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A third-order explicit numerical scheme for stiff ODE equations and its use in reactive 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 particle-point are updated according to the velocity field. By using the DIP method, the incorrect activation 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 perturbation method, Shock-capturing scheme

1. Introduction

The ODE initial value problem

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

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 numerical methods will be 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, Hirschfelder 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 theoretic 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, especially 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 learners still hope to construct explicit A-stable methods in a special nonlinear way, which can break the stability-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 numerical 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 discretization scheme (the first-order explicit Euler scheme is used in this paper); ② constructing modified differential equations of the basic discretization 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 determining suitable coefficients in the perturbation term with the relations of high-order derivatives; ⑤ transporting the coefficients to get the A-stable property.

This paper is organized as follows. In section 2, we give a detailed construction process 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. Conclusions 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 process is given as follows.

- ① The basic discretization scheme

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

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

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

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

Where p is defined as

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

and the a_i are undetermined coefficients.

③ High-order derivatives

For ODEs with a given $f(t, y)$, we need the derivatives 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 derivatives from most ODEs.

In a unified form the derivatives can given as,

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

④ Suitable coefficients in perturbation term

Using Taylor expansion,

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

Equation (2.2) changes to

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

For convenience, the subscript n in y_n is omitted.

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

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

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

$$\begin{aligned} a_1 &= -\frac{y''}{2y'} \\ a_2 &= -\frac{y'''}{6y'} - \frac{a_1 y''}{2y'} \\ a_3 &= -\frac{y^{(4)}}{24y'} - \frac{a_1 y'''}{6y'} - \frac{a_2 y''}{2y'} \\ &\dots \end{aligned} \quad (2.8)$$

a_i can also be written in the form

$$a_i = -\sum_{n=1}^i \frac{y^{(n+1)} a_{i-n}}{(n+1)! y'} \quad (2.9)$$

where, $a_0 = 1$.

Then we can get the N-th order NP schemes as

$$y_{n+1} = y_n + \frac{\Delta t f(t, y_n)}{p_N}, \quad (2.10)$$

where, $p = \sum_{i=0}^N a_i \Delta t^i$

As far, we have constructed the NP schemes, however those schemes may not stable enough in every order. We still can do some skills to tranform p_N with $\overline{p_N}$ to improve the stability, where

$$\overline{p_N} = p_N + O(\Delta t^{n+1}) \quad (2.11)$$

and $\overline{p_N}$ is in the form of

$$\overline{p_N} = \frac{1 + \sum_{i=1}^N b_i \Delta t^i}{1 + \sum_{i=1}^N c_i \Delta t^i} \quad (2.12)$$

The construction of b_i and c_i will be talked in the next section with the analysis of the stability.

3. Stable analysis of the NP schemes

3.1. A-stable and L-stable

In a Dahlquist test equation with $f(t, y) = qy$, the solution of a method can be expressed as

$$y_{n+1} = R(h) x_n \quad (3.1)$$

where, $h = q\Delta t$, and function $R(h)$ is called the stability function of the method. The set

$$S = \{z \in \mathbb{C}; |R(h)| \leq 1\} \quad (3.2)$$

is called the stable domain of the method.

Defination I *A – stable*

Methods are A-stable if the stable domain contains all the positive half-plane.

Defination II *L – stable*

Methods are L-stable if they are A-stable and $R(h) \rightarrow 0$ as $h \rightarrow -\infty$

3.2. *Stable functions of the NP schemes*

In the ODE with a linear $f(t, y) = qy$, the dericatives are in very simple forms as

$$y^{(i)} = q^i y \quad i = 1, 2, \dots \quad (3.3)$$

Then a_i are

$$\begin{aligned} a_1 &= -\frac{q}{2}, a_2 = \frac{q^2}{12}, a_3 = -\frac{q^3}{12}, \\ a_4 &= \frac{29q^4}{720}, a_5 = -\frac{q^5}{72}, a_6 = \frac{53q^6}{15120}, \dots \end{aligned} \quad (3.4)$$

The stability functions of N-th order NP schemes are given as follows in Table 1. As a comprasion, stablity functions of implicit Runge-Kutta methods are also given in the same table.

