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Exponential peer methods with variable step sizes

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Abstract

This paper is concerned with the generalization of the exponential peer method derived in [18] to variable step sizes. Conditions for stiff order p are derived. The zero-stability of the methods is investigated. For a special subclass of methods with only two different arguments of the φ-functions bounds for the step size ratio are given, which ensure zero stability. These bounds are fairly large for practical computations. Different strategies for error estimation and step size control are considered. Numerical tests show that the step size control works reliably and that for special problem classes the methods are superior to classical integrators.

Key words: Exponential peer methods, variable step size, zero-stability.

1 Introduction

Exponential integrators are a well-known class of numerical integration methods for stiff systems of ordinary differential equations, which involve exponential functions (or related functions) of the Jacobian or an approximation to it [4]. Since the first paper about exponential integrators by Certaine [3], there has been a considerable amount of research on methods of this type. Until now the emphasis has been on the development of new methods, see e.g. [9, 2, 11].

Exponential integrators are especially useful for differential equations coming from the spatial discretization of partial differential equations, where the problem often splits into a linear (stiff) and a nonlinear (nonstiff) part.

Linearly-implicit peer methods have been studied e.g. in [12, 13, 14]. They are characterized by a high stage order what makes them attractive for very stiff systems.

Exponential peer methods [18] are based on explicit peer methods, which were introduced by Weiner et al. [16, 17]. They have been derived and investigated in [18] for constant step sizes. A special subclass was identified there, which is optimal zero-stable for constant step sizes and solves linear problems $y' = Ty$ exactly. Order conditions for a stiff order, i.e. the bounds are independent on the stiffness, were given. Due to the high stage order no order reduction occurs, which was illustrated by extensive numerical tests with constant step size.

In this paper we generalize the investigations in [18] for variable step sizes. We derive order conditions for the coefficients which now will depend on the step size ratio. Due to the variable

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step size, zero stability now leads to restrictions of the step size ratio in general. We present one subclass which is optimally zero stable for all step size sequences. For another special class of methods with only two different arguments in the φ-functions we prove stiff order $p = s - 1$, s the number of stages. For this class we compute bounds on the step size ratio which guarantee zero stability. These bounds are fairly large for practical computations.

Furthermore, for the implementation of exponential peer methods an error estimation is included. Two techniques are considered. One technique uses interpolation at $s - 1$ solution points and the other is embedding in different ways. The constructed methods are then tested for problems from [1].

The outline of this paper is as follow: In Section 2 a short overview on exponential peer methods and the formulation for variable step sizes are given.

In Section 3 we derive order conditions for variable step sizes. We show that for all stage numbers s methods of stiff order $p = s - 1$ exist and can be constructed easily. Two special subclasses are discussed. The zero stability of the methods, necessary for convergence, is proved. For a class with only two different arguments in the φ-functions bounds for the step size ratio are derived which guarantee zero-stability. These bounds are sufficiently large for practical computations.

In Section 4 various aspects of the implementation are discussed, especially possibilities of error estimation and step size control. The constructed methods are tested on problems of the Expint package [1]. For comparison we include the results for ode15s and ode45. For special problem types the exponential peer methods turn out to be comparable and superior, but for others the classical codes are more efficient.

2 Exponential Peer Methods

For the initial value problem (IVP) governed by systems of ordinary differential equations

$$\begin{aligned} \frac{dy}{dt} &= f(t,y) = Ty + g(t,y), \quad t \in [t_0, t_{end}] \qquad (1) \\ y(t_0) &= y_0 \in \mathbb{R}^n, \end{aligned}$$

where $g(t,y) = f(t,y) - Ty$, $y : [t_0, t_{end}] \mapsto \mathbb{R}^n$ and $f : [t_0, t_{end}] \times \mathbb{R}^n \mapsto \mathbb{R}^n$, we consider the class of exponential peer methods

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

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 $0 \leq c_i < 1, i = 1, \ldots, s-1$. Further we denote $f_{m,j} = f(t_{mj}, Y_{mj})$. The s stage values Y_{mi} have the same characteristics so we call them *'peer'* [14]. By setting $T_m = 0$ we obtain explicit peer methods, which have been proved to be very efficient for nonstiff systems [17]. In this paper we will consider $T_m = T$.

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

$$\sigma_m = \frac{h_m}{h_{m-1}}, \tag{3}$$

the matrix functions $A_{ij}(h_m T_m)$ and $R_{ij}(h_m T_m)$ are linear combinations of the well known φ-functions and depend on the step size ratio as well.

The φ-functions are defined as follows (e.g. [11]): For integers $l \geq 0$ and complex numbers $z \in \mathbb{C}$, we define $\varphi_l(z)$ through

$$\varphi_0(z) = e^z,$$
$$\varphi_l(z) = \int_0^1 e^{(1-\theta)z} \frac{\theta^{l-1}}{(l-1)!} d\theta, \quad l \geq 1.$$

The φ-functions are related by the recurrence relation

$$\varphi_{l+1}(z) = \frac{\varphi_l(z) - \varphi_l(0)}{z} \quad \text{for } l \geq 0, \quad \text{with } \varphi_l(0) = \frac{1}{l!}. \tag{4}$$

Several methods have been proposed for evaluating these function [10]. We will use the Expint package [1] relying on Padé approximations combined with scaling-and-squaring. For large dimensions, however, Krylov techniques may be advantageous, e.g. [5, 7, 15].

