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A Class of Adaptive Exponentially Fitted Rosenbrock Methods with Variable Coefficients for Symmetric Systems

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Abstract: In several important scientific fields, the efficient numerical solution of symmetric systems of ordinary differential equations, which are usually characterized by oscillation and periodicity, has become an open problem of interest. In this paper, we construct a class of embedded exponentially fitted Rosenbrock methods with variable coefficients and adaptive step size, which can achieve third order convergence. This kind of method is developed by performing the exponentially fitted technique for the two-stage Rosenbrock methods, and combining the embedded methods to estimate the frequency. By using Richardson extrapolation, we determine the step size control strategy to make the step size adaptive. Numerical experiments are given to verify the validity and efficiency of our methods.

Keywords: adaptive exponentially fitted Rosenbrock methods; frequency estimation; variable coefficients; convergence; stability

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1. Introduction

In several important scientific fields such as quantum mechanics, elasticity, and electronics, many problems can be represented by mathematical models of symmetric systems, see, e.g., [1–4], which usually lead to ordinary differential equations characterized by oscillation and periodicity [5,6], i.e.,

$$\begin{cases} y'(t) = f(t, y(t)), & t \in [0, T], \\ y(0) = y_0 \in \mathbb{R}^d. \end{cases} \tag{1}$$

In view of the oscillation and periodicity of the equations in symmetric systems, the exponentially fitted methods, whose theoretical basis was first provided by Gautschi [7] and Lyche [8], have been considered to solve these equations in many studies. For instance, The authors of [9,10] investigated exponentially fitted two-step BDF methods and linear multistep methods. The idea of exponential fitting was first applied to the Runge–Kutta methods by Simos [11], in 1998. Since then, based on Simos' research, a few exponentially fitted Runge–Kutta methods have been constructed [12–14]. Some scholars have also tried to estimate the frequency of the methods by analyzing the local truncation error, and control the step size to improve the effects and efficiency [15,16].

However, the exponentially fitted technique has been mostly applied to Runge–Kutta methods, which have difficulty in solving stiff problems by using the explicit form or cost large amounts of computation by using the implicit form. For this reason, Rosenbrock methods, which are based on the idea introduced by Rosenbrock [17] that a single Newton iteration is enough to preserve the stability properties of the diagonally implicit Runge–Kutta methods, have been considered to solve ordinary differential equations in symmetric systems. The general form of Rosenbrock methods for first-order ordinary differential equations has been given by Hairer and Wanner [18]; then, many scholars developed this form and analyzed the implementation, see, e.g., [19,20] and their references. Rosenbrock methods not only keep the stability of the relative diagonal implicit Runge–Kutta methods, but also reduce the amount of calculation compared against the implicit methods because only a linear system of equations needs to be solved per step. At present, there have been some studies on the exponentially fitted Rosenbrock methods [21–23], but these methods, which use constant frequency and step size, have difficulty in solving the equations efficiently and adaptively.

In this paper, we will combine the exponentially fitted Rosenbrock methods with the embedded Rosenbrock methods to estimate the frequency before each step and control the step size by using Richardson extrapolation. By the frequency estimation and step size control, our methods with variable coefficients can solve the equations with oscillation and periodicity efficiently, and the order of convergence can be improved by one compared with the methods with constant coefficients.

The outline of this paper is as follows. In Section 2, a class of exponentially fitted Rosenbrock methods is constructed, and we give the local truncation error, frequency estimation, and stability analysis of the methods. In Section 3, we combine the exponentially fitted Rosenbrock methods with the embedded Rosenbrock methods to construct a kind of embedded variable coefficient exponentially fitted Rosenbrock (3,2) methods, and perform the frequency estimation and step size control strategy. In Section 4, three numerical tests are presented to verify the validity of our methods by comparing the number of calculation steps, the error and the calculating time with other numerical methods. Section 5 gives some discussion and remarks.

2. A Class of Exponentially Fitted Rosenbrock Methods

In this section, a class of exponentially fitted Rosenbrock methods for the models of the ordinary differential equations is constructed, and we give the local truncation error, frequency estimation, and stability analysis of the methods.

Applying the s-stage Rosenbrock method to solve system (1) yields

$$\begin{cases} k_i = hf(t_n + \alpha_i h, d_i y_n + \sum\limits_{j=1}^{i-1} \alpha_{ij} k_j) + \gamma_i h^2 \dfrac{\partial f}{\partial t}(t_n, y_n) + hJ \sum\limits_{j=1}^{i} \gamma_{ij} k_j, \qquad i = 1, 2, \cdots, s, \\ y_{n+1} = y_n + \sum\limits_{j=1}^{s} b_j k_j, \end{cases}$$

where h is the step size, $y_n \approx y(t_n)$, $J = f_y(t_n, y_n)$, α_{ij}, γ_{ij}, α_i, γ_i and d_i are real coefficients which satisfy $\alpha_i = \sum\limits_{j=1}^{i-1} \alpha_{ij}$ and $\gamma_i = \sum\limits_{j=1}^{i} \gamma_{ij}$ for $i = 1, 2, \cdots, s$.

We can also change the nonautonomous system (1) to an autonomous system by the following transformation,

$$\begin{pmatrix} t \\ y(t) \end{pmatrix}' = \begin{pmatrix} 1 \\ f(t, y(t)) \end{pmatrix}, \quad \begin{pmatrix} t_0 \\ y(t_0) \end{pmatrix} = \begin{pmatrix} 0 \\ y_0 \end{pmatrix}.$$