Table 3.1: The stable functions of N-th order NP schemes

NP schemes	$R(h)$	Implicit Runge-Kutta methods [9]	$R(h)$
2	$\frac{1+h/2}{1-h/2}$	Implicit midpoint	$\frac{1+h/2}{1-h/2}$
3	$\frac{1+h/2+h^2/12}{1-h/2+h^2/12}$	Hammer-Hollingsw 4	$\frac{1+h/2+h^2/12}{1-h/2+h^2/12}$
4	$\frac{1+h/2+h^2/12-h^3/12}{1-h/2+h^2/12-h^3/12}$	Butcher's Lobatto 4	$\frac{1+3h/4+h^2/4+h^3/24}{1-h/4}$
5	$\frac{1+h/2+h^2/12-h^3/12+29h^4/720}{1-h/2+h^2/12-h^3/12+29h^4/720}$	Kuntzm.-Butcher 6	$\frac{1+h/2+h^2/10+h^3/120}{1-h/2+h^2/10-h^3/120}$
6	$\frac{1+h/2+h^2/12-h^3/12+29h^4/720-h^5/72}{1-h/2+h^2/12-h^3/12+29h^4/720-h^5/72}$	Butcher's Lobatto 6	$\frac{1+2h/3+h^2/5+h^3/30+h^4/360}{1-h/3+h^2/30}$
7	$\frac{1+h/2+h^2/12-h^3/12+29h^4/720-h^5/72+53h^6/15120}{1-h/2+h^2/12-h^3/12+29h^4/720-h^5/72+53h^6/15120}$	—	—

3.3. *Stability domains of NP schemes*

The stable domains of N-th order NP schemes and implicit Runge-Kutta methods are given in Fig.1 We can see 2nd-order and 3rd-order NP schemes are A-stable and higher-order schemes also have large stability domains in the positive half-plane. The NP schemes can approach the stability performance of the implicit Runge-Kutta methods.

4. **Transformed coefficients NP method**

Although the NP methods have the similar stability with the implicit Runge-Kutta methods, but not all of them can achieve A-stability and none of them reaches L-stability. We still hope for a more stable property of NP method. A possible way is to construct a new perturbation term \overline{p}_N by transforming the coefficients in it.

