Stiff Order Conditions for Exponential Runge–Kutta Methods of Order Five

Vu Thai Luan and Alexander Ostermann

Abstract Exponential Runge–Kutta methods are tailored for the time discretization of semilinear stiff problems. The actual construction of high-order methods relies on the knowledge of the order conditions, which are available in the literature up to order four. In this short note, we show how the order conditions for methods up to order five are derived; the extension to arbitrary orders will be published elsewhere. Our approach is adapted to stiff problems and allows us to prove highorder convergence results for variable step size implementations, independently of the stiffness of the problem.

1 Introduction

In this paper, we derive the stiff order conditions for exponential Runge–Kutta methods up to order five. These conditions are important for constructing high-order time discretization schemes for semilinear problems

$$
u'(t) = Au(t) + g(u(t)), \quad u(t_0) = u_0,
$$
 (1)

where A has a large norm or is even an unbounded operator. The nonlinearity g, on the other hand, is supposed to be nonstiff with a moderate Lipschitz constant in a strip along the exact solution. Abstract parabolic evolution equations and their spatial discretizations are typical examples of such problems.

Exponential integrators have shown to be very competitive for stiff problems, see $[1, 4, 9]$ $[1, 4, 9]$ $[1, 4, 9]$ $[1, 4, 9]$ $[1, 4, 9]$. They treat the linear part of problem (1) exactly and the nonlinearity in an explicit way. A recent overview of such integrators and their implementation was given in [\[7\]](#page-10-3). The class of exponential Runge–Kutta methods was first considered by Friedli [\[2\]](#page-10-4) who also derived the nonstiff order conditions. For stiff problems, the methods were analyzed in [\[5\]](#page-10-5). In that paper, the stiff order conditions for methods up to order four were derived.

V.T. Luan (\boxtimes) • A. Ostermann

Institut für Mathematik, Universität Innsbruck, Technikerstr. 13, A–6020 Innsbruck, Austria e-mail: [vu.thai-luan@uibk.ac.at;](mailto:vu.thai-luan@uibk.ac.at) alexander.ostermann@uibk.ac.at

[©] Springer International Publishing Switzerland 2014

H.G. Bock et al. (eds.), *Modeling, Simulation and Optimization of Complex Processes - HPSC 2012*, DOI 10.1007/978-3-319-09063-4__11

Motivated by the fact that exponential Runge–Kutta methods can be viewed as small perturbations of the exponential Euler method, we present here a new and simple approach to derive the stiff order conditions. Instead of inserting the exact solution into the numerical scheme and working with defects, as it was done in [\[5,](#page-10-5) [8\]](#page-10-6), we analyze the local error in a direct way. For this purpose, we reformulate the scheme as a perturbation of the exponential Euler method and carry out a perturbation analysis. This allows us to generalize the order four conditions that were given in [\[5\]](#page-10-5) to methods up to order five. The error analysis is performed in the framework of strongly continuous semigroups [\[11\]](#page-10-7) which covers parabolic problems and their spatial discretizations. The work is inspired by our recent paper [\[10\]](#page-10-8), where exponential Rosenbrock methods were constructed up to order five.

The paper is organized as follows. In Sect. [2,](#page-2-0) we introduce a reformulation of exponential Runge–Kutta methods which turns out to be advantageous for the analysis. Our abstract framework is given in Sect. [3.](#page-3-0) The new stiff order conditions are derived in Sect. [4.](#page-4-0) Section [5](#page-9-0) is devoted to the convergence analysis. The main results are given in Table [1](#page-1-0) and Theorem [1.](#page-9-1)

