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Exponential Krylov peer integrators

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Abstract

This paper is concerned with the application of exponential peer methods derived in [5], [28] to stiff ODEs of high dimension. Conditions for stiff order p for variable step size are derived, corresponding methods are given. The methods are combined with Krylov approximations for the φ-functions times a vector using the code `phipm` of [16]. 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 `exp4` [9] for semidiscretized problems show the efficiency of the proposed methods.

MSC: 65L05, 65L06

Keywords. Exponential integrators, peer methods, Krylov methods.

1 Introduction

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

$$\begin{aligned} y' &= f(t,y) \\ y(t_0) &= y_0 \in R^n, \quad t_0 \le t \le t_e. \end{aligned} \tag{1}$$

They involve exponential functions (or related functions) of the Jacobian 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 $g(t,y)$:

$$f(t,y) = Ty + g(t,y). \tag{2}$$

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Since the first paper about exponential integrators by Certaine [4], 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 [11]. There are many papers about the advantages of exponential methods, however, often the numerical results presented consider only the case of constant step size implementation, for instance [2], [24]. In many cases also the constant matrix T in (2) is used as approximation for the Jacobian over the whole integration interval. One exception is the well-established code `exp4` of Hochbruck/Lubich/Selhofer [9]. `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.

In this paper we consider exponential peer methods introduced in [5] and [28] which are based on explicit peer methods [25, 27]. We combine them 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 [16]. The methods are implemented with step size control in MATLAB and tested on large systems, some of them are very stiff. We compare the performance of the exponential peer methods with `exp4`.

The outline of this paper is as follows:

In Section 2 exponential peer methods are considered. Results for stiff order of consistency, zero-stability and convergence are proved. Special methods with 3- and 4-stage methods are given. The computation of the φ-functions times a vector using Krylov approximations is the topic of Section 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 Section 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 Section 5 the results are discussed and conclusions drawn.

2 Exponential Peer Methods

Exponential peer methods for (1) are given by

$$\begin{aligned} Y_{mi} &= \varphi_0(\alpha_i h_m T_m) \sum_{j=1}^{s} b_{ij} Y_{m-1,j} + h_m \sum_{j=1}^{s} A_{ij}(\alpha_i h_m T_m)[f_{m-1,j} - T_m Y_{m-1,j}] \\ &+ h_m \sum_{j=1}^{i-1} R_{ij}(\alpha_i h_m T_m)[f_{mj} - T_m Y_{mj}], \qquad i = 1, 2, ..., s. \end{aligned} \tag{3}$$

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 $0 \le c_i < 1, i = 1, ..., s-1$. Further, we denote $f_{mj} = f(t_{mj}, Y_{mj})$. T_m is an arbitrary matrix, for stability we will use an approximation to the Jacobian $f_y(t_m, Y_{m-1,s})$. The s stage values Y_{mi} have the same characteristics so we call them *'peer'* [21]. By setting $T_m = 0$ we obtain explicit peer methods, which have been proved to be very efficient for nonstiff systems [27].

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

$$\sigma = \frac{h_m}{h_{m-1}}, \tag{4}$$

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 well-known φ-functions and depend on the step size ratio as well.

For integers $l \ge 0$ and complex numbers $z \in \mathbb{C}$ the φ-functions are defined as follows (e.g. [17]):

$$\begin{aligned}\varphi_0(z) &= e^z, \\ \varphi_l(z) &= \int_0^1 e^{(1-\theta)z} \frac{\theta^{l-1}}{(l-1)!} d\theta, \quad l \ge 1.\end{aligned}$$

They are related by the recurrence relation

$$\varphi_{l+1}(z) = \frac{\varphi_l(z) - \varphi_l(0)}{z} \quad \text{for } l \ge 0, \quad \text{with } \varphi_l(0) = \frac{1}{l!}. \tag{5}$$

Several methods have been proposed for evaluating these function [15], for instance methods relying on Padé approximations combined with scaling-and-squaring [2]. For large dimensions Krylov techniques are advantageous, e.g. [9], [22], [16].