Thus, we will focus on the autonomous problems for simplicity of presentation, i.e.,

$$\begin{cases} y'(t) = f(y(t)), \qquad t \in [0, T], \\ y(0) = y_0, \end{cases} \tag{2}$$

where $y(t) : [0, T] \to \mathbb{R}^d$ is assumed to be thrice continuously differentiable and $f(y) : \mathbb{R}^d \to \mathbb{R}^d$ is assumed to be twice continuously differentiable for the subsequent theoretical analysis. We consider the following s-stage Rosenbrock methods for the autonomous system (2),

$$\begin{cases} k_i = hf(d_i y_n + \sum_{j=1}^{i-1} \alpha_{ij} k_j) + hJ \sum_{j=1}^{i} \gamma_{ij} k_j, \qquad i = 1, 2, \cdots, s, \\ y_{n+1} = y_n + \sum_{j=1}^{s} b_j k_j, \end{cases} \tag{3}$$

or, in tableau form,

$$\begin{array}{c|c|cccccc} 0 & d_1 & \gamma & & & & \\ \alpha_2 & d_2 & \beta_{21} & \gamma & & & \\ \alpha_3 & d_3 & \beta_{31} & \beta_{32} & \gamma & & \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \\ \alpha_s & d_s & \beta_{s1} & \beta_{s2} & \beta_{s3} & \cdots & \gamma \\ \hline & & b_1 & b_2 & b_3 & \ldots & b_s \end{array},$$

i.e.,

$$\begin{array}{c|c|c} \alpha & d & A + V \\ \hline & & b^T \end{array}, \tag{4}$$

where $\alpha_1 = 0, \alpha_{ij} + \gamma_{ij} = \beta_{ij}, \alpha_{ii} = 0, \beta_{ii} = \gamma$ for $i, j = 1, 2, \cdots, s$ and

$$A = \begin{pmatrix} 0 & & & \\ \alpha_{21} & 0 & & \\ \vdots & \ddots & \ddots & \\ \alpha_{s1} & \cdots & \alpha_{ss-1} & 0 \end{pmatrix}, \quad V = \begin{pmatrix} \gamma & & & \\ \gamma_{21} & \gamma & & \\ \vdots & \ddots & \ddots & \\ \gamma_{s1} & \cdots & \gamma_{ss-1} & \gamma \end{pmatrix}.$$

Compared with the classic Rosenbrock methods, the methods (4) in which $\gamma_{ii} = \gamma$ for $i = 1, 2, \cdots, s$, need only one LU-decomposition per step and their order conditions can be simplified [18]. Moreover, this kind of method has higher degree of freedom in its coefficient selection due to the extra coefficients d_i in each step.

Let this method exactly integrate the function $y(t) = e^{\pm\lambda t}$, then, we have

$$\begin{cases} (1 \mp \lambda h\gamma)(\pm\lambda h e^{\pm\lambda(t_n + \alpha_i h)}) = d_i(\pm\lambda h e^{\pm\lambda t_n}) + \lambda^2 h^2 \sum_{j=1}^{i-1} \alpha_{ij} e^{\pm\lambda(t_n + \alpha_j h)} \\ \qquad\qquad + \lambda^2 h^2 \sum_{j=1}^{i-1} \gamma_{ij} e^{\pm\lambda(t_n + \alpha_j h)}, \qquad i = 1, 2, \cdots, s, \\ e^{\pm\lambda(t_n + h)} = e^{\pm\lambda t_n} \pm \lambda h \sum_{j=1}^{s} b_j e^{\pm\lambda(t_n + \alpha_j h)}. \end{cases}$$

Let $z = \lambda h$, it follows that

$$\begin{cases} (1 \mp z\gamma) e^{\pm\alpha_i z} = d_i \pm z \sum_{j=1}^{i-1} \beta_{ij} e^{\pm\alpha_j z}, \qquad i = 1, 2, \cdots, s, \\ e^{\pm z} = 1 \pm z \sum_{j=1}^{s} b_j e^{\pm\alpha_j z}. \end{cases} \tag{5}$$

We now try to construct 1–2 stage Rosenbrock methods by (5). If $s = 1$, together with $\alpha_1 = 0$, we have

$$\begin{cases} 1 - z\gamma = d_1, \\ 1 + z\gamma = d_1, \\ e^z = 1 + zb_1, \\ e^{-z} = 1 - zb_1. \end{cases}$$

Solving the system of equations above with $\gamma \neq 0$ derives in $d_1 = 1, z = 0, b_1 = 1,$ which yields a class of 1-stage exponentially fitted Rosenbrock methods, i.e.,

$$\begin{array}{c|c|c} 0 & 1 & \gamma \\ \hline & & 1 \end{array}.$$

If $s = 2$, together with $\alpha_1 = 0$ and $d_1 = 1$, we have

$$\begin{cases} (1 - z\gamma)e^{\alpha_2 z} = d_2 + z\beta_{21}, \\ (1 + z\gamma)e^{-\alpha_2 z} = d_2 - z\beta_{21}, \\ e^z = 1 + zb_1 + zb_2 e^{\alpha_2 z}, \\ e^{-z} = 1 - zb_1 - zb_2 e^{-\alpha_2 z}. \end{cases} \tag{6}$$

In order to obtain the second order methods, Hairer and Wanner provided the following order conditions in [18], i.e.,

$$\begin{cases} b_1 + b_2 = 1, \\ b_2\beta_{21} = \dfrac{1}{2} - \gamma. \end{cases} \tag{7}$$

Combining (6) and (7), and letting the coefficients of the methods satisfy the order conditions when $z \to 0$, then we have $\alpha_2 = \frac{1}{2}$. Therefore, we obtain the following coefficients of the 2-stage exponentially fitted Rosenbrock methods with order 2,

$$\begin{aligned} &\alpha_1 = 0,\ \alpha_2 = \frac{1}{2},\ d_2 = \cosh\frac{z}{2} - \gamma z \sinh\frac{z}{2}, \\ &\beta_{21} = \frac{\sinh\frac{z}{2}}{z} - \gamma\cosh\frac{z}{2},\ b_1 = \frac{\sinh z}{z} - \frac{(\cosh z - 1)\cosh\frac{z}{2}}{z\sinh\frac{z}{2}} = 0,\ b_2 = \frac{\cosh z - 1}{z\sinh\frac{z}{2}}, \end{aligned} \tag{8}$$

where γ is a free coefficient or, in tableau form,

$$\begin{array}{c|c|cc} 0 & 1 & \gamma & \\ \frac{1}{2} & \cosh\frac{z}{2} - \gamma z\sinh\frac{z}{2} & \dfrac{\sinh\frac{z}{2}}{z} - \gamma\cosh\frac{z}{2} & \gamma \\ \hline & & 0 & \dfrac{\cosh z - 1}{z\sinh\frac{z}{2}} \end{array}.$$