3 Consistency and convergence

In this section we will derive order conditions for (2) for variable step sizes and prove zero-stability.

We will assume that the stiffness in (1) is due to the linear part Ty and that the nonlinear part satisfies a global Lipschitz condition

$$\|g(t,u) - g(t,v)\| \leq L_g \|u - v\| \tag{5}$$

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

$$\mu(T) \leq \omega. \tag{6}$$

Often system (1) results from semidiscretization of partial differential equations and this condition is usually satisfied. Assumption (6) implies

$$\|\varphi_0(hT)\| = \|e^{hT}\| \leq e^{\omega h}, \tag{7}$$

see e.g. [8].

Remark 1 *A consequence of (6) is that $\|\varphi_l(h_m T_m)\|$ and $\|h_m T_m \varphi_l(h_m T_m)\|$ 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 $\varphi_l(\alpha_i h_m T_m)$, $l \geq 1$.*

For our investigations of the order of consistency we always assume that the right hand side is sufficiently smooth.

The local residual errors are defined by inserting the exact solution into the numerical method:

$$\Delta_{m,i} = y(t_{mi}) - \varphi_0(\alpha_i h_m T_m) \sum_{j=1}^{s} b_{ij} y(t_{m-1,j}) - h_m \sum_{j=1}^{s} A_{ij}(\alpha_i h_m T_m)[y'(t_{m-1,j}) - T_m y(t_{m-1,j})]$$
$$- h_m \sum_{j=1}^{i-1} R_{ij}(\alpha_i h_m T_m)[y'(t_{mj}) - T_m y(t_{mj})], \quad i = 1, ..., s. \tag{8}$$

Definition 1 *The exponential peer method* (2) *is consistent of nonstiff order p if there are constants $h_0, C > 0$ such that*

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

The method is consistent of stiff order p, if C and h_0 may depend on ω, L_g and bounds for derivatives of the exact solution, but are independent of $\|T\|$.

Note that for peer methods all stage values are of order p, i.e. the order of consistency is equal to the stage order.

To determine the coefficients of the method

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

such that the method has high order, it is advantageous to consider the linear case first.

Theorem 1 *If the exponential peer method satisfies the conditions*

$$\sum_{j=1}^{s} b_{ij} \left(\frac{c_j - 1}{\sigma_m} \right)^l = (c_i - \alpha_i)^l, \quad l = 0, 1, ..., q, \tag{9}$$

then it is of stiff order of consistency $p = q$ for the linear equation $y' = Ty$.

Proof. From (8), for the equation $y' = Ty$ the local residual errors will be

$$\Delta_{m,i} = y(t_m + c_i h_m) - \varphi_0(\alpha_i h_m T_m) \sum_{j=1}^{s} b_{ij} y(t_m + (c_j - 1)h_{m-1})$$
$$= \varphi_0(c_i h_m T_m) y(t_m) - \varphi_0(\alpha_i h_m T_m) \sum_{j=1}^{s} b_{ij} \varphi_0 \left(\frac{(c_j - 1)}{\sigma_m} h_m T_m \right) y(t_m).$$

Using the relation

$$\varphi_0(z) = \sum_{l=0}^{q} \frac{z^l}{l!} + z^{q+1} \varphi_{q+1}(z),$$

which follows from (4), we obtain

$$\Delta_{m,i} = \sum_{l=0}^{q} \left[c_i^l - \sum_{j=1}^{s} b_{ij} \left(\alpha_i + \frac{c_j - 1}{\sigma_m} \right)^l \right] \frac{h_m^l T_m^l}{l!} y(t_m) + h_m^{q+1} \Bigg\{ c_i^{q+1} \varphi_{q+1}(c_i h_m T_m)$$
$$- \sum_{j=1}^{s} b_{ij} \left(\alpha_i + \frac{c_j - 1}{\sigma_m} \right)^{q+1} \varphi_{q+1} \left(\left(\alpha_i + \frac{c_j - 1}{\sigma_m} \right) h_m T_m \right) \Bigg\} T_m^{q+1} y(t_m).$$

With $T_m^{q+1} y(t_m) = y^{(q+1)}(t_m)$ the second term is $\mathcal{O}(h_m^{q+1})$, where the constants are independent of $\|T_m\|$. For the coefficients of $\frac{h_m^l T_m^l}{l!} y(t_m)$ for $l = 0, ..., q$ we have

$$\begin{aligned}
c_i^l - \sum_{j=1}^{s} b_{ij} \left(\alpha_i + \frac{c_j - 1}{\sigma_m} \right)^l &= c_i^l - \sum_{j=1}^{s} b_{ij} \sum_{k=0}^{l} \binom{l}{k} \left(\frac{c_j - 1}{\sigma_m} \right)^k \alpha_i^{l-k} \\
&= c_i^l - \sum_{k=0}^{l} \binom{l}{k} \alpha_i^{l-k} \sum_{j=1}^{s} b_{ij} \left(\frac{c_j - 1}{\sigma_m} \right)^k \\
&= c_i^l - \sum_{k=0}^{l} \binom{l}{k} \alpha_i^{l-k} (c_i - \alpha_i)^k = c_i^l - c_i^l = 0.
\end{aligned}$$