N _o	Order condition	Order
$\mathbf{1}$	$\sum_{i=1}^{s} b_i(Z) = \varphi_1(Z)$	1
$\overline{2}$	$\sum_{i=2}^s b_i(Z)c_i = \varphi_2(Z)$	$\overline{2}$
3	$\sum_{i=1}^{i-1} a_{ii}(Z) = c_i \varphi_1(c_i Z), \quad i = 2, \ldots, s$	2
$\overline{4}$	$\sum_{i=2}^{s} b_i(Z) \frac{c_i^2}{2!} = \varphi_3(Z)$	3
5	$\sum_{i=2}^{s} b_i(Z) J \psi_{2,i}(Z) = 0$	3
6	$\sum_{i=2}^s b_i(Z) \frac{c_i^3}{2!} = \varphi_4(Z)$	4
τ	$\sum_{i=2}^s b_i(Z)J\psi_{3,i}(Z)=0$	$\overline{4}$
8	$\sum_{i=2}^s b_i(Z) J \sum_{i=2}^{i-1} a_{ij}(Z) J \psi_{2,j}(Z) = 0$	4
9	$\sum_{i=2}^{s} b_i(Z) c_i K \psi_{2,i}(Z) = 0$	4
10	$\sum_{i=2}^{s} b_i(Z) \frac{c_i^4}{4!} = \varphi_5(Z)$	5
11	$\sum_{i=2}^{s} b_i(Z) J \psi_{4,i}(Z) = 0$	5
12	$\sum_{i=2}^s b_i(Z) J \sum_{i=2}^{i-1} a_{ij}(Z) J \psi_{3,i}(Z) = 0$	5
13	$\sum_{i=2}^{s} b_i(Z)J \sum_{i=2}^{i-1} a_{ij}(Z)J \sum_{k=2}^{j-1} a_{ik}(Z)J \psi_{2,k}(Z) = 0$	5
14	$\sum_{i=2}^s b_i(Z) J \sum_{i=2}^{i-1} a_{ij}(Z) c_i K \psi_{2,i}(Z) = 0$	5
15	$\sum_{i=2}^{s} b_i(Z) c_i K \psi_{3,i}(Z) = 0$	5
16	$\sum_{i=2}^s b_i(Z)c_i K \sum_{i=2}^{i-1} a_{ij}(Z)J\psi_{2,j}(Z) = 0$	5
17	$\sum_{i=2}^s b_i(Z) B(\psi_{2,i}(Z), \psi_{2,i}(Z)) = 0$	5
18	$\sum_{i=2}^{s} b_i(Z) c_i^2 L \psi_{2i}(Z) = 0$	5

Table 1 Stiff order conditions for explicit exponential Runge–Kutta methods up to order 5. The variables Z , J , K , L denote arbitrary square matrices, and B an arbitrary bilinear mapping of appropriate dimensions. The functions $\psi_{k,l}$ are defined in [\(21\)](#page-6-0)

2 Reformulation of Exponential Runge–Kutta Methods

In order to solve [\(1\)](#page-0-0) numerically, we consider a class of explicit one-step methods, the so-called explicit exponential Runge–Kutta methods

$$
U_{ni} = e^{c_i h_n A} u_n + h_n \sum_{j=1}^{i-1} a_{ij} (h_n A) g(U_{nj}), \quad 1 \le i \le s,
$$
 (2a)

$$
u_{n+1} = e^{h_n A} u_n + h_n \sum_{i=1}^{s} b_i (h_n A) g(U_{ni}).
$$
 (2b)

The stages U_{ni} are approximations to $u(t_n + c_i h_n)$, the numerical solution u_{n+1} approximates the true solution at time t_{n+1} and $h_n = t_{n+1} - t_n$ denotes the step size. The coefficients $a_{ii}(h_nA)$ and $b_i(h_nA)$ are usually chosen as linear combinations of the entire functions $\varphi_k(c_i h_n A)$ and $\varphi_k(h_n A)$, respectively. These functions are given by

$$
\varphi_0(z) = e^z, \quad \varphi_k(z) = \int_0^1 e^{(1-\theta)z} \frac{\theta^{k-1}}{(k-1)!} d\theta, \quad k \ge 1
$$
\n(3)

and thus satisfy the recurrence relation

$$
\varphi_{k+1}(z) = \frac{\varphi_k(z) - \varphi_k(0)}{z}, \quad k \ge 0.
$$
 (4)

It turns out that the equilibria of [\(1\)](#page-0-0) are preserved if the coefficients a_{ij} and b_i of the method fulfill the following simplifying assumptions (see [\[5\]](#page-10-5))

$$
\sum_{i=1}^{s} b_i(h_n A) = \varphi_1(h_n A), \qquad \sum_{j=1}^{i-1} a_{ij}(h_n A) = c_i \varphi_1(c_i h_n A), \quad 1 \le i \le s. \tag{5}
$$

The latter implies in particular that $c_1 = 0$. Without further mention, we will assume throughout the paper that (5) is satisfied.

Following an idea of [\[6,](#page-10-9) [12\]](#page-10-10), we now express the vector $g(U_{ni})$ as

$$
g(U_{ni}) = g(u_n) + D_{ni}, \quad 1 \le i \le s
$$
 (6)

and rewrite [\(2\)](#page-2-2) in terms of D_{ni} . Since $c_1 = 0$, we consequently have $U_{n_1} = u_n$ and $D_{n1} = 0$. The method [\(2\)](#page-2-2) then takes the equivalent form

$$
U_{ni} = u_n + c_i h_n \varphi_1(c_i h_n A) F(u_n) + h_n \sum_{j=2}^{i-1} a_{ij} (h_n A) D_{nj}, \quad 1 \le i \le s,
$$
 (7a)

$$
u_{n+1} = u_n + h_n \varphi_1(h_n A) F(u_n) + h_n \sum_{i=2}^{s} b_i(h_n A) D_{ni}
$$
 (7b)

with $F(u) = Au + g(u)$.