We will assume that the stiffness in (2) is due to the linear part Ty and that the nonlinear part satisfies a global Lipschitz condition

$$\|g(t, u) - g(t, v)\| \le L_g \|u - v\| \tag{6}$$

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

$$\mu(T) \le \omega. \tag{7}$$

Often, systems (1) result from semidiscretization of partial differential equations where this condition is usually satisfied. Assumption (7) implies

$$\|\varphi_0(hT)\| = \|e^{hT}\| \le e^{\omega h}, \tag{8}$$

see e.g. [13].

Remark 1 *With* (6) *condition* (7) *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 method:

$$\Delta_{mi} = y(t_{mi}) - \varphi_0(\alpha_i h_m T_m) \sum_{j=1}^{s} b_{ij} y(t_{m-1,j}) - h_m \sum_{j=1}^{s} A_{ij}(\alpha_i h_m T_m)[y'(t_{m-1,j}) - T_m y(t_{m-1,j})]$$
$$- h_m \sum_{j=1}^{i-1} R_{ij}(\alpha_i h_m T_m)[y'(t_{mj}) - T_m y(t_{mj})], \quad i = 1, ..., s. \tag{9}$$

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

Definition 1 *The exponential peer method* (3) *is consistent of stiff order* q *if there are constants* $h_0, C > 0$ *such that*

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

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 right hand side is sufficiently smooth.

The following theorem gives condition for the coefficients of the method

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

to be of stiff order q.

Theorem 1 *Let the conditions*

$$\sum_{j=1}^{s} b_{ij} \left(\frac{c_j - 1}{\sigma_m} \right)^l = (c_i - \alpha_i)^l, \quad i = 1, ..., s, \tag{10}$$

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

$$\sum_{j=1}^{s} A_{ij}(\alpha_i h_m T_m) \left(\frac{c_j - 1}{\sigma_m} \right)^r + \sum_{j=1}^{i-1} R_{ij}(\alpha_i h_m T_m) c_j^r = \sum_{l=0}^{r} l! \alpha_i^{l+1} \binom{r}{l} (c_i - \alpha_i)^{r-l} \varphi_{l+1}(\alpha_i h_m T_m)$$
$$i = 1, ..., s \tag{11}$$

hold for $r = 0, ..., q$. *Then the exponential peer method is at least of stiff order* q *for* (1).

If in addition (10) *is also satisfied for* $l = q + 1$ *and* $\|T_m y^{(q+1)}\|$ *is of moderate size, then the method is of stiff order* $q + 1$.

Proof. By Taylor expansion of the exact solution in (9) we have

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

Using (10), (11) and the recurrence (5) we obtain

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

i.e. stiff order q. If in addition (10) holds for $l = q+1$ we have

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

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* $\|Ty^{(q+1)}\| \leq C$ *with a constant* C *of moderate size is* $\|T\| \leq C_1$ *(nonstiff order). But* $\|Ty^{(q+1)}\|$ *can be of moderate size 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 [10].*

Corollary 1 *For $q = s-1$ equation* (10) *is equivalent with*

$$B = V_\alpha S V_1^{-1}, \tag{12}$$

where

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

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

Corollary 2 *Let $\alpha = c$, $c_s = 1$. Then, with* (12)*, B will be independent of σ_m, we have*

$$B = \mathbb{1} e_s^T, \quad e_s = (0, 0, ..., 1)^T, \tag{13}$$

and (10) *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 (11) 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. In [28] was therefore a different choice for α investigated. With

$$\alpha = (\alpha^*, ..., \alpha^*, 1)^T, \text{ and } c_i = (s-i)(\alpha_i - 1) + 1, \quad i = 1, ..., s. \tag{14}$$

φ-functions with only two different arguments have to be computed. These methods were tested with constant step size in [28] and with step size control in [6].

However, in combination with Krylov techniques there is no advantage of (14) compared to $\alpha = c$. We will therefore use the methods of Corollary 2, what also simplifies the proof of stiff convergence (cf. Remark 3).

