

SIXTH ORDER EXPLICIT EXPONENTIAL ROSENBROCK-TYPE METHODS FOR SEMILINEAR PARABOLIC PROBLEMS*

Yuhao Cong^{1,†} and Dongping Li^{1,2}

Abstract The paper is concerned with the numerical analysis of high-order exponential Rosenbrock-type integrators for large-scale systems of stiff differential equations. The analysis is performed in a semigroup framework of semilinear evolution equations in Banach space. By expanding the errors of the numerical methods in terms of the solution, we further derive new order conditions and thus allows us to construct higher-order methods. A new and more general stiff error analysis is presented to show the converge results for variable step sizes.

Keywords Exponential Rosenbrock-type methods, stiff order conditions, exponential integrators, variable step size.

MSC(2000) 65M12, 65L06.

1. Introduction

In this paper we consider high order numerical methods for the time integration of large systems of stiff differential equations

$$u'(t) = F(u(t)), \quad u(t_0) = u_0, \quad (1.1)$$

by exponential Rosenbrock-type methods. Such equations typically arise from spatial discretizations of nonlinear time dependent partial differential equations.

The idea of exponential integrators is an old one and has been proposed independently by many authors. Although the first exponential integrators were proposed many years ago, such methods have not been regarded as practical for a long time. This view, however, has changed recently as new methods for computing or approximating the product of a matrix exponential function with a vector have been developed. In recent years, some numerical comparisons presented in [10, 11, 13, 14] reveal exponential integrators turned out to be very competitive for stiff problems. For a detailed overview of such integrators and their implementation, we refer to [9]. The main idea behind these methods is to treat the linear part of problem (1.1) exactly and the nonlinearity in an explicit way.

[†]the corresponding author. Email address: yhcong@shnu.edu.cn (Y. Cong)

¹Department of Mathematics, Shanghai Normal University, Shanghai, 200234, China

²Department of Mathematics, Changchun Normal University, Changchun, 130032, China

*The authors were supported by National Natural Science Foundation of China (10971140).

Motivated by recent interest in exponential integrators for stiff problems [1, 5, 6, 8], in this paper, we consider exponential Rosenbrock-type methods which were introduced in [3, 7], they were based on a continuous linearization of the vector field along the numerical trajectory. In [7], the stiff order conditions were derived up to order 4. Very recently, in [12], a new approach was proposed to derive stiff order conditions for exponential Rosenbrock-type methods up to order five. With these order conditions at hand, we are going to derive stiff order conditions up to sixth-order in this paper. By a careful analysis of the local error, we are able to deduce the desired conditions. A new and more general stiff error analysis is presented to illustrate this procedure for methods up to order 6.

The outline of the paper is organized as follows. In Section 2, we review the problem and the numerical methods for further analysis. In Section 3, the local error analysis of the methods is carried out and some order conditions are derived which eventually guarantee convergence for stiff problems. Section 4 is devoted to the global convergence analysis. For this purpose, we propose a more general method that allows us to prove convergence up to six.

Throughout the paper, C will denote a generic constant that may have different values at different occurrences.

2. Exponential Rosenbrock-type methods

In this paper, we consider the numerical solution of stiff differential equations of the form (1.1). The numerical schemes considered are based on a continuous linearization of (1.1) along the numerical solution. For a given point u_n in the state space, this linearization is

$$u'(t) = J_n u(t) + g_n(u(t)), \quad u(t_0) = u_0. \quad (2.1)$$

where

$$J_n = J(u_n) = \frac{\partial F}{\partial u}(u_n), \quad g_n(u(t)) = F(u) - J_n u(t). \quad (2.2)$$

with J_n denoting the Jacobian of F and g_n the nonlinear remainder, evaluated at u_n , respectively.

Throughout the paper, we restrict our attention to semilinear problems

$$u'(t) = F(u(t)) = Au(t) + g(u(t)), \quad u(t_0) = u_0. \quad (2.3)$$

This implies that (2.2) takes the form

$$J_n = A + \frac{\partial g}{\partial u}(u_n), \quad g_n(u) = F(u) - J_n u = g(u(t)) - \frac{\partial g}{\partial u}(u_n)u. \quad (2.4)$$

Applying an explicit exponential Rosenbrock-type methods to (2.1), we obtain the following class of explicit one-step methods:

$$\begin{cases} U_{ni} = e^{c_i h_n J_n} u_n + h_n \sum_{j=1}^{i-1} a_{ij}(h_n J_n) g_n(U_{nj}), & 1 \leq i \leq s, \\ u_{n+1} = e^{h_n J_n} u_n + h_n \sum_{j=1}^s b_j(h_n J_n) g_n(U_{nj}). \end{cases} \quad (2.5)$$

