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The dual information preserving method for stiff reacting flows

Li Liu[a,b], Yiqing Shen[a,b,*], Shengping Liu[a,b], Ming Yu[c]

[a] LHD, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190, China
[b] School of Engineering Science, Beijing 100049, China
[c] Institute of Applied Physics and Computational Mathematics, Beijing 100094, China

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ABSTRACT

In this paper, we construct a new numerical method to solve the reactive Euler equations to cure the numerical stiffness problem. The species mass equations are first decoupled from the reactive Euler equations, and then they are further fractionated into the convection step and the reaction step. In the convection step, by introducing two kinds of Lagrangian points (cell-point and particle-point), a dual information preserving (DIP) method is proposed to resolve the convection characteristics. In this new method, the information (including the transport value and the relative coordinates to the center of the current cell) of the cell-point and that of the particle-point are updated according to the velocity field. The information of the cell-point in a cell can effectively restrict the incorrect reaction activation caused by the numerical dissipation, while the information of the particle-point can help to preserve the sharp shock front once the strong shock waves are formed. Hence, by using the DIP method, the spurious numerical propagation phenomenon in stiff reacting flows is effectively eliminated. In addition, a numerical perturbation method is also developed to solve the fractional reaction step (ODE equation) to improve the stability and efficiency. A series of numerical examples are presented to validate the accuracy and robustness of the new method.

1. Introduction

In simulating problems governed by the reactive Euler equations, such as combustion and high-speed chemical reaction, the difference between the timescales of reaction and convection, which limits both the time step and grid spacing, may cause the numerical stiffness problems, for example, the spurious numerical propagation phenomenon of the shock waves in flow fields [1–3]. In order to attenuate the influence of the limited time step, the implicit time method or fractional step method is usually used to calculate the reaction ODE equations. However, if the mesh is not fine enough, the time method cannot remove the incorrect reaction activation caused by the spatial discretization, especially in the flows with shock waves. This is because the numerical dissipation introduced to capture shocks smears the shock front and also leads to the reaction activation in incorrect cells. Although the applications of high order shock capturing schemes can effectively reduce the numerical dissipation and sharpen the discontinuity, the incorrect reaction activation and spurious propagation may still occur.

Wang et al. [4] gave a comprehensive overview of the last two decades of efforts contributed to overcome the spurious numerical phenomenon. Since there is difference between timescales of the convection and the reaction, the fractional step method is usually used to solve the reactive Euler equations. Bao and Jin [3,5,6] developed a random projection method in the reaction terms to capture the detonations, but the assumption of a priori stiff source limits the application of this method. Zhang et al. [7] proposed an equilibrium state method (ESM) by using appropriate equilibrium states to activate the stiff source terms. The main defect of the ESM in applications is that it is difficult to determine the equilibrium states, especially in a complex chemical system. Based on the idea of Harten ENO subcell resolution method [8], Chang [9] developed a finite volume ENO method in the convection step, while Wang et al. [4,10] proposed high order finite difference methods with subcell resolution reconstructing the reaction step. However, as pointed out by Yee et al. [11], the subcell resolution method and its nonlinear filter counterparts [12] can delay the onset of the wrong speed of propagation for the stiff detonation problem with coarse grids and moderate stiff source terms, but this kind of method has additional spurious behavior as the grid is refined and the stiffness is further increased.

Ideally, the shock wave front can be regarded as an interface, hence, the interface tracking methods, such as the level set

* Corresponding author at: LHD, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190, China.
E-mail address: yqshen@imech.ac.cn (Y. Shen).

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method, the VOF method and the front tracking method, have been used in the premixed combustion with the instantaneous flame viewed as an infinitely thin interface between fresh and burned gases [13,14], and also used in alleviating the nonphysical phenomena [15] in the simple two-phase detonations by tracking the inert shock as an interface. However, since the general chemical dynamic model is composed of multi-species and finite rate reactions, there are continuous reacting regions other than a traditional two-phase interface, hence, these interface tracking methods mentioned above cannot solve the stiff problem generated in general reacting flows well.

For solving the interface/free surface fluid flow problems, the marker and cell (MAC) method is regarded as the basis of the interfacial tracking techniques [16]. The essence of the MAC method is the Lagrangian virtual marker particles and the cells defined on an Eulerian grid. Marker particles, often as many as 16 per cell, are moved from their coordinates at time t_n to their new coordinates at time t_{n+1} according to the newly computed velocity u at the cell center. The cell classification is updated every time step using information provided by the virtual Lagrangian mesh constituted by the marker particles. The MAC method has been applied to interface/free surface flow problems successfully [17–19]. The main advantages of the MAC method are that it eliminates all logic problems associated with interfaces and readily extended to three-dimension. However, because a large number of particle coordinates must be stored, the storage increases significantly. Another limitation in the MAC method as well as in the level set and the VOF methods is that it is difficult to extend to the case that the interface (free surface) is generated by the flow itself, such as the shock waves and the chemical reaction.