Since the vectors D_{ni} are small in norm, in general, exponential Runge–Kutta methods can be interpreted as small perturbations of the exponential Euler scheme

$$
u_{n+1} = u_n + h_n \varphi_1(h_n A) F(u_n).
$$

The reformulated scheme [\(7\)](#page-2-3) can be implemented more efficiently than [\(2\)](#page-2-2), and it offers advantages in the error analysis, see below.

3 Analytic Framework

For the error analysis of [\(7\)](#page-2-3), we work in an abstract framework of strongly continuous semigroups on a Banach space X with norm $\|\cdot\|$. Background information on semigroups can be found in the monograph [\[11\]](#page-10-7).

Throughout the paper we consider the following assumptions.

Assumption 1. The linear operator A is the infinitesimal generator of a strongly continuous semigroup e^{tA} on X.

This implies (see [\[11,](#page-10-7) Thm. 2.2]) that there exist constants M and ω such that

$$
\|e^{tA}\|_{X\leftarrow X} \le M e^{\omega t}, \quad t \ge 0. \tag{8}
$$

Under the above assumption, the expressions $\varphi_k(h_nA)$ and consequently the coefficients $a_{ij}(h_nA)$ and $b_i(h_nA)$ of the method are bounded operators, see [\(3\)](#page-2-4). This property is crucial in our proofs.

For high-order convergence results, we require the following regularity assumption.

Assumption 2. We suppose that (1) possesses a sufficiently smooth solution u : $[0, T] \rightarrow X$ 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](#page-3-1) implies that g is locally Lipschitz in a strip along the exact solution. It is well known that semilinear reaction-diffusion-advection equations can be put into this abstract framework, see [\[3\]](#page-10-11).

4 A New Approach to Construct the Stiff Order Conditions

In this section, we present a new approach to derive the stiff order conditions for exponential Runge–Kutta methods. It is the well-known that the exponential Euler method

$$
u_{n+1} = u_n + h_n \varphi_1(h_n A) F(u_n)
$$
 (9)

has order one. In view of [\(7b\)](#page-3-2), exponential Runge–Kutta methods can be considered as small perturbations of [\(9\)](#page-4-1). This observation motivates us to investigate the vectors D_{ni} in order to get a higher-order method.

Let \tilde{u}_n denote the exact solution of [\(1\)](#page-0-0) at time t_n , i.e., $\tilde{u}_n = u(t_n)$. In order to study the local error of scheme [\(7\)](#page-2-3), we consider one step with initial value \tilde{u}_n , i.e.

$$
\hat{U}_{ni} = \tilde{u}_n + c_i h_n \varphi_1(c_i h_n A) F(\tilde{u}_n) + h_n \sum_{j=2}^{i-1} a_{ij} (h_n A) \hat{D}_{nj},
$$
\n(10a)

$$
\hat{u}_{n+1} = \tilde{u}_n + h_n \varphi_1(h_n A) F(\tilde{u}_n) + h_n \sum_{i=2}^s b_i (h_n A) \hat{D}_{ni}
$$
\n(10b)

with

$$
\hat{D}_{ni} = g(\hat{U}_{ni}) - g(\tilde{u}_n), \quad \hat{U}_{ni} \approx u(t_n + c_i h_n). \tag{11}
$$

Let $\tilde{u}_h^{(k)}$ denote the k-th derivative of the exact solution $u(t)$ of [\(1\)](#page-0-0), evaluated at $t \in \mathcal{F}$. For $k = 1, 2$ we use the corresponding potations \tilde{u}' , \tilde{u}'' for simplicity. We time t_n . For $k = 1, 2$ we use the corresponding notations \tilde{u}'_n , \tilde{u}''_n for simplicity. We further denote the *k*-th derivative of $g(u)$ with respect to *u* by $g^{(k)}(u)$ further denote the k-th derivative of $g(u)$ with respect to *u* by $g^{(k)}(u)$.