Here, $h_n = t_{n+1} - t_n > 0$ denotes the time step size and c_i are the nodes. The methods are fully explicit and don't require the solution of linear or nonlinear systems of equations. As usual in exponential integrators, the coefficients $a_{ij}(z)$, $b_i(z)$ are linear combinations of the $\varphi_j(c_i z)$, $\varphi_j(z)$ functions, respectively. These φ functions are given by

$$\varphi_j(z) = \int_0^1 e^{(1-\theta)z} \frac{\theta^{j-1}}{(j-1)!} d\theta, \quad j \geq 1. \quad (2.6)$$

They satisfy the following recurrence relations

$$\varphi_{j+1}(z) = \frac{\varphi_j(z) - \frac{1}{j!}}{z}, \quad \varphi_0(z) = e^z. \quad (2.7)$$

A desirable property of numerical methods (2.5) is that they preserve equilibria u^* of the autonomous problems (2.3). Requiring $U_{ni} = u_n = u^*$ for all i and $n \geq 0$ immediately yields the necessary and sufficient conditions. It turns out that the coefficients of the methods have to satisfy

$$\sum_{j=1}^{i-1} a_{ij}(z) = c_i \varphi_1(c_i z), \quad \sum_{j=1}^s b_j(z) = \varphi_1(z), \quad 1 \leq i \leq s, \quad (2.8)$$

which implies $c_1 = 0$ and consequently $U_{n1} = u_n$.

Without further mention, we will assume throughout the paper that the conditions (2.8) are fulfilled. With the help of (2.8), the numerical scheme (2.5) then takes the equivalent form

$$\begin{cases} U_{ni} = u_n + c_i h_n \varphi_1(c_i h_n J_n) F(u_n) + h_n \sum_{j=2}^{i-1} a_{ij}(h_n J_n) D_{nj}, \\ u_{n+1} = u_n + h_n \varphi_1(h_n J_n) F(u_n) + h_n \sum_{j=1}^s b_j(h_n J_n) D_{nj}, \end{cases} \quad (2.9)$$

with $D_{nj} = g_n(U_{ni}) - g_n(u_n)$, $2 \leq j \leq s$.

3. Local error analysis

Our analysis will be based on an abstract framework of analytic semigroups on a Banach space X with norm $\|\cdot\|$. Background information on semigroups can be found in the textbook [4]. Throughout the paper we consider the following assumptions.

Assumption 1. The linear operator J is the infinitesimal generator of an analytic semigroup e^{tJ} on X . This assumption implies that there exist constants C and ω such that

$$\|e^{tJ}\|_{X \leftarrow X} \leq C e^{\omega t}, \quad t \geq 0, \quad (3.1)$$

holds uniformly in a neighborhood of the exact solution of (2.3). In particular, the expressions $\varphi_k(z)$ and consequently the coefficients $a_{ij}(h_n J)$ and $b_i(h_n A)$ of the methods are bounded operators. This property is crucial in our proofs.

Assumption 2. We suppose that (2.3) possesses a sufficiently smooth solution $u : [t_0, T] \rightarrow X$ with derivatives in X and that $g : X \rightarrow X$ is sufficiently often

Fréchet differentiable in a strip along the exact solution. All occurring derivatives are assumed to be uniformly bounded. Assumption 2 implies that the Jacobian of $F(u)$ satisfies the Lipschitz condition

$$\|J(u) - J(v)\|_{X \leftarrow X} \leq C\|u - v\|. \quad (3.2)$$

For the local error analysis of scheme (2.9), as usual, we consider one step with initial value $\tilde{u}_n = u(t_n)$ on the exact solution, i.e.

$$\begin{cases} \hat{U}_{ni} = \tilde{u}_n + c_i h_n \varphi_1(c_i h_n \tilde{J}_n) F(\tilde{u}_n) + h_n \sum_{j=2}^{i-1} a_{ij}(h_n \tilde{J}_n) \tilde{D}_{nj}, \\ \hat{u}_{n+1} = \tilde{u}_n + h_n \varphi_1(h_n \tilde{J}_n) F(\tilde{u}_n) + h_n \sum_{j=2}^s b_j(h_n \tilde{J}_n) \tilde{D}_{nj}, \end{cases} \quad (3.3)$$

with

$$\begin{aligned} \tilde{J}_n &= \frac{\partial F}{\partial u}(\tilde{u}_n) = A + \frac{\partial g}{\partial u}(\tilde{u}_n), \\ \tilde{g}_n(u) &= F(u) - \tilde{J}_n u, \\ \tilde{D}_{nj} &= \tilde{g}_n(\hat{U}_{nj}) - \tilde{g}_n(\tilde{u}_n), \quad 2 \leq j \leq s. \end{aligned} \quad (3.4)$$

Let $\tilde{u}_n^{(k)}$ denote the k th derivative of the exact solution $u(t)$ of (2.3), evaluated at time t_n . For $k = 1, 2$, we use the common notation $\tilde{u}'_n, \tilde{u}''_n$ for simplicity.

