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Exponential Krylov peer integrators

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Abstract This paper is concerned with the application of exponential peer methods to stiff ODEs of high dimension. Conditions for stiff order p for variable step size are derived, and corresponding methods are given. The methods are combined with Krylov approximations for the φ-functions times a vector using the code `phipm` of Niesen and Wright. The structure of the peer methods is exploited to reduce the Krylov dimensions. Numerical tests with step size control of three exponential peer methods and comparisons with the exponential W-method `exp4` for semidiscretized problems show the efficiency of the proposed methods.

Keywords Exponential integrators · Peer methods · Krylov methods

Mathematics Subject Classification 65L05 · 65L06

1 Introduction

Exponential integrators are a well-known class of numerical integration methods for stiff initial value problems

$$\begin{aligned} y' &= f(t, y) \\ y(t_0) &= y_0 \in \mathbb{R}^n, \quad t_0 \le t \le t_e. \end{aligned} \tag{1.1}$$

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They involve exponential functions (or related functions) of the Jacobian f_y or an approximation to it. They are especially useful for differential equations coming from the spatial discretization of partial differential equations, where the problem often splits into a linear stiff part Ty and a nonlinear (nonstiff) part $g(t, y)$:

$$f(t, y) = Ty + g(t, y). \tag{1.2}$$

Since the first paper about exponential integrators by Certaine [3], there has been a considerable amount of research on methods of this type. A comprehensive overview about different aspects of exponential integrators is given in [10]. Exponential integrators have several nice properties, for instance in contrast to BDF methods large imaginary parts of the eigenvalues of the Jacobian cause no problems. There are many papers about the advantages of exponential methods, however, the numerical results given are often not convincing. The reason is the large effort for the computation of the φ-functions. This effort is reasonable as long as the approximation for the Jacobian can be held constant and also the step size is kept fixed. This is the reason why in many papers only the case of constant step size implementation is considered, for instance [2,20]. If the problem is nonlinear, and changes of the Jacobian of the stiff part and of the solution behavior require variable step sizes and adaptation of T, then exponential integrators are in general no longer competitive. One exception is the well-established code `exp4` of Hochbruck/Lubich/Selhofer [8]. `exp4` is an exponential W-method combined with Krylov approximations for $\varphi_1(h\gamma f_y)v$, which has proved to be an efficient integrator for large systems. However, it suffers from order reduction for very stiff problems.

The aim of this paper is the presentation of an efficient class of exponential integrators, so called exponential peer methods, for nonlinear, large stiff problems. Exponential peer methods for problems of moderate dimension with exact computation of the φ-functions were introduced in [4] and [24]. They are based on explicit peer methods [21,23]. The order of peer methods is equal to their stage-order. So we can overcome the order reduction for very stiff problems occuring in `exp4`. In this paper we combine exponential peer methods with Krylov approximations for products of the form $\varphi_l(c_i hT)v$. For this purpose we use a modified version of the code `phipm` of Niesen and Wright [13]. The methods are implemented with step size control in MATLAB and tested on large nonlinear problems, some of which are very stiff. We compare the performance of the exponential peer methods with `exp4` [8].

The outline of this paper is as follows:

In Sect. 2 exponential peer methods are considered. Results for stiff order of consistency, zero-stability and convergence are proved. Special 3- and 4-stage methods are given. The computation of the φ-functions times a vector using Krylov approximations is the topic of Sect. 3. We give an overview about theoretical results and show how the special structure of the peer methods can be exploited to reduce the Krylov dimensions. In Sect. 4 numerical tests are presented. We consider three partial differential equations and discretize them in space. For two problems we use different spatial resolutions leading to semidiscrete problems of similar type but different number of equations and stiffness. Three exponential peer methods are tested and compared with `exp4`. Finally, in Sect. 5 the results are discussed and conclusions are drawn.

2 Exponential peer methods

Peer methods were first considered in [16]. Here we study exponential peer methods which belong to the class of exponential integrators and were introduced in [24]. They require the computation of the well-known φ-functions of a matrix but are otherwise explicit, no nonlinear systems need to be solved.

Exponential peer methods for (1.1) are given by

$$Y_{mi} = \varphi_0(\alpha_i h_m T_m) \sum_{j=1}^{s} b_{ij} Y_{m-1,j} + h_m \sum_{j=1}^{s} A_{ij}(\alpha_i h_m T_m)[f_{m-1,j} - T_m Y_{m-1,j}] + h_m \sum_{j=1}^{i-1} R_{ij}(\alpha_i h_m T_m)[f_{mj} - T_m Y_{mj}], \qquad i = 1, \ldots, s. \tag{2.1}$$

Here we assume $\alpha_i \geq 0$. The values Y_{mi} approximate the exact solution $y(t_m + c_i h_m)$ at points $t_{mi} = t_m + c_i h_m$, where the nodes c_i are assumed to be pairwise distinct. They are chosen such that $c_s = 1$ and the other nodes satisfy $0 \leq c_i < 1, \quad i = 1, \ldots, s-1$.

In contrast to Runge–Kutta methods which have one distinguished variable of higher order and stage values of lower order, in peer methods all stage values share the same accuracy and stability properties (with minor modifications), so we call them *'peer'* [17]. For the computation of the new stage values all stage values from the previous step are used.

The coefficients $b_{ij} \in \mathbb{R}$ will depend on the step size ratio

$$\sigma_m = \frac{h_m}{h_{m-1}}, \tag{2.2}$$

the matrix functions $A_{ij}(\alpha_i h_m T_m)$ and $R_{ij}(\alpha_i h_m T_m)$ are linear combinations of the φ-functions and depend on the step size ratio as well. We collect the coefficients in matrices and vectors

$$B = (b_{ij})_{i,j=1}^{s}, \quad A = (A_{ij})_{i,j=1}^{s}, \quad R = (R_{ij})_{i,j=1}^{s}, \quad c = (c_i)_{i=1}^{s}, \quad \alpha = (\alpha_i)_{i=1}^{s}.$$

Further, here and in the following we use the abbreviations

$$f_{mj} = f(t_{mj}, Y_{mj}), \quad g_{mj} = f_{mj} - T_m Y_{mj}.$$

T_m is an arbitrary matrix, for stability we will use an approximation to the Jacobian $f_y(t_m, Y_{m-1,s})$. By setting $T_m = 0$ we obtain explicit peer methods, which have been proved to be very efficient for nonstiff systems [23].

