Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2022-0122

Vol. **33**, No. 3, pp. 849-883
March 2023

Adaptive Multi-Resolution Method for 3D Reactive Flows with Level Set Front Capturing

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Communicated by Kun Xu

Received 21 April 2022; Accepted (in revised version) 28 December 2022

Abstract. For compressible reactive flows with stiff source terms, a new block-based adaptive multi-resolution method coupled with the adaptive multi-resolution representation model for ZND detonation and a conservative front capturing method based on a level-set technique is presented. When simulating stiff reactive flows, under-resolution in space and time can lead to incorrect propagation speeds of discontinuities, and numerical dissipation makes it impossible for traditional shock-capturing methods to locate the detonation front. To solve these challenges, the proposed method leverages an adaptive multi-resolution representation model to separate the scales of the reaction from those of fluid dynamics, achieving both high-resolution solutions and high efficiency. A level set technique is used to capture the detonation front sharply and reduce errors due to the inaccurate prediction of detonation speed. In order to ensure conservation, a conservative modified finite volume scheme is implemented, and the front transition fluxes are calculated by considering a Riemann problem. A series of numerical examples of stiff detonation simulations are performed to illustrate that the present method can acquire the correct propagation speed and accurately capture the sharp detonation front. Comparative numerical results also validate the approach's benefits and excellent performance.

AMS subject classifications: 35L65, 76V05

Key words: Compressible reactive flows, reactive Euler equations, three-dimensional simulation, adaptive multi-resolution, level set method, sharp front capturing.

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1 Introduction

Detonation waves are supersonic combustion waves that involve an exothermic process driving by a shock discontinuity. The well-known CJ model [7] is the simplest, as its detonation front consists of a single discontinuity and its reaction finishes instantaneously. The ZND model [12] is more complex, proposed by Zelovich, Neumann and Doering [12], describing the detonation front as a single jump discontinuity followed by a chemical reaction zone [35]. This paper focuses on the simulations of reactive flows utilizing the ZND model.

In the ZND model, the hydrodynamics of inviscid flow is described by the homogeneous conservation laws and the mass fraction of reactant is introduced in addition to the single reaction rate equation. Colella et al. [8] identified for the first time the phenomenon of spurious propagation of the detonation front in 1986. LeVeque and Yee [22] discovered that numerical dissipation in traditional shock-capturing schemes leads to propagation error, which smears the detonation front and activates the source term in a non-physical manner. In actually, the time scale of the reaction rate equation is frequently quicker than that of the hydrodynamics, and the rapid temporal changes can result in rapid spatial variations of the flow states around the detonation front and reactive zone. Moreover, the reaction rate term is a temperature-sensitive function. Inadequate spatial and temporal resolution can therefore result in non-physical fluid states and incorrect propagation speed of the detonation front [40].

The methods to overcome this difficulty can be divided into three categories, the fractional step method [6,29,37,38,41,42], the front-tracking method [15,17,20,21,26,28,39], and the adaptive technique [1–4,11,13,24].

The first is the fractional step method, which separately solves the homogeneous conservation laws and the reaction rate equation. Chang [6] combined the finite volume ENO method and Harten's subcell resolution method for reactive flows and obtained correct solutions for one-dimensional instances. However, it is difficult to apply this strategy to high-dimensional systems. Wang [37,38] proposed a high-order finite difference method utilizing the idea of Harten's ENO subcell resolution method to solve two-dimensional cases. Nonetheless, this method achieves only second order accuracy in time and is hard to be applied in a Runge-Kutta method with more than two stages. Zhang [42] utilized a two-equilibrium-states reconstruction in the reaction step to calculate the accurate propagation speed of the discontinuity. Although these approaches can obtain the correct propagation speed, as mentioned in [9], extra steps are still required to solve the reaction rate equation. Moreover, the detonation front remains diffusive due to the numerical diffusion errors produced by the shock-capturing schemes around discontinuities.

The second is to avoid numerical dissipation by tracking the discontinuities [17,20, 21], such as the front tracking technique and the level set method. LeVeque [20] utilized a front tracking technique based on a high-resolution wave propagation method to solve one-dimensional problems and then extended it to two dimensions [21]. In high dimen-