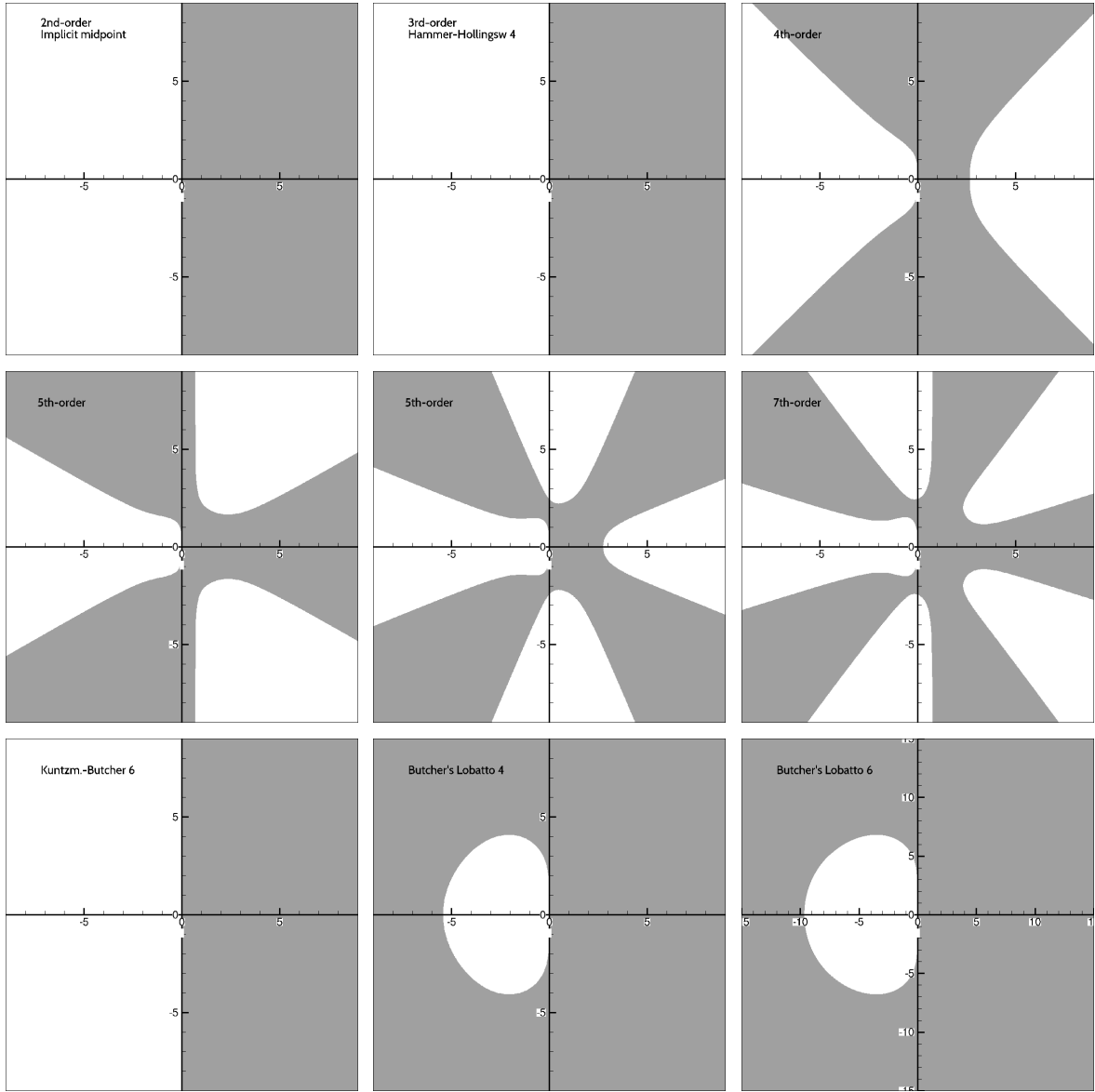


Figure 1: Stability domains for NP schemes

As $p_N = p + O(\Delta t^N)$, if $\overline{p_N} = p_N + O(\Delta t^N)$, the new NP scheme has the same truncation error order with the old one. Here, we assume the new $\overline{p_N}$ with the form

$$\overline{p_N} = \frac{1 + b_1 \Delta t + b_2 \Delta t + \cdots + b_{N-1} \Delta t^{N-1}}{1 + c_1 \Delta t + c_2 \Delta t^2 + \cdots + c_{N-2} \Delta t^{N-2}}. \quad (4.1)$$

and $c_{N-2} = -b_{N-1}/f'_y$. Here we have $2N - 4$ coefficients and $N - 1$ power series relations, so $N - 3$ coefficients are undetermined. In follows, we will consider the transformed NP method in different orders.

4.1. The third-order transformed NP method

The second order method has too little coefficients, there is no space to transform, so we begin with the third-order method. For the third-order method with p_3 , there is no undetermined coefficients, the new

$$\overline{p_3} = \frac{1 + b_1 \Delta t + b_2 \Delta t^2}{1 + c_1 \Delta t} = 1 + a_1 \Delta t + a_2 \Delta t^2 + O(\Delta t^3), \quad (4.2)$$

where $c_1 = -b_2/f'_y$. The transformed coefficients can be solved by the relations

$$\begin{aligned} b_1 &= a_1 + c_1 \\ b_2 &= a_2 + a_1 c_1 \end{aligned} \quad (4.3)$$

Then the transformed coefficients b_1 and b_2 are

$$b_1 = a_1 - \frac{a_2}{f'_y + a_1}, \quad b_2 = \frac{a_2}{1 + a_1/f'_y} \quad (4.4)$$

It is easy to get the stability function as

$$R(h) = \frac{1 + h/3}{1 - 2h/3 + h^2/6} \quad (4.5)$$

4.2. The fourth-order transformed NP method

The perturbation term for the fourth-order NP method is in the form

$$\overline{p_4} = \frac{1 + b_1 \Delta t + b_2 \Delta t^2 + b_3 \Delta t^3}{1 + c_1 \Delta t + c_2 \Delta t^2} \quad (4.6)$$

and $c_2 = -b_3/f'_y$. By the relation

$$\overline{p_4} = 1 + a_1 \Delta t + a_2 \Delta t^2 + a_3 \Delta t^3 + O(\Delta t^4). \quad (4.7)$$

We can get the relations

$$\begin{aligned} b_1 &= a_1 + c_1 \\ b_2 &= a_2 + a_1 c_1 + c_2 \\ b_3 &= a_3 + a_2 c_1 + a_1 c_2 \end{aligned} \quad (4.8)$$