Expanding \tilde{D}_{ni} in (3.4) in a Taylor series at \tilde{u}_n and substituting it into the second equation of (3.3). Note that

$$\frac{\partial \tilde{g}_n}{\partial u}(\tilde{u}_n) = 0. \quad (3.5)$$

We get the representation

$$\begin{aligned} \hat{u}_{n+1} &= \tilde{u}_n + h_n \varphi_1(h_n \tilde{J}_n) F(\tilde{u}_n) \\ &+ \sum_{i=2}^s b_i(h_n \tilde{J}_n) \sum_{q=2}^k \frac{h_n^{q+1}}{q!} \frac{\partial^q \tilde{g}_n}{\partial u^q}(\tilde{u}_n)(V_i, V_i, \dots, V_i) + O(h_n^{k+2}). \end{aligned} \quad (3.6)$$

with

$$V_i = \frac{1}{h_n}(\hat{U}_{ni} - \tilde{u}_n) = c_i h_n \varphi_1(c_i h_n \tilde{J}_n) F(\tilde{u}_n) + h_n \sum_{j=2}^{i-1} a_{ij}(h_n \tilde{J}_n) \tilde{D}_{nj}. \quad (3.7)$$

In order to derive stiff order conditions up to 6, we set $k = 5$.

Let

$$\psi_j(z) = \sum_{i=2}^s b_i(z) \frac{c_i^{j-1}}{(j-1)!} - \varphi_j(z), \quad (3.8)$$

$$\psi_{j,i}(z) = \sum_{k=2}^{i-1} a_{ik}(z) \frac{c_k^{j-1}}{(j-1)!} - c_i^j \varphi_j(c_i z). \quad (3.9)$$

The following two lemmas are important to deriving the order conditions. They are straightforward by some adjustments for Lemma 3.1 and Lemma 3.2 in [12], respectively. We omit the details.

Lemma 3.1. *Under Assumptions 1 and 2, we have for all $t \geq 0$*

$$\begin{aligned} \varphi_1(t\tilde{J}_n)\tilde{u}'_n &= \tilde{u}'_n + \frac{t}{2!}\tilde{u}''_n + \frac{t^2}{3!}\left(\tilde{u}_n^{(3)} - 3!\varphi_3(t\tilde{J}_n)\frac{\partial^2\tilde{g}_n}{\partial u^2}(\tilde{u}'_n, \tilde{u}'_n)\right) \\ &+ t^3\varphi_4(t\tilde{J}_n)\left(\tilde{u}_n^{(4)} - \frac{\partial^3\tilde{g}_n}{\partial u^3}(\tilde{u}'_n, \tilde{u}'_n, \tilde{u}'_n) - 3\frac{\partial^2\tilde{g}_2}{\partial u^2}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}''_n)\right). \end{aligned} \quad (3.10)$$

Lemma 3.2. *Under Assumptions 1 and 2, we have*

$$\begin{aligned} V_i &= c_i\tilde{u}'_n + \frac{c_i^2h_n}{2}\tilde{u}''_n + \frac{c_i^3h_n^2}{3!}\tilde{u}_n^{(3)} + h_n^2\psi_{3,i}\frac{\partial^2\tilde{g}_n}{\partial u^2}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}'_n) + c_i^4h_n^3\varphi_4(c_ih_n\tilde{J}_n)\tilde{u}_n^{(4)} \\ &+ h_n^3\psi_{4,i}\left(\frac{\partial^3\tilde{g}_n}{\partial u^3}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}'_n, \tilde{u}'_n) + 3\frac{\partial^2\tilde{g}_n}{\partial u^2}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}''_n)\right) + O(h_n^4). \end{aligned} \quad (3.11)$$