For integers $l \geq 0$ and complex numbers $z \in \mathbb{C}$ the φ-functions are defined as follows (e.g. [14]):

$$\varphi_0(z) = e^z,$$

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

They are related by the recurrence relation

$$\varphi_{l+1}(z) = \frac{\varphi_l(z) - \varphi_l(0)}{z} \quad \text{for } l \geq 0, \quad \text{with } \varphi_l(0) = \frac{1}{l!}. \tag{2.3}$$

Several methods have been proposed for evaluating these function [12], for instance methods relying on Padé approximations combined with scaling-and-squaring [2]. For large dimensions Krylov techniques are advantageous, e.g. [8,13,18].

We will assume that the stiffness in (1.2) is due to the linear part Ty and that the nonlinear part satisfies a global Lipschitz condition

$$\|g(t,u) - g(t,v)\| \leq L_g \|u - v\| \tag{2.4}$$

with Lipschitz constant L_g of moderate size. We assume that T has a bounded logarithmic norm

$$\mu(T) \leq \omega. \tag{2.5}$$

Often, systems (1.1) result from semidiscretization of partial differential equations where this condition is usually satisfied. Assumption (2.5) implies

$$\|\varphi_0(hT)\| = \|e^{hT}\| \leq e^{\omega h}, \tag{2.6}$$

see e.g. [11].

Remark 1 With (2.4), condition (2.5) will also be satisfied for $T_m = T + g_y(t_m, Y_{m-1,s})$ with some ω of moderate size. An immediate consequence is that $\|\varphi_l(\alpha_i h_m T_m)\|$ and $\|h_m T_m \varphi_l(\alpha_i h_m T_m)\|$ are uniformly bounded for $l \geq 1$. This also holds for the matrix coefficients $A_{ij}(\alpha_i h_m T_m)$ and $R_{ij}(\alpha_i h_m T_m)$ which we always choose as linear combinations of the $\varphi_l(\alpha_i h_m T_m)$, $l \geq 1$.

We define the local residual errors by inserting the exact solution into the numerical scheme (2.1):

$$\begin{aligned}\Delta_{mi} = {} & y(t_{mi}) - \varphi_0(\alpha_i h_m T_m) \sum_{j=1}^{s} b_{ij}\, y(t_{m-1,j}) - h_m \sum_{j=1}^{s} A_{ij}(\alpha_i h_m T_m) \\ & \times [y'(t_{m-1,j}) - T_m y(t_{m-1,j})] \\ & - h_m \sum_{j=1}^{i-1} R_{ij}(\alpha_i h_m T_m)[y'(t_{mj}) - T_m y(t_{mj})], \quad i = 1, \ldots, s. \end{aligned} \tag{2.7}$$

We are interested in the stiff order of the exponential peer method.

Definition 1 The exponential peer method (2.1) is consistent of stiff order q if there are constants $h_0, C > 0$ such that

$$\|\Delta_{mi}\| \le C h_m^{q+1} \quad \text{for all } h_m \le h_0, \quad \text{and for all } 1 \le i \le s,$$

where C and h_0 may depend on ω, L_g and bounds for derivatives of the exact solution, but are independent of $\|T_m\|$.

Note that for peer methods all stage values are of order q, i.e. the stiff order of consistency is equal to the stage order. In the following we always assume that the exact solution $y(t)$ is sufficiently smooth.

Conditions for stiff order of exponential peer methods for variable step sizes were studied in [4] and [24] in detail. For completeness we give here a compact formulation and proof of the main result.

Theorem 1 ([24]) *Let the conditions*

$$\sum_{j=1}^{s} b_{ij} \left(\frac{c_j - 1}{\sigma_m} \right)^l = (c_i - \alpha_i)^l, \quad i = 1, \ldots, s, \tag{2.8}$$

be satisfied for $l = 0, \ldots, q$. Let further

$$\begin{aligned} &\sum_{j=1}^{s} A_{ij}(\alpha_i h_m T_m) \left(\frac{c_j - 1}{\sigma_m} \right)^r + \sum_{j=1}^{i-1} R_{ij}(\alpha_i h_m T_m) c_j^r \\ &\quad = \sum_{l=0}^{r} l! \alpha_i^{l+1} \binom{r}{l} (c_i - \alpha_i)^{r-l} \varphi_{l+1}(\alpha_i h_m T_m) i = 1, \ldots, s \end{aligned} \tag{2.9}$$

hold for $r = 0, \ldots, q$. Then the exponential peer method is at least of stiff order q for (1.1).

If in addition (2.8) is also satisfied for $l = q + 1$ and $\|T_m y^{(q+1)}\| \le C$, where the constant C is independent of $\|T_m\|$, then the method is of stiff order $q + 1$.

Proof By Taylor expansion of the exact solution in (2.7) we have

$$\begin{aligned} \Delta_{mi} = \sum_{r=0}^{q+1} \Bigg\{ & c_i^r I - \varphi_0(\alpha_i h_m T_m) \sum_{j=1}^{s} b_{ij} \left(\frac{c_j - 1}{\sigma_m} \right)^r - r \sum_{j=1}^{s} A_{ij}(\alpha_i h_m T_m) \left(\frac{c_j - 1}{\sigma_m} \right)^{r-1} \\ & + h_m T_m \sum_{j=1}^{s} A_{ij}(\alpha_i h_m T_m) \left(\frac{c_j - 1}{\sigma_m} \right)^r - r \sum_{j=1}^{i-1} R_{ij}(\alpha_i h_m T_m) c_j^{r-1} \\ & + h_m T_m \sum_{j=1}^{i-1} R_{ij}(\alpha_i h_m T_m) c_j^r \Bigg\} \frac{h_m^r}{r!} y^{(r)}(t_m) + \mathcal{O}(h_m^{q+2}) \end{aligned}$$