The method is therefore of stiff order $p = q$ for $y' = Ty$. ■

Writing (9) for $q = s - 1$ as matrix equation and solving for B we obtain

Corollary 1 *Let*

$$B = V_\alpha S V_1, \tag{10}$$

where

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

Then the exponential peer method has stiff order $p = s - 1$ for the equation $y' = Ty$.

Corollary 2 *Let $\alpha = c$, $c_s = 1$. Then with* (10) *we have $B = \mathbb{1} e_s^T$, $e_s = (0, 0, ..., 1)^T$, and*

$$\sum_{j=1}^{s} b_{ij} \left(\frac{c_j - 1}{\sigma_m} \right)^l = (c_s - 1)^l.$$

Therefore (9) *is satisfied for all l, the exponential peer method solves the system $y' = Ty$ with exact starting values exactly.*

In the following we will always assume B to be defined by (10), the coefficients b_{ij} are therefore determined by c and α. We now will consider the general case (1) to obtain conditions for the matrix coefficients $A_{ij}(\alpha_i hT)$ and $R_{ij}(\alpha_i hT)$.

Theorem 2 *Let the conditions* (9) *be satisfied for $l = 0, ..., q$. Let further*

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

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

Proof. By Taylor expansion of the exact solution in (8) and using $g(t,y) = y' - Ty$ we have

$$\Delta_{m,i} = \sum_{r=0}^{q} \left\{ c_i^r I - \varphi_0(\alpha_i h_m T_m) \sum_{j=1}^{s} b_{ij} \left(\frac{c_j - 1}{\sigma_m} \right)^r - r \sum_{j=1}^{s} A_{ij}(\alpha_i h_m T_m) \left(\frac{c_j - 1}{\sigma_m} \right)^{r-1} \right.$$
$$+ h_m T_m \sum_{j=1}^{s} A_{ij}(\alpha_i h_m T_m) \left(\frac{c_j - 1}{\sigma_m} \right)^r - r \sum_{j=1}^{i-1} R_{ij}(\alpha_i h_m T_m) c_j^{r-1}$$
$$\left. + h_m T_m \sum_{j=1}^{i-1} R_{ij}(\alpha_i h_m T_m) c_j^r \right\} \frac{h_m^r}{r!} y^{(r)}(t_m) + \mathcal{O}(h_m^{q+1}) \tag{12}$$

The coefficients of $y^{(r)}(t_m)$ should be equal to zero for $r = 0, ..., q$. For $r = 0$ using (9) and (11) we obtain

$$I - \varphi_0(\alpha_i h_m T_m) \sum_{j=1}^{s} b_{ij} + h_m T_m \sum_{j=1}^{s} A_{ij}(\alpha_i h_m T_m) + h_m T_m \sum_{j=1}^{i-1} R_{ij}(\alpha_i h_m T_m)$$
$$= I - \varphi_0(\alpha_i h_m T_m) + \alpha_i h_m T_m \varphi_1(\alpha_i h_m T_m) = 0 \quad \text{by (4)}.$$

For $r = 1, ..., q$ holds for the coefficients

$$c_i^r I - \varphi_0(\alpha_i h_m T_m) \sum_{j=1}^{s} b_{ij} \left(\frac{c_j - 1}{\sigma_m} \right)^r - r \sum_{j=1}^{s} A_{ij}(\alpha_i h_m T_m) \left(\frac{c_j - 1}{\sigma_m} \right)^{r-1}$$
$$+ h_m T_m \sum_{j=1}^{s} A_{ij}(\alpha_i h_m T_m) \left(\frac{c_j - 1}{\sigma_m} \right)^r - r \sum_{j=1}^{i-1} R_{ij}(\alpha_i h_m T_m) c_j^{r-1} + h_m T_m \sum_{j=1}^{i-1} R_{ij}(\alpha_i h_m T_m) c_j^r$$
$$= c_i^r I - \varphi_0(\alpha_i h_m T_m)(c_i - \alpha_i)^r - r \sum_{l=0}^{r-1} \alpha_i^{l+1} \binom{r-1}{l} (c_i - \alpha_i)^{r-1-l} l! \varphi_{l+1}(\alpha_i h_m T_m)$$
$$+ h_m T_m \sum_{l=0}^{r} \alpha_i^{l+1} \binom{r}{l} (c_i - \alpha_i)^{r-l} l! \varphi_{l+1}(\alpha_i h_m T_m) \quad \text{by (11)}$$
$$= c_i^r I - \varphi_0(\alpha_i h_m T_m)(c_i - \alpha_i)^r - r \sum_{l=1}^{r} \alpha_i^{l} \binom{r-1}{l-1} (c_i - \alpha_i)^{r-l} (l-1)! \varphi_{l}(\alpha_i h_m T_m)$$
$$+ \sum_{l=0}^{r} \alpha_i^{l} \binom{r}{l} (c_i - \alpha_i)^{r-l} (l! \varphi_{l}(\alpha_i h_m T_m) - I) \quad \text{by (4)}$$
$$= c_i^r I - \varphi_0(\alpha_i h_m T_m)(c_i - \alpha_i)^r - \sum_{l=1}^{r} \alpha_i^{l} \binom{r}{l} (c_i - \alpha_i)^{r-l} l! \varphi_{l}(\alpha_i h_m T_m)$$
$$+ \sum_{l=0}^{r} \alpha_i^{l} \binom{r}{l} (c_i - \alpha_i)^{r-l} l! \varphi_{l}(\alpha_i h_m T_m) - c_i^r I = 0. \qquad \blacksquare$$