Substituting the above expansion of V_i into (3.6), as

$$\begin{aligned} &\frac{\partial^2\tilde{g}_n}{\partial u^2}(\tilde{u}_n)(V_i, V_i) \\ &= \frac{\partial^2\tilde{g}_n}{\partial u^2}(\tilde{u}_n)\left(c_i^2(\tilde{u}'_n, \tilde{u}'_n) + c_i^3h_n(\tilde{u}'_n, \tilde{u}''_n) + \frac{2c_i^4h_n^2}{3!}(\tilde{u}'_n, \tilde{u}_n^{(3)})\right. \\ &+ 2c_ih_n^2\left(\tilde{u}'_n, \psi_{3,i}\frac{\partial^2\tilde{g}_n}{\partial u^2}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}'_n)\right) + 2c_i^4h_n^3\left(\tilde{u}'_n, \varphi_4(c_ih_n\tilde{J}_n)\tilde{u}_n^{(4)}\right) \\ &+ 2c_ih_n^3\left(\tilde{u}'_n, \psi_{4,i}\frac{\partial^3\tilde{g}_n}{\partial u^3}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}'_n, \tilde{u}'_n)\right) + 6c_ih_n^3\left(\tilde{u}'_n, \psi_{4,i}\frac{\partial^2\tilde{g}_n}{\partial u^2}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}''_n)\right) \\ &\left. + \frac{c_i^4h_n^2}{4}(\tilde{u}''_n, \tilde{u}''_n) + \frac{2c_i^5h_n^3}{3!}(\tilde{u}''_n, \tilde{u}_n^{(3)}) + 2c_i^2h_n^3\left(\tilde{u}''_n, \psi_{3,i}\frac{\partial^2\tilde{g}_n}{\partial u^2}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}'_n)\right)\right), \end{aligned} \quad (3.12)$$

$$\begin{aligned} &\frac{\partial^3\tilde{g}_n}{\partial u^3}(\tilde{u}_n)(V_i, V_i, V_i) \\ &= \frac{\partial^3\tilde{g}_n}{\partial u^3}(\tilde{u}_n)\left(c_i^3(\tilde{u}'_n, \tilde{u}'_n, \tilde{u}'_n) + \frac{3c_i^4h_n}{2}(\tilde{u}'_n, \tilde{u}'_n, \tilde{u}''_n) + \frac{3c_i^5h_n^2}{4}(\tilde{u}'_n, \tilde{u}''_n, \tilde{u}''_n)\right. \\ &\left. + \frac{c_i^5h_n^2}{2!}(\tilde{u}'_n, \tilde{u}'_n, \tilde{u}_n^{(3)}) + 3c_i^2h_n^2\left(\tilde{u}'_n, \tilde{u}'_n, \psi_{3,i}\frac{\partial^2\tilde{g}_n}{\partial u^2}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}'_n)\right)\right), \end{aligned} \quad (3.13)$$

$$\begin{aligned} &\frac{\partial^4\tilde{g}_n}{\partial u^4}(\tilde{u}_n)(V_i, V_i, V_i, V_i) \\ &= \frac{\partial^4\tilde{g}_n}{\partial u^4}(\tilde{u}_n)\left(c_i^4(\tilde{u}'_n, \tilde{u}'_n, \tilde{u}'_n, \tilde{u}'_n) + 2c_i^5h_n(\tilde{u}'_n, \tilde{u}'_n, \tilde{u}'_n, \tilde{u}''_n)\right), \end{aligned} \quad (3.14)$$

$$\frac{\partial^5\tilde{g}_n}{\partial u^5}(\tilde{u}_n)(V_i, V_i, V_i, V_i, V_i) = c_i^5\frac{\partial^5\tilde{g}_n}{\partial u^5}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}'_n, \tilde{u}'_n, \tilde{u}'_n, \tilde{u}'_n). \quad (3.15)$$

Then

$$\begin{aligned} \hat{u}_{n+1} &= \tilde{u}_n + h_n\varphi_1(h_n\tilde{J}_n)\tilde{u}_n + h_n^3\sum_{i=1}^s b_i\frac{c_i^2}{2}\frac{\partial^2\tilde{g}_n}{\partial u^2}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}'_n) + h_n^4\sum_{i=1}^s b_i\frac{c_i^3}{3!}M_n \\ &+ h_n^5\sum_{i=1}^s b_i\frac{c_i^4}{4!}N_n + h_n^5\hat{N}_n + h_n^6\sum_{i=1}^s b_i\frac{c_i^5}{5!}L_n + h_n^6\hat{L}_n + O(h_n^7), \end{aligned} \quad (3.16)$$

with

$$M_n = 3 \frac{\partial^2 \tilde{g}_n}{\partial u^2}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}''_n) + \frac{\partial^3 \tilde{g}_n}{\partial u^3}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}''_n, \tilde{u}'''_n), \quad (3.17)$$

$$N_n = 4 \frac{\partial^2 \tilde{g}_n}{\partial u^2}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}_n^{(3)}) + 3 \frac{\partial^2 \tilde{g}_n}{\partial u^2}(\tilde{u}_n)(\tilde{u}''_n, \tilde{u}''_n) + 6 \frac{\partial^3 \tilde{g}_n}{\partial u^3}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}''_n, \tilde{u}'''_n) \\ + \frac{\partial^4 \tilde{g}_n}{\partial u^4}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}''_n, \tilde{u}'''_n, \tilde{u}^{(4)}), \quad (3.18)$$