Using (2.8), (2.9) and the recurrence (2.3) we obtain

$$\begin{aligned}\Delta_{mi} = \Bigg\{ & c_i^{q+1} I - \varphi_0(\alpha_i h_m T_m) \sum_{j=1}^{s} b_{ij} \left(\frac{c_j - 1}{\sigma_m}\right)^{q+1} \\ & -(q+1) \sum_{j=1}^{s} A_{ij}(\alpha_i h_m T_m) \left(\frac{c_j - 1}{\sigma_m}\right)^{q} \\ & -(q+1) \sum_{j=1}^{i-1} R_{ij}(\alpha_i h_m T_m) c_j^q + h_m T_m \sum_{j=1}^{i-1} R_{ij}(\alpha_i h_m T_m) c_j^{q+1} \\ & + h_m T_m \sum_{j=1}^{s} A_{ij}(\alpha_i h_m T_m) \left(\frac{c_j - 1}{\sigma_m}\right)^{q+1} \Bigg\} \frac{h_m^{q+1}}{(q+1)!} y^{(q+1)}(t_m) + \mathcal{O}(h_m^{q+2}),\end{aligned}$$

i.e. stiff order q.

By the assumption $\|T_m y^{(q+1)}\| \le C$ we get for the last two terms

$$\begin{aligned}\left(\sum_{j=1}^{i-1} R_{ij}(\alpha_i h_m T_m) c_j^{q+1} + \sum_{j=1}^{s} A_{ij}(\alpha_i h_m T_m) \left(\frac{c_j - 1}{\sigma_m}\right)^{q+1} \right) \\ \times \frac{h_m^{q+2}}{(q+1)!} T_m y^{(q+1)} = \mathcal{O}(h_m^{q+2}),\end{aligned}$$

and if in addition (2.8) holds for $l = q+1$ we have

$$\begin{aligned}\Delta_{mi} = \Bigg\{ & c_i^{q+1} I - \varphi_0(\alpha_i h_m T_m) \sum_{j=1}^{s} b_{ij} \left(\frac{c_j - 1}{\sigma_m}\right)^{q+1} \\ & -(q+1) \sum_{j=1}^{s} A_{ij}(\alpha_i h_m T_m) \left(\frac{c_j - 1}{\sigma_m}\right)^{q} \\ & -(q+1) \sum_{j=1}^{i-1} R_{ij}(\alpha_i h_m T_m) c_j^q \Bigg\} \frac{h_m^{q+1}}{(q+1)!} y^{(q+1)}(t_m) + \mathcal{O}(h_m^{q+2}) \\ = & \left\{ c_i^{q+1} I - \sum_{l=0}^{q+1} l! \alpha_i^l \binom{q+1}{l} (c_i - \alpha_i)^{q+1-l} \varphi_l(\alpha_i h_m T_m) \right\} \frac{h_m^{q+1}}{(q+1)!} y^{(q+1)}(t_m) \\ & + \mathcal{O}(h_m^{q+2}).\end{aligned}$$

With $\varphi_l(\alpha_i h_m T_m) = \alpha_i h_m T_m \varphi_{l+1}(\alpha_i h_m T_m) + \frac{1}{l!} I$ and $\sum_{i=0}^{q+1} \alpha_i^l \binom{q+1}{l} (c_i - \alpha_i)^{q+1-l} = c_i^{q+1}$ we finally obtain $\Delta_{mi} = \mathcal{O}(h_m^{q+2})$. ■

Remark 2 A sufficient condition for $\|Ty^{(q+1)}\| \le C$, where C is independent of $\|T\|$, is $\|T\| \le C_1$ (nonstiff order). But $\|Ty^{(q+1)}\|$ can be bounded independently of $\|T\|$ also if $\|T\| \gg 1$, for instance for autonomous problems with sufficiently smooth function $g(y)$ or for special semidiscretized partial differential equations with homogeneous Dirichlet boundary conditions. Order conditions for explicit exponential Runge–Kutta methods for parabolic problems are studied in [9].

For $q = s - 1$ equation (2.8) is equivalent to

$$B = V_\alpha S V_1^{-1}, \tag{2.10}$$

where

$$S = \mathrm{diag}(1, \sigma_m, \ldots, \sigma_m^{s-1}), \quad \mathbb{1} = (1, \ldots, 1)^T$$
$$V_\alpha = \left(\mathbb{1},\ c - \alpha,\ \ldots,\ (c-\alpha)^{s-1}\right), \quad V_1 = \left(\mathbb{1},\ c - \mathbb{1},\ \ldots,\ (c-\mathbb{1})^{s-1}\right).$$

A natural choice for α is $\alpha = c$:

Corollary 1 *Let $\alpha = c$, $c_s = 1$. Then, with (2.10), B will be independent of σ_m, we have*

$$B = \mathbb{1} e_s^T, \quad e_s = (0, 0, \ldots, 1)^T, \tag{2.11}$$

and (2.8) is satisfied for all l. The exponential peer method solves the system $y' = Ty$ with $T_m = T$ and exact starting values exactly.

Note that for $q = s - 1$ for any given strictly lower triangular matrix R we can solve (2.9) for A, due to the regularity of V_1. Therefore we can construct exponential peer methods of any order.

If we apply exponential peer methods with exact computation of $\varphi_l(\alpha_i h_m T_m)$, for instance with the methods in EXPINT, then with the choice $\alpha = c$ we have s different arguments resulting in high computational costs. Therefore, in [24] a different choice for α was investigated. With

$$\alpha = (\alpha^*, \ldots, \alpha^*, 1)^T, \text{ and } c_i = (s - i)(\alpha_i - 1) + 1, \quad i = 1, \ldots, s, \tag{2.12}$$

φ-functions with only two different arguments have to be computed. These methods were tested with constant step size in [24] and with step size control in [5].

In [5] for methods (2.12) of stiff order of consistency q zero-stability, i.e.

$$\|B_{m+l} B_{m+l-1} \ldots B_m\| \le K \quad \text{for all } m, l \ge 0,$$

was proved under a restriction of the step size ratio $\sigma_m \le \sigma^*$ with some $\sigma^* > 1$. Stiff order of convergence q could be shown under the additional assumption

$$\sum_{j=1}^{N-1} |\sigma_j - 1| \le K, \quad t_N = t_e. \tag{2.13}$$

In combination with Krylov techniques there is no advantage of (2.12) compared to $\alpha = c$. We will therefore use the methods of Corollary 1. Here B is constant and this simplifies the proof of stiff convergence, no additional assumption (2.13) is needed.

