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High Order Finite Difference Methods with Subcell Resolution for Stiff Multispecies Discontinuity Capturing

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Abstract. In this paper, we extend the high order finite-difference method with subcell resolution (SR) in [34] for two-species stiff one-reaction models to multispecies and multireaction inviscid chemical reactive flows, which are significantly more difficult because of the multiple scales generated by different reactions. For reaction problems, when the reaction time scale is very small, the reaction zone scale is also small and the governing equations become very stiff. Wrong propagation speed of discontinuity may occur due to the underresolved numerical solution in both space and time. The present SR method for reactive Euler system is a fractional step method. In the convection step, any high order shock-capturing method can be used. In the reaction step, an ODE solver is applied but with certain computed flow variables in the shock region modified by the Harten subcell resolution idea. Several numerical examples of multispecies and multireaction reactive flows are performed in both one and two dimensions. Studies demonstrate that the SR method can capture the correct propagation speed of discontinuities in very coarse meshes.

AMS subject classifications: 65M06, 76V05, 80A32

Key words: Stiff reaction term, shock capturing, detonation, WENO, ENO subcell resolution, multispecies, multireactions.

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1 Introduction

When simulating high speed reactive flows, a wide range of reaction rates may be present, and the chemical time-scales are often orders of magnitude smaller than the typical relaxation time of fluid dynamics, leading to the stiffness of the problem.

The mathematical model for inviscid chemical reactive flows can be described by the reactive Euler equations coupled with source terms. Consider the reactive Euler equations in two dimensions in the form

$$U_t+F(U)_x+G(U)_y=S(U), \tag{1.1}$$

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. The stiff source term is one of the sources lead to problems of numerical stiffness. Insufficient spatial resolution 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. [12] 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 [22] 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.

Numerically resolving all the chemical small scales will result in tremendous computational cost. Therefore, many works have contributed to the analysis and development of underresolved numerical methods which are able to capture the correct shock/discontinuities location and speed without resolving the small chemical scales. Examples include the level set and front tracking methods [6,19,23,26,30], random choice method [10–12,24], random projection method [1–3] and many other works [4,5,7–9,13,14,16,17,25,27,31,32]. See Wang et al. [33] for a comprehensive overview of the last two decades of this development. Wang et al. [33] also proposed a new high order finite difference method with subcell resolution for advection equations with stiff source terms for a single reaction to overcome the difficulty.

In this work, we extend the subcell resolution method to multispecies and multireaction problems, which are significantly more difficult because of the multiple scales generated by different reactions. The proposed SR method for the reactive Euler system is a fractional step method. In the convection step, any high order shock-capturing method can be used. However shock-capturing schemes will produce transition points due to the numerical dissipation. Here, transition points mean the smeared numerical solution in the shock region. In the reaction step, an ODE solver is applied but with the values of certain computed flow variables at the transition points in the shock region modified by a reconstructed polynomial using the idea of Harten's subcell resolution method. It