We now consider the following 2-stage exponentially fitted Rosenbrock methods of order 2 and analyze the local truncation error, i.e.,

$$\begin{cases} k_1 = (I - \gamma hJ)^{-1} hf(d_1 y_n), \\ k_2 = (I - \gamma hJ)^{-1}[hf(d_2 y_n + \alpha_2 k_1) + hJ\gamma_{21}k_1], \\ y_{n+1} = y_n + b_1 k_1 + b_2 k_2, \end{cases} \tag{9}$$

where the coefficients are given by (8). Based on Bui's idea in [24], we expand $(I - \gamma hJ)^{-1}$ in the geometrical series, i.e.,

$$(I - \gamma hJ)^{-1} = I + \gamma hJ + \gamma^2 h^2 J^2 + O(h^3). \tag{10}$$

If we assume that y_n in (9) is the exact solution $y(t_n)$ at t_n and expand the hyperbolic functions in the coefficients in Taylor series, we can obtain a one-step approximation $\tilde{y}_{n+1}$ of the solution at t_n+h by (9) and (10), i.e.,

$$\begin{aligned}\tilde{y}_{n+1} = {} & y(t_n) + hf(y(t_n)) + \frac{1}{2}Jf(y(t_n))h^2 + \frac{1}{8}f''(y(t_n))f(y(t_n))^2h^3 \\ & + (\gamma-\gamma^2)J^2f(y(t_n))h^3 - \frac{4\gamma-1}{8}J\lambda^2h^3y(t_n) + \frac{\lambda^2}{24}f(y(t_n))h^3 + O(h^4).\end{aligned} \tag{11}$$

Meanwhile, for the exact solution at t_n+h, we have

$$\begin{aligned}y(t_n+h) = {} & y(t_n) + hf(y(t_n)) + \frac{1}{2}Jf(y(t_n))h^2 \\ & + \frac{1}{6}[f''(y(t_n))f(y(t_n))^2 + J^2f(y(t_n))]h^3 + O(h^4).\end{aligned} \tag{12}$$

Based on (11) and (12), the local truncation error LTE^{EFRB} of exponentially fitted Rosenbrock methods (9) can be expressed as

$$\begin{aligned}LTE^{EFRB} &= y(t_n+h) - \tilde{y}_{n+1} \\ &= \frac{h^3}{24}[y''' - (24\gamma - 24\gamma^2 - 3)f'y'' - D(y' - (12\gamma-3)f'y)] + O(h^4) \\ &= h^3(\psi_1(t,y,f) + \psi_2(t,y,f,\lambda)) + O(h^4),\end{aligned} \tag{13}$$

where $h^3\psi_1(t,y,f) = \frac{h^3}{24}[y''' - (24\gamma-24\gamma^2-3)f'y'']$, $h^3\psi_2(t,y,f,\lambda) = h^3D\psi_3(t,y,f) + O(h^4)$, $h^3\psi_3(t,y,f) = -\frac{h^3}{24}[y' - (12\gamma-3)f'y]$, $\lambda = diag(\lambda_1,\lambda_2,\cdots,\lambda_d) \in \mathbb{R}^{d\times d}$, $D = \lambda^2$ and all functions in (13) are evaluated at $t=t_n$ and $y=y(t_n)$.

If we let the principle local truncation error in (13) be zero, we can approximate and renew the frequency λ in each step to make the coefficients variable by the following equation,

$$\begin{pmatrix} h^3\psi_{11} \\ h^3\psi_{12} \\ \vdots \\ h^3\psi_{1d}\end{pmatrix} + \begin{pmatrix}\lambda_1^2 & & & \\ & \lambda_2^2 & & \\ & & \ddots & \\ & & & \lambda_d^2\end{pmatrix}\begin{pmatrix} h^3\psi_{31} \\ h^3\psi_{32} \\ \vdots \\ h^3\psi_{3d}\end{pmatrix} = \begin{pmatrix}0 \\ 0 \\ \vdots \\ 0\end{pmatrix}, \tag{14}$$

where $h^3\psi_{1i}$ and $h^3\psi_{3i}$ for $i=1,2,\cdots,d$ are respectively the ith-component of $h^3\psi_1(t,y,f)$ and $h^3\psi_3(t,y,f)$, then the order of the methods can be improved by one.

On the other hand, we consider the stability of (9). Let $z\to 0$, then we get a class of constant coefficient exponentially fitted Rosenbrock methods, i.e.,

$$\begin{array}{c|c|cc} 0 & 1 & \gamma & \\ \frac{1}{2} & 1 & \frac{1}{2}-\gamma & \gamma \\ \hline & & 0 & 1 \end{array}. \tag{15}$$

By analogy with the definition of the stability function of Runge–Kutta methods in [25], the definition of the stability function of Rosenbrock methods is as follows.

Definition 1. *Applying the Rosenbrock methods (3) to the following linear test equations*

$$\begin{cases} y' = \lambda y, & \lambda \in \mathbb{C}, \\ y(0) = y_0 \end{cases}$$

yields $y_{n+1} = R(z)y_n$ *with*

$$R(z) = 1 + zb^{\mathrm{T}}(I - z(A+V))^{-1}d,$$

then $R(z)$ *is called the stability function of Rosenbrock methods* (3).

It is obvious that
$$R(z) = \frac{det(I - z(A+V) + zdb^{\mathrm{T}})}{det(I - z(A+V))}, \tag{16}$$
where the numerator and denominator of $R(z)$ are polynomials of degree no more than s. It means that $R(z)$ can be expressed as
$$R(z) = \frac{P(z)}{Q(z)},$$
where $P(z) = \sum_{k=0}^{l} a_k z^k$, $Q(z) = \sum_{k=0}^{m} b_k z^k$ are two polynomials with real coefficients, l, $m \le s$, a_l, $b_m \ne 0$, $a_0 = b_0 = 1$, and $P(z)$ and $Q(z)$ contain no common factors. Li pointed out in [25] that the A-stability of single-step methods was equivalent to the A-acceptability of the rational approximations to the function e^z. The following lemma gives the necessary and sufficient condition for the A-acceptability of $R(z)$.