Corollary 3 *Let $\alpha = c$, $c_s = 1$ and B given by (10). Let*

$$\sum_{j=1}^{s} A_{ij}(c_i h_m T_m) \left(\frac{c_j - 1}{\sigma_m} \right)^r + \sum_{j=1}^{i-1} R_{ij}(c_i h_m T_m) c_j^r = r! c_i^{r+1} \varphi_{r+1}(c_i h_m T_m) \tag{13}$$

for $r = 0, ..., q$. Then the exponential peer method is consistent of stiff order at least $p = q$.

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 allow the bounds to depend on $T_m y^{(q+1)}$ (nonstiff order), then the order of the methods will be $p = q+1$,

Theorem 3 *Let the solution $y(t)$ be $(q+2)$-times continuously differentiable. Let the conditions (9) be satisfied for $l = 0, ..., q+1$, and (11) for $l = 0, ..., q$. Then the method is of nonstiff order $p = q+1$.*

Proof. Considering one more term in (12) gives for the term with h_m^{q+1}

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

With $\varphi_l(\alpha_i h_m T_m) = \alpha_i h_m T_m \varphi_{l+1}(\alpha_i h_m T_m) + \frac{1}{l!} I$ we finally obtain

$$= \left\{ c_i^{q+1} I - \sum_{l=0}^{q+1} \alpha_i^{l} \binom{q+1}{l} (c_i - \alpha_i)^{q+1-l} \right\} \frac{h_m^{q+1}}{(q+1)!} y^{(q+1)}(t_m) + \mathcal{O}\left(h_m^{q+2}\right)$$
$$= \mathcal{O}\left(h_m^{q+2}\right).$$

So $\Delta_{m,i} = \mathcal{O}\left(h_m^{q+2}\right)$ and the method is of nonstiff order $p = q+1$. ∎

Remark 2 *Note that $\|T_m y^{(q+1)}\|$ can be of moderate size although $\|T_m\|$ is very large, 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 [6].*

Due to the two-step character, for convergence of the method, we have in addition to show zero-stability.

Definition 2 *The exponential peer method* (2) *is called stable (zero stable) if*

$$\|B_{m+l}B_{m+l-1}...B_m\| \le K \qquad \text{for all } m, l \ge 0. \tag{14}$$

In general B_m depends on the step ratio σ_m (i.e. $B_m = B(\sigma_m)$). Therefore, condition (14) will usually lead to restrictions on the step size ratio. The proof of zero-stability and the computation of corresponding intervals for the step size ratio is in general a difficult task for linear multistep and general linear methods. Here we will consider two special classes of exponential peer methods. The first is given with the choice of Corollary 2:

Theorem 4 *Let $\alpha = c$, $c_s = 1$ and B given by* (10)*. Then the exponential peer method is stable for all step size sequences.*

Proof. From $B_m = \mathbb{1}e_s^T$ we have $B_{m+l}B_{m+l-1}...B_m = \mathbb{1}e_s^T$. ■

The choice $\alpha = c$ is optimal with respect to stability. However, this class of methods requires the computation of φ-functions with s different arguments whenever the step size changes. Because this is in general the most time consuming part in these methods we are interested in methods with a smaller number of different arguments. An efficient class with only two different arguments was proposed in [18] for constant step sizes. We will consider here the stability of this class for variable step sizes.