4.1 Taylor Expansion of the Exact and the Numerical Solution

On the one hand, expressing the exact solution of [\(1\)](#page-0-0) at time t_{n+1} by the variationof-constants formula

$$
\tilde{u}_{n+1} = u(t_{n+1}) = e^{h_n A} \tilde{u}_n + h_n \int_0^1 e^{(1-\theta)h_n A} g(u(t_n + \theta h_n)) d\theta \tag{12}
$$

and then expanding $g(u(t_n + \theta h_n))$ in a Taylor series at \tilde{u}_n gives

$$
\tilde{u}_{n+1} = \tilde{u}_n + h_n \varphi_1(h_n A) F(\tilde{u}_n)
$$
\n
$$
+ \sum_{q=1}^k h_n^{q+1} \int_0^1 e^{(1-\theta)h_n A} \frac{\theta^q}{q!} g^{(q)}(\tilde{u}_n) (\underbrace{V, \dots, V}_{q \text{ times}}) d\theta + \mathcal{R}_k
$$
\n(13)

with $V = \frac{1}{\theta h_n} \big(u(t_n + \theta h_n) - u(t_n) \big)$ and the remainder hn

$$
\mathscr{R}_k=h_n^{k+2}\int_0^1e^{(1-\theta)h_nA}\int_0^1\frac{\theta^{k+1}(1-s)^k}{k!}g^{(k+1)}(\tilde{u}_n+s\theta h_nV)(\underbrace{V,\ldots,V}_{k+1 \text{ times}})\,ds\,d\theta.
$$

It is easy to see that $\|\mathcal{R}_k\| \leq Ch_h^{\kappa+2}$ where the constant C only depends on values
that are uniformly bounded by Assumptions 1 and 2. From now on, we will use the that are uniformly bounded by Assumptions [1](#page-3-3) and [2.](#page-3-1) From now on, we will use the Landau notation for such remainder terms. Thus, we will write $\mathcal{R}_k = \mathcal{O}(h_n^{k+2})$.

Expanding $u(t_n + \theta h_n)$ in a Taylor series at t_n gives

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

Inserting these expressions into [\(13\)](#page-4-2) for $k = 4$, using [\(3\)](#page-2-4) and the symmetry of the multilinear mappings in (13) , we obtain

$$
\tilde{u}_{n+1} = \tilde{u}_n + h_n \varphi_1(h_n A) F(\tilde{u}_n) + h_n^2 \varphi_2(h_n A) \mathbf{L} + h_n^3 \varphi_3(h_n A) \mathbf{M}
$$
\n
$$
+ h_n^4 \varphi_4(h_n A) \mathbf{N} + h_n^5 \varphi_5(h_n A) \mathbf{P} + \mathcal{O}(h_n^6)
$$
\n(14)

with

$$
\mathbf{L} = g'(\tilde{u}_n)\tilde{u}'_n, \quad \mathbf{M} = g'(\tilde{u}_n)\tilde{u}''_n + g''(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}'_n), \n\mathbf{N} = g'(\tilde{u}_n)\tilde{u}^{(3)}_n + 3g''(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}''_n) + g^{(3)}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}'_n, \tilde{u}'_n), \n\mathbf{P} = g'(\tilde{u}_n)\tilde{u}^{(4)}_n + 3g''(\tilde{u}_n)(\tilde{u}''_n, \tilde{u}''_n) + 4g''(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}^{(3)}_n) \n+ 6g^{(3)}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}'_n, \tilde{u}''_n) + g^{(4)}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}'_n, \tilde{u}'_n, \tilde{u}'_n).
$$
\n(15)

On the other hand, expanding \hat{D}_{ni} in [\(11\)](#page-4-3) in a Taylor series at \tilde{u}_n , we obtain

$$
\hat{D}_{ni} = \sum_{q=1}^{k} \frac{h_n^q}{q!} g^{(q)}(\tilde{u}_n) (\underbrace{V_i, \dots, V_i}_{q \text{ times}}) + \mathcal{O}(h_n^{k+1})
$$
\n(16)

with

$$
V_i = \frac{1}{h_n} (\hat{U}_{ni} - \tilde{u}_n) = c_i \varphi_1(c_i h_n A) F(\tilde{u}_n) + \sum_{j=2}^{i-1} a_{ij} (h_n A) \hat{D}_{nj}.
$$
 (17)

Inserting (16) into $(10b)$, we get

$$
\hat{u}_{n+1} = \tilde{u}_n + h_n \varphi_1(h_n A) F(\tilde{u}_n) + \sum_{i=2}^s b_i(h_n A) \sum_{q=1}^k \frac{h_n^{q+1}}{q!} g^{(q)}(\tilde{u}_n) (\underbrace{V_i, \dots, V_i}_{q \text{ times}}) + \mathcal{O}(h_n^{k+2}).
$$
\n(18)

In order to construct methods of order 5 we set $k = 4$ and compute V_i .

