Martin–Luther–Universität
Halle–Wittenberg
Institut für Mathematik

Exponential Peer Methods

R. Weiner and T. El Azab

Report No. 14 (2009)

Editors:
Professors of the Institute for Mathematics, Martin-Luther-University Halle-Wittenberg.

Electronic version: see `http://www2.mathematik.uni-halle.de/institut/reports/`

Exponential Peer Methods

R. Weiner and T. El Azab

Report No. 14 (2009)

Prof. Dr. Rüdiger Weiner
Tamer El Azab
Martin-Luther-Universität Halle-Wittenberg
Naturwissenschaftliche Fakultät III
Institut für Mathematik
Theodor-Lieser-Str. 5
D-06120 Halle/Saale, Germany
Email: rüdiger.weiner@mathematik.uni-halle.de
Email: tamer.el-azab@mathematik.uni-halle.de

Exponential Peer Methods

Rüdiger Weiner*and Tamer El-Azab †

Abstract

We present a new class of exponential integrators, *exponential peer methods*, for the solution of stiff differential systems. Order conditions are derived. For a special class of methods of order $p = s - 1$, s the number of stages, we show optimal zero stability and prove that for a wide class of stiff systems the methods are of order $p \geq s - 1$. Numerical tests and comparison with exponential integrators of the Expint package are given. The numerical tests confirm the theoretical results, no order reduction is observed.

Keywords: Exponential integrators, peer methods, Expint.

1 Introduction

In the past few years exponential integrators have attracted a lot of interest. 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) and a nonlinear (nonstiff) part. Exponential integrators can be considered as numerical methods which involve exponential functions (or related functions) of the Jacobian or an approximation to it [2]. A historical survey is given by Minchev and Wright [6]. Recently exponential Rosenbrock-type methods were considered by Hochbruck et al. [4], exponential general linear methods have been studied by Ostermann et al. [8].

In this paper we present a new class of exponential integrators, exponential peer methods (EPM). Linearly-implicit peer methods have been studied e.g. in [9], [10], [11]. They are characterized by a high stage order what makes them attractive for very stiff systems. Exponential peer methods are based on explicit peer methods, which were introduced by Weiner et al. [13], [14].

The outline of this paper is as follow: In Section 2 we will define the new methods.

In Section 3 we investigate consistency and zero stability of the methods. We formulate simplifying conditions which guarantee order $p = s - 1$, where s is the number of stages.

*Institut für Mathematik, Martin-Luther-Universität Halle-Wittenberg, Postfach, 06099 Halle, Germany. E-mail: weiner@mathematik.uni-halle.de

†Institut für Mathematik, Martin-Luther-Universität Halle-Wittenberg, Postfach, 06099 Halle, Germany. E-mail: elazab@mathematik.uni-halle.de

For the nonstiff case the order is $p = s$. Due to the two step character of the methods zero stability has to be discussed.

In Section 4 we consider a special class of EPM of stiff order $p = s - 1$ with only 2 different arguments for the exponential functions. By a special choice of the nodes we obtain optimally zero stable methods. We show that the methods solve linear problems $y' = Ty$ exactly.

In Section 5 we present numerical results obtained using the framework of the Expint package by Berland et al. [1]. We compare the new methods with other exponential integrators implemented in Expint. The results confirm our theoretical results and show the potential of the new class of methods. Finally, we give some conclusions and an outlook for future work.

2 Exponential Peer Methods

We consider the initial value problem

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

$y(t) : \mathbb{R} \mapsto \mathbb{R}^n$ and $f : \mathbb{R} \times \mathbb{R}^n \mapsto \mathbb{R}^n$. For the formulation of exponential peer methods we assume as usual in exponential integrators a linearization of the form

$$\begin{aligned} \frac{dy}{dt} &= f(t, y) = Ty + g(t, y), \quad t \in [t_0, t_{end}] \\ y(t_0) &= y_0 \in \mathbb{R}^n. \end{aligned} \tag{2}$$

where $g(t, y) = f(t, y) - Ty$. Here $T \in \mathbb{R}^{n\times n}$ is an arbitrary matrix which should approximate the Jacobian f_y for stability reasons. In our tests with the Expint package [1] T is constant over the whole integration interval, in principle, however, T may change in every step.

We consider the following class of exponential peer methods

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

where we assume $\alpha_i \geq 0$ and the nodes c_i to be pairwise distinct. In this paper we will assume constant stepsizes. By setting $T = 0$ we obtain explicit peer methods, which have been proved to be very efficient for nonstiff systems [14]. The values $Y_{mi} \approx y(t_m + c_i h)$ have the same characteristics so we call them *'peer'* [11], $f_{m,j} = f(t_{mj}, Y_{mj})$, $t_{mj} = t_m + c_j h$.

The coefficients b_{ij} are constant, the matrix functions $A_{ij}\,(hT)$ and $R_{ij}\,(hT)$ are linear combinations of the well known φ-functions. These are defined as follows (e.g. [8]):

For integers $l \geq 0$ and complex numbers $z \in \mathbb{C}$, we define $\varphi_l(z)$ through

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

The φ-functions are related by the recurrence relation

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

Several methods have been proposed for evaluating these function [7]. We will use the Expint package relying on Padé approximations combined with scaling-and-squaring. For large dimensions, however, Krylov techniques will be advantageous, e.g. [3], [4], [12].

3 Consistency and convergence

In this section we will derive order conditions for EPM. We are interested in the application of exponential peer methods to stiff systems. We will assume that the stiffness is due to the linear part Ty. Therefore we want error estimates, which may depend on bounds of derivatives of the exact solution, but not on the norm of T. We assume that T has a bounded logarithmic matrix

$$\mu(T) \leq \omega. \tag{5}$$

If we use different matrices T in different steps, then we will assume (5) for all steps. If the system (2) comes from semidiscretization of parabolic equations then this condition is usually satisfied. Assumption (5) implies

$$\|\varphi_0(hT)\| = \|e^{hT}\| \leq e^{\omega h}, \tag{6}$$

see e.g. [5]. A further consequence is, that $\|\varphi_l(hT)\|$ and $\|hT\varphi_l(hT)\|$ are uniformly bounded. Furthermore, we will assume that the Lipschitz constant of $g(t, y)$ is of moderate size.