Lemma 1 ([25]). *Assume that* $p \ge 2m - 3$, *then* $R(z)$ *is A-acceptable iff the three inequalities hold*

(i) $|R(\infty)| \le 1$;

(ii) $Q(z) > 0$ *when* $z \le 0$;

(iii) $b_{m-1}^2 - a_{m-1}^2 + 2(a_m a_{m-2} - b_m b_{m-2}) \ge 0$,

where $m \ge 2$, *and we add the definitions that* $a_{l+1} = a_{l+2} = \cdots = a_m = 0$ *if* $l < m$.

Based on Lemma 1, we can give the following theorem for the A-stability of method (15).

Theorem 1. *If* $\gamma \ge \frac{1}{4}$, *the 2-stage Rosenbrock method* (15) *with single coefficient* γ *is A-stable.*

Proof. According to (16), the stability function of the method (15) is
$$R(z) = \frac{1 + (1-2\gamma)z + (\gamma^2 - 2\gamma + \frac{1}{2})z^2}{1 - 2\gamma z + \gamma^2 z^2}. \tag{17}$$

Let $z \to \infty$, then we have $|R(\infty)| = |\frac{\gamma^2 - 2\gamma + \frac{1}{2}}{\gamma^2}|$. When $\gamma \ge \frac{1}{4}$, we have $|R(\infty)| \le 1$, which means that the condition (i) in Lemma 1 holds if $\gamma \ge \frac{1}{4}$.

According to (17), we have $Q(z) = (1 - \gamma z)^2$. For $\forall z \le 0$, we have $Q(z) > 0$, which means that the condition (ii) in Lemma 1 holds.

Consider the condition (iii) in Lemma 1 when $l = m = 2$, it is easy to find in (17) that $b_0 = 1$, $b_1 = -2\gamma$, $b_2 = \gamma^2$ and $a_0 = 1$, $a_1 = 1 - 2\gamma$, $a_2 = \gamma^2 - 2\gamma + \frac{1}{2}$. If $\gamma \ge \frac{1}{4}$, we have
$$b_{m-1}^2 - a_{m-1}^2 + 2(a_m a_{m-2} - b_m b_{m-2}) = 2\gamma(2\gamma - 1) \ge 0,$$
which means that the condition (iii) in Lemma 1 holds.

To sum up, if $\gamma \ge \frac{1}{4}$, $R(z)$ is A-acceptable as the rational approximation to the function e^z, which means that the 2-stage Rosenbrock method (15) with single coefficient γ is A-stable. □

3. Frequency Estimation and Step Size Control

This section will combine the exponentially fitted Rosenbrock methods with the embedded Rosenbrock methods to construct a kind of embedded variable coefficient exponentially fitted Rosenbrock (3,2) methods, and perform the frequency estimation and step size control strategy.

We consider the embedded Rosenbrock methods for system (2). This kind of method combines two Rosenbrock methods with different orders, which have the same coefficients of the lower stage part. The tableau form of the methods is as follows,

$$
\begin{array}{c|c|cccccc}
0 & d_1 & \gamma & & & & \\
\alpha_2 & d_2 & \beta_{21} & \gamma & & & \\
\alpha_3 & d_3 & \beta_{31} & \beta_{32} & \gamma & & \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \\
\alpha_s & d_s & \beta_{s1} & \beta_{s2} & \beta_{s3} & \cdots & \gamma \\
\hline
 & & b_1 & b_2 & b_3 & \dots & b_s \\
\hline
 & & \hat{b}_1 & \hat{b}_2 & \hat{b}_3 & \dots & \hat{b}_s
\end{array},
$$

and we define $y_1 = y_0 + \sum_{j=1}^{s} b_j k_j$ and $\hat{y}_1 = y_0 + \sum_{j=1}^{s} \hat{b}_j k_j$. To estimate the local truncation error of the embedded methods, we give the following lemma referred to in [26].

Lemma 2 ([26]). *Whenever a starting step h has been chosen, the Rosenbrock methods with order p and q respectively compute two approximations to the solution, y_1 and $\hat{y}_1$, where $p < q$, then the error of y_1 is estimated by $\hat{y}_1 - y_1$, i.e.,*

$$y(t_0 + h) - y_1 = \hat{y}_1 - y_1 + O(h^{p+2}).$$

Now, we construct a class of embedded Rosenbrock methods by using the coefficients of the 2-stage Rosenbrock methods (8). It can be expressed in the following tableau form

$$
\begin{array}{c|c|ccc}
0 & 1 & \gamma & & \\
\frac{1}{2} & \cosh\frac{z}{2} - \gamma z \sinh\frac{z}{2} & \frac{\sinh\frac{z}{2}}{z} - \gamma\cosh\frac{z}{2} & \gamma & \\
\alpha_3 & 1 & \beta_{31} & \beta_{32} & \gamma \\
\hline
 & & 0 & \frac{\cosh z - 1}{z\sinh\frac{z}{2}} & \\
\hline
 & & \hat{b}_1 & \hat{b}_2 & \hat{b}_3
\end{array}, \tag{18}
$$

where γ is a free coefficient. Together with the order conditions for order 3 in [18]

$$
\begin{cases}
b_1 + b_2 + b_3 = 1, \\
\hat{b}_2(\frac{1}{2} - \gamma) + \hat{b}_3\beta_{31} + \hat{b}_3\beta_{32} = \frac{1}{2} - \gamma, \\
\hat{b}_2 \times \frac{1}{4} + \hat{b}_3\alpha_3^2 = \frac{1}{3}, \\
\hat{b}_3\beta_{32} = \frac{\frac{1}{3} - 2\gamma + 2\gamma^2}{1 - 2\gamma},
\end{cases} \tag{19}
$$

when we let $\hat{b}_2 = 0$ and $\alpha_3 = \frac{2}{3}$, the coefficients of method (18) are determined by (19), i.e.,