$$\hat{N}_n = \sum_{i=1}^s b_i c_i \frac{\partial^2 \tilde{g}_n}{\partial u^2}(\tilde{u}_n) \left(\tilde{u}'_n, \psi_{3,i} \frac{\partial^2 \tilde{g}_n}{\partial u^2}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}''_n) \right), \quad (3.19)$$

$$L_n = 10 \frac{\partial^2 \tilde{g}_n}{\partial u^2}(\tilde{u}_n)(\tilde{u}''_n, \tilde{u}_n^{(3)}) + 15 \frac{\partial^3 \tilde{g}_n}{\partial u^3}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}''_n, \tilde{u}'''_n) \\ + 10 \frac{\partial^3 \tilde{g}_n}{\partial u^3}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}'_n, \tilde{u}_n^{(3)}) + 10 \frac{\partial^4 \tilde{g}_n}{\partial u^4}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}'_n, \tilde{u}''_n, \tilde{u}'''_n) \\ + \frac{\partial^5 \tilde{g}_n}{\partial u^5}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}'_n, \tilde{u}''_n, \tilde{u}''_n, \tilde{u}'''_n) + 5 \frac{\partial^2 \tilde{g}_n}{\partial u^2}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}_n^{(4)}), \quad (3.20)$$

$$\hat{L}_n = \sum_{i=1}^s b_i c_i \frac{\partial^2 \tilde{g}_n}{\partial u^2}(\tilde{u}_n) \left(\tilde{u}'_n, \psi_{4,i} \frac{\partial^3 \tilde{g}_n}{\partial u^3}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}''_n, \tilde{u}'''_n) \right) \\ + 3 \sum_{i=1}^s b_i c_i \frac{\partial^2 \tilde{g}_n}{\partial u^2}(\tilde{u}_n) \left(\tilde{u}'_n, \psi_{4,i} \frac{\partial^2 \tilde{g}_n}{\partial u^2}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}''_n) \right) \\ + \sum_{i=1}^s b_i c_i^2 \frac{\partial^2 \tilde{g}_n}{\partial u^2}(\tilde{u}_n) \left(\tilde{u}''_n, \psi_{3,i} \frac{\partial^2 \tilde{g}_n}{\partial u^2}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}''_n) \right) \\ + \sum_{i=1}^s b_i \frac{c_i^2}{2} \frac{\partial^3 \tilde{g}_n}{\partial u^3}(\tilde{u}_n) \left(\tilde{u}'_n, \tilde{u}'_n, \psi_{3,i} \frac{\partial^2 \tilde{g}_n}{\partial u^2}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}''_n) \right). \quad (3.21)$$

By the variation of constants formula, the exact solution (2.3) at t_{n+1} can be expressed

$$\tilde{u}_{n+1} = e^{h_n \tilde{J}_n} \tilde{u}_n + h_n \int_0^1 e^{(1-\theta)h_n \tilde{J}_n} \tilde{g}_n(u(t_n + \theta h_n)) d\theta \\ = \tilde{u}_n + h_n \varphi_1(h_n \tilde{J}_n) \tilde{u}'_n + \sum_{q=2}^k h_n^{q+1} \int_0^1 e^{(1-\theta)h_n \tilde{J}_n} \frac{\theta^q}{q!} \frac{\partial^q \tilde{g}_n}{\partial u^q}(\tilde{u}_n)(V, V, \dots, V) d\theta \\ + O(h_n^{k+2}) \quad (3.22)$$

with

$$V = \frac{1}{\theta h_n} (u(t_n + \theta h_n) - u(t_n)) = \sum_{r=1}^m \frac{(\theta h_n)^{r-1}}{r!} \tilde{u}_n^{(r)} + O(h_n^m). \quad (3.23)$$

Then

$$\tilde{u}_{n+1} = \tilde{u}_n + h_n \varphi_1(h_n \tilde{J}_n) \tilde{u}'_n + h_n^3 \varphi_3(h_n \tilde{J}_n) \frac{\partial^2 \tilde{g}_n}{\partial u^2}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}''_n) + h_n^4 \varphi_4(h_n \tilde{J}_n) M_n \\ + h_n^5 \varphi_5(h_n \tilde{J}_n) N_n + h_n^6 \varphi_6(h_n \tilde{J}_n) L_n + O(h_n^7), \quad (3.24)$$

Table 1. Stiff order conditions for exponential Rosenbrock-type methods.

Here J, K denote arbitrary square matrices, the functions φ_i, φ_{ji} , are defined in (3.8) and (3.9), respectively.