We insert the exact solution $y(t_m + c_i h)$ into the numerical method and drop the argument hT of the matrix functions to simplify the presentation. Then by Taylor expansion at t_m, assuming that the righthand side is sufficiently differentiable, we obtain for the local residual errors

$$\begin{aligned}\Delta_{m,i} = \sum_{l=0} \Bigg\{ & c_i^l I - \varphi_0 \sum_{j=1}^{s} b_{ij} (c_j - 1)^l - l \sum_{j=1}^{s} A_{ij} (c_j - 1)^{l-1} - l \sum_{j=1}^{i-1} R_{ij} c_j^{l-1} \\ & + hT \sum_{j=1}^{s} A_{ij} (c_j - 1)^l + hT \sum_{j=1}^{i-1} R_{ij} c_j^l \Bigg\} \frac{h^l}{l!} y^{(l)}(t_m).\end{aligned} \tag{7}$$

Definition 1 *The exponential peer method* (3) *is consistent of order* p *if*

$$\Delta_{m,i} = \mathcal{O}(h^{p+1}) \quad \textit{for all } 1 \leq i \leq s.$$

Note, that for peer methods 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 condition*

$$\sum_{j=1}^{s} b_{ij}(c_j-1)^l=(c_i-\alpha_i)^l,\quad l=0,1,...,q, \tag{8}$$

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

Proof. From (7), for the equation $y'=Ty$ the local residual errors will be

$$\Delta_{m,i}=\sum_{l=0}\left\{c_i^l I-\varphi_0\sum_{j=1}^{s} b_{ij}\,(c_j-1)^l\right\}\frac{h^l}{l!}y^{(l)}(t_m),\qquad y^{(l)}(t_m)=T^l y(t_m).$$

With $\varphi_0(\alpha_i hT)=\sum_{k=0}\frac{\alpha_i^k h^k}{k!}T^k$ and comparison of the coefficients of $T^r y(t_m)$ we get the condition

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

With (8) the right hand side is just

$$\begin{aligned}\sum_{j=1}^{s} b_{ij}\sum_{l=0}^{r}\binom{r}{l}(c_j-1)^l\alpha_i^{r-l} &= \sum_{l=0}^{r}\binom{r}{l}\alpha_i^{r-l}\sum_{j=1}^{s} b_{ij}(c_j-1)^l\\ &=\sum_{l=0}^{r}\binom{r}{l}\alpha_i^{r-l}(c_i-\alpha_i)^l=c_i^r.\end{aligned}$$

The method is therefore of order $p=q$. ■

Corollary 1 *Let*

$$B=V_\alpha V_1^{-1}. \tag{10}$$

where

$$c=\begin{pmatrix}c_1\\ \vdots\\ c_s\end{pmatrix},\quad \alpha=\begin{pmatrix}\alpha_1\\ \vdots\\ \alpha_s\end{pmatrix},\quad V_\alpha=\left(\mathbb{1},\ \ c-\alpha,\ \ \ldots,\ \ (c-\alpha)^{s-1}\right),\quad \mathbb{1}=\begin{pmatrix}1\\ \vdots\\ 1\end{pmatrix}.$$

Then the exponential peer method has 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*

$$\sum_{j=1}^{s} b_{ij}(c_j - 1 + \alpha_i)^r = \alpha_i^r = c_i^r.$$

Therefore (8) is satisfied for all r, the exponential peer method solves the system $y' = Ty$ with exact starting values exactly.

Proof. By (3), we have

$$\begin{aligned} Y_{1i} &= e^{\alpha_i hT} \sum_{j=1}^{s} b_{ij} Y_{0j} = e^{\alpha_i hT} Y_{0s} \\ &= e^{\alpha_i hT} e^{hT} y(t_0) = e^{(1+c_i)hT} y(t_0), \end{aligned}$$

i.e. Y_{1i} is exact. ■

The coefficients b_{ij} are determined by Theorem 1 for given α and c . Using these order conditions we now will consider the general case (2) to obtain conditions for the matrix coefficients $A_{ij}(hT)$ and $R_{ij}(hT)$.

Theorem 2 *Let the conditions (8) be satisfied for $l = 0, ..., q$. Let further*

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

for $r = 0, ..., q$. Then the exponential peer method is at least of order $p = q$ for (2).

Proof. From (7), we get for the coefficient of $\frac{h^r}{r!} y^{(r)}(t_m)$:

$$\begin{aligned} c_i^r I - \varphi_0 \sum_{j=1}^{s} b_{ij}(c_j - 1)^r - r \sum_{j=1}^{s} A_{ij}(c_j - 1)^{r-1} + hT \sum_{j=1}^{s} A_{ij}(c_j - 1)^r \\ - r \sum_{j=1}^{i-1} R_{ij} c_j^{r-1} + hT \sum_{j=1}^{i-1} R_{ij} c_j^r \end{aligned} \tag{12}$$

This coefficient should be equal to zero. We will prove this by induction.
Let $r = 0$. With (10) and (11) we have

