FOURTH-ORDER TIME-STEPPING FOR STIFF PDEs

LIU YU TING

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1 Introduction

Many numerical time-stepping methods have been developed to solve stiff partial differential equations (PDEs). In this paper, we focus on the exponential time-differencing fourth-order Runge–Kutta (ETDRK4) method proposed by Cox and Matthews. However, the evaluation of the Runge–Kutta coefficients may suffer from cancellation errors when the linear operator has eigenvalues close to zero. In existing implementations, these coefficients are typically evaluated in a diagonal setting. To solve the cancellation error and extend the method to non-diagonal linear operators, the authors modify the method of evaluating the coefficients of Runge-Kutta by using contour integrals in the complex plane.

2 Method Explanation

2.1 Integrating factor formulation

After discretizing the spatial part of PDE, we can get a system of ordinary differential equations

$$u_t = \mathbf{L}u + \mathbf{N}(u, t)$$

where $\mathbf{L}$ is the discretized linear operator represented as a matrix and $\mathbf{N}$ is the nonlinear function.
To solve the stiff problem, we apply an integrating factor $e^{-\mathbf{L}t}$ and then integrate from t_n to $t_n + h$. We get

$$u_{n+1} = e^{\mathbf{L}h}u_n + e^{\mathbf{L}h}\int_0^h e^{-\mathbf{L}\tau}\mathbf{N}(u(t_n+\tau), t_n+\tau)d\tau.$$

Since the linear part is solved exactly, the step of time is not restricted by linear stability constraints.
To evaluate the solution at the next time step, the integral term must be approximated.

2.2 ETDRK4 coefficients and cancellation errors

Following Cox and Matthews, we use the ETDRK4 scheme here to solve the u_{n+1} by

$$\begin{aligned}
\alpha &= h^{-2}\mathbf{L}^{-3}\big[-4-\mathbf{L}h+e^{\mathbf{L}h}\big(4-3\mathbf{L}h+(\mathbf{L}h)^2\big)\big],\\
\beta &= h^{-2}\mathbf{L}^{-3}\big[2+\mathbf{L}h+e^{\mathbf{L}h}\big(-2+\mathbf{L}h\big)\big],\\
\gamma &= h^{-2}\mathbf{L}^{-3}\big[-4-3\mathbf{L}h-(\mathbf{L}h)^2+e^{\mathbf{L}h}\big(4-\mathbf{L}h\big)\big].\\
a_n &= e^{\mathbf{L}h/2}u_n+\mathbf{L}^{-1}(e^{\mathbf{L}h/2}-\mathbf{I})\mathbf{N}(u_n,t_n),\\
b_n &= e^{\mathbf{L}h/2}u_n+\mathbf{L}^{-1}(e^{\mathbf{L}h/2}-\mathbf{I})\mathbf{N}(a_n,t_n+h/2),\\
c_n &= e^{\mathbf{L}h/2}a_n+\mathbf{L}^{-1}(e^{\mathbf{L}h/2}-\mathbf{I})(2\mathbf{N}(b_n,t_n+h/2)-\mathbf{N}(u_n,t_n)),\\
u_{n+1} &= e^{Lh}u_n+h^{-2}\mathbf{L}^{-3}[\alpha\mathbf{N}(u_n,t_n)+2\beta[\mathbf{N}(a_n,t_n+h/2)+\mathbf{N}(b_n,t_n+h/2)]+\gamma\mathbf{N}(c_n,t_n+h)].
\end{aligned}$$

Unfortunately, α, β and γ have the cancellation error problem when $\mathbf{L}$ has eigenvalues close to zero since they are higher-order analogues of $\frac{e^z-1}{z}$. Cox and Matthews solved this problem using a cutoff function. When there is an eigenvalue close to zero, they apply Taylor expansions to the diagonal elements of the operator. However, their approach mainly relies on the diagonal structure of the linear operator. Here, instead of assuming a diagonal linear operator, we propose an alternative approach to evaluate the coefficients.

2.3 Evaluation of Matrix Functions via Contour Integrals

In this paper, the authors modify the method for computing the coefficients by using contour integrals in the complex plane, which resolves the cancellation error problem.