No.	Order	Order Condition
1	1	$\psi_1(z) = 0$
2	2	$\psi_{1,i}(z) = 0, \quad 2 \leq i \leq s$
3	3	$\psi_3(z) = 0$
4	4	$\psi_4(z) = 0$
5	5	$\psi_5(z) = 0$
6	5	$\sum_{i=1}^s b_i(z) c_i J \psi_{3,i} = 0$
7	6	$\sum_{i=1}^s b_i(z) c_i^2 K \psi_{3,i} = 0$
8	6	$\sum_{i=1}^s b_i(z) c_i J \psi_{4,i} = 0$
9	6	$\psi_6(z) = 0$

where M_n, N_n, L_n are defined as (3.17), (3.18), (3.20), respectively.

Let $\bar{e}_{n+1} = \hat{u}_{n+1} - \tilde{u}_{n+1}$ denote the local error, i.e., the difference between the numerical solution \hat{u}_{n+1} after one step starting from \tilde{u}_n and the corresponding exact solution of (2.3) at t_{n+1} , then

$$\begin{aligned} \bar{e}_{n+1} = & h_n^3 \psi_3(h_n \tilde{J}_n) \frac{\partial^2 \tilde{g}_n}{\partial u^2}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}'_n) + h_n^4 \psi_4(h_n \tilde{J}_n) M_n + h_n^5 \psi_5(h_n \tilde{J}_n) N_n + h_n^5 \hat{N}_n \\ & + h_n^6 \psi_6(h_n \tilde{J}_n) L_n + h_n^6 \hat{L}_n + O(h_n^7). \end{aligned} \quad (3.25)$$

By zeroing the corresponding terms in (3.25), the stiff order conditions for methods of order six can easily be identified and reported in Table 1. Until now, all of the order conditions derived are listed in Table 1. Note that the first two conditions of Table 1 are automatically satisfied in our context since they are used to derive our reformulated scheme (2.9), and the first six conditions were already derived by Hochbruck and Luan et al. [7, 12].

4. Convergence bounds

The purpose of this section is to give a global error analysis of scheme (2.9). We will derive uniform error bounds on bounded time intervals. In order to bound the global error, we begin with the following lemma.

Lemma 4.1. ([12]) *Under Assumptions 1 and 2, the following estimates*

$$\|\varphi_k(tJ(u)) - \varphi_k(tJ(v))\|_{X \leftarrow X} \leq Ct \|u - v\|, \quad (4.1)$$

$$\|a_{ij}(tJ(u)) - a_{ij}(tJ(v))\|_{X \leftarrow X} \leq Ct \|u - v\|, \quad (4.2)$$

$$\|b_k(tJ(u)) - b_k(tJ(v))\|_{X \leftarrow X} \leq Ct \|u - v\|. \quad (4.3)$$

hold for all i, j, k in a neighborhood of the exact solution.

In order to get our main results, the further assumption on the estimate

$$\left\| \prod_{j=0}^{n-\nu} e^{h_{n-j} J_{n-j}} \right\|_{X \leftarrow X} \leq \mathcal{C}, \quad t_0 \leq t_\nu \leq t_n = T \quad (4.4)$$

holds uniformly in ν and n , where \mathcal{C} is a constant. It was shown in [7] that such a stability bound holds for variable step sizes, under a mild restriction on the step size sequence. For details, we refer the reader to [7].

Lemma 4.2. *Let the initial value problem (1.1) satisfy Assumptions 1, 2, and the stability estimates (4.4), y_0 and z_0 be two input values to a step with exponential Rosenbrock-type methods (2.5), using variable step size h_n , $n = 0, 1, \dots$, and y_n, z_n be the corresponding output values. Then*

$$\|y_n - z_n\| \leq C \|y_0 - z_0\|. \quad (4.5)$$

Proof. Denote the stage values by Y_{ni} and Z_{ni} at time t_n , respectively.

The equation

$$\begin{aligned} E_{ni} = Y_{ni} - Z_{ni} &= e^{c_i h_n \bar{J}_n} y_n - e^{c_i h_n \hat{J}_n} z_n \\ &+ h \sum_{j=1}^{i-1} \left(a_{ij}(h_n \bar{J}_n) \bar{g}_n(Y_{nj}) - a_{ij}(h_n \hat{J}_n) \hat{g}_n(Z_{nj}) \right). \end{aligned} \quad (4.6)$$

Here,

$$\begin{aligned} \bar{J}_n &= \frac{\partial F}{\partial u}(y_n) = A + \frac{\partial g}{\partial u}(y_n), \\ \hat{J}_n &= \frac{\partial F}{\partial u}(z_n) = A + \frac{\partial g}{\partial u}(z_n), \\ \bar{g}_n(u) &= F(u) - \bar{J}_n u, \\ \hat{g}_n(u) &= F(u) - \hat{J}_n u. \end{aligned} \quad (4.7)$$