Theorem 2 *Let the exponential peer method be of stiff order of convergence q. Let $\alpha = c$, $c_s = 1$ and $B = \mathbb{1}e_s^\top$. Let the starting values be of order q and let the coefficients of the method be bounded for $\sigma_m \le \sigma^*$ with $\sigma^* > 1$. Then the method is convergent of stiff order q.*

Proof We consider the global error $\varepsilon_m = Y(t_m) - Y_m$. For the i-th component there holds

$$\begin{aligned}\varepsilon_{mi} &= \varphi_0(c_i h_m T_m)(y(t_{m-1,s}) - Y_{m-1,s}) \\ &\quad + h_m \sum_{j=1}^{s} A_{ij}(c_j h_m T_m)(g(t_{m-1,j}, y(t_{m-1,j})) - g_{m-1,j}) \\ &\quad + h_m \sum_{j=1}^{i-1} R_{ij}(c_j h_m T_m)(g(t_{mj}, y(t_{mj})) - g_{mj}) + \Delta_{mi}.\end{aligned}$$

With (2.4), (2.6) and the boundedness of the coefficients A_{ij} and R_{ij} by Remark 1 follows

$$\|\varepsilon_{mi}\| \le e^{c_i h_m \omega}\|\varepsilon_{m-1,s}\| + h_m L_g C_A \sum_{j=1}^{s}\|\varepsilon_{m-1,j}\| + h_m L_g C_R \sum_{j=1}^{i-1}\|\varepsilon_{mj}\| + C h_m^{q+1}.$$

Defining $\|\varepsilon_m\| = \max_i \|\varepsilon_{mi}\|$ we obtain

$$\|\varepsilon_m\| \le (1 + C_1 h_m)\|\varepsilon_{m-1}\| + C_2 h_m \|\varepsilon_m\| + C h_m^{q+1},$$

and for $h \le h_0$

$$\|\varepsilon_m\| \le (1 + C_3 h_m)\|\varepsilon_{m-1}\| + C_4 h_m^{q+1},$$

where h_0 and the constants are independent of $\|T_m\|$. Stiff order of convergence q follows in standard manner. ■

In our numerical tests we use two methods with 3 and 4 stages with $\alpha = c$, $c_s = 1$ and $B = \mathbb{1}e_s^\top$. The coefficients A_{ij} and R_{ij} are computed by (2.9) with $q = s - 1$, where we have chosen the free parameters to have an upper triangular matrix A and a strictly lower triangular matrix R. This gives a unique solution for the coefficients, but may be not the best choice. The methods are of stiff order $s - 1$. If $\|T_m y^{(s)}\| = \mathcal{O}(1)$ the stiff order is $q = s$, which is also the nonstiff order.

The 3-stage method `Peer3a` is given by:

$$c = \alpha = (1/4, 1/2, 1)^\top, \quad B = \mathbb{1}e_s^\top,$$

$$A_{11} = \frac{1}{6}\sigma\varphi_2 + \frac{1}{6}\sigma^2\varphi_3, \quad A_{12} = -\frac{3}{8}\sigma\varphi_2 - \frac{1}{4}\sigma^2\varphi_3,$$
$$A_{13} = \frac{1}{4}\varphi_1 + \frac{5}{24}\sigma\varphi_2 + \frac{1}{12}\sigma^2\varphi_3,$$
$$A_{22} = -\frac{1}{2(\sigma+2)}\sigma^2\varphi_2 + \frac{2}{\sigma+2}\sigma^2\varphi_3, \quad A_{23} = \frac{1}{2}\varphi_1 + \frac{1}{4}(2\sigma-4)\varphi_2 - 2\sigma\varphi_3,$$
$$A_{33} = \varphi_1 - 6\varphi_2 + 16\varphi_3,$$
$$R_{21} = \frac{2}{\sigma+2}\varphi_2 + \frac{4\sigma}{\sigma+2}\varphi_3, \quad R_{31} = 8\varphi_2 - 32\varphi_3, \quad R_{32} = -2\varphi_2 + 16\varphi_3.$$

Here (for the integration step from t_m to t_{m+1}) σ denotes the step size ratio h_m/h_{m-1}. The 4-stage method `Peer4a` is constructed analogously with $c = \alpha = (\frac{1}{4}, \frac{1}{2}, \frac{3}{4}, 1)^\top$.

3 Computation of the φ-functions

The implementation of exponential peer methods using Krylov techniques requires an efficient computation of sums of φ-functions times a vector in (2.1). Our implementation uses the code `phipm` of [13]. This code computes the sum

$$\varphi_0(A)u_0 + \sum_{k=1}^{p} \varphi_k(A)u_k \tag{3.1}$$

by exploiting the following property:

Theorem 3 (see Al-Mohy/Higham [1]) *Let $A \in \mathbb{C}^{n,n}$, $W = [w_1, \ldots, w_p] \in \mathbb{C}^{n,p}$ and*

$$\widetilde{A} = \begin{bmatrix} A & W \\ 0 & J \end{bmatrix} \in \mathbb{C}^{n+p,n+p}, \quad J = \begin{bmatrix} 0 & I_{p-1} \\ 0 & 0 \end{bmatrix} \in \mathbb{C}^{p,p}.$$

Then the $(n+j)$-th column of $X = \varphi_l(\widetilde{A})$ is

$$X(1:n, n+j) = \sum_{k=1}^{j} \varphi_{l+k}(A)w_{j-k+1}, \quad j = 1, \ldots, p.$$

With $l = 0$ and

$$\widetilde{A} = \begin{bmatrix} A & u_p & u_{p-1} & \ldots & u_3 & u_2 & u_1 \\ 0 & & & J & & & \end{bmatrix}$$

we get $\varphi_0(A)$ in the upper left $n \times n$-submatrix of $\varphi_0(\widetilde{A})$ and the remaining terms of (3.1) in the column $n+p$ of $\varphi_0(\widetilde{A})$.

