}{\partial x}(\rho u Y_k) = \frac{\partial}{\partial x}\left(\rho D_k \frac{\partial Y_k}{\partial x}\right) + \dot{\omega}_k, \tag{4}$$

$$\rho E = \frac{\rho R T}{\gamma - 1} + \frac{1}{2}\rho u u + \rho \sum_{k=1}^{N_{sp}} Y_k h_k^0, \tag{5}$$

where ρ is the density, p is the pressure, E is the total energy (per unit mass), γ is the ratio of specific heats, R is the gas constant, T is the gas temperature, λ is the thermal conductivity, μ_l is the fluid viscosity, N_{sp} is the number of species, Y_k is the mass fraction of the kth species, h_k^0 is the enthalpy of formation of kth species, D_k is the diffusivity of kth species and $\dot{\omega}_k$ is its reaction rate. Ideal gas law has been assumed here for simplicity.