Since

$$\begin{aligned} \|\bar{g}_n(Y_{nj}) - \hat{g}_n(Z_{nj})\| &\leq \|\bar{g}_n(Y_{nj}) - \bar{g}_n(Z_{nj})\| + \|\bar{g}_n(Z_{nj}) - \hat{g}_n(Z_{nj})\| \\ &\leq C(\|E_{nj}\| + \|y_n - z_n\|). \end{aligned} \quad (4.8)$$

By Lemma 4.1, we have

$$\begin{aligned} \|E_{ni}\| &\leq \|e^{c_i h_n \bar{J}_n} (y_n - z_n)\| + \|(e^{c_i h_n \bar{J}_n} - e^{c_i h_n \hat{J}_n}) z_n\| \\ &\quad + h_n \left\| \sum_{j=1}^{i-1} \left(a_{ij}(h_n \bar{J}_n) - a_{ij}(h_n \hat{J}_n) \right) \bar{g}_n(Y_{nj}) \right\| \\ &\quad + h_n \left\| \sum_{j=1}^{i-1} a_{ij}(h_n \hat{J}_n) \left(\bar{g}_n(Y_{nj}) - \hat{g}_n(Z_{nj}) \right) \right\| \\ &\leq C \|y_n - z_n\| + C h_n \|y_n - z_n\| + C h_n^2 \|y_n - z_n\| \\ &\quad + C h_n \sum_{j=1}^{i-1} (\|E_{nj}\| + \|y_n - z_n\|) \\ &= C(1 + h_n + h_n^2) \|y_n - z_n\| + C h_n \sum_{j=1}^{i-1} \|E_{nj}\|. \end{aligned} \quad (4.9)$$

An application of a discrete Gronwall lemma 4 in [5] yields

$$\|E_{ni}\| \leq C(1 + h_n + h_n^2)\|y_n - z_n\|. \quad (4.10)$$

Then

$$\begin{aligned} e_{n+1} &= y_{n+1} - z_{n+1} \\ &= e^{h_n \bar{J}_n} y_n - e^{h_n \hat{J}_n} z_n + h_n \sum_{j=1}^s \left(b_j(h_n \bar{J}_n) \bar{g}_n(Y_{nj}) - b_j(h_n \hat{J}_n) \hat{g}_n(Z_{nj}) \right) \\ &= e^{h_n \bar{J}_n} (y_n - z_n) + (e^{h_n \bar{J}_n} - e^{h_n \hat{J}_n}) z_n \\ &\quad + h_n \sum_{j=1}^s \left(b_j(h_n \bar{J}_n) - b_j(h_n \hat{J}_n) \right) \bar{g}_n(Y_{nj}) \\ &\quad + h_n \sum_{j=1}^s b_j(h_n \hat{J}_n) \left(\bar{g}_n(Y_{nj}) - \hat{g}_n(Z_{nj}) \right) \\ &= e^{h_n \bar{J}_n} e_n + P_n, \end{aligned} \quad (4.11)$$

where

$$\begin{aligned} P_n &= (e^{h_n \bar{J}_n} - e^{h_n \hat{J}_n}) z_n + h_n \sum_{j=1}^s \left(b_j(h_n \bar{J}_n) - b_j(h_n \hat{J}_n) \right) \bar{g}_n(Y_{nj}) \\ &\quad + h_n \sum_{j=1}^s b_j(h_n \hat{J}_n) \left(\bar{g}_n(Y_{nj}) - \hat{g}_n(Z_{nj}) \right). \end{aligned} \quad (4.12)$$

Applying this estimate (4.10), we have

$$\begin{aligned} \|P_n\| &\leq \|(e^{h_n \bar{J}_n} - e^{h_n \hat{J}_n}) z_n\| + h_n \sum_{j=1}^s \left\| \left(b_j(h_n \bar{J}_n) - b_j(h_n \hat{J}_n) \right) \bar{g}_n(Y_{nj}) \right\| \\ &\quad + h_n \sum_{j=1}^s \left\| b_j(h_n \hat{J}_n) \left(\bar{g}_n(Y_{nj}) - \hat{g}_n(Z_{nj}) \right) \right\| \\ &\leq Ch_n(1 + h_n + h_n^2)\|e_n\|. \end{aligned} \quad (4.13)$$

Solving the recursion (4.11) yields

$$e_{n+1} = \sum_{v=0}^n \prod_{j=1}^{n-v} e^{h_{n-j} \bar{J}_{n-j}} P_v + \prod_{j=0}^n e^{h_j \bar{J}_j} e_0. \quad (4.14)$$