Using the recurrence relation

$$\varphi_k(A) = A\varphi_{k+1}(A) + \frac{1}{k!}I$$

in `phipm` the computation of the sum (3.1) is transformed into the approximation of only one single function $\varphi_p(A)v$. Building the Krylov subspace $\mathcal{K}_m = \text{span}\{v_1, \ldots, v_m\}$ by the Arnoldi algorithm (see e.g. [15]) and using $v_1 = v/\|v\|$ we arrive at the approximation ([13])

$$\varphi_p(A)v \approx \beta V_m \varphi_p(H_m)e_1.$$

Here V_m is the n-by-m orthogonal matrix with columns $v_1, \ldots, v_m$ and $\beta = \|v\|$. To compute $\varphi_p(H_m)e_1$ we apply Theorem 3 with $J \in \mathbb{R}^{p+1,p+1}$

$$\widetilde{H}_m = \begin{bmatrix} H_m & e_1 & 0 & \cdots & 0 \\ 0 & & & J & \end{bmatrix}$$

and obtain

$$\varphi_0(\widetilde{H}_m) = \begin{bmatrix} \varphi_0(H_m) & \varphi_1 e_1 & \cdots & \varphi_p e_1 & \varphi_{p+1} e_1 \\ 0 & * & * & * & * \end{bmatrix}. \tag{3.2}$$

The additional column allows the error estimation ([13,18])

$$\varphi_p(A)v - \beta V_m \varphi_p(H_m)e_1 \approx \beta h_{m+1,m} e_m^\top \varphi_{p+1}(H_m)e_1 v_{m+1}. \tag{3.3}$$

In `phipm` the error estimator is also used to improve the approximation:

$$\varphi_p(A)v \approx \beta V_m \varphi_p(H_m)e_1 + \beta h_{m+1,m} e_m^\top \varphi_{p+1}(H_m)e_1 v_{m+1}.$$

$\varphi_0(\widetilde{H}_m)$ for the extended matrix $\widetilde{H}_m$ (see Theorem 3) is computed by the MATLAB function `expm`.

We will now describe how the special structure of peer methods is exploited to reduce the numerical costs for the Krylov approximations. The idea is to rearrange the computation that the vectors which are multiplied by the φ-functions have small norms. We start with the exponential peer-method (2.1). With $c_i = \alpha_i$, $c_s = 1$ and $B = \mathbb{1}e_s^T$ (see Corollary 1) we get

$$\begin{aligned} Y_{mi} &= \varphi_0(c_i hT)Y_{m-1,s} + c_i h\varphi_1(c_i hT)g_{m-1,s} \\ &\quad + h\sum_{j=1}^{s} A_{ij}(c_i hT)g_{m-1,j} + h\sum_{j=1}^{i-1} R_{ij}(c_i hT)g_{mj} - c_i h\varphi_1(c_i hT)g_{m-1,s}, \\ &\quad i = 1, \ldots, s. \end{aligned}$$

By the order condition (2.9) for $r = 0$ we have

$$\sum_{j=1}^{s} A_{ij}(\alpha_i hT) + \sum_{j=1}^{i-1} R_{ij}(c_i hT) = c_i \varphi_1(c_i hT)$$

and with $g_{mj} = g_{m-1,s} + \mathcal{O}(h)$, $g_{m-1,j} = g_{m-1,s} + \mathcal{O}(h)$, $hT\varphi_1(hT) = \varphi_0(hT) - I$ this results in

$$\begin{aligned}
Y_{mi} &= \varphi_0(c_i hT) Y_{m-1,s} + c_i h \varphi_1(c_i hT)(f_{m-1,s} - T Y_{m-1,s}) \\
&\quad + h \left(\sum_{j=1}^{s} A_{ij}(c_i hT) g_{m-1,j} + \sum_{j=1}^{i-1} R_{ij}(c_i hT) g_{mj} - c_i h \varphi_1(c_i hT) g_{m-1,s} \right) \\
&= Y_{m-1,s} + c_i h \varphi_1(c_i hT) f_{m-1,s} \\
&\quad + h \left(\sum_{j=1}^{s} A_{ij}(c_i hT) g_{m-1,j} + \sum_{j=1}^{i-1} R_{ij}(c_i hT) g_{mj} - c_i \varphi_1(c_i hT) g_{m-1,s} \right) \\
&= Y_{m-1,s} + c_i h \varphi_1(c_i hT) f_{m-1,s} \\
&\quad + h \sum_{j=1}^{s} A_{ij}(c_i hT) \underbrace{(g_{m-1,j} - g_{m-1,s})}_{\mathcal{O}(h)} + h \sum_{j=1}^{i-1} R_{ij}(c_i hT) \underbrace{(g_{mj} - g_{m-1,s})}_{\mathcal{O}(h)}.
\end{aligned} \tag{3.4}$$

We thus can avoid φ_0 and the terms $\varphi_1(c_i hT)v$ appear with different arguments $c_i hT$ but with the same vector $v = f_{m-1,s}$ in all stages. All other vectors are of size $\mathcal{O}(h^2)$.

We get a further simplification similar to `exp4`, if the arguments $c_i hT$ of φ_1 are multiples of $c_1 hT$. With $e^z = \varphi_0(z) = 1 + z\varphi_1(z)$ it holds

$$\begin{aligned}
1 + 2z\varphi_1(2z) = e^{2z} = e^z e^z = (1 + z\varphi_1(z))^2 &= 1 + 2z\varphi_1(z) + z^2 \varphi_1^2(z) \\
\varphi_1(2z) &= \frac{1}{2}(2 + z\varphi_1(z))\varphi_1(z) \\
&= \frac{1}{2}(1 + \varphi_0(z))\varphi_1(z)
\end{aligned}$$

and analogously

$$\begin{aligned}
\varphi_1(3z) &= \frac{1}{3}\varphi_1(z) + \frac{2}{3}\varphi_1(2z)\varphi_0(z) \\
\varphi_1(4z) &= \frac{1}{2}\varphi_1(2z)(1 + \varphi_0^2(z)).
\end{aligned}$$

