# A third-order explicit numerical scheme for stiff ODE equations

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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. First, the species mass equations are decoupled from the reactive Euler equations, and they are further fractionated into the convection step and reaction step. In the species convection step, by introducing two kinds of virtual Lagrangian point (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 location to the centre of current cell) of cell-point and paticle-point are updated according to the velocity field. By using the DIP method, the incorrect activate position of the reaction, which may be caused by the numerical dissipation, can be effectively avoided. In addition, a numerical perturbation method is also developed to solve the fractionated 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.

*Keywords:* Stiff reacting flow, Dual information preserving method, Numerical pertutbation method, Shock-capturing scheme

## 1. Introduction

In simulating problems governed by reactive Euler equations, such as combustion and high speed chemical reaction, the difference of 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[**?** **?** **?** ]. In order to attenuate the influence of limited time step, the implicit time method or fraction 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 flow 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

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reduce numerical dissipation and sharpen the discontinuity, the incorrect reaction activation and spurious propagation may still occur.

Wang et al.[**?** ] gave a comprehensive overview of the last two decades of efforts contributed to overcome the spurious numerical phenomenon. Bao and Jin [**?** **?** **?** ] 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.[**?** ] proposed an equilibrium state method (ESM) by using appropriate equilibrium states to activate the stiff source terms. The main defect of ESM in application is that it is difficult to determine the equilibrium states, especially in complex chemical system. Based on the idea of Harten ENO subcell resolution method[**?** ], Chang[**?** ] developed a finite volume ENO method in the convection step, while Wang et al.[**?** **?** ] proposed high order finite difference methods with subcell resolution reconstructing the reaction step. However, as pointed out by Yee et al.[**?** ], the subcell resolution method and its nonlinear filter counterparts[**?** ] 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 interfacial tracking methods, such as the level set method, the VOF method and the front tracking method, seem as a good option for simulating reacting flows. In fact, they have been used in the premixed combustion with the instantaneous flame viewed as an infinitely thin interface between fresh and burned gases[**?** **?** ], and also used in alleviating the nonphysical phenomena[**?** ] in the simple two-phases detonations by tracking the inert shock as an interface. However, since the general chemical dynamic model comprises of multi-species with a finite rate of reactions, there is a continuous reacting region other than a traditional two-phases interface, hence, these interfacial tracking methods mentioned above cannot solve the stiff problem generated in chemical flows well.

For solving the interface/free surface fluid flow problems, the marker and cell (MAC) method is regarded as the basis of interfacial tracking techniques[**?** ]. 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 centre. The cell classification is updated at each 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[**?** **?** **?** ]. The main advantages of the MAC method are that it eliminates all logic problems associated with interfaces and readily extended to three-dimensional computations. However, the storage increase significantly, because a large number of particle coordinates must be stored. 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 wave and the chemical reaction.

In this paper, by introducing two kinds of virtual Lagrangian points, we propose a dual information preserving method to cure the spurious numerical propagation phenomenon in simulating 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 virtual 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 and one Lagrangian cell-point are introduced in each cell at the beginning, and all particle-points are tracked in the whole computation, and the information on the cell-point is determined as: if there are particle-points in current cell, the information is updated by averaging all particle-points' information; else if there are cell-points entered, the information is updated by averaging all entered cell-points' information; otherwise a new cell-point is set at the cell center and its transport value is obtained by interpolating those of contiguous cell-points. 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 it as dual information preserving (DIP) method. In addition, this paper developed a numerical perturbation method to solve the fractionated 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 fractionated reaction step, analysis of stability and numerical examples are also presented. A series of examples, including one- and two- dimensional problems, simplified reaction model 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.

Our task in this study is to develop a new numerical method for the systems of ordinary differential equations

$$\boldsymbol{y}' = \boldsymbol{f}(t, \boldsymbol{y}(t)), \quad \boldsymbol{y}(0) = \boldsymbol{y}_0. \tag{1.1}$$

This eqautions is really easy to solve for

## 2. Numerical perturbation method

For Eq(**??**), one of the simplest scheme is the first-order explcit Euler scheme

$$\boldsymbol{y}_{n+1} - \boldsymbol{y}_n = \Delta t f(t, \boldsymbol{y}), \tag{2.1}$$

## 3. Conclusions

The dual information preserving method is firstly proposed to cure the numerical stiff problem generated in simulating the reacting flows. First, the species mass fraction equations are decoupled from the reactive Euler equations, and then they are further fractionated into the convection step and reaction step. The DIP method is actually proposed to deal with the species convection step. Two kinds of virtual Lagrangian point are introduced, one is limited in each Eulerian cell, and another one is tracked in the whole computation

domain. The number of each kind of virtual point is the same as the cell (grid) number.The DIP method can effectively eliminate the spurious propagation speed caused by the intermediate state generated by the numerical dissipation.

In this paper, the numerical perturbation (NP) methods are also developed to solve the fractionated reaction step (ODE equations). The NP schemes show several advantages, such as no iteration, high order accuracy and large stable region.

A series of numerical examples are used to demonstrate the reliability and robustness of the new methods.

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**References**