Lemma 1. *Under Assumptions [1](#page-3-3) and [2,](#page-3-1) we have*

$$
\varphi_1(c_i h_n A) F(\tilde{u}_n) = \tilde{u}'_n + \frac{c_i h_n}{2!} \mathbf{X}_i + \frac{c_i^2 h_n^2}{3!} \mathbf{Y}_i + \frac{c_i^3 h_n^3}{4!} \mathbf{Z}_i + \mathcal{O}(h_n^4)
$$
(19)

with

$$
\mathbf{X}_{i} = \tilde{u}_{n}'' - 2! \varphi_{2}(c_{i}h_{n}A) \mathbf{L}, \quad \mathbf{Y}_{i} = \tilde{u}_{n}^{(3)} - 3! \varphi_{3}(c_{i}h_{n}A) \mathbf{M},
$$

$$
\mathbf{Z}_{i} = \tilde{u}_{n}^{(4)} - 4! \varphi_{4}(c_{i}h_{n}A) \mathbf{N}.
$$
 (20)

Proof. It is easy to see from [\(1\)](#page-0-0) that $Au^{(k)}(t) = u^{(k+1)}(t) - \frac{d^k}{dt^k} g(u(t))$. Thus $Au^{(k)}(t)$ is bounded for all k. Evaluating it at $t = t$, for $k = 1, 2, 3$ by using the chain rule. is bounded for all k. Evaluating it at $t = t_n$ for $k = 1, 2, 3$ by using the chain rule,
we obtain expressions for $4\tilde{\nu}'$, $4\tilde{\nu}''$, and $4\tilde{\nu}^{(3)}$. Using $E(\tilde{\nu}) = \tilde{\nu}'$ and employing we obtain expressions for $A\tilde{u}'_n$, $A\tilde{u}''_n$, and $A\tilde{u}^{(3)}_n$. Using $F(\tilde{u}_n) = \tilde{u}'_n$ and employing
the recurrence relation $\omega_1(h, A) = \frac{1}{h} + h \cdot A\omega_1 + (h \cdot A)$, we get the recurrence relation $\varphi_k(h_nA) = \frac{1}{k!} + h_nA\varphi_{k+1}(h_nA)$, we get

$$
\varphi_1(c_i h_n A) F(\tilde{u}_n) = \tilde{u}'_n + \frac{c_i h_n}{2!} \mathbf{X}_i + \frac{c_i^2 h_n^2}{3!} \mathbf{Y}_i + \frac{c_i^3 h_n^3}{4!} \mathbf{Z}_i + h_n^4 c_i^4 \varphi_5(c_i h_n A) A \tilde{u}_n^{(4)}.
$$

In the subsequent analysis, we use the abbreviations $a_{ij} = a_{ij}(h_nA)$, $b_i = b_i(h_nA)$, and

$$
\psi_{j,i} = \psi_{j,i}(h_n A) = \sum_{k=2}^{i-1} a_{ik}(h_n A) \frac{c_k^{j-1}}{(j-1)!} - c_i^j \varphi_j(c_i h_n A). \tag{21}
$$

Lemma 2. *Under Assumptions [1](#page-3-3) and [2,](#page-3-1) the following holds*

$$
V_{i} = c_{i}\tilde{u}'_{n} + h_{n}\left(\frac{c_{i}^{2}}{2!}\tilde{u}''_{n} + \psi_{2,i} \mathbf{L}\right)
$$

+ $h_{n}^{2}\left(\frac{c_{i}^{3}}{3!}\tilde{u}^{(3)}_{n} + \psi_{3,i} \mathbf{M} + \sum_{j=2}^{i-1} a_{ij}g'(\tilde{u}_{n})\psi_{2,j} \mathbf{L}\right) + h_{n}^{3}\left(\frac{c_{i}^{4}}{4!}\tilde{u}^{(4)}_{n} + \psi_{4,i} \mathbf{N} + \sum_{j=2}^{i-1} a_{ij}g'(\tilde{u}_{n})\psi_{3,j} \mathbf{M} + \sum_{j=2}^{i-1} a_{ij}g'(\tilde{u}_{n})\sum_{k=2}^{j-1} a_{jk}g'(\tilde{u}_{n})\psi_{2,k} \mathbf{L} + \sum_{j=2}^{i-1} a_{ij}c_{j}g''(\tilde{u}_{n})(\tilde{u}'_{n}, \psi_{2,j} \mathbf{L}) + \mathcal{O}(h_{n}^{4}).$ \n(22)