In the 4th-order method the c_1 is undetermined, we set $c_1 = -6a_1$. Then the transformed coefficients are

$$\begin{aligned} c_1 &= -6a_1, c_2 = -b_3/f'_y \\ b_1 &= -5a_1, b_2 = a_2 - 6a_1^2 - \frac{a_3 - 6a_1a_2}{f'_y + a_1}, b_3 = \frac{a_3 - 6a_1a_2}{1 + a_1/f'_y} \end{aligned} \quad (4.9)$$

t The stability function is given as

$$R(h) = \frac{1 + 7h/2 + 5h^2/4}{1 + 5h/2 - 7h^2/4 + h^3/3} \quad (4.10)$$

4.3. The fifth-order transformed NP methods

The perturbation term for the fifth-order NP method is

$$\overline{p}_5 = \frac{1 + b_1\Delta t + b_2\Delta t^2 + b_3\Delta t^3 + b_4\Delta t^4}{1 + c_1\Delta t + c_2\Delta t^2 + c_3\Delta t^3}, \quad (4.11)$$

and $c_3 = -b_4/f'_y$. The transformed coefficients are obtained as follows

$$\begin{aligned} b_1 &= a_1 + c_1 \\ b_2 &= a_2 + a_1c_1 + c_2 \\ b_3 &= a_3 + a_2c_1 + a_1c_2 + c_3 \\ b_4 &= a_4 + a_3c_1 + a_2c_2 + a_1c_3 \end{aligned} \quad (4.12)$$

We set the undetermined coefficients as $c_1 = -6a_1, c_2 = -144a_2$. Then the transformed coefficients are get as

$$\begin{aligned} c_1 &= -6a_1, c_2 = -144a_2, c_3 = -b_4/f'_y \\ b_1 &= -5a_1, b_2 = -6a_1^2 - 143a_2, b_3 = a_3 - 150a_1a_2 - \frac{a_4 - 4a_1a_3 + 29a_2^2}{f'_y + a_1}, b_4 = \frac{a_4 - 6a_1a_3 - 144a_2^2}{1 + a_1/f'_y} \end{aligned} \quad (4.13)$$

The stability function is

$$R(h) = \frac{1 + 7h/2 - 125h^2/12 - 1229h^3/360}{1 + 5h/2 - 161h^2/12 + 3091h^3/360 - 871h^4/360} \quad (4.14)$$

4.4. The sixth-order transformed NP method

The perturbation term for the sixth-order NP method is

$$\overline{p}_6 = \frac{1 + b_1\Delta t + b_2\Delta t^2 + b_3\Delta t^3 + b_4\Delta t^4 + b_5\Delta t^5}{1 + c_1\Delta t + c_2\Delta t^2 + c_3\Delta t^3 + c_4\Delta t^4} \quad (4.15)$$

and $c_4 = -b_5/f'_y$. The transformed coefficients are obtained as follows

$$\begin{aligned}
b_1 &= a_1 + c_1 \\
b_2 &= a_2 + a_1c_1 + c_2 \\
b_3 &= a_3 + a_2c_1 + a_1c_2 + c_3 \\
b_4 &= a_4 + a_3c_1 + a_2c_2 + a_1c_3 + c_4 \\
b_5 &= a_5 + a_4c_1 + a_3c_2 + a_2c_3 + a_1c_4
\end{aligned} \tag{4.16}$$

We use the undetermined coefficients $c_1 = -6a_1, c_2 = 144a_2,$ and $c_3 = 600a_3$. Then the stability function is

$$R(h) = \frac{1 + 7h/2 - 125h^2/12 - 263h^3/6 - 2029h^4/144}{1 + 5h/2 - 161h^2/12 - 335h^3/6 + 5171h^4/144 - 3643h^5/360} \tag{4.17}$$

