Journal of Computational Physics 291 (2015) 52–59

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Short note

A short note on the counter-intuitive spurious behaviors in stiff reacting flow

Bin Zhang [a,b,*], Jian-Hang Wang [b]

[a] Department of Mathematics, Shanghai Jiao Tong University, Shanghai, 200240, China
[b] School of Aeronautics and Astronautics, Shanghai Jiao Tong University, Shanghai, 200240, China

ARTICLE INFO

Article history:
Received 31 March 2014
Received in revised form 17 February 2015
Accepted 5 March 2015
Available online 16 March 2015

Keywords:
Counter-intuitive spurious behaviors
Wrong propagation speed of discontinuities
Stiff source term
Simplified 2×2 system
Reactive Euler equations

ABSTRACT

A well known spurious numerical phenomenon may occur in solving stiff detonation problems due to the under-resolved numerical solution in both space and time. Most people believe that decreasing numerical dissipation or stiffness will delay or eliminate the onset of spurious numerical phenomenon. However, several counter-intuitive spurious behaviors were observed by H.C. Yee et al. (2013) [10] recently and the mechanism of the generation of these strange phenomena remains an open question. The goal of this short note is to give a reasonable explanation for these counter-intuitive spurious behaviors existing in the detonation problems (the simplified 2×2 system and the reactive Euler equations) with stiff reacting source terms and discontinuities. In developing the mechanism of spurious numerical phenomenon in detonation problems, we find the parameters of the intermediate state are very important because they determine whether the spurious phenomenon will happen or not. Furthermore, these counter-intuitive spurious behaviors are mainly due to the oscillation of those intermediate state parameters as the time step or grid is refined gradually. These findings may help us to get a further understanding of some of the difficulties in numerical combustion and problems with stiff nonlinear source terms and discontinuities in general.

1. Introduction

The spurious numerical phenomenon in reactive Euler equations was first observed by Colella et al. [1] who derived analytically the conditions at which these spurious solutions may be produced, but did not provide a reasonable explanation. Lafon and Yee [2,3] pointed out that this spurious numerical phenomenon, which is greatly influenced by the different combination of time step, grid spacing and initial conditions, may be linked to the existence of some stable spurious steady-state numerical solutions. By analyzing a properly defined scalar equation with a stiff source term, LeVeque and Yee [4] found that the propagation error is mainly due to numerical dissipation contained in the scheme, which smears the discontinuity front and activates the source term in a nonphysical manner. A nonequilibrium state induced by the smearing will restore to equilibrium immediately if the source term is very stiff. This means a discontinuity will shift to a cell boundary after one time step and finally leads to incorrect propagation speed of the discontinuity. During the last two decades, this issue has attracted a great deal of attention and many innovative numerical methods have been proposed successively to overcome some of the difficulties [5–9].

* Corresponding author at: Department of Mathematics, Shanghai Jiao Tong University, Shanghai, 200240, China.
E-mail address: sjtuzhangbin@gmail.com (B. Zhang).

http://dx.doi.org/10.1016/j.jcp.2015.03.017
0021-9991/

It is generally recognized that the degree of wrong propagation speed of the discontinuity is highly dependent on the dissipation of the advection scheme and the stiffness of the source term. Therefore, most people believe that the wrong propagation speed can be improved towards the correct propagation speed by decreasing the numerical viscosity in advection scheme or the stiffness of the source term. However, the latest researches [10,11] show that there are several surprising counter-intuitive spurious numerical results for compressible Euler and Navier–Stokes equations containing stiff reacting source terms and discontinuities: Smaller CFL numbers (corresponding to less stiffness) may exhibit more spurious behaviors which have clashed with some traditional concepts (a small CFL number gives more accurate solutions for non-reacting problems). These counter-intuitive spurious numerical results imply that the traditional concept of the CFL guideline needs to be revised for problems with nonlinear stiff source terms. Unfortunately, the generation mechanism for spurious numerical phenomenon in stiff scalar problems cannot be used directly to explain these counter-intuitive spurious behaviors in stiff reacting Euler equations. Therefore, the main objective of this short note is to explain the cause of these several counter-intuitive spurious numerical behaviors by developing the generation mechanism of the spurious numerical phenomenon for detonation problems (the simplified 2×2 system and the reactive Euler equations). The rest of this note is organized as follows. In Section 2, two standard spurious numerical results for the simplified 2×2 system and the reactive Euler equations are presented respectively. In Section 3, the mechanism of generation of the spurious numerical phenomenon for detonation problems is reported. Several counter-intuitive spurious numerical results are obtained and their corresponding explanations are given in Section 4. Finally, some concluding remarks are drawn in Section 5.

2. Spurious numerical phenomenon

We first introduce the spurious numerical phenomenon by two simple detonation problems (the simplified 2×2 system and the reactive Euler equations): A one-dimensional detonation wave propagates at a constant speed from left to right. Both these two governing equations are solved with the standard fractional step method [9] which solves the convection step and reaction step separately. This method is widely used in combustion and reactive flow simulations [9,10]. Second-order upwind schemes (the Upstream Non-Oscillatory advection scheme [12] for the simplified 2×2 system and the AUSM scheme plus a TVD Minmod limiter for reactive Euler equations) are used for the current study. On one hand, the solution behavior for a different scheme can be different, based on the combination of time step size, grid spacing, initial condition and numerical boundary condition; on the other hand, the counter-intuitive spurious behaviors are common resulting from the generation mechanism which will be discussed later.

2.1. The simplified 2×2 system

The 2×2 system is a nonlinear hyperbolic system with stiff source terms. This system is an effective, though rather simplified, mathematical model for the motion of detonation:

$$\begin{cases} \frac{\partial T}{\partial t} + \frac{\partial}{\partial x}\left(\frac{1}{2}T^2\right) = Q\,\omega\,(T,z) \\ \frac{\partial z}{\partial t} = -\omega\,(T,z) \end{cases} ;\ \omega = \begin{cases} Da \cdot z & ,\ T < T_{ig} \\ 0 & ,\ T \geq T_{ig} \end{cases} \tag{1}$$

where T represents temperature and z is the mass fraction. Positive parameter $Q = 2$ represents the heat release of the chemical reaction. The reaction rate ω is given by the ignition temperature model which is often used in fast chemical processes. $Da = 200$ and $T_{ig} = 0.05$ are the Damkohler number and ignition temperature respectively. The computational domain is $[0, L = 200]$ and the initial condition is given as follows:

$$\left(T^0(x), z^0(x)\right) = \begin{cases} (6,0) & x < 5 \\ (0,1) & x > 5 \end{cases} \tag{2}$$

Both the exact solution ($N = 200\,000$ and $\Delta t = 1 \times 10^{-6}$) and the non-physical solution ($N = 400$ and $\Delta t = 0.001$) at time $t = 5$ are compared in Fig. 1 (left). It can be found that there is only one detonation with the Von Neuman spike in the correct solution. However, the spurious numerical solution consists of a weak detonation and a shock wave (bifurcating wave pattern) connected by a gradually increasing intermediate zone ($T_x \approx 2.09$). The Von Neuman spike cannot be seen in this solution because there are inadequate grids in the reactive zone. At $t = 5$, the detonation location of the wrong solution is at about $x = 130.0$ which is much larger than the theoretical value of $x = 27.47$. This discrepancy of detonation location in these two solutions will grow as time goes on.

2.2. The reactive Euler equations

Consider the simplest reactive Euler equations with only two chemical states: the burnt gas and the unburnt gas. The unburnt gas is converted to burnt gas via a single irreversible reaction.