Because in all stages the function φ_1 is multiplied with the same vector $v = f_{m-1,s}$, we can compute approximations for $\varphi_1(2A)v$, $\varphi_1(3A)v$ and $\varphi_1(4A)v$ very efficiently from $\varphi_1(A)v$. First

$$\varphi_1(A)v \approx \beta V_m \varphi_1(H) e_1$$

were $\varphi_1(H)e_1$ is explicitly available from (3.2). Because of

$$\begin{aligned}\varphi_1(2A)v &\approx \beta V_m \varphi_1(2H)e_1\\ &= \beta V_m \frac{1}{2}\left(I + \varphi_0(H)\right)\varphi_1(H)e_1\\ &= \beta V_m \frac{1}{2}\left(\varphi_1(H)e_1 + \varphi_0(H)\varphi_1(H)e_1\right)\\ &= \beta V_m \frac{1}{2}(X_1 + X_2)\end{aligned}$$

with $X_1 = \varphi_1(H)e_1$, $X_2 = \varphi_0(H)X_1 = \varphi_0(H)\varphi_1(H)e_1$ and the explicitly given $\varphi_0(H)$ (see (3.2)) an approximation for the product $\varphi_1(2A)v$ is also available. In the same way we get the expressions

$$\begin{aligned}\varphi_1(3A)v &\approx \beta V_m \varphi_1(3H)e_1\\ &= \beta V_m \frac{1}{3}(X_1 + X_2 + X_3)\\ \varphi_1(4A)v &\approx \beta V_m \varphi_1(4H)e_1\\ &= \beta V_m \frac{1}{4}(X_1 + X_2 + X_3 + X_4)\end{aligned}$$

with $X_3 = \varphi_0(H)X_2 = \varphi_0^2(H)\varphi_1(H)e_1$ und $X_4 = \varphi_0(H)X_3 = \varphi_0^3(H)\varphi_1(H)e_1$.

To summarize, we need one expensive computation of $c_1 h\varphi_1(c_1 hT)f_{m-1,s}$ with a possibly high Krylov dimension per step and the less expensive computation of $c_i h\varphi_1(c_i hT)f_{m-1,s}$ for $i = 2, \ldots, s$. Furthermore we need for each stage one sum of φ-functions multiplied with vectors of small norms, where we may expect small Krylov dimensions.

Niesen and Wright use their code `phipm` to solve linear autonomous problems in [13] using just one large integration step. To avoid large Krylov dimensions they use time-stepping inside of `phipm`. However, for nonlinear problems it is more natural and more efficient to use no time-stepping within the computation of the φ-functions but to rely on the local error estimation and step size control of the exponential peer method. This was observed also in our numerical tests. We therefore disabled the internal time-stepping of `phipm`.

Furthermore we observed that due to the recursive computation of $\varphi_1(rH)e_1$, $r = 2, \ldots, s$, it is advantageous to use a sharper tolerance in `phipm` here. If the integration tolerance is *tol* we use for the internal tolerances $10^{-4}tol$ for $\varphi_1(rH)e_1$ and *tol* for the part (3.4).

4 Numerical tests

We implemented the methods `Peer3a`, `Peer4a` with Krylov approximation as described in Sect. 3. For comparison we also included a 3-stage exponential peer method `Peer3alfa` with property (2.12) and `exp4` ([8], http://na.math.kit.edu/research/software.php). In our tests we used the exact Jacobian resp. exact Jacobian times vector products. In all codes we restricted the maximal Krylov dimension to

36. The starting values for the exponential peer Krylov methods were computed with ROWMAP [22].

In our tests we used absolute and relative tolerances $atol = rtol$. The step size control is done by estimating the local error by an embedded solution and taking into account the Krylov error $kryerr$ obtained from (3.3). For our methods of stiff order $q = s - 1$ we compute an embedded solution $\widehat{Y}_{m,s-1}$ at $t_{m,s-1}$ of stiff order $\widehat{q} = s - 2$ by the interpolation polynomial using (t_{m1}, Y_{m1}), (t_{m3}, Y_{m3}) for the 3-stage methods, and (t_{m1}, Y_{m1}), (t_{m2}, Y_{m2}), (t_{m4}, Y_{m4}) for Peer4a. The local error of the embedded solution is then estimated by

$$err = \frac{1}{\sqrt{n}} \left(\sum_{i=1}^{n} \left(\frac{Y_{m,s-1,i} - \widehat{Y}_{m,s-1,i}}{sk_i} \right)^2 \right)^{\frac{1}{2}},$$

where the scaling factors are given by

$$sk_i = atol + rtol|Y_{m-1,s-1,i}|.$$

The factor fac for the computation of the new step size is

$$fac = err^{\frac{-1}{s-1}}.$$

If the Krylov dimension for the computation of $c_1 h_m \varphi(c_1 h_m T_m) f_{m-1,s}$ is >27, fac is changed by taking into account the corresponding Krylov error

$$fac := \min(fac, \frac{1}{\sqrt{kryerr}}). \tag{4.1}$$

The same is done if the Krylov dimension for (3.4) is >27. As usual some safety factors are introduced giving finally

$$fac := \min(1.5, \max(0.2, 0.9 fac)), \quad h_{new} = fac \cdot h_{old}.$$

If $err > 1$ the step is repeated. Furthermore, the step size will not be increased for one step after a rejection occurred.

We used the following test problems:

Brusselator:

This is the two-dimensional Brusselator with diffusion:

$$\begin{aligned} u_t &= 1 + u^2 v - (B+1)u + \alpha \left(u_{xx} + u_{yy} \right) + f(x, y, t) \\ v_t &= -u^2 v + Bu + \alpha(v_{xx} + v_{yy}), \quad (x, y) \in \Omega = [0, 1]^2, \quad t \in [0, t_e]. \end{aligned}$$

We consider two versions of this example, both with homogeneous Neumann boundary conditions

$$\frac{\partial u}{\partial \mathbf{n}} = 0 \quad \frac{\partial v}{\partial \mathbf{n}} = 0 \quad \text{at} \quad x = 0, 1 \quad \text{or} \quad y = 0, 1.$$

Version 1: [6, pp. 248–249]

- $t_e = 1, \quad B = 3, \quad \alpha = 0.02.$
- Initial conditions: $u(x, y, 0) = 0.5 + y, \quad v(x, y, 0) = 1 + 5x$
- $f\,(x, y, t) = 0.$
- Spatial discretization with central differences of second order with $M = 100$ grid points in each spatial direction, dimension of the ODE-system: $n = 2M^2 = 20{,}000$.