4.5. The seven-order transformed NP methods

$$\overline{p_7} = \frac{1 + b_1\Delta t + b_2\Delta t^2 + b_3\Delta t^3 + b_4\Delta t^4 + b_5\Delta t^5 + b_6\Delta t^6}{1 + c_1\Delta t + c_2\Delta t^2 + c_3\Delta t^3 + c_4\Delta t^4 + c_5\Delta t^5}, \tag{4.18}$$

and $c_5 = -b_6/f'_y$. The transformed coefficients are obtained as follows

$$\begin{aligned}
b_1 &= a_1 + c_1 \\
b_2 &= a_2 + a_1c_1 \\
b_3 &= a_3 + a_2c_1 + a_1c_2 + c_3 \\
b_4 &= a_4 + a_3c_1 + a_2c_2 + a_1c_3 + c_4 \\
b_5 &= a_5 + a_4c_1 + a_3c_2 + a_2c_3 + a_1c_4 + c_5 \\
b_6 &= a_6 + a_5c_1 + a_4c_2 + a_3c_3 + a_2c_4 + a_1c_5
\end{aligned} \tag{4.19}$$

The undetermined coefficients are set as $c_1 = -6a_1, c_2 = 144a_2, c_3 = -144a_3$ and $c_4 = 1440a_4$. The stability function is

$$R(h) = \frac{1 + 7h/2 + 163h^2/12 + 109h^3/6 + 39449h^4/720 + 52063h^5/3024}{1 + 5h/2 + 127h^2/12 + 37h^3/6 + 30809h^4/720 - 15207h^5/494 + 52091h^6/7560} \tag{4.20}$$

5. The stability analysis of the transformed NP method

The stability functions of the transformed NP methods are collected in Table 5.1, and the stability domains are showed in Fig.2. It is obviously that all the 3rd-order to 7th-order transformed NP methods are A-stable and L-stable and their unstability domains are limited in finite regions.

6. Numerical tests for the NP methods and the transformed NP methods

Some numerical tests are considered in this section. There are two purposes, one is to show the construction process of the NP methods in the real coding and using background as the new methods are far from the

Table 5.1: The stable functions of N-th order transformed NP methods

Order	$R(h)$
3	$\frac{1+h/3}{1-2h/3+h^2/6}$
4	$\frac{1+7h/2+5h^2/4}{1+5h/2-7h^2/4+h^3/3}$
5	$\frac{1+7h/2-125h^2/12-1229h^3/360}{1+5h/2-161h^2/12+3091h^3/360-871h^4/360}$
6	$\frac{1+7h/2-125h^2/12-263h^3/6-2029h^4/144}{1+5h/2-161h^2/12-335h^3/6+5171h^4/144-3643h^5/360}$
7	$\frac{1+7h/2+163h^2/12+109h^3/6+39449h^4/720+52063h^5/3024}{1+5h/2+127h^2/12+37h^3/6+30809h^4/720-15207h^5/494+52091h^6/7560}$