Now, using the stability estimate (4.13) and the bound (4.4), we obtain

$$\|e_{n+1}\| \leq Ch_n \sum_{v=0}^n (1 + h_n + h_n^2) \|e_n\| + C \|e_0\|. \quad (4.15)$$

An application of a Gronwall lemma again, we concludes the desired bound (4.5). \square

Next, we consider the cumulative effect of errors in many steps leading to an error in a final output point. Denote the approximations computed by an exponential Rosenbrock-type methods by u_1, u_2, \dots, u_n , with $u_0 = u(t_0)$, and a variable stepsize is adopted. By Lemma 4.2, the error committed in the ν step is bounded by $C\bar{e}_\nu$, and \bar{e}_ν is the local truncation error at step ν . Then the total contribution to the error would be

$$\|u(t_n) - u_n\| \leq C \sum_{\nu=0}^{n-1} \bar{e}_\nu.$$

Such an idea can be found in [2]. This leads to the following

Theorem 4.1. *Let the initial value problem (1.1) satisfy Assumptions 1, 2, and the stability estimates (4.4). Consider for its numerical solution an explicit exponential Rosenbrock-type methods (2.5) that satisfies the local truncation error at step $k = 1, 2, \dots, n$ bounded by $\delta_k \leq Ch_k^{p+1}$. Then the global truncation error is bounded by*

$$\|u(t_n) - u_n\| \leq C \sum_{j=0}^{n-1} h_j^{p+1}$$

uniformly in $t_0 \leq t_n \leq T$. The constant C depends on T , but it is independent of n and h .

Corollary 4.1. *Let the initial value problem (1.1) satisfy Assumptions 1 and 2. Consider for its numerical solution an explicit exponential Rosenbrock-type methods (2.5) that fulfills the order conditions 1-9 of Table 1. Then, under the stability assumption (4.4), the scheme (2.5) is convergent of order 6. In particular, the global truncation error is bounded by*

$$\|u(t_n) - u_n\| \leq C \sum_{j=0}^{n-1} h_j^7$$

uniformly in $t_0 \leq t_n \leq T$. The constant C depends on T , but it is independent of n and h .

References

- [1] H. Berland, B. Owren and B. Skaflestad, *B-series and order conditions for exponential integrators*, SIAM J. Numer. Anal., 43 (2005), 1715-1727.
- [2] J. C. Butcher, *Numerical methods for ordinary differential equations*, John Wiley and Sons Ltd, Chichester, 2008.
- [3] M. Caliari and A. Ostermann, *Implementation of exponential Rosenbrocktype integrators*, Appl. Numer. Math., 59 (2009), 568C581.
- [4] K. J. Engel and R. Nagel, *One-Parameter semigroups for linear evolution equations*, Springer, New York, 2000.
- [5] M. Hochbruck and A. Ostermann, *Exponential Runge-Kutta methods for parabolic problems*, Appl. Numer. Math. 53 (2005), 323-339.
- [6] M. Hochbruck and A. Ostermann, *Explicit exponential Runge-Kutta methods for semilinear parabolic problems*, SIAM J. Numer. Anal., 43 (2006), 1069-1090.

-
- [7] M. Hochbruck, A. Ostermann and J. Schweitzer, *Exponential Rosenbrock-Type methods*, SIAM J. Numer. Anal., 47 (2009), 786-803.
 - [8] M. Hochbruck, C. Lubich and H. Selhofer, *Exponential integrators for large systems of differential equations*, SIAM J. Sci. Comput., 19 (1998), 1552-1574.
 - [9] M. Hochbruck and A. Ostermann, *Exponential integrators*, Acta Numerica, 19 (2010), 209-286.
 - [10] A. K. Kassam and L.N. Trefethen, *Fourth-order time stepping for stiff PDEs*, SIAM J. Sci. Comput., 26 (2005), 1214C1233.
 - [11] S. Krogstad, *Generalized integrating factor methods for stiff PDEs*, J. Comput. Phys., 203 (2005), 72C88.
 - [12] V. T. Luan and A. Ostermann, *Exponential Rosenbrock methods of order five-construction, analysis and numerical comparisons*, J. Comput. Appl. Math., 255 (2014), 417-431.
 - [13] J. Loffeld and M. Tokman, *Comparative performance of exponential, implicit, and explicit integrators for stiff systems of ODEs*, J. Comput. Appl. Math., 241 (2013), 45-67.
 - [14] M. Tokman, *Efficient integration of large stiff systems of ODEs with exponential propagation iterative (EPI) methods*, J. Comput. Phys., 213 (2006), 748C776.