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 $\sigma \leq \sigma^*$ 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 holds

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

with $g_{mj} = f(t_{mj}, Y_{mj}) - T_m Y_{mj}$. With (6), (8) 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. ■

Remark 3 *In [6] for methods* (14) *of stiff order of consistency q zero-stability for $\sigma \le \sigma^*$ with $\sigma^* > 1$ was proved. Stiff order of convergence q could be shown under the additional assumption*

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

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 (11) 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:

$$\begin{aligned}
&c = \alpha = (1/4, 1/2, 1)^\top, \quad B = \mathbb{1} e_s^\top \\
&A_{11} = \frac{1}{6}\sigma\varphi_2 + \frac{1}{6}\sigma^2\varphi_3, \quad A_{12} = -\frac{3}{8}\sigma\varphi_2 - \frac{1}{4}\sigma^2\varphi_3, \quad A_{13} = \frac{1}{4}\varphi_1 + \frac{5}{24}\sigma\varphi_2 + \frac{1}{12}\sigma^2\varphi_3, \\
&A_{22} = -\frac{1}{2(\sigma+2)}\sigma^2\varphi_2 + \frac{2}{\sigma+2}\sigma^2\varphi_3, \quad A_{23} = \frac{1}{2}\varphi_1 + \frac{1}{4}(2\sigma - 4)\varphi_2 - 2\sigma\varphi_3, \\
&A_{33} = \varphi_1 - 6\varphi_2 + 16\varphi_3, \\
&R_{21} = \frac{2}{\sigma+2}\varphi_2 + \frac{4\sigma}{\sigma+2}\varphi_3, \quad R_{31} = 8\varphi_2 - 32\varphi_3, \quad R_{32} = -2\varphi_2 + 16\varphi_3.
\end{aligned}$$

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 (3). Our implementation uses the code `phipm` of [16]. This code computes the sum

$$\varphi_0(A)u_0 + \sum_{k=1}^{p} \varphi_k(A)u_k \tag{15}$$

by exploiting the following property:

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

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

With $l = 0$ and

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

we get $\varphi_0(A)$ in the upper left $n \times n$-submatrix of $\varphi_0(\widetilde{A})$ and the remaining terms of (15) 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 (15) is transformed into the approximation of only one single function $\varphi_p(A)v$. Building the Krylov subspace $\mathcal{K}_m = \text{span}\{v_1, ..., v_m\}$ by the Arnoldi algorithm (see e.g. [19]) and using $v_1 = v/\|v\|$ we arrive at the approximation ([16])

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

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

$$\widetilde{H} = \begin{bmatrix} H & e_1 & 0 & \dots & 0 \\ 0 & & & J & \end{bmatrix}$$

and obtain

$$\varphi_0(\widetilde{H}) = \begin{bmatrix} \varphi_0(H) & \varphi_1 e_1 & \dots & \varphi_p e_1 & \varphi_{p+1} e_1 \\ 0 & * & * & * & * \end{bmatrix}. \tag{16}$$

The additional column allows the error estimation ([22], [16])

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

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 (3). With $c_i = \alpha_i$, $c_s = 1$ and $B = \mathbb{1}e_s^T$ (see Corollary 2) we get

$$\begin{aligned} Y_{mi} \;=\; & \varphi_0(c_ihT)Y_{m-1,s} + c_ih\varphi_1(c_ihT)g_{m-1,s} \\ & + h\sum_{j=1}^{s} A_{ij}(c_ihT)g_{m-1,j} + h\sum_{j=1}^{i-1} R_{ij}(c_ihT)g_{mj} - c_ih\varphi_1(c_ihT)g_{m-1,s} \qquad i = 1,\dots,s. \end{aligned}$$

By the order condition (11) for $r = 0$ we have

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

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

$$\begin{aligned} Y_{mi} &= \varphi_0(c_ihT)Y_{m-1,s} + c_ih\varphi_1(c_ihT)(f_{m-1,s} - TY_{m-1,s}) \\ &\quad + h\left(\sum_{j=1}^{s} A_{ij}(c_ihT)g_{m-1,j} + \sum_{j=1}^{i-1} R_{ij}(c_ihT)g_{mj} - c_ih\varphi_1(c_ihT)g_{m-1,s}\right) \\ &= Y_{m-1,s} + c_ih\varphi_1(c_ihT)f_{m-1,s} \\ &\quad + h\left(\sum_{j=1}^{s} A_{ij}(c_ihT)g_{m-1,j} + \sum_{j=1}^{i-1} R_{ij}(c_ihT)g_{mj} - c_i\varphi_1(c_ihT)g_{m-1,s}\right) \\ &= Y_{m-1,s} + c_ih\varphi_1(c_ihT)f_{m-1,s} \\ &\quad + h\sum_{j=1}^{s} A_{ij}(c_ihT)\underbrace{(g_{m-1,j} - g_{m-1,s})}_{\mathcal{O}(h)} + h\sum_{j=1}^{i-1} R_{ij}(c_ihT)\underbrace{(g_{mj} - g_{m-1,s})}_{\mathcal{O}(h)}. \end{aligned} \tag{17}$$