Proof. Using [\(16\)](#page-5-0) and [\(17\)](#page-5-1) repeatedly, one obtains the following representations

$$
\hat{D}_{nj} = h_n g'(\tilde{u}_n) V_j + \frac{h_n^2}{2!} g''(\tilde{u}_n) (V_j, V_j) + \frac{h_n^3}{3!} g^{(3)}(\tilde{u}_n) (V_j, V_j, V_j) + \mathcal{O}(h_n^4),
$$
\n
$$
V_j = c_j \varphi_1(c_j h_n A) F(\tilde{u}_n) + \sum_{k=2}^{j-1} a_{jk} \Big(h_n g'(\tilde{u}_n) V_k + \frac{h_n^2}{2!} g''(\tilde{u}_n) (V_k, V_k) \Big) + \mathcal{O}(h_n^3),
$$
\n
$$
V_k = c_k \varphi_1(c_k h_n A) F(\tilde{u}_n) + h_n \sum_{l=2}^{k-1} a_{kl} g'(\tilde{u}_n) V_l + \mathcal{O}(h_n^2) \text{ and}
$$
\n
$$
V_l = c_l \varphi_1(c_l h_n A) F(\tilde{u}_n) + \mathcal{O}(h_n).
$$

Applying Lemma [1](#page-6-1) to the first terms of V_i , V_k , V_l and then sequentially inserting V_l into V_k , V_k into V_j , and V_j into \hat{D}_{nj} , we obtain the full expression of \hat{D}_{nj} with the remainder $\mathcal{O}(h_n^4)$. Substituting this into [\(17\)](#page-5-1), employing Lemma [1](#page-6-1) once more and combining all obtained terms we get (22) combining all obtained terms we get (22) .

The following result follows immediately from Lemma [2.](#page-6-3)

Lemma 3. *Under Assumptions [1](#page-3-3) and [2](#page-3-1) we have*

$$
g^{(4)}(\tilde{u}_n)(V_i, V_i, V_i, V_i) = c_i^4 g^{(4)}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}'_n, \tilde{u}'_n, \tilde{u}'_n) + \mathcal{O}(h_n),
$$

\n
$$
g^{(3)}(\tilde{u}_n)(V_i, V_i, V_i) = c_i^3 g^{(3)}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}'_n, \tilde{u}'_n) + h_n(\frac{3}{2}c_i^4 g^{(3)}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}'_n, \tilde{u}''_n)
$$

\n
$$
+ 3c_i^2 g^{(3)}(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}'_n, \psi_{2,i} \mathbf{L}) + \mathcal{O}(h_n^2),
$$

\n
$$
g''(\tilde{u}_n)(V_i, V_i) = c_i^2 g''(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}'_n) + h_n(c_i^3 g''(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}''_n)
$$

\n
$$
+ 2c_i g''(\tilde{u}_n)(\tilde{u}'_n, \psi_{2,i} \mathbf{L}) + h_n^2(\frac{c_i^4}{3}g''(\tilde{u}_n)(\tilde{u}'_n, \tilde{u}^{(3)}_n) + 2c_i g''(\tilde{u}_n)(\tilde{u}'_n, \psi_{3,i} \mathbf{M})
$$

\n
$$
+ 2c_i g''(\tilde{u}_n)(\tilde{u}'_n, \sum_{j=2}^{i-1} a_{ij} g'(\tilde{u}_n) \psi_{2,j} g'(\tilde{u}_n) \tilde{u}'_n) + \frac{c_i^4}{4} g''(\tilde{u}_n)(\tilde{u}''_n, \tilde{u}''_n)
$$

\n
$$
+ c_i^2 g''(\tilde{u}_n)(\tilde{u}''_n, \psi_{2,i} \mathbf{L}) + g''(\tilde{u}_n)(\psi_{2,i} \mathbf{L}, \psi_{2,i} \mathbf{L}) + \mathcal{O}(h_n^3).
$$

Employing the results of Lemma [3,](#page-7-0) we get the expansion of the numerical solution

$$
\hat{u}_{n+1} = \tilde{u}_n + h_n \varphi_1(h_n A) F(\tilde{u}_n) + h_n^2 \Big(\sum_{i=2}^s b_i c_i \Big) \mathbf{L} + h_n^3 \Big(\sum_{i=2}^s b_i \frac{c_i^2}{2!} \Big) \mathbf{M} + h_n^4 \Big(\sum_{i=2}^s b_i \frac{c_i^3}{3!} \Big) \mathbf{N} + h_n^5 \Big(\sum_{i=2}^s b_i \frac{c_i^4}{4!} \Big) \mathbf{P} + \mathbf{R} + \mathcal{O}(h_n^6)
$$
\n(23)

with **L**, **M**, **N** and **P** as in [\(15\)](#page-5-2), and the remaining terms

$$
\mathbf{R} = h_n^3 \sum_{i=2}^s b_i g'(\tilde{u}_n) \psi_{2,i} \mathbf{L} + h_n^4 \sum_{i=2}^s b_i g'(\tilde{u}_n) \psi_{3,i} \mathbf{M}
$$