$$
\begin{aligned}
&\alpha_1 = 0,\ \alpha_2 = \frac{1}{2},\ \alpha_3 = \frac{2}{3},\ d_2 = \cosh\frac{z}{2} - \gamma z \sinh\frac{z}{2},\ d_3 = 1, \\
&\beta_{21} = \frac{\sinh\frac{z}{2}}{z} - \gamma\cosh\frac{z}{2},\ \beta_{31} = \frac{2}{9(1-2\gamma)},\ \beta_{32} = \frac{4(6\gamma^2 - 6\gamma + 1)}{9(1-2\gamma)}, \\
&b_1 = 0,\ b_2 = \frac{\cosh z - 1}{z\sinh\frac{z}{2}},\ \hat{b}_1 = \frac{1}{4},\ \hat{b}_2 = 0,\ \hat{b}_3 = \frac{3}{4},
\end{aligned}
$$

where $\gamma \neq \dfrac{1}{2}$ or, in tableau form,

$$
\begin{array}{c|c|ccc}
0 & 1 & \gamma & & \\
\frac{1}{2} & \cosh\frac{z}{2} - \gamma z \sinh\frac{z}{2} & \frac{\sinh\frac{z}{2}}{z} - \gamma\cosh\frac{z}{2} & \gamma & \\
\frac{2}{3} & 1 & \frac{2}{9(1-2\gamma)} & \frac{4(6\gamma^2-6\gamma+1)}{9(1-2\gamma)} & \gamma \\
\hline
 & & 0 & \frac{\cosh z - 1}{z\sinh\frac{z}{2}} & \\
\hline
 & & \frac{1}{4} & 0 & \frac{3}{4}
\end{array}. \tag{20}
$$

We now choose one of the methods above to introduce the frequency estimation and step size control strategy. We record the exponentially fitted Rosenbrock (3,2) method (20) as EFRB(3,2) when $\gamma = \frac{1}{4}$, i.e.,

$$
\begin{array}{c|c|ccc}
0 & 1 & \frac{1}{4} & & \\
\frac{1}{2} & \cosh\frac{z}{2} - \frac{z}{4} \sinh\frac{z}{2} & \frac{\sinh\frac{z}{2}}{z} - \frac{1}{4}\cosh\frac{z}{2} & \frac{1}{4} & \\
\frac{2}{3} & 1 & \frac{4}{9} & -\frac{1}{9} & \frac{1}{4} \\
\hline
 & & 0 & \frac{\cosh z - 1}{z\sinh\frac{z}{2}} & \\
\hline
 & & \frac{1}{4} & 0 & \frac{3}{4}
\end{array}. \tag{21}
$$

We also record the Rosenbrock (3,2) method (21) as RB(3,2) when $z \to 0$, i.e.,

$$
\begin{array}{c|c|ccc}
0 & 1 & \frac{1}{4} & & \\
\frac{1}{2} & 1 & \frac{1}{4} & \frac{1}{4} & \\
\frac{2}{3} & 1 & \frac{4}{9} & -\frac{1}{9} & \frac{1}{4} \\
\hline
 & & 0 & 1 & \\
\hline
 & & \frac{1}{4} & 0 & \frac{3}{4}
\end{array}. \tag{22}
$$

Suppose that y_{n+1}^{class} and LTE^{class} are the numerical solution and the local truncation error for the second-order component of RB(3,2), and y_{n+1}^{EFRB} and LTE^{EFRB} are the numerical solution and the local truncation error for the second-order component of EFRB(3,2), then we have

$$LTE^{class} = y(t_n + h) - y_{n+1}^{class} = h^3\psi_1(t, y, f) + O(h^4), \tag{23}$$

$$LTE^{EFRB} = y(t_n + h) - y_{n+1}^{EFRB} = h^3(\psi_1(t, y, f) + \psi_2(t, y, f, \lambda)) + O(h^4), \tag{24}$$

where $h^3\psi_1(t, y, f) = h^3(\dfrac{1}{24}y''' - \dfrac{1}{16}f'y'')$, $h^3\psi_2(t, y, f, \lambda) = h^3 D\psi_3(t, y, f) + O(h^4)$, $h^3\psi_3(t, y, f) = -\dfrac{h^3}{24}y'$ and all functions in (23) and (24) are evaluated at $t = t_n$ and $y = y(t_n)$. Together with (23) and (24), we have

$$h^3\psi_2(t, y, f, \lambda) \approx LTE^{EFRB} - LTE^{class} = y_{n+1}^{class} - y_{n+1}^{EFRB}.$$

For each integration step, we can estimate $h^3\psi_3(t, y, f)$ by the following equation,

$$
\begin{pmatrix} h^3\psi_{31} \\ h^3\psi_{32} \\ \vdots \\ h^3\psi_{3d} \end{pmatrix} \approx \begin{pmatrix} \lambda_1^2 & & & \\ & \lambda_2^2 & & \\ & & \ddots & \\ & & & \lambda_d^2 \end{pmatrix}^{-1} \begin{pmatrix} h^3\psi_{21} \\ h^3\psi_{22} \\ \vdots \\ h^3\psi_{2d} \end{pmatrix}, \tag{25}
$$

where $h^3\psi_{2i}$ and $h^3\psi_{3i}$ for $i = 1, 2, \cdots, d$ are respectively the ith-component of $h^3\psi_2(t, y, f, \lambda)$ and $h^3\psi_3(t, y, f)$. For the first integration step, λ is set as a suitable starting frequency $\lambda^{(0)}$.

On the other hand, if we suppose that the numerical solution for the third-order component of RB(3,2) is $\hat{y}^{class}_{n+1}$, we can estimate $h^3\psi_1(t,y,f)$ based on lemma 2 by

$$LTE^{class} = h^3\psi_1(t,y,f) + O(h^4) \approx \hat{y}^{class}_{n+1} - y^{class}_{n+1}. \tag{26}$$

After obtaining the approximations of $h^3\psi_1(t,y,f)$ and $h^3\psi_3(t,y,f)$ by (25) and (26), we substitute them into (14) to estimate and renew the frequency λ. In addition, if the estimate of $h^3\psi_{1i}$ is close to zero, the estimate of λ_i is zero, which means that the coefficients of the EFRB(3,2) method (21) are equal to the coefficients of the RB(3,2) method (22). If the estimate of $h^3\psi_{3i}$ is close to zero, it means that the principle local truncation error is not related to λ_i. In this case, we do not renew the frequency. If we estimate the frequency before each step of the method, we will get a variable coefficient method and its order will be increased by one.