Theorem 5 *Let $\alpha = (\alpha^*, ..., \alpha^*, 1)^T$ and $c_i = (s-i)(\alpha_i - 1) + 1$, $i = 1, ..., s$. Let B given by* (10)*. Then there exist constants $\sigma_{min} < 1 < \sigma_{max}$ so that the exponential peer method is stable for all step size sequences satisfying $\sigma_{min} \le \sigma \le \sigma_{max}$.*

Proof. In [18] it was shown that all c_i are distinct with $c_s = 1$ and that the matrix $B(1)$ for constant step sizes has the form

$$B(1) = e_s e_s^T + F_0^T = \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ & & \cdots & & \\ 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & \cdots & 0 & 1 \end{pmatrix}$$

with $F_0 = (\delta_{i-1,j})$. $B(1)$ is optimally zero stable, i.e. one eigenvalue is one and all other eigenvalues are zero. The matrix

$$Q = \mathbb{1}e_1^T + F_0^T \Lambda$$

with $\Lambda = \mathrm{diag}(0, 1, \varepsilon, ..., \varepsilon^{s-2})$, with a parameter $0 < \varepsilon < 1$, transforms $B(1)$ to Jordan canonical form

$$Q^{-1}B(1)Q = \psi = \begin{pmatrix} 1 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & \epsilon & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & \epsilon \\ 0 & 0 & 0 & \dots & 0 & 0 \end{pmatrix}. \tag{15}$$

This follows from

$$B(1)Q = \mathbb{1}e_1^T + F_0^T F_0^T \Lambda \quad \text{and}$$
$$Q\psi = \mathbb{1}e_1^T + \varepsilon F_0^T \Lambda F_0^T = \mathbb{1}e_1^T + F_0^T F_0^T \Lambda.$$

We now apply this transformation to $B(\sigma)$. The first column of Q is $\mathbb{1}$, leading to

$$Q^{-1}B(\sigma)Qe_1 = e_1.$$

Because the last row of Q is e_1^T we obtain

$$e_1^T Q^{-1}B(\sigma)Q = e_s^T B(\sigma)Q = e_s^T Q = e_1^T.$$

This results in

$$Q^{-1}B(\sigma)Q = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & \widehat{B}(\sigma) & \\ 0 & & & \end{pmatrix},$$

where $\|\widehat{B}(1)\| = \|\psi\| < 1$ for $0 < \varepsilon < 1$. This means, that for an interval $[\sigma_{min}, \sigma_{max}]$ around 1 we have

$$\|Q^{-1}B(\sigma)Q\| = \max(\|\widehat{B}(\sigma)\|, 1)$$

for instance for the norms $\|\cdot\|_l$, $l = 1, 2, \infty$. This implies that for all $\sigma_j \in [\sigma_{min}, \sigma_{max}]$ we have

$$\|B_{m+k}B_{m+k-1}\cdots B_{m+1}B_m\| \le \|Q\| \cdot \|Q^{-1}\|$$

for all $m, k \ge 0$, i.e. zero stability. ■

For $s = 3, 4, 5$ we have computed the following bounds for σ_{min} and σ_{max} with MAPLE:

1. $s = 3 : \|\widehat{B}(\sigma)\|_1 \le 1$ for $\varepsilon = 1/4$ and $0 < \sigma \le 2$.
2. $s = 4 : \|\widehat{B}(\sigma)\|_\infty \le 1$ for $\varepsilon = 1/5$ and $0 < \sigma \le 1.5$.
3. $s = 5 : \|\widehat{B}(\sigma)\|_2 \le 1$ for $\varepsilon = 1/2$ and $0 < \sigma \le 1.3313$.

These bounds are sufficiently large for practical computations.

Remark 3 *By considering the special case of increasing h in each step by σ_{max} we found numerically $\sigma_{max} = \frac{s-1}{s-2}$. So, we suppose that there exists some norm such that*

$$\|\widehat{B}\| \le 1 \quad \textit{for} \quad 0 < \sigma \le \frac{s-1}{s-2}.$$

Remark 4 *If we perform $s-1$ consecutive steps with constant step size, then $[B(1)]^{s-1} = \mathbb{1}e_s^T$. and because of $B(\sigma)\mathbb{1} = \mathbb{1}$ all further products will be uniformly bounded independent of σ. Thus, by trying to keep the step size constant for some steps the stability of the exponential peer methods is strongly improved. This strategy is used in our implementation.*

4 Implementation issues and numerical tests

We constructed exponential peer methods with variable step size due to Theorems 1 and 2 with $s = 3, 4, 5$ stages of stiff order $p = s - 1$. The nodes c_i are determined by Theorem 5 with

$$\alpha^* = \frac{s-1}{s}$$

For simplicity the free parameters are chosen so that R is strictly lower triangular and A is upper triangular. For constant step sizes these methods reduce to those used in [18].

For error estimation we consider 2 possibilities

1. By interpolation using Y_{mi}, $i = 1, ..., s-1$, we compute a solution $\widetilde{Y}_{ms}$ of order $p = s - 2$.
2. We compute an embedded solution $\widetilde{Y}_{ms}$. Here we consider two cases.
   (a) We use an $(s-1)$-stage method with same α^* and $c = (c_2, ..., c_s)$ and compute $\widetilde{Y}_{ms}$ of order $s - 2$.
   (b) We solve the equations (11) for $i = s$ up to $r = s$. Because for $i = s$ (9) is also satisfied for $l = 0, ..., s$ we have $\widetilde{Y}_{ms}$ of local order $p = s$. We use $\widetilde{Y}_{ms}$ for error estimation and continue with $Y_{m1}, ..., Y_{m,s-1}, \widetilde{Y}_{ms}$.