+ $h_n^4 \sum_{i=2}^s b_i g'(\tilde{u}_n) \sum_{j=2}^{i-1} a_{ij} g'(\tilde{u}_n) \psi_{2,j} \mathbf{L} + h_n^4 \sum_{i=2}^s b_i c_i g''(\tilde{u}_n) (\tilde{u}'_n, \psi_{2,i} \mathbf{L})$
+ $h_n^5 \sum_{i=2}^s b_i g'(\tilde{u}_n) \psi_{4,i} \mathbf{N} + h_n^5 \sum_{i=2}^s b_i g'(\tilde{u}_n) \sum_{j=2}^{i-1} a_{ij} g'(\tilde{u}_n) \psi_{3,j} \mathbf{M}$
+ $h_n^5 \sum_{i=2}^s b_i g'(\tilde{u}_n) \sum_{j=2}^{i-1} a_{ij} g'(\tilde{u}_n) \sum_{k=2}^{j-1} a_{jk} g'(\tilde{u}_n) \psi_{2,k} \mathbf{L}$
+ $h_n^5 \sum_{i=2}^s b_i g'(\tilde{u}_n) \sum_{j=2}^{i-1} a_{ij} c_j g''(\tilde{u}_n) (\tilde{u}'_n, \psi_{2,j} \mathbf{L}) + h_n^5 \sum_{i=2}^s b_i c_i g''(\tilde{u}_n) (\tilde{u}'_n, \psi_{3,i} \mathbf{M})$
+ $h_n^5 \sum_{i=2}^s b_i c_i g''(\tilde{u}_n) (\tilde{u}'_n, \sum_{j=2}^{i-1} a_{ij} g'(\tilde{u}_n) \psi_{2,j} \mathbf{L}) + h_n^5 \sum_{i=2}^s \frac{b_i}{2!} g''(\tilde{u}_n) (\psi_{2,i} \mathbf{L}, \psi_{2,i} \mathbf{L})$
+ $h_n^5 \sum_{i=2}^s b_i \frac{c_i^2}{2!} g''(\tilde{u}_n) (\tilde{u}''_n, \psi_{2,i} \mathbf{L}) + h_n^5 \sum_{i=2}^s b_i \frac{$

4.2 Local Error and Derivation of Stiff Order Conditions

Now we are ready to study the order conditions. Let $\tilde{e}_{n+1} = \hat{u}_{n+1} - \tilde{u}_{n+1}$ 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 [\(1\)](#page-0-0) at t_{n+1} , and let

$$
\psi_j(h_n A) = \sum_{i=2}^s b_i(h_n A) \frac{c_i^{j-1}}{(j-1)!} - \varphi_j(h_n A), \quad j \ge 2.
$$

Subtracting (14) from (23) gives

$$
\tilde{e}_{n+1} = h_n^2 \psi_2(h_n A) \mathbf{L} + h_n^3 \psi_3(h_n A) \mathbf{M} + h_n^4 \psi_4(h_n A) \mathbf{N} + h_n^5 \psi_5(h_n A) \mathbf{P} + \mathbf{R} + \mathcal{O}(h_n^6).
$$
\n(24)

The stiff order conditions can easily be identified from [\(24\)](#page-8-0). They are summarized in Table [1.](#page-1-0) Note that the last two terms in **R** give rise to the same order condition, which is labeled 18 in Table [1.](#page-1-0)

The first nine conditions in Table [1](#page-1-0) are the same as in [\[5\]](#page-10-5). Note that the method satisfies $c_1 = 0$ $c_1 = 0$ $c_1 = 0$ and $\psi_{i,1} = 0$ for all j. Therefore, all sums in Table 1 with the very exception of the first one start with the lower index 2.

5 Convergence Analysis

With the above local error analysis at hand, we are now ready to prove convergence.