Now, we try to control its step size by Richadson extrapolation. We first give the following lemma referred to in [26].

Lemma 3 ([26])**.** *Assume that y_{n+1} is the numerical solution of one step with step size h of a Rosenbrock method of order p from (t_n, y_n), and ω_{n+1} is the numerical solution of two steps with step size $\frac{h}{2}$, then the error of ω_{n+1} can be expressed as*

$$y(x_{n+1}) - \omega_{n+1} = \frac{\omega_{n+1} - y_{n+1}}{2^p - 1} + O(h^{p+2}).$$

Based on Lemma 3, we give the following step size control strategy. Let $error = \dfrac{\omega_{n+1} - y_{n+1}}{2^p - 1}$, we compare $error$ with the tolerance tol which is given by user. If $|error| \leq tol$, then we accept the step and progress with the ω_{n+1} value; if $|error| > tol$, then we reject the step and repeat the whole procedure with a new step size. In both cases, referred to in [18], the new step size is given by

$$h_{new} = h_{old}\, min(facmax, max(facmin, fac(tol/error)^{\frac{1}{p+1}})),$$

where $facmax$ and $facmin$ are the maximum and minimum acceptable factors, respectively, and fac is the safety factor. In this paper, we let $facmax = 2, facmin = 0.5$ and $fac = 0.8$.

4. Numerical Experiments

In this section, we present three numerical experiments to test the performance of our methods and compare the error and computational efficiency with other numerical methods. All the numerical experiments were executed by using MATLAB® on a Windows 11 PC with an Intel® Core™ i5-10210U CPU.

Example 1. *Consider the following ODE system in [27],*

$$\begin{cases} y''(t) = -\omega y(t) + (\omega^2 - 1)\sin t, & t \geq 0, \\ y(0) = 1,\; y'(0) = \omega + 1, \end{cases} \tag{27}$$

with exact solution $y(t) = \cos\omega t + \sin\omega t + sint$. Let $y'(t) = x(t), Y(t) = (x(t), y(t))^T$, then we get a new ODE system

$$\begin{cases} Y'(t) = \begin{pmatrix} 0 & -\omega^2 \\ 1 & 0 \end{pmatrix} Y(t) + \begin{pmatrix} (\omega^2 - 1)\sin t \\ 0 \end{pmatrix}, & t \geq 0, \\ Y(0) = \begin{pmatrix} \omega + 1 \\ 1 \end{pmatrix}. \end{cases} \tag{28}$$

Problem (28) *has been solved in the interval* $0 \le t \le 10$ *with* $\lambda_i^{(0)} = 10$ *for each component of the solution when* $\omega = 10$.

Example 2. *Consider the following ODE system in [28],*

$$\begin{cases} y'(t) = \begin{pmatrix} -21 & 19 & -20 \\ 19 & -21 & 20 \\ 40 & -40 & -40 \end{pmatrix} y(t), \quad 0 \le t \le 100, \\ y(0) = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}, \end{cases} \tag{29}$$

with the following solution:

$$y(t) = \frac{1}{2}\begin{pmatrix} 1 & 1 & 1 \\ 1 & -1 & -1 \\ 0 & -2 & 2 \end{pmatrix}\begin{pmatrix} e^{-2t} \\ e^{-40t}\cos 40t \\ e^{-40t}\sin 40t \end{pmatrix}.$$

Problem (29) *has been solved in the interval* $0 \le t \le 100$ *with* $\lambda_i^{(0)} = -40$ *for each component of the solution.*

Example 3. *Consider the following PDE system in [29],*

$$\begin{cases} \dfrac{\partial u}{\partial t} = \dfrac{\partial^2 u}{\partial x^2} - u + 2e^{-t}, & 0 < x < 1,\ t > 0, \\ u(0,t) = u(1,t) = 0, & t > 0, \\ u(x,0) = x(1-x), & 0 < x < 1, \end{cases} \tag{30}$$

with exact solution $u(x,t) = x(1-x)e^{-t}$. *The PDE system* (30) *can be transformed into an ODE system by spatial discretization with central finite difference of second order, which results in*

$$\begin{cases} u_i'(t) = \dfrac{1}{\Delta x^2}[u_{i-1}(t) - 2u_i(t) + u_{i+1}(t)] - u_i(t) + 2e^{-t}, \ \ i = 1,2,\cdots,M-1,\ t > 0, \\ u_i(0) = i\Delta x(1 - i\Delta x),\ \ i = 1,2,\cdots,M-1, \end{cases} \tag{31}$$

where $\Delta x = 1/M, x_i = i\Delta x$, $u_i(t)$ *is meant to approximate the solution of* (30) *at the point* (t, x_i) *and we define* $u_0(t) = u_M(t) = 0$. *Then, problem* (31) *has been solved in the interval* $0 \le t \le 10$ *with* $\lambda_i^{(0)} = -2$ *for each component of the solution when* $M = 10$.

We first solve Example 1 by the EFRB(3,2) method with constant step size to test the order of our method. We use the following formula to estimate the order of our method,

$$p \approx log_2[\frac{error(h)}{error(h/2)}],$$

where $error(h) = \max\limits_{1 \le n \le N} ||\varepsilon(h)||$, $\varepsilon(h) = y(t_n) - y_n$ represents the error of y_n when h is the step size and $t_N = 10$. Let $h = 1/2^k, k = 4,5,\cdots,9$, then the error and the order of convergence of our method are shown in Table 1. The results in Table 1 imply that the EFRB(3,2) method can achieve third order convergence.