In our tests we denote the corresponding s-stage methods by *epmsi* if interpolation is used and by *epmsea* or *epmseb* if embedding of type (a) or (b) is used, resp.

The error is estimated by

$$err = \frac{1}{\sqrt{n}} \frac{\|Y_{ms} - \bar{Y_m}\|_2}{atol + rtol \cdot \max(\|Y_{ms}\|_2, \|\widetilde{Y}_{ms}\|_2)}.$$

We then compute $fac = err^{-1/(s-1)}$. With respect to Remark 4 the new step size is computed as follows

$$h_{new} = \begin{cases} h, & 1 \le fac \le \sigma_{max} \\ \sigma_{max} h, & fac > \sigma_{max} \\ \max(0.2, fac) h, & fac < 1, \end{cases}$$

with $\sigma_{max} = (s-1)/(s-2)$. In the last case the step is repeated.

We use the framework of Expint [1] to test our methods. We have adapted our methods to the structure required and we use the computation of the φ-functions implemented in Expint. Expint contains several semidiscretized PDEs as test problems and a collection of well-known exponential integrators implemented with constant step size. In contrast to [18] we compare our exponential peer methods with *ode15s* and *ode45* at these test problems. By N the number of Fourier nodes or the number of inner points in a finite difference discretization is denoted. We give only a short overview about the problems here, for more detailed information we refer to [1] and the description in the package.

1. 1D Gray-Scott equation

$$\begin{aligned} u_t &= D_1 u_{xx} - uv^2 + a(1-u) \\ v_t &= D_2 v_{xx} + uv^2 - (a+b)v, \quad t \in [0, 10] \\ a &= 0.035, \quad b = 0.065, \quad D_1 = 2.e-5, \quad D_2 = 1.e-5, \end{aligned}$$

with periodic boundary conditions and scaled Gauss curves as initial conditions, see [1]. Fourier space discretization gives a diagonal matrix T of dimension 128.

2. Allen-Cahn equation

$$u_t = 0.001u_{xx} + u - u^3, \quad x \in [-1,1], \quad t \in [0,10],$$
$$u(0,x) = 0.53x + 0.47\sin(-1.5\pi x), \quad u(t,-1) = -1, \quad u(t,1) = 1.$$

The linear part $0.001u_{xx}$ is discretized using a Chebyshev differentiation matrix resulting in a full matrix T of dimension 64.

3. Kuramoto-Sivashinsky equation

$$u_t = -u_{xx} - u_{xxxx} - uu_x, \quad x \in [0, 32\pi], \quad t \in [0,10].$$

Spectral discretization with periodic boundary conditions and dimension $N = 128$ is used.

4. Nonlinear Schrödinger equation

$$iu_t = -u_{xx} + (V(x) + \lambda|u|^2)u, \quad x \in [-\pi,\pi], \quad t \in [0,10].$$

Periodic boundary conditions and the initial condition $u(0,x) = e^{\sin(2x)}$ are considered. We used $\lambda = 1$, $V(x) = \frac{1}{1+\sin^2(x)}$ and a spectral semi-discretization with $N = 128$.

5. Schrödinger type equation

$$iu_t = u_{xx} - uu_x + \phi(t,x), \quad x \in [0,1], \quad t \in [0,10].$$

6. Hyperbolic test equation (cf. [11])

$$iu_t = u_{xx} - \frac{1}{1+u^2} + \phi(t,x), \quad x \in [0,1], \quad t \in [0,10].$$

In the problems (5) and (6) $\phi(t,x)$ is chosen to give the exact solution $u(t,x) = x(1-x)e^{-t}$. Standard finite differences with $N = 64$, Dirichlet boundary conditions and exact initial conditions are used. T is defined by the space discretization of u_{xx}.

The s starting values for the exponential peer methods are computed with ode15s.

In the following figures we present the accuracy of the numerical solution Y at t_{end} versus the computing time. The error is computed by

$$error = \frac{\|Y - Y_{ref}\|_\infty}{\max_i \max(|Y_{ref,i}|, 1)},$$

where Y_{ref} is a reference solution which is computed with ode15s and high accuracy.