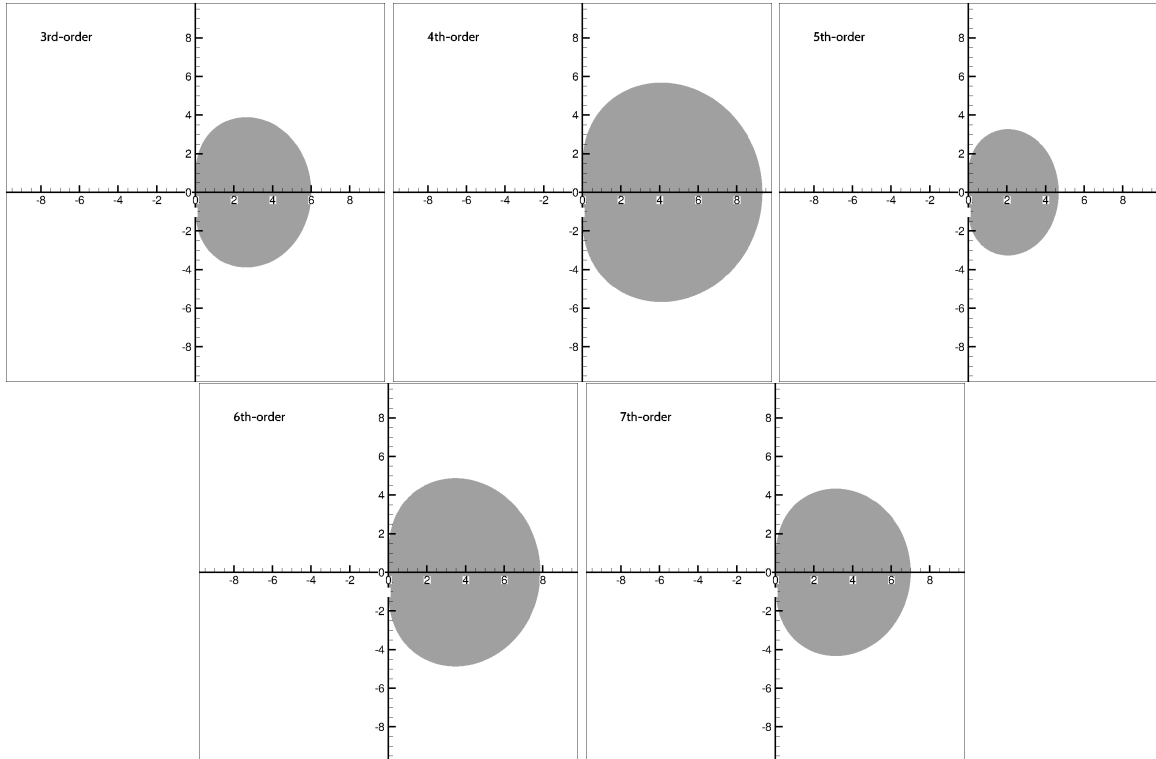


Figure 2: Stability domains for the transformed NP methods

methods frequently used; the other one purpose is to test the real performance of the new method espially in the computing of the nolinear ODE and ODEs.

Example 1 [10, 11]

$$\begin{aligned} y'(x) &= g'(x) + \lambda(y - g(x)), \quad y = g(0) \text{ at } x = 0 \\ g(x) &= 10 - (10 + x)e^{-x}, \quad \lambda \text{ real.} \end{aligned} \quad (6.1)$$

In this example we consider the error and the convergence order changing with different stiffness which is determined by $\Delta x \lambda$. For the method without stiff stability, the error will be significantly increasing and even breakup when $\Delta x \lambda$ is large.

For Eq.(6.1) the high-order derivatives are

$$y^{(n)} = g^{(n)} + \lambda^n(y - g), \quad n = 2, 3, \dots \quad (6.2)$$

and

$$\begin{aligned} g' &= (9 + x)e^{-x}, g'' = -(8 + x)e^{-x}, g^{(3)} = (7 + x)e^{-x} \\ g^{(4)} &= -(6 + x)e^{-x}, g^{(5)} = (5 + x)e^{-x}, g^{(6)} = -(4 + x)e^{-x}. \end{aligned} \quad (6.3)$$

Then we can get the Perturbation coefficients a_i by Eq.(2.8).

$$a_1 = -\frac{y''}{2y'}, \quad a_2 = \frac{y''^2}{4y'} - \frac{y'''}{6y'}, \quad \dots \quad (6.4)$$

Also the transformed Perturbation coefficients b_i can be constructed through the process in Chapter 4.

In this example, the step is fixed as $\Delta x = 0.2$ and the final time is $t = 5.0$ The errors

$$Err = \frac{|y(x) - \text{Exact}(t)|}{|y(x)|} \quad (6.5)$$

and the convergence orders

$$\text{Order} = \log_2 \frac{Err(\Delta x)}{Err(\Delta x/2)} \quad (6.6)$$

of different order NP methods and transformed NP methods are plotted in Fig.3 and Fig.4. with a slight stiffness as $-\Delta x \lambda < 1$ all the methods can get their theoretical convergence orders. But when $-\Delta x \lambda > 10$, there are significant errors appair with the NP methods, and the results become unacceptable. While the errors computed by the transformed NP methods will increase and then hold steady to a value near 10^{-3} and the order all convergence to 1 no matter how huge the λ becomes.

Example 2 [12, 13]

$$\begin{aligned} y_1' &= y_2, \quad y_1(0) = 2, \\ \varepsilon y_2' &= (1 - y_1^2)y_2 - y_1, \quad y_2(0) = 0, \quad \varepsilon = 10^{-6} \end{aligned} \quad (6.7)$$

This exmaple is known as the famous Van der Pol's equation which is very stiff.