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

Let the statement be correct up to $r - 1$. Then for r holds

$$c_i^r I - \varphi_0 \sum_{j=1}^{s} b_{ij}(c_j - 1)^r - r \sum_{j=1}^{s} A_{ij}(c_j - 1)^{r-1} + hT \sum_{j=1}^{s} A_{ij}(c_j - 1)^r$$

$$
\begin{aligned}
&- r\sum_{j=1}^{i-1} R_{ij}c_j^{r-1} + hT\sum_{j=1}^{i-1} R_{ij}c_j^r \\
=&c_i^r I - \varphi_0(c_i-\alpha_i)^r - r\sum_{l=0}^{r-1}\alpha_i^{l+1}\binom{r-1}{l}(c_i-\alpha_i)^{r-1-l}l!\varphi_{l+1} \\
&+ hT\sum_{l=0}^{r}\alpha_i^{l+1}\binom{r}{l}(c_i-\alpha_i)^{r-l}l!\varphi_{l+1} \\
=&c_i^r I - \varphi_0(c_i-\alpha_i)^r - r\sum_{l=1}^{r}\alpha_i^{l}\binom{r-1}{l-1}(c_i-\alpha_i)^{r-l}(l-1)!\varphi_{l} \\
&+ \sum_{l=0}^{r}\alpha_i^{l}\binom{r}{l}(c_i-\alpha_i)^{r-l}(l!\varphi_l - I) \\
=&c_i^r I - \varphi_0(c_i-\alpha_i)^r - \sum_{l=1}^{r}\alpha_i^{l}\binom{r}{l}(c_i-\alpha_i)^{r-l}l!\varphi_{l} \\
&+ \sum_{l=0}^{r}\alpha_i^{l}\binom{r}{l}(c_i-\alpha_i)^{r-l}l!\varphi_{l} - c_i^r I = 0. \qquad \blacksquare
\end{aligned}
$$

Corollary 3 *Let $\alpha = c$, $c_s = 1$ and $B = 1\!\!1 e_s^T$. Let*

$$\sum_{j=1}^{s} A_{ij}(c_j-1)^r + \sum_{j=1}^{i-1} R_{ij}c_j^r = r!\alpha_i^{r+1}\varphi_{r+1} \quad \text{for } r = 0, ..., q. \tag{13}$$

Then the exponential peer method is consistent of 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 (nonstiff case), then the order of the methods will be $p = q+1$,

Theorem 3 *Let the assumptions of Theorem 2 be satisfied. If in addition for the solution of (1), $y^{(l)}(t_m)$, $Ty^{(l)}(t_m)$ are bounded for all l, then the method is of order $p = q+1$.*

Proof. For the term with h^{q+1} in (7), we have

$$
\begin{aligned}
&\Bigg\{c_i^{q+1}I - \varphi_0\sum_{j=1}^{s} b_{ij}(c_j-1)^{q+1} - (q+1)\sum_{j=1}^{s} A_{ij}(c_j-1)^q - (q+1)\sum_{j=1}^{i-1} R_{ij}c_j^q \\
&+ hT\sum_{j=1}^{i-1} R_{ij}c_j^{q+1} + hT\sum_{j=1}^{s} A_{ij}(c_j-1)^{q+1}\Bigg\}\frac{h^{q+1}}{(q+1)!}y^{(q+1)}(t_m) \\
=&\left\{c_i^{q+1}I - \varphi_0(c_i-\alpha_i)^{q+1} - (q+1)\sum_{l=0}^{q} l!\alpha_i^{l+1}\binom{q}{l}(c_i-\alpha_i)^{q-l}\varphi_{l+1}\right\}\frac{h^{q+1}}{(q+1)!}y^{(q+1)}(t_m) + O\left(h^{q+2}\right)
\end{aligned}
$$

$$
\begin{aligned}
&=\left\{c_i^{q+1}I-\varphi_0\left(c_i-\alpha_i\right)^{q+1}-\sum_{l=1}^{q+1}l!\alpha_i^l\binom{q+1}{l}\left(c_i-\alpha_i\right)^{q+1-l}\varphi_l\right\}\frac{h^{q+1}}{(q+1)!}y^{(q+1)}\left(t_m\right)+O\left(h^{q+2}\right)\\
&=\left\{c_i^{q+1}I-\sum_{l=0}^{q+1}l!\alpha_i^l\binom{q+1}{l}\left(c_i-\alpha_i\right)^{q+1-l}\varphi_l\right\}\frac{h^{q+1}}{(q+1)!}y^{(q+1)}\left(t_m\right)+O\left(h^{q+2}\right)\\
&=\left\{c_i^{q+1}I-\sum_{l=0}^{q+1}\alpha_i^l\binom{q+1}{l}\left(c_i-\alpha_i\right)^{q+1-l}\right\}\frac{h^{q+1}}{(q+1)!}y^{(q+1)}\left(t_m\right)+O\left(h^{q+2}\right)\\
&=O\left(h^{q+2}\right). \qquad \blacksquare
\end{aligned}
$$

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

For the convergence of the method we need in addition zero-stability. Consider the linear test problem $y'=Ty$. By applying the EPM we obtain

$$
Y_m=M\left(z\right)Y_{m-1}=\left(M\left(z\right)\right)^m Y_0,\quad M\left(z\right)=\Phi(B\otimes I),\quad z=hT, \tag{14}
$$

where $\Phi=\mathrm{diag}(\varphi_0(\alpha_1 hT),...,\varphi_0(\alpha_s hT))$ and $Y_m=\left(Y_{mi}\right)_{i=1}^{s}$. $M\left(z\right)$ is the stability matrix of the method. For zero-stability we consider $z=0$.

Definition 2 *The exponential peer method* (3) *is zero-stable if the spectral radius of the stability matrix at $z=0$ is one (i.e. $\varrho(M\left(0\right))=1$) and all eigenvalues on the unit circle are simple.*

From (14) we have $M\left(0\right)=B$. Analogously to Adams methods we will consider methods where the matrix B has the eigenvalues

$$
\lambda_1=1,\qquad \lambda_2=\lambda_3=....=\lambda_s=0, \tag{15}
$$

i.e. the parasitic roots are zero, a property also shared by the exponential general linear methods of Ostermann et al. [8]. We call such methods optimally zero-stable. The nodes c_i are chosen such that $c_s=1$ and the other nodes satisfy $c_i<1, i=1,...,s-1$. Since the matrix B is constant, zero-stability implies that powers of B are uniformly bounded.

For convergence consider first the nonstiff case. Then for sufficiently small h we have

$$
\Phi=I+\mathcal{O}(h)
$$

for $h\to 0$. With our assumption on $g(t,y)$ follows by standard arguments (e.g. [14])

Theorem 4 *Let the exponential peer method be consistent of order p and zero-stable. Let for the starting values hold $Y_{0i}-y(t_0+c_i h)=\mathcal{O}(h^p)$. Then the method is convergent of order p.* $\square$

Note that here the $\mathcal{O}(h)$-terms may depend on $\|T\|$. For special methods this can be avoided.