Version 2: [7, pp. 151–152]

- $t_e = 11.5, \quad B = 3.4, \quad \alpha = 0.1.$
- Initial conditions: $u(x, y, 0) = 22y\,(1 - y)^{3/2}\,, \quad v(x, y, 0) = 27x\,(1 - x)^{3/2}.$
- $f\,(x, y, t) = \begin{cases} 5 & \text{if} \quad (x - 0.3)^2 + (y - 0.6)^2 \le 0.1^2 \quad \text{and} \quad t \ge 1.1 \\ 0 & \text{else} \end{cases}$
- Spatial discretization with central differences of second order. We used $M = 128$ grid points in each spatial direction resulting in $n = 2M^2 = 32{,}768$ ODEs, and $M = 256$, $n = 2M^2 = 131{,}072$.

Laser:
This example is from [8].

$$\begin{aligned} i \cdot u_t &= H(t, x)u \\ H(t, x) &= -\frac{1}{2}\frac{d^2}{dx^2} + Kx^2/2 + \mu x \sin^2(wt) \end{aligned}$$

with $\mu = 100$, $w = 1$, $K = 10$, periodic boundary conditions and initial conditions

$$u(x, 0) = e^{-\sqrt{K}x^2/2}, \quad x \in [-10, 10], \quad t \in [0, 1].$$

Space discretization is done with the pseudo-spectral method with $n = 512$ Fourier modes.

Combustion:
This is a very stiff nonlinear 3D problem from combustion theory [19]:

$$\begin{aligned} c_t &= \Delta c - Dce^{-\delta/T} \\ L\,T_t &= \Delta T + \alpha Dce^{-\delta/T}, \quad (x, y) \in \Omega = [0, 1]^3\,, \quad t \in [0, 0.3], \end{aligned} \tag{4.2}$$

where we used $L = 0.9$, $\alpha = 1$, $\delta = 20$, $D = \frac{Re^{\delta}}{\alpha\delta}$ and $R = 5$, and initial conditions

$$c\,(x, y, z, 0) = T\,(x, y, z, 0) = 1.$$

The boundary conditions are of homogeneous Neumann type for $x = 0$, $y = 0$, $z = 0$ and of Dirichlet type

$$c\,(x, y, z, t) = T\,(x, y, z, t) = 1 \quad \text{for} \quad x = 1, \quad y = 1, \quad z = 1\,.$$

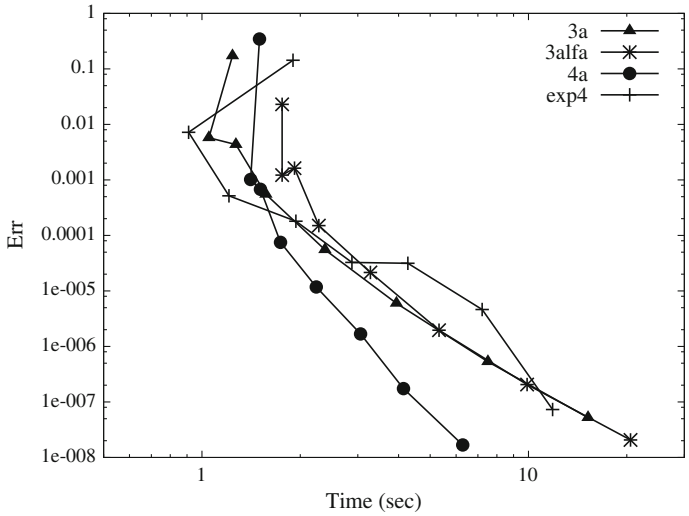

Fig. 1 Results for Brusselator I, $m = 100$

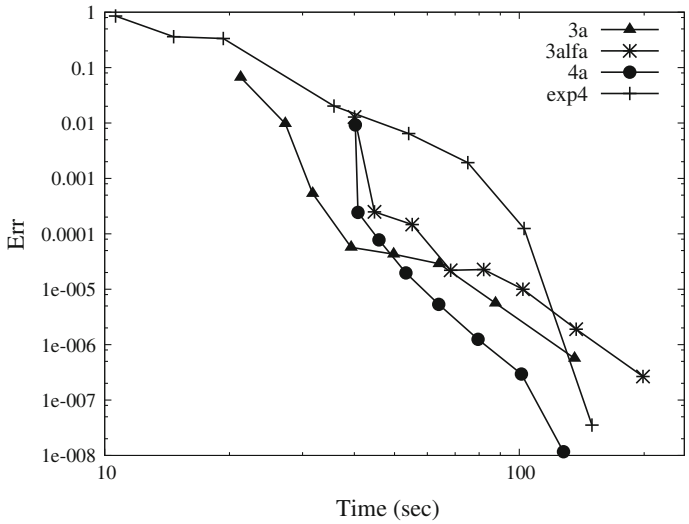

Fig. 2 Results for Brusselator II, $m = 128$

We discretized this problem on a uniform three-dimensional mesh by second-order central differences. We used $M = 40$ and $M = 80$ resulting in 128,000 and 1,024,000 ODEs.

