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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 of 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

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more clear glance at the numerical stiffness. Although it is still difficult to define "stiffness" in a precise 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 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. For this reason, some leaners still hope to construct explicit A-stable methods in a special nonlinear way, which can break the stablility-barrier of explicit methods and solve the stiff equations more easily. As an example, Wu[4, 5] constructed a sixth-order A-stable explicit one-step method by adding an exponential term into the traditional Taylor series methods[6, 7]. In our previous work [8], a third-order A-stable numercal perturbation (NP) method has been proposed and used in solving the stiff reacting ODE equations. But there is still no universal way to construct A-stable explicit method in arbitrary orders.

In this paper, we give a general study of the numerical perturbation method and construct 2nd-order to 7th-order A-stable one-step NP method. The main process of constructing a numerical perturbation method for ODEs is as follows: ① constructing a basic disretization scheme (the first-order explicit Euler scheme is used in this paper); ② constructing modified differential equations of the bacis disretization scheme by plusing a perturbation term which is power-series of Δt with undetermined coefficients; ③ using the original ODEs to obtain high-order derivatives; ④ eliminating truncated errors in the modified differential equations by determing suitable coeffients in the perturbation term with the relations of high-order derivatives; ⑤ transporting the coeffients to get the A-stable property.

This paper is organized as follows. In section 2, we give a detailed construction processs of NP method. In section 3, 2nd-order to 7th-order NP schemes is constructed. In section 4, we study the stability of NP schemes. A series of numerical examples are used to test the actual performance of the NP method in section 5. Conclutions are showned in section 6.

2. The numerical perturbation method

The NP method was first proposed by Gao and co-workers to solve the convective-diffusion equations. The significant difficulty of the NP method is how to get high-order derivatives of the original differential equations. For ODEs, every order derivative.can be obtained easily and mathematically. Then the construct pocess is given as follows.

① The basic disretization scheme

The simplest scheme to solve the ODEs (**??**) is the first order explicit Euler scheme

$$y_{n+1} - y_n = \Delta t f(t, y_n). \tag{2.1}$$

And we use it as the basic discretization scheme of the NP schemes.

② Perturbation term

In order to improve the accuracy orders of the basic discretization scheme (2.1), one common way is to add substeps between t and $t + \Delta t$. While we choose a very different and special way, adding a perturbation term p into the basic discretization scheme as

$$p(y_{n+1} - y_n) = \Delta t f(t, y_n). \tag{2.2}$$

Where p is defined as

$$p = 1 + \sum_{i=1}^{\infty} a_i \Delta t^i, \tag{2.3}$$

and the a_i are undetermined coefficients.

③ High-order derivatives

For ODEs with a given $f(t, y)$, we need the dericatives beforehand. Different from Runge-Kutta methods, the final NP schemes changes with different $f(t, y)$. This step may increase some theoretical and preparatory work. Fortunately, it's very easy to get the high-order dericatives from most ODEs.

In a unified form the dericatives can given as,

$$\begin{aligned} &\frac{dy}{dt} = f \\ &\frac{d^2y}{dt^2} = f'_t + f'_y f \\ &\frac{d^3y}{dt^3} = f''_{tt} + 2f''_{yt} f + f''_{yy} f^2 + {f'_y}^2 f + f'_y f'_t \\ &\dots \end{aligned} \tag{2.4}$$

④ Suitable coefficients in perturbation term

Using Taylor expasion,

$$y_{n+1} = y_n + \Delta t y'_n + \frac{\Delta t^2}{2} y''_n + \frac{\Delta t^3}{6} y'''_n + O(\Delta t^4) \tag{2.5}$$

Equation (2.2) changes to

$$\begin{aligned} \frac{dy}{dt} =& f(t, y) - \left(\frac{1}{2} \frac{d^2y}{dt^2} + a_1 \frac{dy}{dt} \right) \Delta t - \left(\frac{1}{6} \frac{d^3y}{dt^3} + \frac{a_1}{2} \frac{d^2y}{dt^2} + a_2 \frac{dy}{dt} \right) \Delta t^2 \\ &- \left(\frac{1}{24} \frac{d^4y}{dt^4} + \frac{a_1}{6} \frac{d^3y}{dt^3} + \frac{a_2}{2} \frac{d^2y}{dt^2} + a_3 \frac{dy}{dt} \right) \Delta t^3 + O(\Delta t^4) \end{aligned} \tag{2.6}$$

For convenience, the subscript n in y_n is omitted.

Clearly, if the second term in the right hand side becomes zero,

$$\frac{1}{2}\frac{d^2y}{dt^2} + a_1\frac{dy}{dt} = 0, \tag{2.7}$$

then equation (2.2) has second-order accuracy. Similarly, we can get higher order schemes by elimination more terms, thus we have

$$\begin{aligned} a_1 =& -\frac{y''}{2y'} \\ a_2 =& \frac{y''^2}{4y'^2} - \frac{y'''}{6y'} \\ a_3 =& -\frac{y^{(4)}}{24y'} - \frac{y''^3}{8y'^3} + \frac{y'''y''}{12y'^2} \\ & \cdots \end{aligned} \tag{2.8}$$

Then we can get the NP schemes as

$$y_{n+1} = y_n + \frac{\Delta t f(t, y_n)}{p}, \tag{2.9}$$

where, $p = 1 + a_1\Delta t + a_2\Delta t^2 + \cdots$

⑤ Transforming the coeffiecient a_i

As far, we have get the NP schemes, however they maybe not have enough stability. Consdier a special linear ODE $f = qy$, the dericatives are

$$y^{(i)} = q^i y \quad i = 1, 2, \cdots . \tag{2.10}$$

Then a_i are

$$a_1 = -\frac{q}{2}a_1 = -\frac{q}{2}$$

2.1. The Taylor series method

$$y_{n+1} = y_n + \frac{dy}{dt}\Delta t + \frac{1}{2}\frac{d^2y}{dt^2} + \cdots \tag{2.11}$$

$$\begin{aligned} f &= Ay \\ \frac{dy}{dt} &= f = Ay \\ \frac{d^2y}{dt^2} &= A^2y \end{aligned} \tag{2.11}$$

$$y_{n+1} = y_n + Ay_n\Delta t + A^2\Delta t\frac{1}{2}\frac{d^2y}{dt^2} + \cdots \tag{2.11}$$

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

3. Numerical perturbation method

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

$$\boldsymbol{y}_{n+1} - \boldsymbol{y}_n = \Delta t f(t, \boldsymbol{y}) \tag{3.0}$$

If we want to improve the accuracy order of scheme (3), 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

4. 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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