Theorem 5 *Let the exponential peer method be consistent of order p and zero-stable. Let for the starting values hold $Y_{0i} - y(t_0 + c_i h) = \mathcal{O}(h^p)$. Let $b_{ij} \geq 0$ for all $1 \leq i, j \leq s$. Then the method is convergent of stiff order p.*

Proof. For the global error

$$\varepsilon_{mi} = y(t_{mi}) - Y_{mi}$$

holds

$$\varepsilon_{mi} = \varphi_0(\alpha_i hT) \sum_{j=1}^{s} b_{ij} \varepsilon_{m-1,j} + h \sum_{j=1}^{s} A_{ij}(g(t_{m-1,j}, y(t_{m-1,j})) - g(t_{m-1,j}, Y_{m-1,j})$$
$$+ h \sum_{j=1}^{i-1} R_{ij}(g(t_{mj}, y(t_{mj})) - g(t_{mj}, Y_{mj})) + \Delta_{m,i}$$

From (8) we have for $l = 0$ the relation $\sum_{j=1}^{s} b_{ij} = 1$. With the assumptions on b_{ij} and on g for $\|\varepsilon_m\| = \max_i \|\varepsilon_{mi}\|$, (6) then follows

$$\|\varepsilon_m\| \leq (1 + C_\alpha h)\|\varepsilon_{m-1}\| + h(C_A L_g \|\varepsilon_{m-1}\| + C_R L_g \|\varepsilon_m\|) + Ch^{p+1}.$$

Here the constants are independent on $\|T\|$. The order of convergence p follows by standard arguments. ■

4 A special class of methods

In our numerical tests we will use the framework of Expint. Although there exist relations between φ-functions of special arguments, it seems to be advantageous to have the number of different arguments as small as possible. In this section we will therefore consider a special class with only two different values of α_i:

$$\alpha = \begin{pmatrix} \alpha^* \\ \vdots \\ \alpha^* \\ 1 \end{pmatrix}, \quad c_i = (s - i)(\alpha_i - 1) + 1. \tag{16}$$

Furthermore we will always assume that B is defined by (10). By Corollary 1 the conditions (8) are fulfilled up to $s - 1$. For this choice we immediately obtain

Theorem 6 *For*

$$\frac{s-2}{s-1} \leq \alpha^* < 1$$

the nodes c_i are distinct and satisfy $0 \leq c_i \leq 1$ with $c_s = 1$. Due to $B = V_\alpha V_1^{-1}$ the exponential peer methods are of order $p \geq s - 1$ for $y' = Ty$.

With (10) and (16) the methods are also optimally zero stable.

Theorem 7 *The methods defined by* (10), (16) *are optimally zero-stable, the matrix B is given by*

$$B = \begin{pmatrix} 0 & 1 & 0 & \dots & 0 & 0 \\ 0 & 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & \ddots & 0 \\ 0 & 0 & 0 & \dots & 0 & 1 \\ 0 & 0 & 0 & \dots & 0 & 1 \end{pmatrix}. \tag{17}$$

Proof. (17) is equivalent to

$$BV_1 = \begin{pmatrix} 1 & c_2 - 1 & \dots & (c_2 - 1)^{s-1} \\ \vdots & \vdots & & \vdots \\ 1 & c_{s-1} - 1 & \dots & (c_{s-1} - 1)^{s-1} \\ 1 & 0 & \dots & 0 \\ 1 & 0 & \dots & 0 \end{pmatrix}$$

This is equal to V_α iff

$$\begin{aligned} c_{s-1} &= \alpha_{s-1} \\ c_{i+1} - 1 &= c_i - \alpha_i, \quad i = 1, ..., s-1. \end{aligned} \tag{18}$$

Inserting (16) immediately proves the statement. ■

Exponential integrators are designed to solve the linear system $y' = Ty$ exactly. However, due to their two-step character this is not trivial for peer methods. For the choice $\alpha = c$ this was proved in Corollary 2. Here we will prove this property also for the choice (16).

Theorem 8 *Let the starting values Y_{0i} be exact. Then $Y_{1i} = e^{(1+c_i)hT}y(t_0)$, i.e. the exact solution of $y' = Ty$.*

Proof. By (3) we have

$$Y_{1i} = e^{\alpha_i hT} \sum_{j=1}^{s} b_{ij} Y_{0j} = e^{\alpha_i hT} \sum_{j=1}^{s} b_{ij} e^{c_j hT} y(t_0)$$

Due to the structure of B for $i = 1, ..., s-1$ this simplifies to

$$\begin{aligned} Y_{1i} &= e^{(c_{i+1}h + \alpha_i h)T} y(t_0) \\ &= e^{(c_i h + h)T} y(t_0) \quad \text{(by (18))} \\ &= e^{(1+c_i)hT} y(t_0), \end{aligned}$$

i.e. Y_{1i} is exact. For the last stage we have

$$Y_{1s} = e^{hT} Y_{0s} = e^{hT} e^{hT} y(t_0) = e^{2hT} y(t_0). \qquad ■$$

The matrix coefficients A and R can be computed by solving the system of algebraic equations (11) for $r = 0, ..., s-1$ using Maple. We have done this for $s = 3, 4, 5, 6, 7$. The corresponding methods are called epm3 – epm7. By Theorem 2 the methods are of order and stage order $p \geq s-1$. There are free parameters when solving (11), which we set to zero for simplicity to obtain an upper triangular matrix A and a strictly lower triangular matrix R. However, this may be not the best choice. For instance it is possible to set $R = 0$ and to obtain parallel methods. As example we present the coefficients of epm4.