Figures 1, 2, 3, 4, 5 and 6 (in logarithmic scale) show the error at the endpoint t_e

$$\mathrm{Err} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(\frac{y_i - yref_i}{1 + |yref_i|}\right)^2},$$

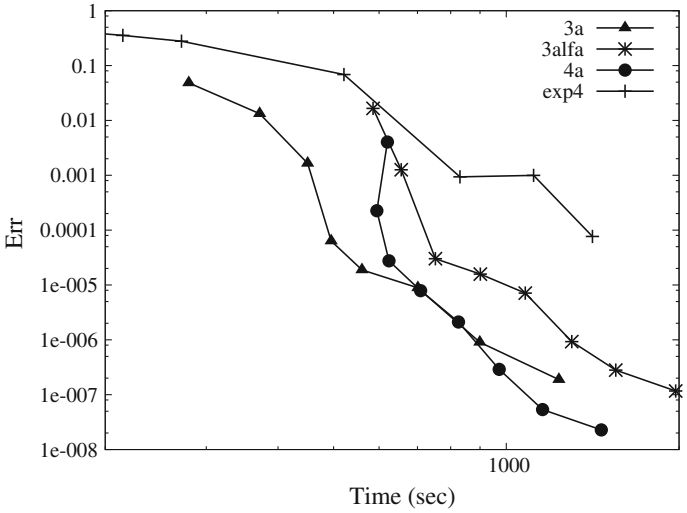

Fig. 3 Results for Brusselator II, $m = 256$

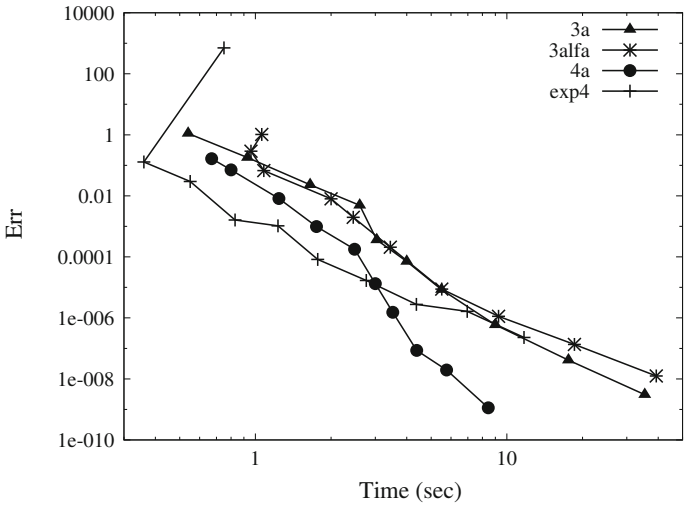

Fig. 4 Results for Laser

vs. computing time for tolerances $atol = rtol = 10^{-1}, \ldots, 10^{-8}$, for Laser $10^{-1}, \ldots, 10^{-10}$. Here the ODE reference solution *yref* has been computed with high accuracy.

5 Conclusions and outlook

The peer methods solve all problems reliably. The results show that they are also applicable for large problems which are nonlinear and may be very stiff. As expected,

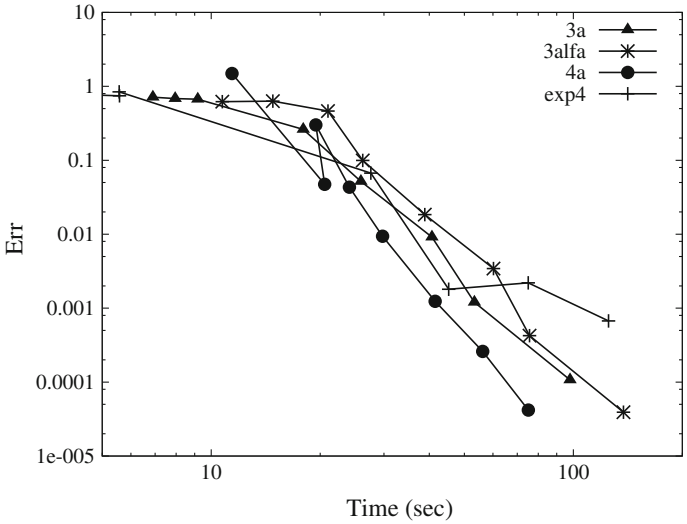

Fig. 5 Results for combustion, $m = 40$

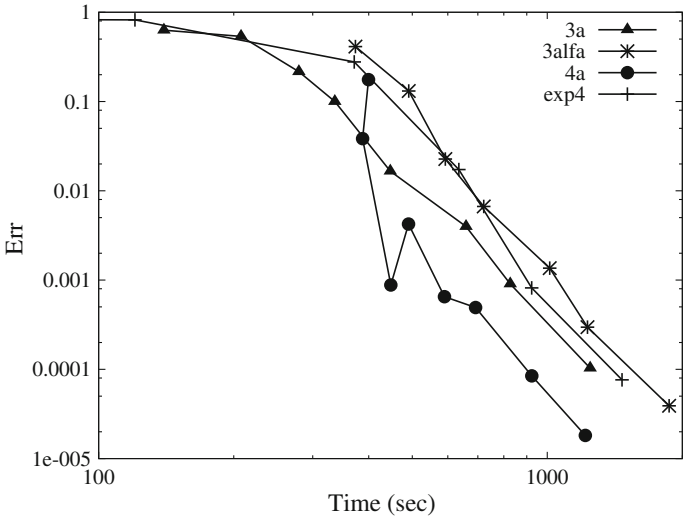

Fig. 6 Results for combustion, $m = 80$

the average Krylov dimensions for the approximation of $c_1 h_m \varphi(c_1 h_m T_m) f_{m-1,s}$ were much larger than for (3.4) (here the dimension for stage s was always largest). For $atol = 10^{-6}$ for instance the average Krylov dimensions were 22.8 for $c_1 h_m \varphi(c_1 h_m T_m) f_{m-1,s}$ and 11.9 for the last stage for (3.4) for Combustion with $m = 80$, 31.2 vs. 5.1 for Brusselator II with $m = 256$ and 7.0 vs. 1.8 for Laser. The limit $krymax = 36$ was reached in some steps for the first Krylov subspace for Brusselator II and for Combustion for all tolerances, for Laser for crude tolerances only, and it was never hit for Brusselator I.

The numerical tests indicate:

- The higher stiff order of the peer methods (no order reduction) pays off. Method `Peer4a` performed well in all examples and seems to be the most promising exponential peer method tested in this paper.
- As expected, the smaller number of arguments for methods satisfying (2.12) (`Peer3alfa`) has no advantage in combination with Krylov techniques.

Improvements of the performance may be achieved by keeping the Jacobian constant for some steps which has not been tested yet. Also the test of a matrix-free version with difference approximation for Jacobian times vector products is a topic of future research.

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