Recent years, the Lagrangian–Eulerian (LE) approaches with the combination of Lagrangian particles and the Eulerian background grids have attracted great attention in solving the convection-diffusion problems [20–24]. The LE method takes advantage of appropriate operator splitting techniques to solve different aspects of the physical model with most suitable Lagrangian or Eulerian formalism [24]. Shipilova et al. [25] applied a LE method (the particle transform method) to solve the convection-diffusion-reaction problems, numerical results showed that the PTM can avoid the numerical oscillation even for a very sparse grid. So far, there is no attempt to use the LE approaches to deal with the spurious numerical propagation phenomenon generated in simulating the reacting flows.

In this paper, by introducing two kinds of Lagrangian points, we propose the dual information preserving method to cure the spurious numerical propagation in the chemical reacting flows. In this method, the information includes the transport value and the relative coordinates to the center of the Eulerian cell containing the point. The species mass fraction equations are first decoupled from the reactive Euler equations, and then they are further fractionated into the convection step and reaction step. In the species convection step, one Lagrangian particle-point is introduced in each cell at the beginning of the whole computation, and one Lagrangian cell-point is introduced in each cell at the beginning of each time step. All the particle-points are tracked in the whole computation, and the information of the cell-point is determined as: if there are particle-points in current cell, the information is updated by averaging all the particle-points' information; else if there are cell-points entered, the information is updated by averaging all the entered cell-points' information; otherwise a new cell-point is set at the cell center and its transport value is obtained by interpolating its neighboring cell-points' values. The information of the cell-point in a cell can effectively restrict the incorrect reaction activation possibly caused by the numerical dissipation, while the information of the particle-point can help to preserve the sharp shock front once the strong shock waves are formed. Hence, the new method can effectively eliminate the spurious numerical propagation phenomenon in the stiff reacting flows. Different from the MAC method, the new method does not need cell classification and has only two times of the cell number's points to be stored. As it contains information on two kinds of Lagrangian points, we call the method as dual information preserving (DIP) method. In addition, by multiplying a power-series of the time step to the explicit Euler scheme, a numerical perturbation method is developed to solve the fractional reaction step (ODE equation) to improve the stability and efficiency.

This paper is organized as follows. In Section 2, we briefly introduce the decoupling method for solving the reactive Euler equations. In Section 3, a dual information preserving method is proposed to solve the convection step of species mass fraction equations. In Section 4, a numerical perturbation method is developed to solve the fractional reaction step, and analysis of stability and numerical examples are also presented. A series of examples, including one- and two-dimensional problems, simplified reaction and multi-species reaction models, are given to validate the accuracy and robustness of the new method in Section 5. Conclusions are shown in Section 6.

2. Spurious reaction activation and the decoupling method for reactive Euler equations

The one-dimensional governing equations of reacting flows without consideration of heat conduction and viscosity are the reactive Euler equations given as

$$\frac{\partial U}{\partial t}+\frac{\partial F}{\partial x}=S, \tag{2.1}$$

where

$$U=\begin{pmatrix}\rho\\ \rho u\\ E\\ \rho z_1\\ \rho z_2\\ \vdots\\ \rho z_{ns-1}\end{pmatrix}, F=\begin{pmatrix}\rho u\\ \rho u^2+p\\ u(E+p)\\ \rho u z_1\\ \rho u z_2\\ \vdots\\ \rho u z_{ns-1}\end{pmatrix}, S=\begin{pmatrix}0\\ 0\\ 0\\ \omega_1\\ \omega_2\\ \vdots\\ \omega_{ns-1}\end{pmatrix},$$

ns is the number of reaction species, z_i and ω_i are the mass fraction and the production rate of the ith species. The mass fraction of the nsth species is given by

$$z_{ns}=1-\sum_{i=1}^{ns-1} z_i.$$

And the pressure is

$$p=(\gamma-1)\left(E-\frac{1}{2}\rho u^2-\rho\sum_{i=1}^{ns} q_i z_i\right),$$

where q_i is the formation enthalpy of species i and the ratio of specific heats γ is independent of temperature in this paper.

In the shock-dominant reaction flows, such as the detonation flows, the reaction follows the shock with a process of reaction heat release. Obviously, if a shock-capturing method is used, the numerical dissipation of the reaction is unavoidable. Especially if the computational grid is not fine enough, then the numerical dissipation results in a relatively thick reaction region with large temperature variation, and hence the reaction may be activated at a wrong location. In order to avoid the presence of the wrong reaction, a natural idea is to deal with the shock and the reaction, separately.