Example 1 *Method epm4 with 4 stages of order* $p \geq 3$*:*

$$\alpha = \left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}, 1\right]^T, \quad C = \left[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}, 1\right]^T, \quad B = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$A = \begin{pmatrix} A_{11} & A_{12} & A_{13} & A_{14} \\ 0 & A_{11} & A_{12} & A_{13} \\ 0 & 0 & A_{11} & A_{12} \\ 0 & 0 & 0 & A_{44} \end{pmatrix}, R = \begin{pmatrix} 0 & 0 & 0 & 0 \\ A_{14} & 0 & 0 & 0 \\ A_{13} & A_{14} & 0 & 0 \\ R_{41} & R_{42} & R_{43} & 0 \end{pmatrix}$$

where

$$\begin{aligned} A_{11} &= \frac{3}{4}\phi_2 + \frac{27}{4}\phi_3 - \frac{81}{4}\phi_4, & A_{12} &= \frac{3}{4}\phi_1 - \frac{9}{8}\phi_2 - \frac{27}{2}\phi_3 + \frac{243}{4}\phi_4, \\ A_{13} &= \frac{9}{4}\phi_2 + \frac{27}{4}\phi_3 - \frac{243}{4}\phi_4, & A_{14} &= -\frac{3}{8}\phi_2 + \frac{81}{4}\phi_4 \\ A_{44} &= \phi_1 - \frac{22}{3}\phi_2 + 32\phi_3 - 64\phi_4, & R_{41} &= 12\phi_2 - 80\phi_3 + 192\phi_4 \\ R_{42} &= -6\phi_2 + 64\phi_3 - 192\phi_4, & R_{43} &= \frac{4}{3}\phi_2 - 16\phi_3 + 64\phi_4. \end{aligned}$$

5 Numerical Tests

In this section we use the framework of Expint [1] to test our methods. We have put our methods in 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 stepsize. We compare our exponential peer methods with some of the exponential integrators included in Expint at these test problems. In our figures we will use the same names for the integrators and problems as in Expint, see [1] for references of problems and methods.

The s starting values for the exponential peer methods are computed with either Hochost4 (one of the integrators included in the package) or ode15s. To avoid computations with negative stepsizes we proceed as follows:

$$h_{peer} = \frac{t_{end} - t_0}{n_{steps} + 1 - c_1} \qquad h_{start} = (c_i - c_1)h_{peer}, \quad i = 1, ..., s.$$

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

$$error = \max_{i=1,\ldots,n} \frac{|Y_i - Y_{ref,i}|}{|Y_{ref,i}|},$$

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

In the following figures we present our test results. The dimension of the problems is denoted by ND. Figure 1 shows the results of the peer methods for the Gray-Scott problem. It

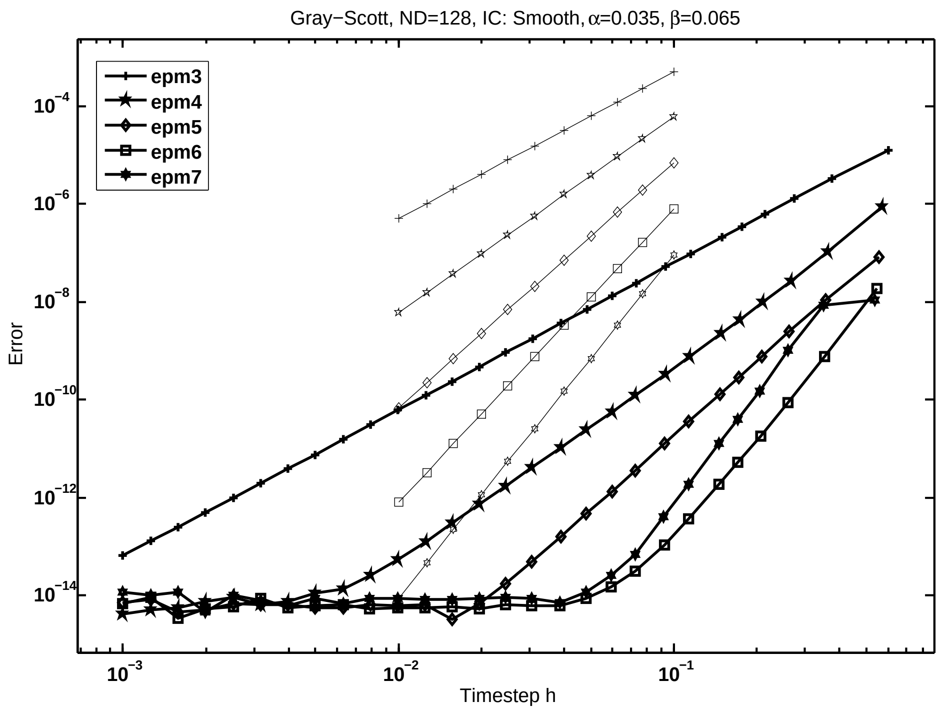

Figure 1: Exponential peer methods for Gray-Scott

confirms our theoretical order results for the peer methods. For comparison we included lines with slopes corresponding to 3–7 into the figure.

In Figures 2–8 we compare the 4- and 5-stage peer methods epm4 and epm5 with exponential integrators of the Expint package. The results show that the peer methods in general give very accurate results.

Some methods, e.g. lawson4, suffer from order reduction when applied to some test problems (see Fig. 6–8), but for peer methods no order reduction is observed. This is also the case for the peer methods of higher order, as illustrated in Figure 9, where we apply all methods to the parabolic test problem.