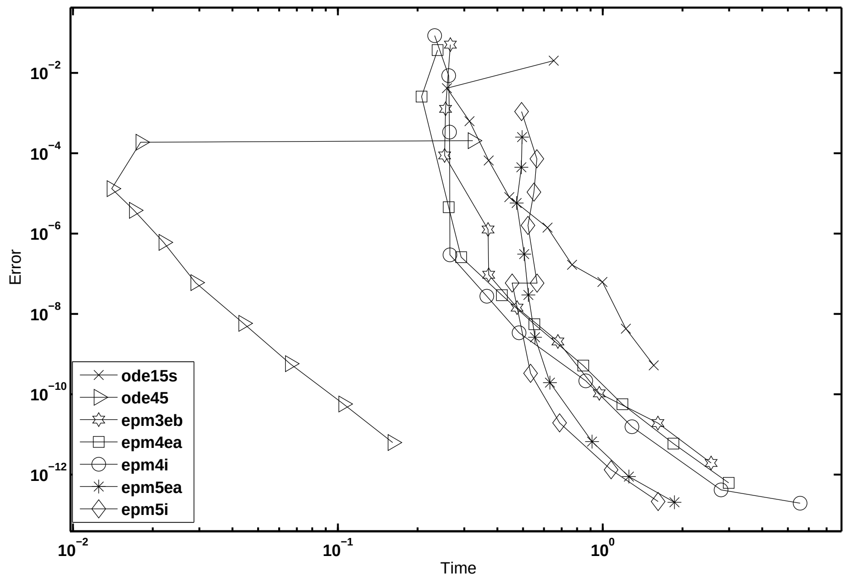

Figure 1: Results for Gray-Scott

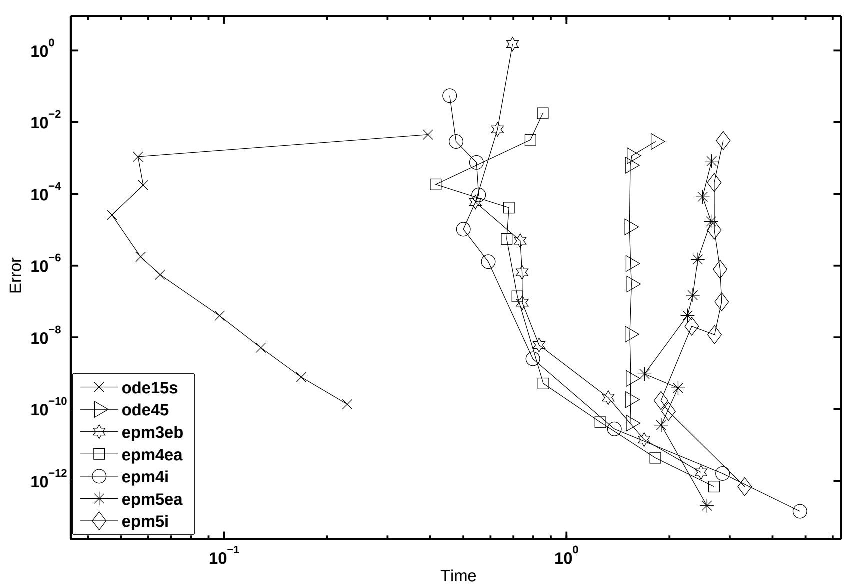

Figure 2: Results for the Allen-Cahn equation

5 Conclusions

The results of the exponential peer methods show that the proposed kinds of error estimation and step size control work reliably. For crude tolerances the 3- and 4-stage methods are more