Table 1. The error and the order of convergence of the EFRB(3,2) method for problem (27).

h	1/16	1/32	1/64	1/128	1/256	1/512
$error(h)$	3.9592×10^{-1}	3.0439×10^{-2}	2.8673×10^{-3}	3.5307×10^{-4}	4.3312×10^{-5}	5.4082×10^{-6}
p	-	3.7012	3.4082	3.0217	3.0271	3.0016

We now compare the EFRB(3,2) method with the stiff ODE solvers in MATLAB® such as ode23s, ode23t, and ode23tb, which have the same stage as our method. For each stiff ODE solver in MATLAB®, the relative tolerance $RelTol$ is set as tol and the absolute tolerance $AbsTol$ is set as $10^{-3}tol$. The error for each component of the solution was calculated as the maximum of the absolute value of the difference between the numerical and exact solutions, and we use the largest error across all components as the error of the problems. Figures 1–3 show the relationship between the error and the average calculating time for each method when $tol = 10^{-k}, k = 2, 3, \cdots, 10$. Tables 2–4 show the calculating steps, the error, and the calculating time for each method when $tol = 10^{-5}, 10^{-7}$ and 10^{-9}. From the figures and tables, we conclude that the EFRB(3,2) method achieves better performance than all the stiff ODE solvers for ODE Examples 1 and 2. For the PDE Example 3, the EFRB(3,2) method achieves similar performance with ode23tb and better performance than other stiff ODE solvers. Furthermore, our method performs better than ode23tb in the small-tolerance range for Example 3. The performance of the EFRB(3,2) method in these three examples verifies the effectiveness and efficiency of our method, making it possible to be applied to the stiff ODE systems and PDE systems.

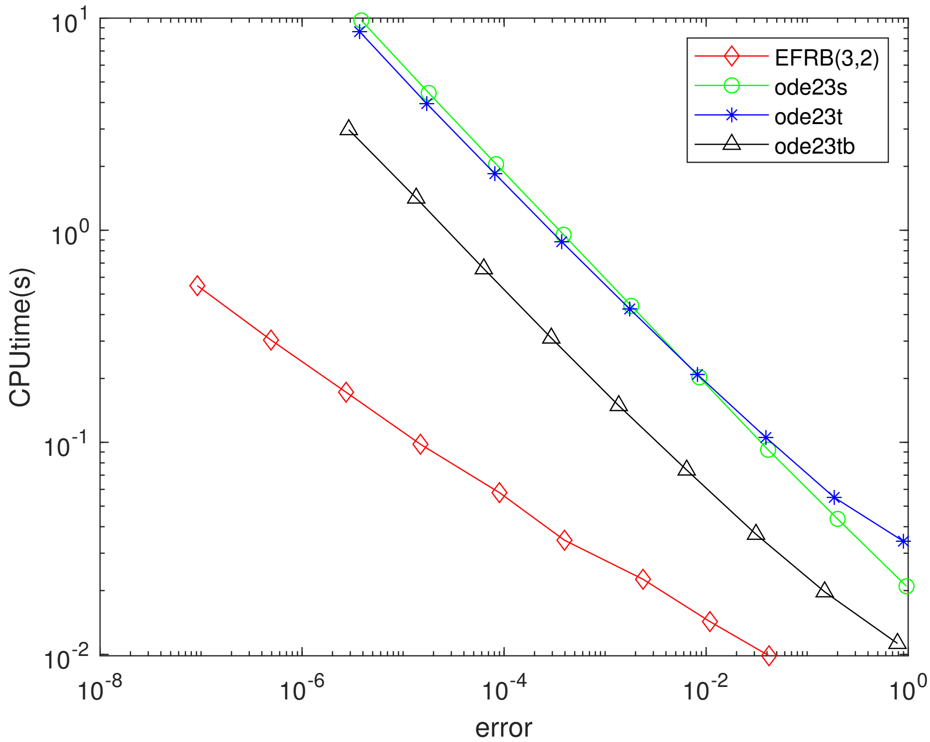

Figure 1. CPUtime−error of each method for Example 1.

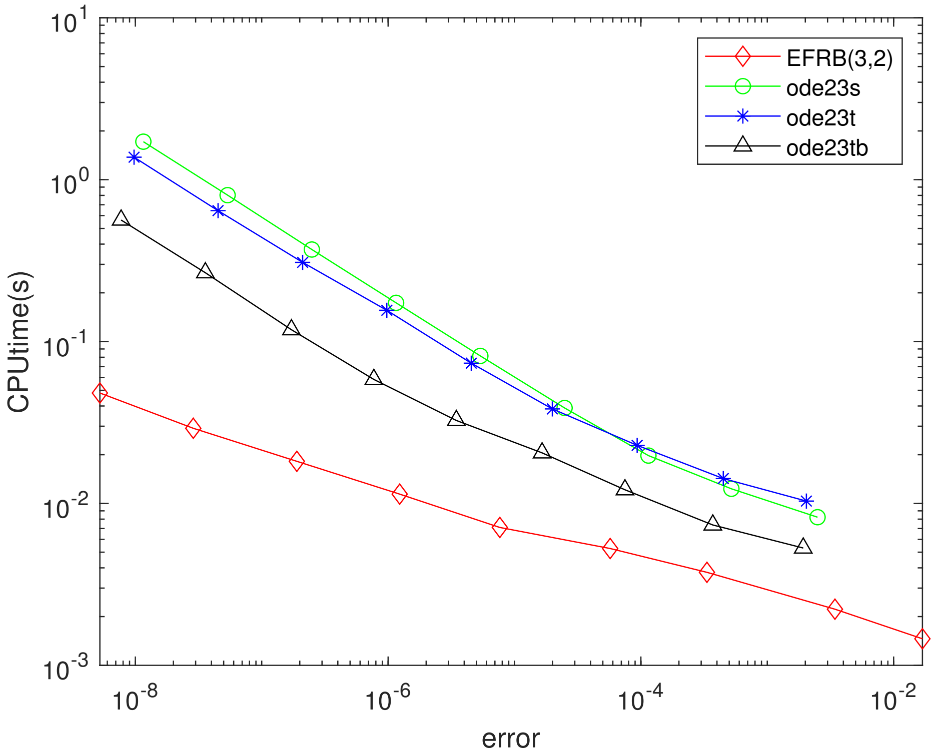

Figure 2. CPUtime−error of each method for Example 2.