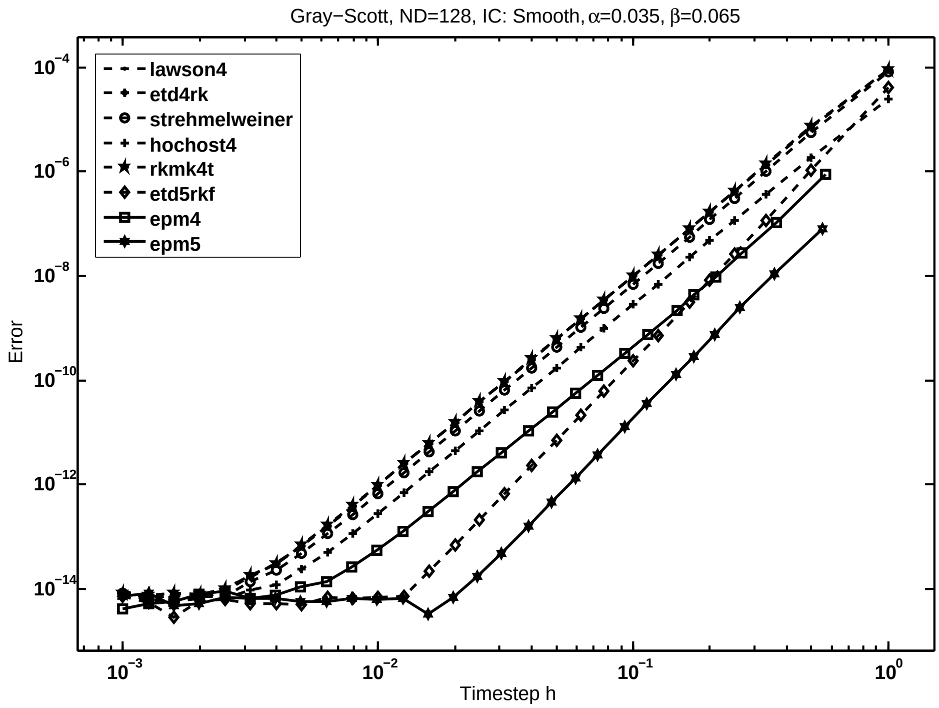

Figure 2: Results for Gray-Scott

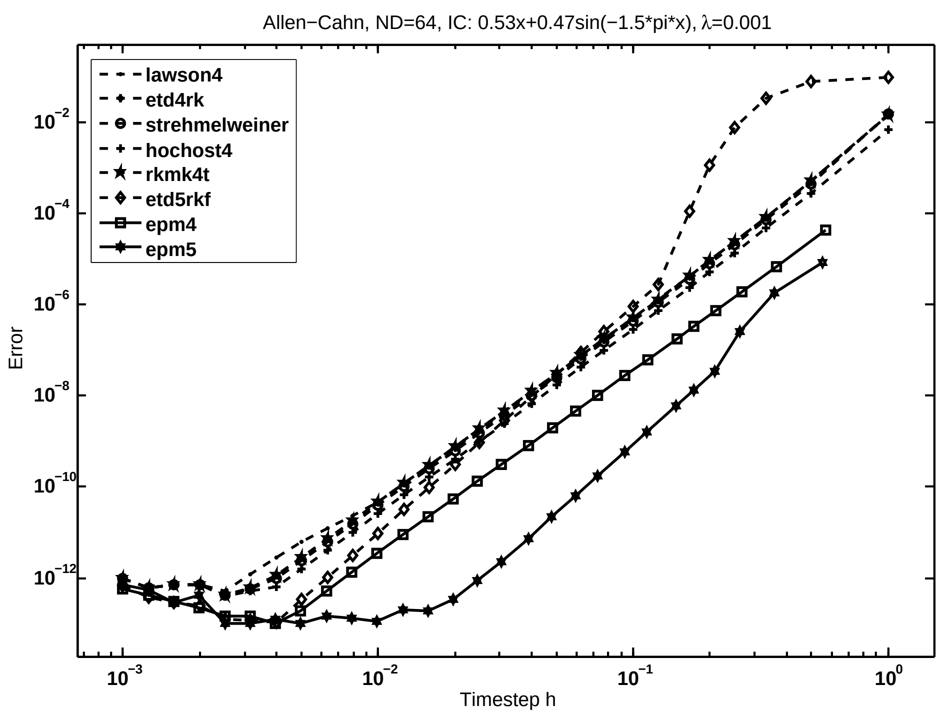

Figure 3: Results for the Allen-Cahn equation

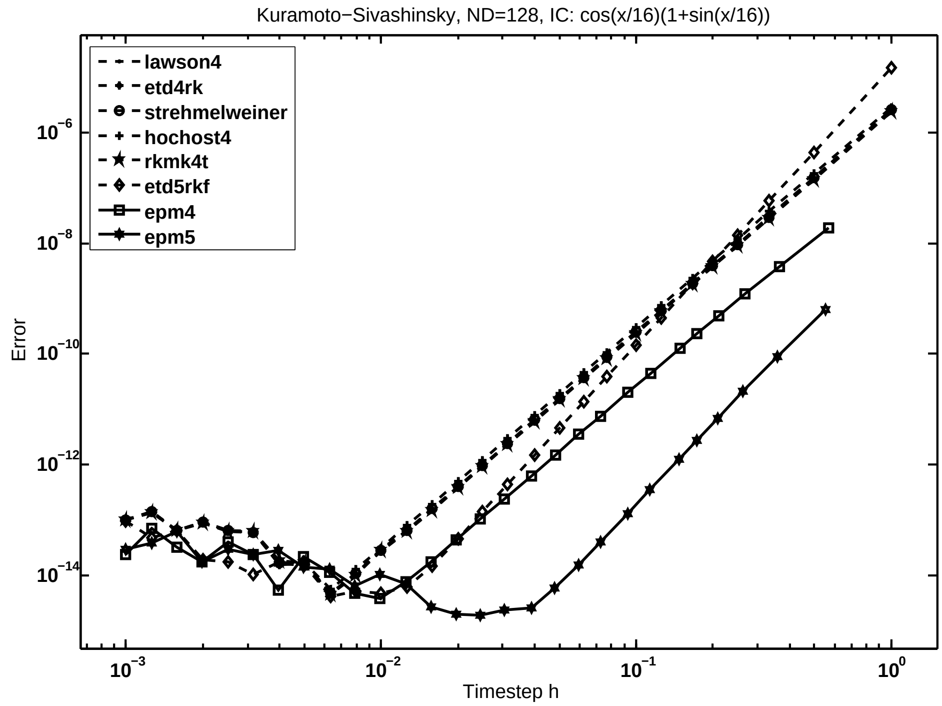

Figure 4: Results for the Kuramoto-Sivashinsky equation

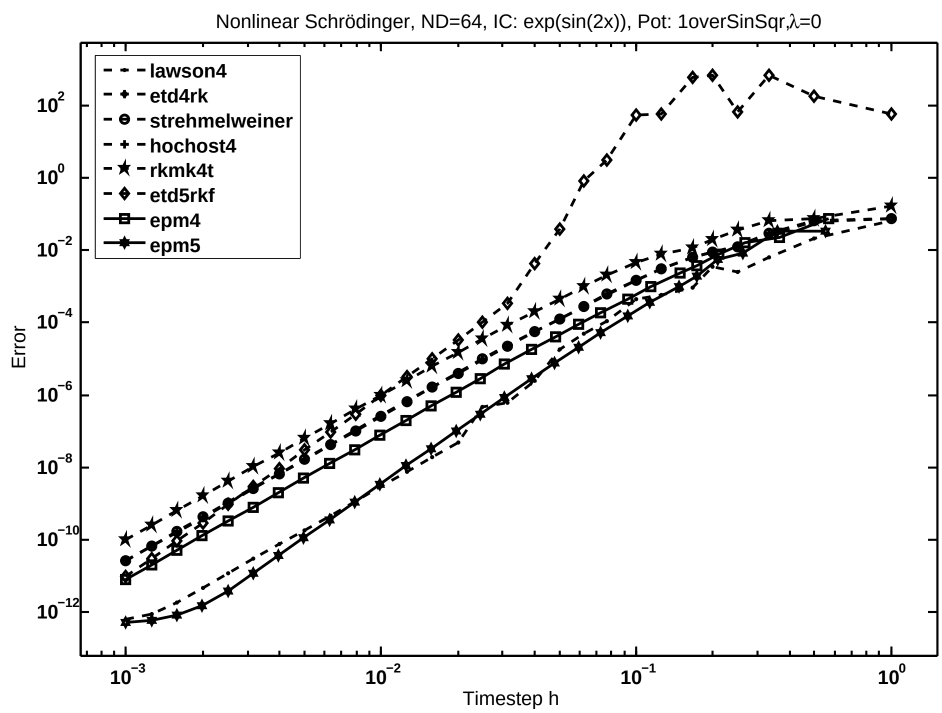

Figure 5: Results for the Nonlinear Schrödinger equation

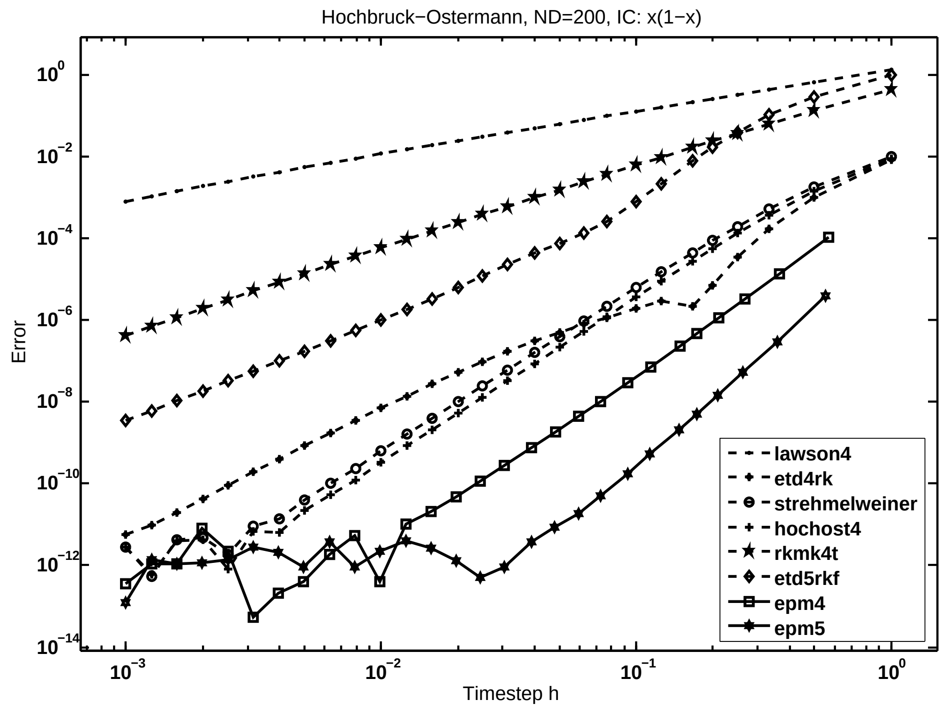

Figure 6: Results for the Hochbruck-Ostermann equation