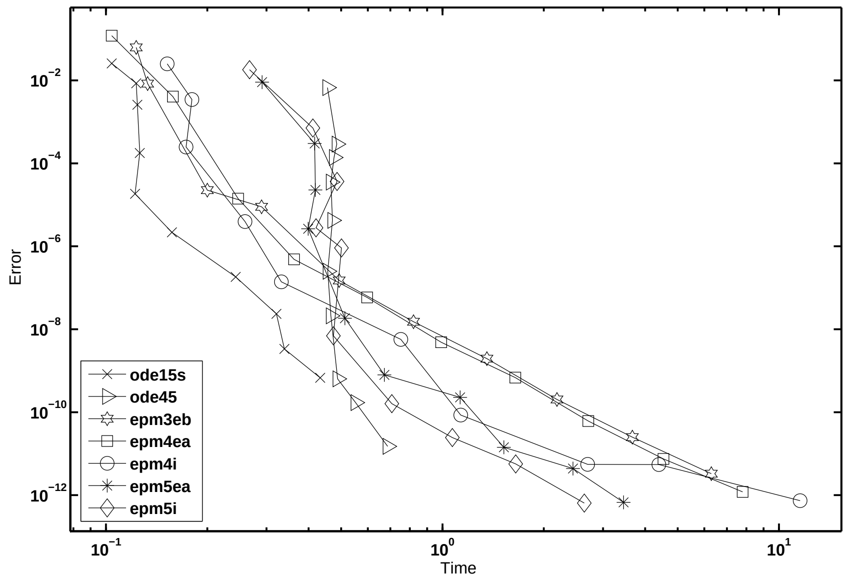

Figure 3: Results for the Kuramoto-Sivashinsky equation

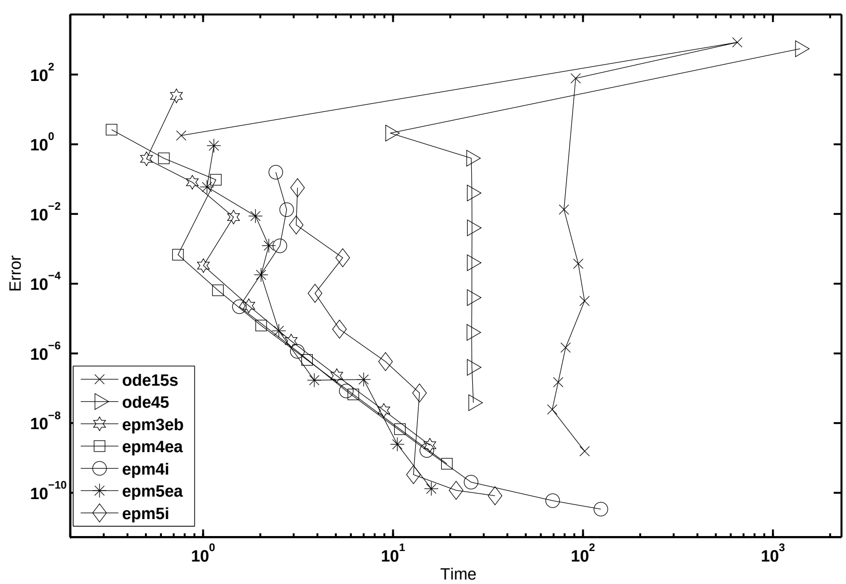

Figure 4: Results for the Nonlinear Schrödinger equation

efficient than the 5-stage methods which may be due to the larger value of σ_{max}. ode45 is the

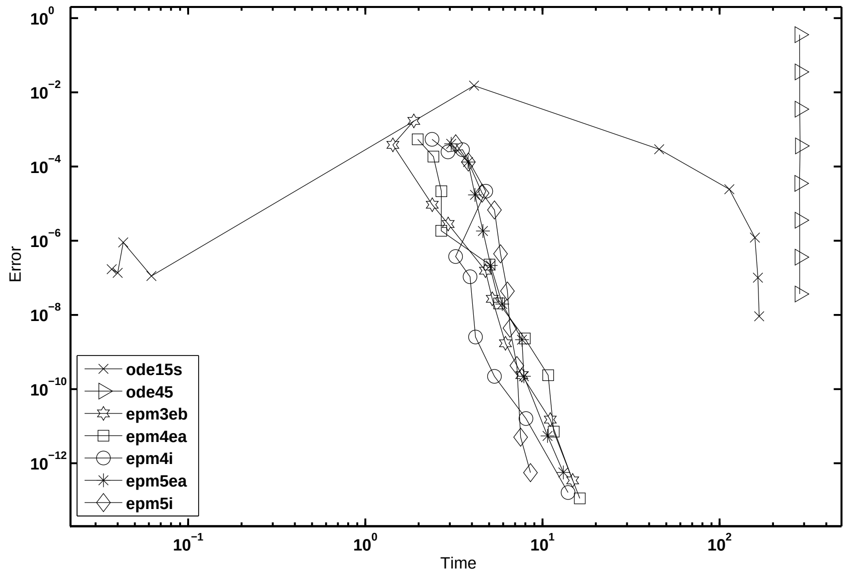

Figure 5: Results for the Schrödinger type equation

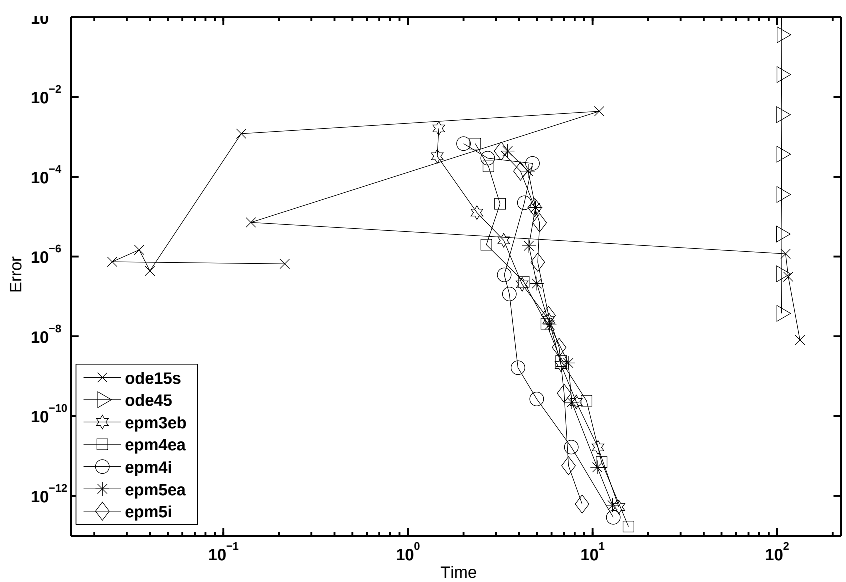

Figure 6: Results for the hyperbolic test equation

most efficient code for the nonstiff Gray-Scott problem, for Allen-Cahn and Kuramoto-Sivashinski ode15s is superior. The exponential peer methods seem to be the method of choice if the Jacobian has eigenvalues with large imaginary part. Here they are more efficient than the classical codes, especially for sharper tolerances.

The computing time of the exponential peer methods is in general determined by the computation of the φ-functions, which require a large number of squaring for problems with a large norm of the Jacobian. Here the strategy of trying to keep the step size constant pays off. The situation may change for large scale problems where Krylov methods are used to approximate products of φ-functions times a vector. This will be the topic of future research.

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