The Cauchy integral formula states that, if f is holomorphic on the curve Γ and its interior, then

$$f(z)=\frac{1}{2\pi i}\int_\Gamma \frac{f(t)}{t-z}dt$$

for all z in the interior of Γ.
We define the matrix function f($\mathbf{L}$) by

$$f(\mathbf{L})=\frac{1}{2\pi i}\int_\Gamma f(t)(t\mathbf{I}-\mathbf{L})^{-1}dt.$$

where all eigenvalues of $\mathbf{L}$ are in the interior of Γ.
Since Γ does not intersect the spectrum of $\mathbf{L}$, the resolvent $(t\mathbf{I}-\mathbf{L})^{-1}$ is well-defined for all $t \in \Gamma$. Notice that Γ need to stay away from zero to avoid the cancellation error, since zero is the removable singularity of coefficients and $\mathbf{L}^{-1}(e^{\mathbf{L}h/2}-\mathbf{I})$.
From the contour integral formula, cancellation errors are avoided because the integrand does not contain terms of the form $\frac{0}{0}$ along the contour.
From the formula of α, β, γ and $\mathbf{L}^{-1}(e^{\mathbf{L}h/2}-\mathbf{I})$, we find that they are all holomorphic in $\mathbb{C} \setminus \{0\}$, where 0 is the removable singularity. Thus after we extend all of them with $f(0) = \lim_{x\to 0} f(x)$, we can use the contour integral to compute them.
For both integrals, we use trapezoidal rule to approximate them with 32 or 64 equally spaced points. If $\mathbf{L}$ is diagonal, the coefficients can be evaluated directly as scalar functions of the diagonal entries. If not, then the coefficients are evaluated through the corresponding matrix functions defined by the contour integral. Since $\mathbf{L}^{-1}(e^{\mathbf{L}h/2}-\mathbf{I})$ also suffers from cancellation error, it is evaluated using a contour integral as well.

From the formula of α, β, γ and $\mathbf{L}^{-1}(e^{\mathbf{L}h/2}-\mathbf{I})$, we know that they are independent in time. Thus they only need to be computed once before the time-stepping procedure. Therefore, this method requires only a little additional computational cost.

3 Experience

First, since the behavior of γ has already been compared in the paper, we compare the coefficients α and β by contour integral and direct evaluation for different values of z. To avoid the cancellation error happen in contour integral, we choose $R = 2$ except $R = 1$.

Table 1: Computation of α using the direct formula, contour integral, and high-precision exact evaluation ($h = 1$, $R = 2$, $M = 32$).

z	Formula	Contour ($R = 2, M = 32$)	Exact
10	$1.62994446881570 \times 10^{3}$	$1.62994446881570 \times 10^{3}$	$1.62994446881570 \times 10^{3}$
1	$4.36563656918090 \times 10^{-1}$	$4.36563656918088 \times 10^{-1}$	$4.36563656918090 \times 10^{-1}$
10^{-1}	$1.84106060653555 \times 10^{-1}$	$1.84106060652688 \times 10^{-1}$	$1.84106060652688 \times 10^{-1}$
10^{-2}	$1.68340855921656 \times 10^{-1}$	$1.68340855605248 \times 10^{-1}$	$1.68340855605248 \times 10^{-1}$
10^{-3}	$1.66833657999632 \times 10^{-1}$	$1.66833408355561 \times 10^{-1}$	$1.66833408355561 \times 10^{-1}$
10^{-4}	$1.66977542903624 \times 10^{-1}$	$1.66683334083356 \times 10^{-1}$	$1.66683334083356 \times 10^{-1}$
10^{-5}	0	$1.66668333340833 \times 10^{-1}$	$1.66668333340833 \times 10^{-1}$
10^{-6}	0	$1.66666833333408 \times 10^{-1}$	$1.66666833333408 \times 10^{-1}$
10^{-7}	0	$1.66666683333334 \times 10^{-1}$	$1.66666683333334 \times 10^{-1}$
10^{-8}	0	$1.66666668333333 \times 10^{-1}$	$1.66666668333333 \times 10^{-1}$
10^{-9}	0	$1.66666666833333 \times 10^{-1}$	$1.66666666833333 \times 10^{-1}$

Table 2: Computation of β using the direct formula, contour integral, and high-precision reference values ($h = 1$, $R = 2$, $M = 32$).

