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A third-order explicit numerical scheme for stiff ODE equations and it use in **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

The ODE initial value problem

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

is considered in this paper. Having a history over two centuries, developing numerical methods for the ODE equations seems to be an old topic. However, if "some components of the solution decay much more rapidly than others"[1], the numercial methods will beset by the stiffness, which is still bothering us with stable and efficient problems in many disciplines, for instance in simulating the chemical kinetics and control theory.

About in the 1960s, explosion prosperity has happened in the study of the ODE equations. Especially the numerical stability researches done by Dahlquist, Hirshfelder and many other mathematicians, give a more clear glance at the numerical stiffness. Although it is still difficult to define "stiffness" in a precise

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way, many important theories proposed in that period, such as the famous A-stability[2] and the following L-stability[3], are powerful rulers to measure the stiffness of equations and the stable property of a numerical method. With those theoritic study, a fact is revealed that the explicit one-step methods, for instance, the Runge-Kutta methods, and all the multistep methods cannot be A-stable. Under this background and with the popular use of one-step methods, espcially Runge-Kutta class of methods, nearly a common sense have been achieved, that if we want to solve stiff equations stably with relatively large time steps, we must bear the cost of iteration in an implicit method, for the reason that only implicit methods can achieve both the A-stability and the high-order accuracy at the same time.

However, this statement may not be true beyond the frames of the one-step or the multistep methods. In fact, only linear methods have been thoroughly studied but few unlinear ODE methods have been considered or applied. For this reason, a few leaners hope to construct unlinear explicit A-stable methods to break the stablility-barrier of explicit methods and to apply more easily than using the implicit methods.

In this paper, we try to develop a high-order stiff-stable explicit numerical method

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. This equations is easy to solve for

2. Numerical perturbation method

For Eq(1.1), one of the simplest scheme is the first-order explcit Euler scheme

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

If we want to improve the accuracy order of scheme (2.1), one common method is add

But as proved by

A common way to get higher-order accuracy it to use sub-timestep in the intercal $[t, t + \Delta t]$, with the stable property in an explicit scheme is to construct unlinear schemes with more derivative informations from the original differential equation (1.1)

First, more dericative information can be get from the original differential equation (1.1) theoretically

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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