We thus can avoid φ_0 and the terms $\varphi_1(c_ihT)v$ appear with different arguments c_ihT 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_ihT of φ_1 are multiples of c_1hT. 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 the functions φ_1 in all stages are multiplied with the same vector $v = f_{m-1,s}$, we can compute $\varphi_1(2A)v$, $\varphi_1(3A)v$ and $\varphi_1(4A)v$ very efficiently from $\varphi_1(A)v$. First it holds

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

were $\varphi_1(H)e_1$ is explicitly available from (16). Because of

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

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 explicit given $\varphi_0(H)$ (see (16)) the product $\varphi_1(2A)v$ is also available. In the same way we get the expressions

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

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 $c_1h\varphi_1(c_1hT)f_{m-1,s}$ with a possibly high Krylov dimension per step and the less expensive computation of $c_ih\varphi_1(c_ihT)f_{m-1,s}$

for $i = 2, ..., s$. 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 [16] 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 $\varphi_1(rH)e_1$, $r = 2, ..., s$, 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 (17).

4 Numerical tests

We implemented `Peer3a`, `Peer4a` with Krylov approximation as described in Section 3. For comparison we also included a 3-stage exponential peer method `Peer3alfa` with property (14) and `exp4` ([9], 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` [26]. For step size control we estimate the local error $Y_{m,s-1} - \widehat{Y}_{m,s-1}$, where an embedded solution $\widehat{Y}_{m,s-1}$ is computed by interpolation using the values Y_{mi}, $i = 1, \ldots, s-2, s$. We used the following test problems:

Brusselator:
This is the two-dimensional Brusselator with diffusion:

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

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: [7, p.248-249]

- $t_e = 1, \quad B = 3, \quad \alpha = 0.02.$
- Initial conditions: $u(x,y,0) = 0.5 + y, \quad v(x,y,0) = 1 + 5x$
- $f\,(x,y,t) = 0.$
- Number of grid points in each spatial direction: $M = 100$, dimension of the ODE-system: $n = 2M^2 = 20000$.

Version 2: [8, p.151-152]

- $t_e = 11.5, \quad B = 3.4, \quad \alpha = 0.1.$
- Initial conditions: $u(x,y,0) = 22y\,(1-y)^{3/2}, \quad v(x,y,0) = 27x\,(1-x)^{3/2}$.
- $f\,(x,y,t) = \begin{cases} 5 & \text{if } \ (x-0.3)^2 + (y-0.6)^2 \le 0.1^2 \ \text{ and } \ t \ge 1.1 \\ 0 & \text{else} \end{cases}$
- We used $M = 128$ grid points in each spatial direction resulting in $n = 2M^2 = 32768$ ODEs, and $M = 256$, $n = 2M^2 = 131072$.

Laser:
This example is from [9].

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

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 [23]:

$$\begin{aligned} c_t &= \Delta c - Dce^{-\delta/T} \\ L\,T_t &= \Delta T + \alpha Dce^{-\delta/T}, \quad (x,y) \in \Omega = [0,1]^3\,, \quad t \in [0,0.3], \end{aligned} \tag{18}$$

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

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

We discretized this problem on a uniform three-dimensional mesh by second-order central differences. We used $M = 40$ and $M = 80$ resulting in 128000 and 1024000 ODEs.

