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High order finite difference methods with subcell resolution for advection equations with stiff source terms ☆

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ABSTRACT

A new high order finite-difference method utilizing the idea of Harten ENO subcell resolution method is proposed for chemical reactive flows and combustion. In reaction problems, when the reaction time scale is very small, e.g., orders of magnitude smaller than the fluid dynamics time scales, the governing equations will become very stiff. Wrong propagation speed of discontinuity may occur due to the underresolved numerical solution in both space and time. The present proposed method is a 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. For numerical experiments, a fifth-order finite-difference WENO scheme and its anti-diffusion WENO variant are considered. A wide range of 1D and 2D scalar and Euler system test cases are investigated. Studies indicate that for the considered test cases, the new method maintains high order accuracy in space for smooth flows, and for stiff source terms with discontinuities, it can capture the correct propagation speed of discontinuities in very coarse meshes with reasonable CFL numbers.

1. Introduction

In simulating hyperbolic conservation laws in conjunction with an inhomogeneous stiff source term, if the solution is discontinuous, spurious numerical results may be produced due to different time scales of the transport part and the source term. This numerical issue often arises in combustion and high speed chemical reacting flows.

The reactive Euler equations in two dimensions have the form

$$U_t + F(U)_x + G(U)_y = S(U), \tag{1}$$

where U, $F(U)$, $G(U)$ and $S(U)$ are vectors. If the time scale of the ordinary differential equation (ODE) $U_t = S(U)$ for the source term is orders of magnitude smaller than the time scale of the homogeneous conservation law $U_t + F(U)_x + G(U)_y = 0$ then the problem is said to be stiff. In high speed chemical reacting flows, the source term represents the chemical reactions which may be much faster than the gas flow. This leads to problems of numerical stiffness. Insufficient spatial/temporal resolution

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may cause an incorrect propagation speed of discontinuities and nonphysical states for standard dissipative numerical methods.

This numerical phenomenon was first observed by Colella et al. [13] in 1986 who considered both the reactive Euler equations and a simplified system obtained by coupling the inviscid Burgers' equation with a single convection/reaction equation. LeVeque and Yee [23] showed that a similar spurious propagation phenomenon can be observed even with scalar equations, by properly defining a model problem with a stiff source term. They introduced and studied the simple one-dimensional scalar conservation law with an added nonhomogeneous parameter dependent source term

$$u_t + u_x = S(u), \tag{2}$$

$$S(u) = -\mu u\left(u - \frac{1}{2}\right)(u-1), \tag{3}$$

where the parameter $\frac{1}{\mu}$ can be described as the reaction time. When μ is very large, a wrong shock speed phenomenon will be observed in a coarse mesh. In order to isolate the problem, LeVeque and Yee solve (2) and (3) by the fractional step method. For the particular source term, the reaction (ODE) step of the fractional step method can be solved exactly. They found that the propagation error is due to the numerical dissipation contained in the scheme, which smears the discontinuity front and activates the source term in a nonphysical manner. By increasing the spatial resolution by an order of magnitude, they were able to improve towards the correct propagation speed.

It is noted that, in a general stiff source term problem, a sufficient spatial resolution is as important as temporal resolution when the reaction step of the fractional step method cannot be solved exactly. A study linking spurious numerical standing waves for (2) and (3) by first and second-order spatial and temporal discretizations can be found in Lafon and Yee [22,21] and Griffiths et al. [15].

For the last two decades, this spurious numerics phenomenon has attracted a large volume of research work in the literature (see, e.g., [5,28,6,32,8,15,24,1,7,27]). Various strategies have been proposed to overcome this difficulty. Since numerical dissipation that spreads the discontinuity front is the cause of the wrong propagation speed of discontinuities, a natural strategy is to avoid any numerical dissipation in the scheme. In combustion, level set and front tracking methods were used to track the wave front to minimize this spurious behavior [24,1,7,27]. In [11,12], Chorin introduced the random choice method which is based on the exact solution of Riemann problems at randomly chosen locations within the computational cells and does not need to introduce any viscosity. It has been successfully used in [13,25] for the solution of underresolved detonation waves. However, it is difficult to eliminate all numerical viscosity in a shock-capturing scheme. There are also many works on modifying shock-capturing methods for this problem in the literature. Fractional step methods are commonly used for allowing an underresolved meshsize. Such methods solve the homogeneous conservation law (i.e., the convection step) and the ODE system (i.e., the reaction step) separately. In [9,10], Chang applied Harten's subcell resolution method [16] in a finite volume ENO method in the convection step with exact time evolution, which is able to produce a zero viscosity shock profile in the nonreacting flow. The time evolution is advanced along the characteristic line. Correct results were shown in the one-dimensional scalar case. However it seems difficult to extend this method to one-dimensional systems or multi-dimensional scalar equations or systems, due to the requirement of exact time evolution. In [14], Engquist and Sjögreen proposed a simple temperature extrapolation method based on a finite difference ENO scheme with implicit Runge–Kutta time discretization, which uses a first/second order extrapolation of the temperature value from outside the shock profile. Their approach is easily extended to multi-dimensions. However, their method is not a fractional step method, and it does not work well in the situation of insufficient spatial resolution. Helzel et al. [17] presented a modified fractional step method for detonation waves in which the exact Riemann solution is used to determine where burning should occur. Bao and Jin [2–4] proposed a random projection method based on the fractional step method where in the convection step a standard shock-capturing scheme is used, and in the reaction step a projection is performed to make the ignition temperature random. They have successfully applied this method to various problems in one- and two-dimensions. However they assume an *a priori* stiff source. In [33], Tosatto and Vigevano proposed a MinMax scheme, which is based on a two-value variable reconstruction within each cell, where the appropriate maximum and minimum values of the unknown are considered. The scheme may be applied with no difficulties to both stiff and nonstiff problems. Only one-dimensional problems were tested. However, it seems difficult to generalize either the random projection method or the MinMax method to higher order accuracy. There are other works in the literature for stiff source hydrodynamics, e.g. [26].

Our objective in this study is to develop a high order finite difference method which can capture the correct detonation speed in an underresolved mesh and will maintain high order accuracy in the smooth part of the flow. The first step of the proposed fractional step method is the convection step which solves the homogeneous hyperbolic conservation law in which any high-resolution shock-capturing method can be used. The aim in this step is to produce a sharp wave front, but some numerical dissipation is allowed. The second step is the reaction step where an ODE solver is applied with modified transition points. Here, by transition points, we refer to the smeared numerical solution in the shock region, which is due to the dissipativity of a shock-capturing scheme. Because the transition points in the convection step will result in large erroneous values of the source term if the source term is stiff, we first identify these points and then extrapolate them by a reconstructed polynomial using the idea of Harten's subcell resolution method. Unlike Chang's approach, we apply Harten's subcell resolution in the reaction step. Thus our approach is flexible in allowing any shock-capturing scheme as the convection operator. In the reaction step, since the extrapolation is based on the high order reconstruction, high order accuracy can be