z	Formula	Contour ($R = 2, M = 32$)	Exact
10	$1.76223726358454 \times 10^{2}$	$1.76223726358454 \times 10^{2}$	$1.76223726358454 \times 10^{2}$
1	$2.81718171540955 \times 10^{-1}$	$2.81718171540955 \times 10^{-1}$	$2.81718171540955 \times 10^{-1}$
10^{-1}	$1.75255656269524 \times 10^{-1}$	$1.75255656269513 \times 10^{-1}$	$1.75255656269513 \times 10^{-1}$
10^{-2}	$1.67502505643569 \times 10^{-1}$	$1.67502505565491 \times 10^{-1}$	$1.67502505565491 \times 10^{-1}$
10^{-3}	$1.66749725138970 \times 10^{-1}$	$1.66750025005557 \times 10^{-1}$	$1.66750025005557 \times 10^{-1}$
10^{-4}	$1.66977542903624 \times 10^{-1}$	$1.66675000250006 \times 10^{-1}$	$1.66675000250006 \times 10^{-1}$
10^{-5}	$4.44089209850063 \times 10^{-1}$	$1.66667500002500 \times 10^{-1}$	$1.66667500002500 \times 10^{-1}$
10^{-6}	0	$1.66666750000025 \times 10^{-1}$	$1.66666750000025 \times 10^{-1}$
10^{-7}	0	$1.66666675000000 \times 10^{-1}$	$1.66666675000000 \times 10^{-1}$
10^{-8}	0	$1.66666667500000 \times 10^{-1}$	$1.66666667500000 \times 10^{-1}$
10^{-9}	0	$1.66666666750000 \times 10^{-1}$	$1.66666666750000 \times 10^{-1}$

From the tables, the coefficients computed by the contour integral have smaller errors. However, the directly evaluated coefficients have larger errors when z is close to zero due to cancellation errors.

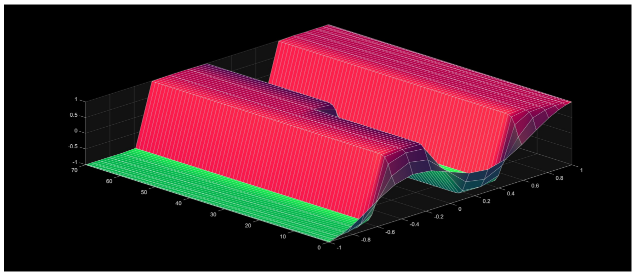
Next, we apply the same method, ETDRK4, with time step = 0.01 and two different approaches for evaluating the coefficients of Runge-Kutta: contour integral and direct evaluation.

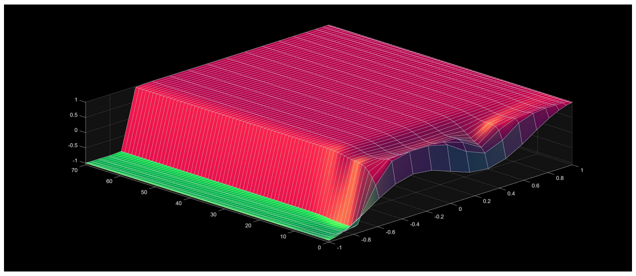
We take the Allen–Cahn equation as a test example.

$$u_t = 0.002u_{xx} + u - u^3, \quad -1 \le x \le 1, \quad t \ge 0$$

with initial and boundary conditions

$$u(x,0) = 0.53x + 0.47\sin(-1.5\pi x), \quad u(-1,t) = -1, \qquad u(1,t) = 1, \quad t \ge 0.$$


(a) contour integral


(b) direct evaluation

The solution obtained by direct evaluation is incorrect due to cancellation error.

4 Conclusion

Since the original way to evaluate the coefficients of Runge-Kutta might have cancellation error when the linear operator has eigenvalues close to 0, this paper proposes a new way to evaluate coefficients of Runge-Kutta using contour integrals.

This evaluation generalizes the ETDRK4 method which can be applied not only to the diagonal linear operator but also to the non-diagonal operator. Moreover, it does not need much additional computational cost since the coefficients only need to be evaluated once before time-stepping.

However, in the implementation, the contour needs to be chosen carefully, especially the radius of the contour. The eigenvalues of the matrix should lie inside the contour, and the contour should stay away from zero to avoid cancellation errors. In fact, we can just choose a sufficiently large radius to solve this problem and it only increases a little computational cost since we use the trapezoidal rule with 32 or 64 points to approximate the integral.

Overall, the contour integral approach provides a simple and effective way to generalize the ETDRK4 method for solving stiff PDEs.