The following figures (in logarithmic scale) show the error at the endpoint t_e

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

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

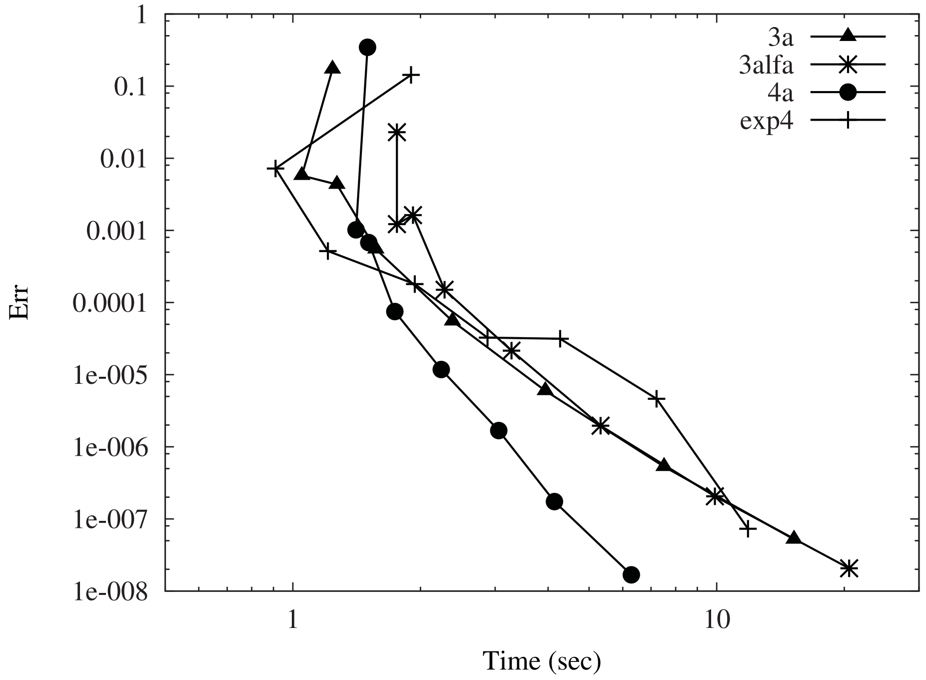

Figure 1: Results for Brusselator I, $m = 100$

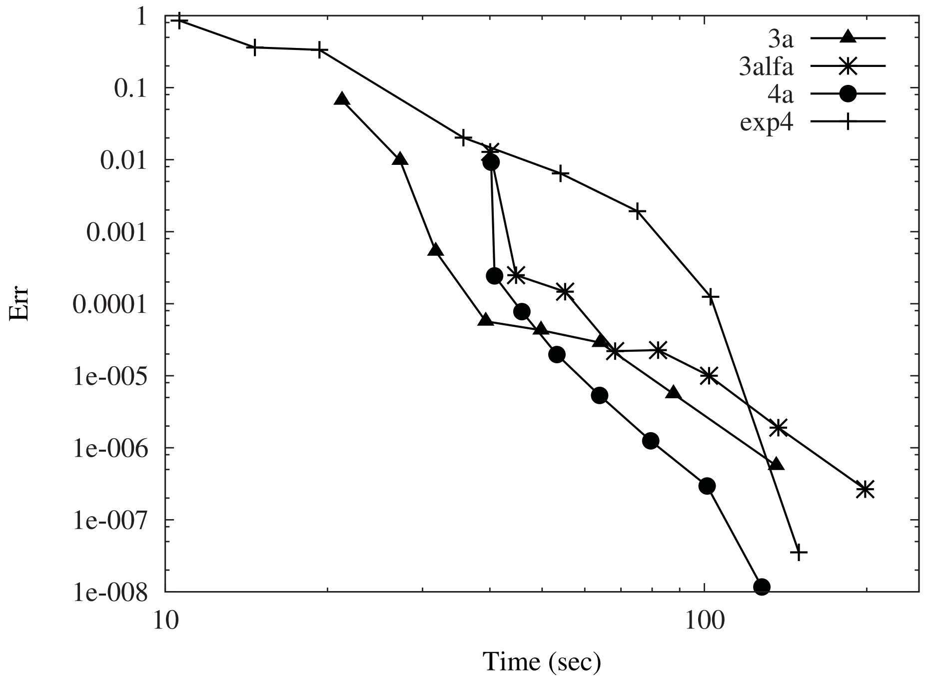