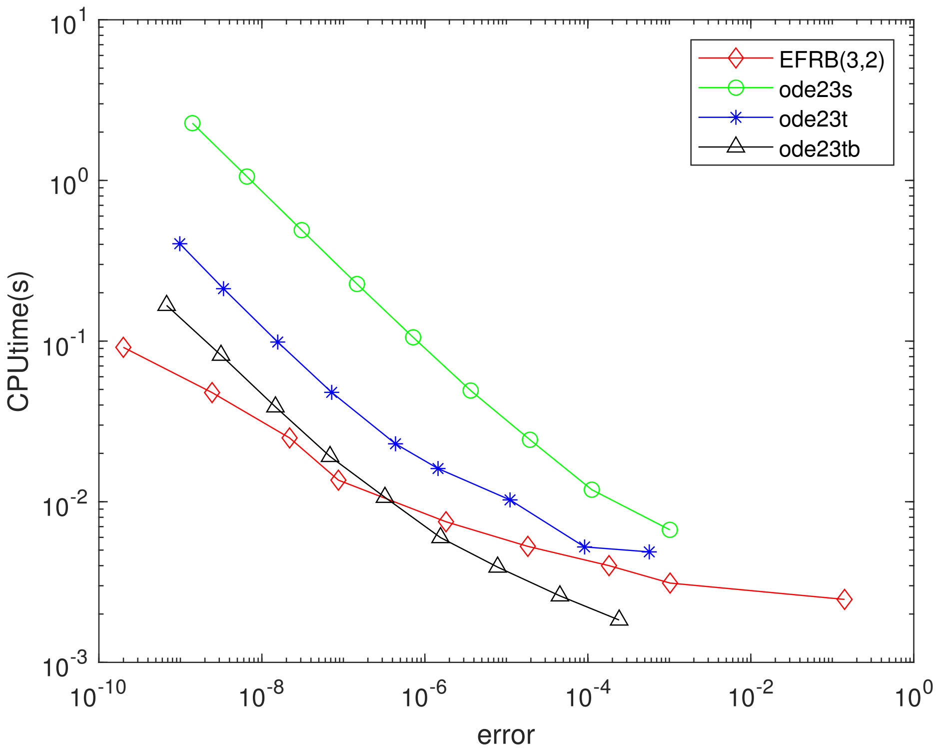

Figure 3. CPUtime−error of each method for Example 3.

Table 2. The accepted steps, rejected steps, error, and calculating time of each method for Example 1.

Method	Tol	Accepted Steps	Rejected Steps	Error	Time(s)
EFRB(3,2)	10^{-5}	622	44	3.9582×10^{-4}	0.0387
	10^{-7}	1915	23	1.4846×10^{-5}	0.0965
	10^{-9}	6038	70	4.9237×10^{-7}	0.3006
ode23s	10^{-5}	3009	68	8.5624×10^{-3}	0.1937
	10^{-7}	14404	71	3.8814×10^{-4}	0.9061
	10^{-9}	67396	42	1.7927×10^{-5}	4.2465
ode23t	10^{-5}	4444	44	8.2055×10^{-3}	0.2010
	10^{-7}	21148	40	3.7150×10^{-4}	0.8442
	10^{-9}	98805	19	1.7141×10^{-5}	3.7756
ode23tb	10^{-5}	3477	55	6.4195×10^{-3}	0.0708
	10^{-7}	16583	38	2.9314×10^{-4}	0.2978
	10^{-9}	77627	26	1.3478×10^{-5}	1.3235

Table 3. The accepted steps, rejected steps, error, and calculating time of each method for Example 2.

Method	Tol	Accepted Steps	Rejected Steps	Error	Time(s)
EFRB(3,2)	10^{-5}	49	4	6.3863×10^{-5}	0.0176
	10^{-7}	150	25	1.0545×10^{-6}	0.0246
	10^{-9}	372	20	2.9298×10^{-8}	0.0423
ode23s	10^{-5}	529	18	2.4912×10^{-5}	0.0446
	10^{-7}	2478	115	1.1568×10^{-6}	0.2064
	10^{-9}	11540	521	5.3705×10^{-8}	0.8153
ode23t	10^{-5}	783	5	1.9925×10^{-5}	0.0544
	10^{-7}	3546	3	9.7763×10^{-7}	0.1946
	10^{-9}	16431	3	4.5192×10^{-8}	0.6497
ode23tb	10^{-5}	608	5	1.6531×10^{-5}	0.0198
	10^{-7}	2788	3	7.7115×10^{-7}	0.6134
	10^{-9}	13251	3	3.5798×10^{-8}	0.2668

Table 4. The accepted steps, rejected steps, error, and calculating time of each method for Example 3.

Method	Tol	Accepted Steps	Rejected Steps	Error	Time(s)
EFRB(3,2)	10^{-5}	58	4	2.3242×10^{-5}	0.0079
	10^{-7}	139	4	9.9917×10^{-8}	0.0299
	10^{-9}	543	4	1.4384×10^{-8}	0.0703
ode23s	10^{-5}	471	1	3.6454×10^{-6}	0.0570
	10^{-7}	2293	1	1.4693×10^{-7}	0.2551
	10^{-9}	10792	1	6.5482×10^{-9}	1.1690
ode23t	10^{-5}	256	0	1.4514×10^{-6}	0.0164
	10^{-7}	1156	0	7.1862×10^{-8}	0.0567
	10^{-9}	5341	0	3.3804×10^{-9}	0.2405
ode23tb	10^{-5}	178	0	1.5574×10^{-6}	0.0083
	10^{-7}	846	0	6.8615×10^{-8}	0.0314
	10^{-9}	3948	0	3.1499×10^{-9}	0.0848

5. Conclusions

In this paper, a class of variable coefficient exponentially fitted embedded Rosenbrock methods with adaptive step size has been developed. By the frequency estimation and step size control strategy, the order of convergence will be increased by one and the methods can renew the step size adaptively. The numerical experiments show that compared with other methods such as ode23s, ode23t, and ode23tb in MATLAB®, our methods can achieve lower error with fewer calculating steps and shorter time, and these advantages will be much more significant if the tolerance is lower. We believe that this kind of methods can be applied to more complex symmetric systems, and the Rosenbrock methods of higher order can be constructed by our frequency estimation and step size control strategy.

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