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

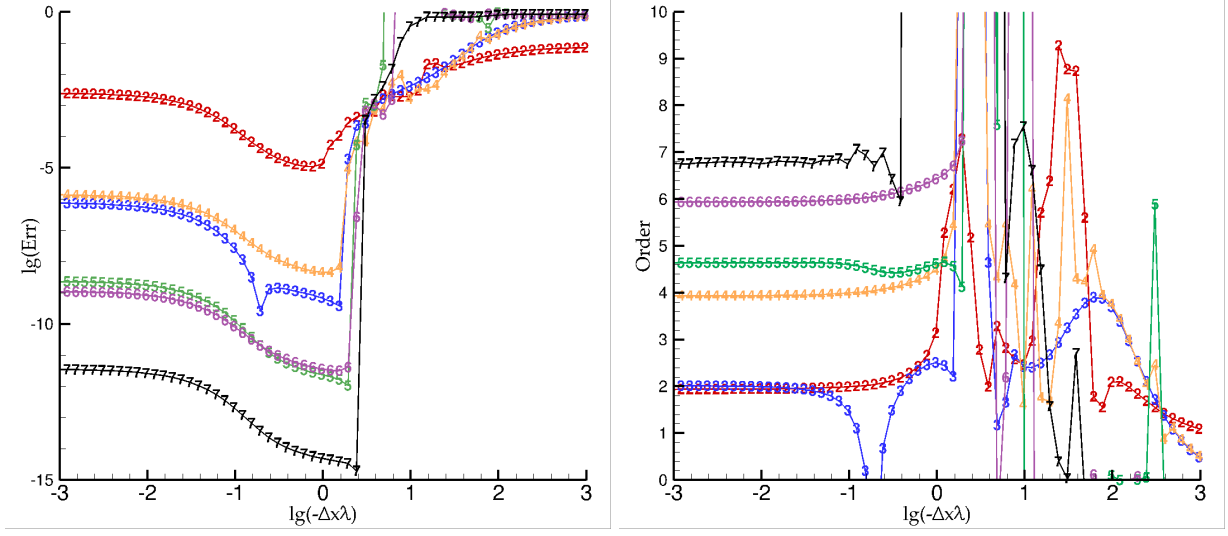


Figure 3: Errors and convergence orders for the Example 1 by the NP methods

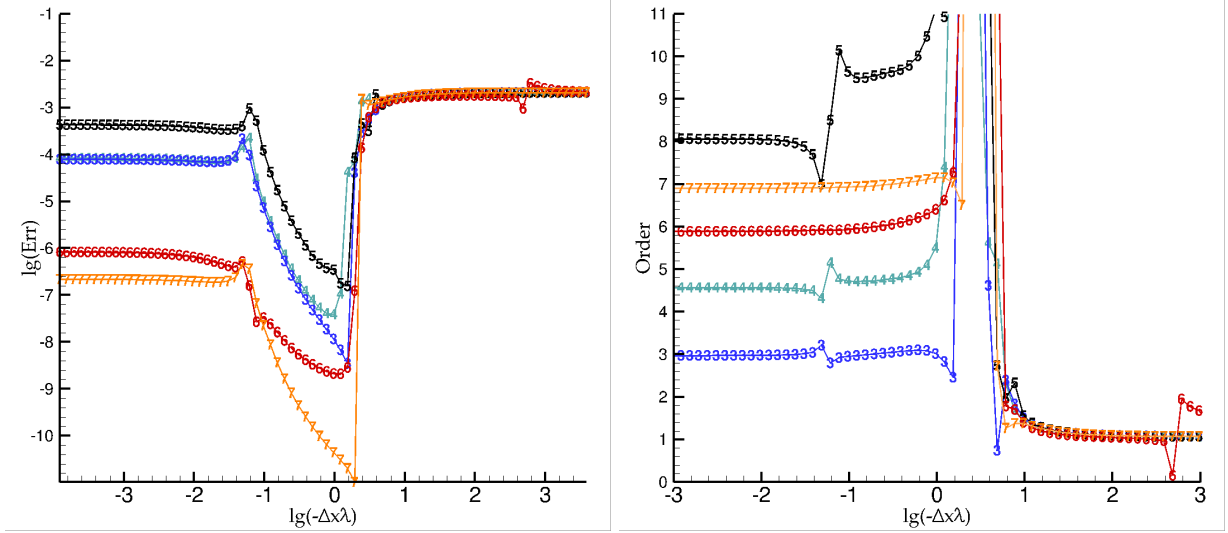


Figure 4: Errors and convergence orders for the Example 1 by the transformed NP methods

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

$$\frac{\partial u}{\partial t} + \nabla \cdot F = S(u) \quad (6.8)$$

7. 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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