Figure 2: Results for Brusselator II, $m = 128$

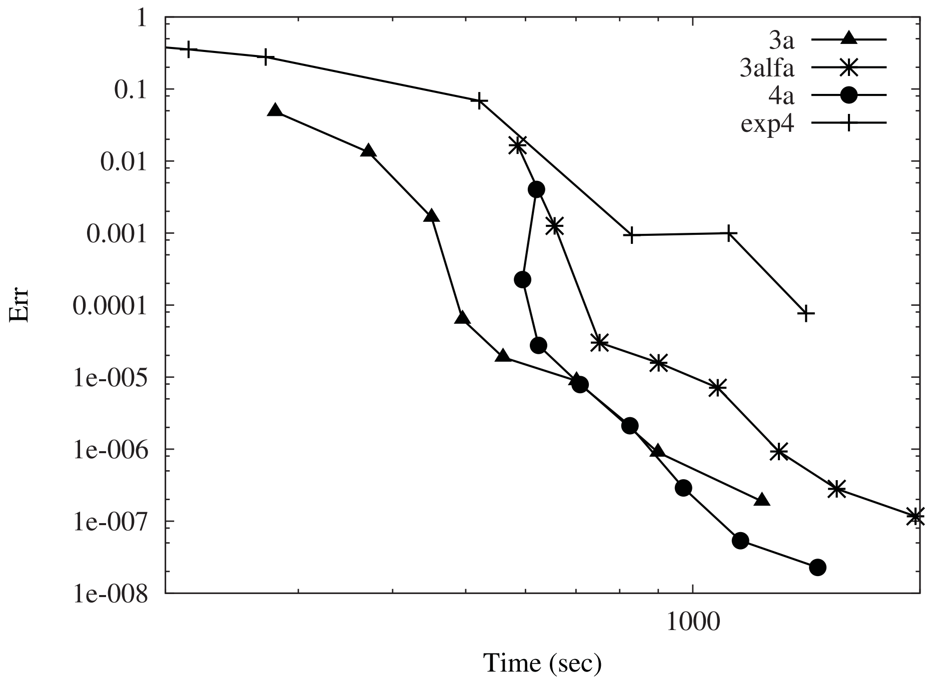

Figure 3: Results for Brusselator II, $m = 256$

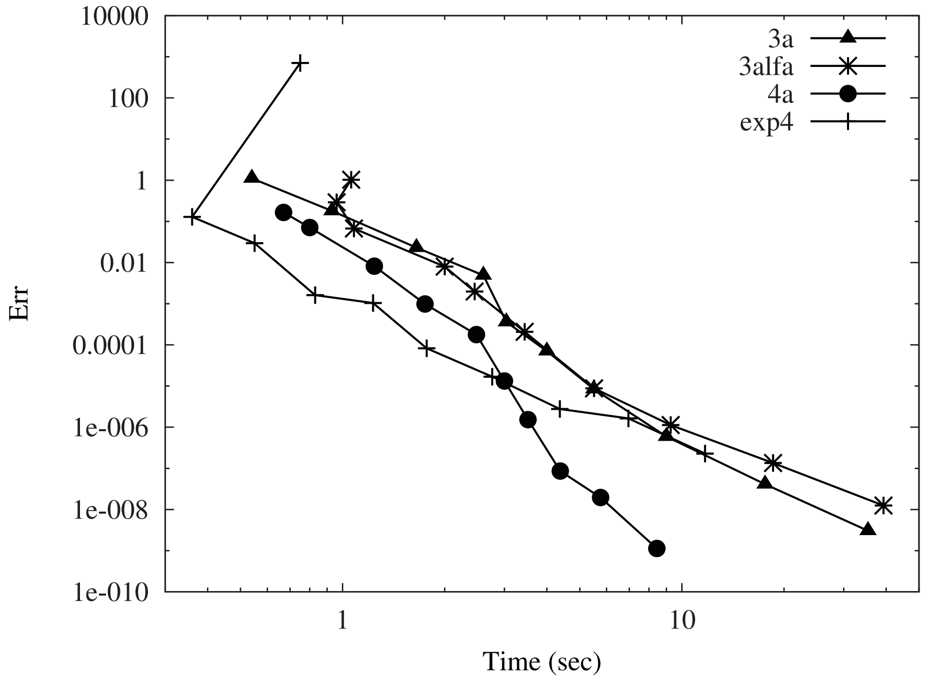

Figure 4: Results for Laser

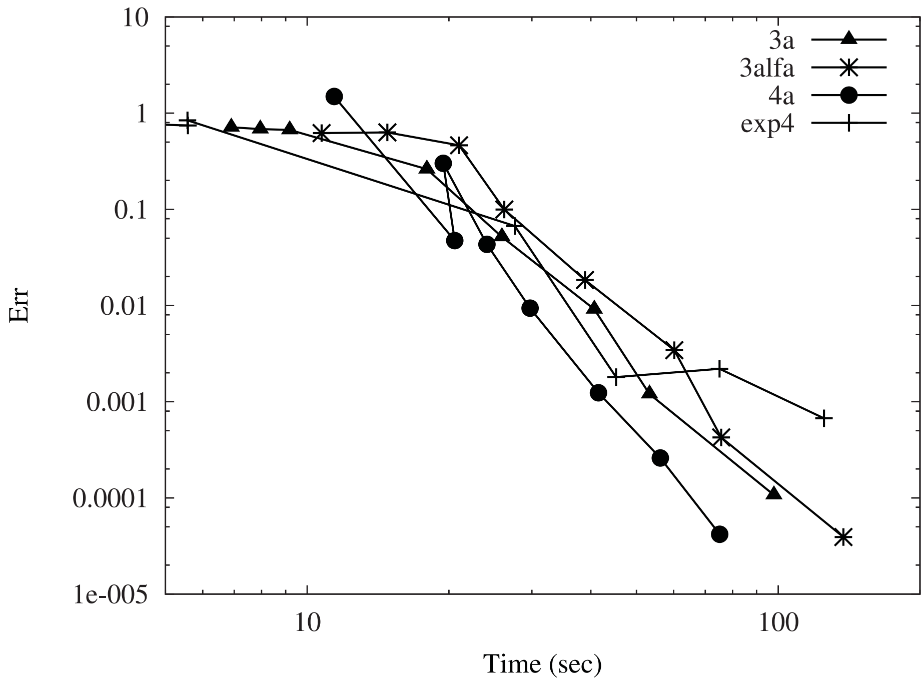

Figure 5: Results for Combustion, $m = 40$

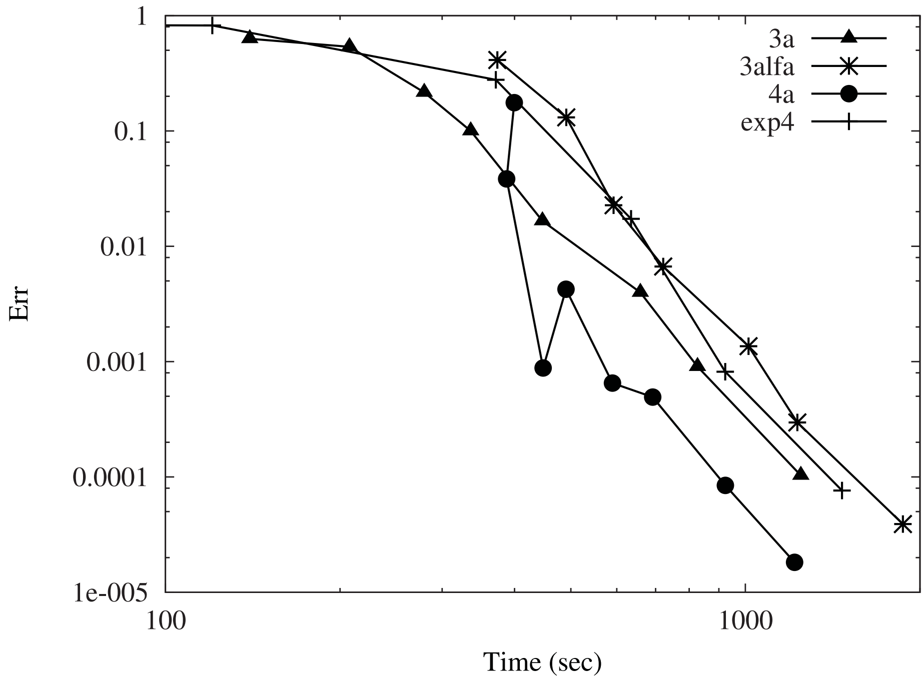

Figure 6: Results for Combustion, $m = 80$

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. 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 (14) (`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 was not yet tested. 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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