Theorem 1. *Let the initial value problem [\(1\)](#page-0-0) satisfy Assumptions [1](#page-3-3) and [2.](#page-3-1) Consider for its numerical solution an explicit exponential Runge–Kutta method [\(7\)](#page-2-3) that fulfills the order conditions of Table [1](#page-1-0) up to order p for some* $2 \leq p \leq 5$. Then,
the numerical solution u_n satisfies the error bound *the numerical solution u*n *satisfies the error bound*

$$
||u_n - u(t_n)|| \le C \sum_{i=0}^{n-1} h_i^{p+1},
$$
\n(25)

 $uniformly$ on $t_0 \leq t_n \leq T$. In particular, the constant C can be chosen independently
of the step size sequence h_1 in $[t_0, T]$ *of the step size sequence* h_i *in* $[t_0, T]$ *.*

Proof. The proof is quite standard. It only remains to verify that the numerical scheme [\(7\)](#page-2-3) is stable. For this, let v_k and w_k denote two approximations to $u(t_k)$ at time t_k . Performing $n - k$ steps $(n > k)$ gives

$$
v_n = e^{(h_{n-1} + \ldots + h_k)A} v_k + \sum_{m=k}^{n-1} h_m e^{(h_{n-1} + \ldots + h_{m+1})A} \sum_{i=1}^s b_i (h_m A) g(V_{mi})
$$

and a similar expression for w_n . Using the Lipschitz condition of g and the stability estimate [\(8\)](#page-3-4) on the semigroup shows the bound

$$
||v_n - w_n|| \leq \tilde{C} (||v_k - w_k|| + \sum_{m=k}^{n-1} h_m ||v_m - w_m||)
$$

with a constant C that can be chosen uniformly in n and k for $t_0 \le t_k \le t_n \le T$.
The application of a standard Gronwall inequality thus proves stability The application of a standard Gronwall inequality thus proves stability.

We now make use of the fact that the global error $u_n - u(t_n)$ can be estimated by the sum of the propagated local errors $\hat{u}_k - \tilde{u}_k$, $k = 1, \ldots, n$. Due to the stability of the error propagation we obtain at once (25) the error propagation, we obtain at once (25) .

A discussion of the solvability of the order conditions given in Table [1,](#page-1-0) sample methods and numerical experiments will be published elsewhere.

Acknowledgements This work was supported by the FWF doctoral program 'Computational Interdisciplinary Modelling' W1227. The work of the first author was partially supported by the Tiroler Wissenschaftsfond grant UNI-0404/1284.

References

- 1. Cox, S., Matthews, P.: Exponential time differencing for stiff systems. J. Comput. Phys. **176**, 430–455 (2002)
- 2. Friedli, A.: Verallgemeinerte Runge–Kutta Verfahren zur Lösung steifer Differentialgleichungssysteme. In: Burlirsch, R., Grigorieff, R., Schrödinger, J. (eds.) Numerical Treatment of Differential Equations. Lecture Notes in Mathematics, vol. 631, pp. 35–50. Springer, Berlin (1978)
- 3. Henry, D.: Geometric Theory of Semilinear Parabolic Equations. Lecture Notes in Mathematics, vol. 840. Springer, Berlin/Heidelberg (1981)
- 4. Hochbruck, M., Lubich, C., Selhofer, H.: Exponential integrators for large systems of differential equations. SIAM J. Sci. Comput. **19**, 1552–1574 (1998)
- 5. Hochbruck, M., Ostermann, A.: Explicit exponential Runge–Kutta methods for semilinear parabolic problems. SIAM J. Numer. Anal. **43**, 1069–1090 (2005)
- 6. Hochbruck, M., Ostermann, A.: Explicit integrators of Rosenbrock-type. Oberwolfach Rep. **3**, 1107–1110 (2006)
- 7. Hochbruck, M., Ostermann, A.: Exponential integrators. Acta Numer. **19**, 209–286 (2010)
- 8. Hochbruck, M., Ostermann, A., Schweitzer, J.: Exponential Rosenbrock-type methods. SIAM J. Numer. Anal. **47**, 786–803 (2009)
- 9. Kassam, A.-K., Trefethen, L.N.: Fourth-order time stepping for stiff PDEs. SIAM J. Sci. Comput. **26**, 1214–1233 (2005)
- 10. Luan, V.T., Ostermann, A.: Exponential Rosenbrock methods of order five – construction, analysis and numerical comparisons. J. Comput. Appl. Math. **255**, 417–431 (2014)
- 11. Pazy, A.: Semigroups of Linear Operators and Applications to Partial Differential Equations. Springer, New York (1983)
- 12. Tokman, M.: Efficient integration of large stiff systems of ODEs with exponential propagation iterative (EPI) methods. J. Comput. Phys. **213**, 748–776 (2006)