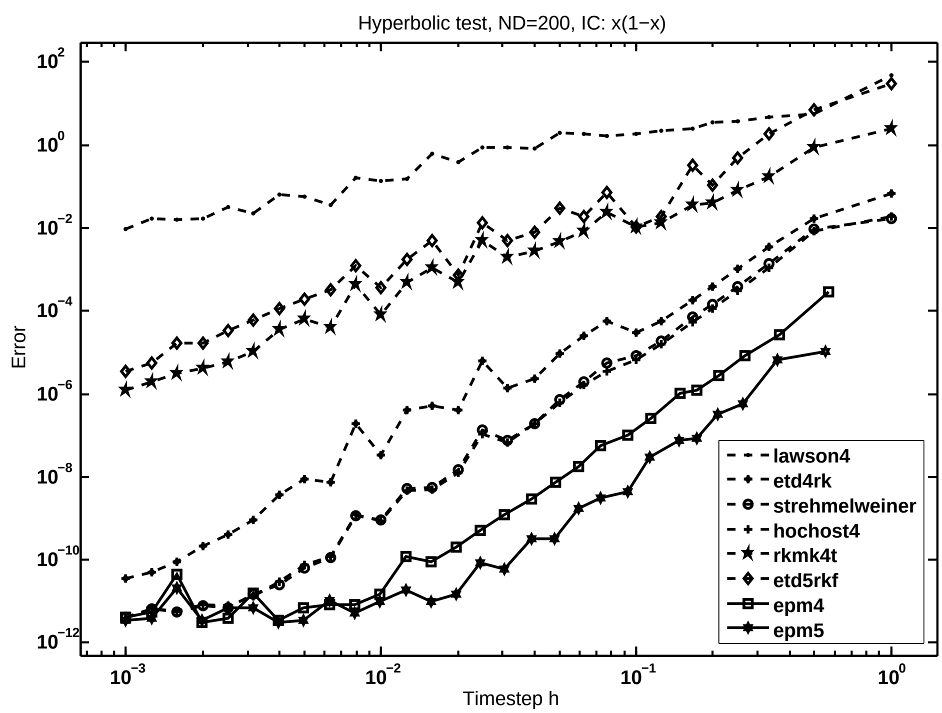

Figure 7: Results for the hyperbolic test equation

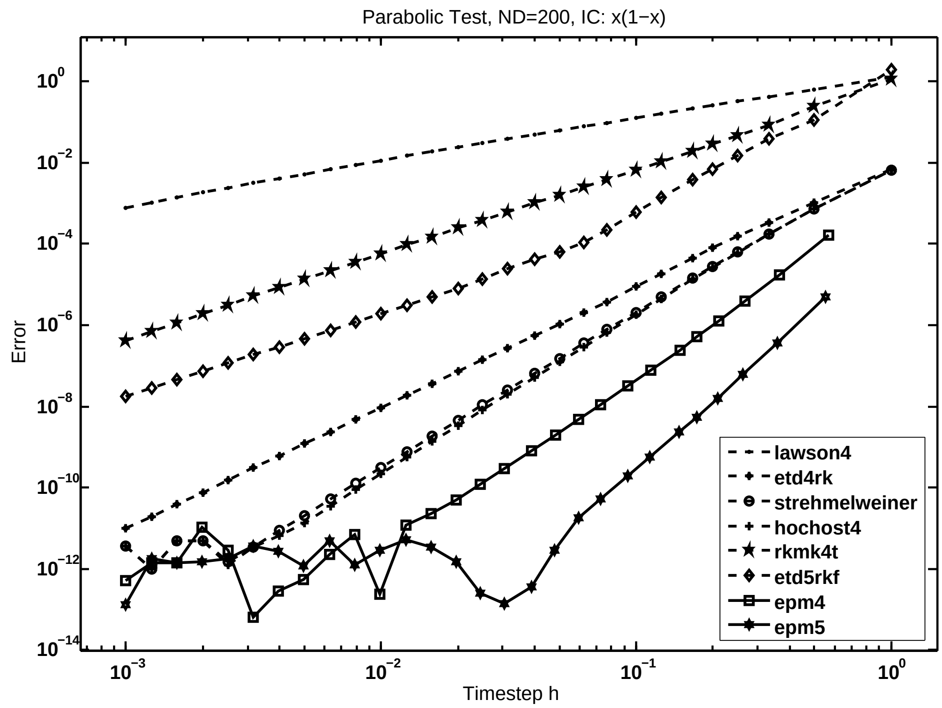

Figure 8: Results for the parabolic test equation

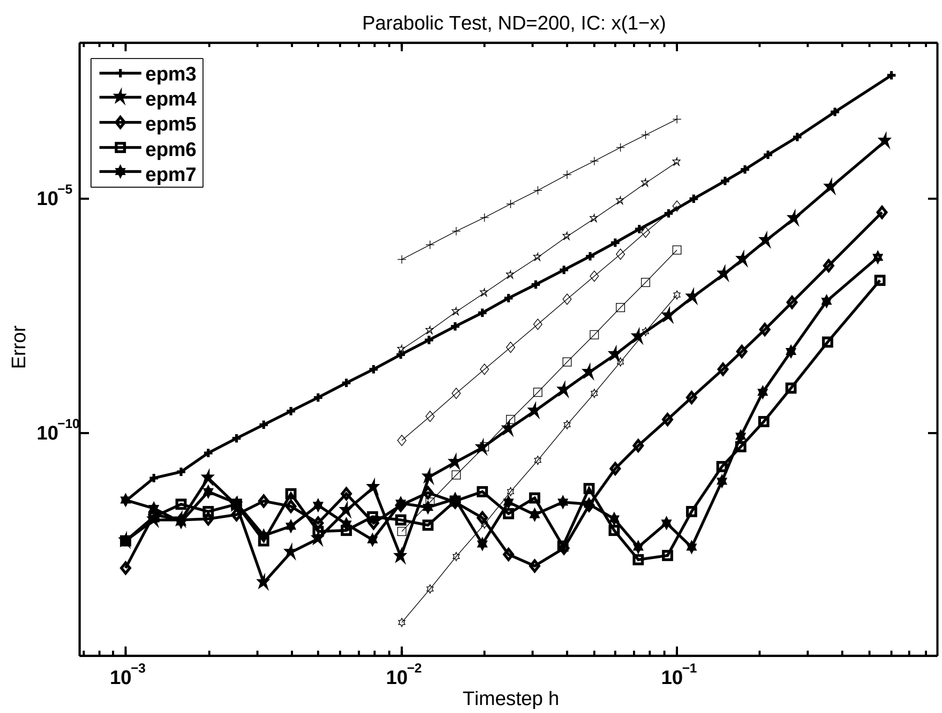

Figure 9: Results of exponential peer methods for the parabolic test problem

6 Conclusion

In this paper we have constructed and analyzed exponential peer methods with constant stepsize. We have presented a special class of methods which are optimally zero stable. We have derived order conditions, which allow to construct methods of arbitrary high order, in this paper we have considered methods up to 7 stages.

We have proved that for a wide class of stiff problems an s-stage method is of order and stage order $p \geq s-1$. These results are confirmed by our numerical tests.

The aim of the present work was to look if peer methods can be used successfully in exponential integrators. The results obtained in our numerical tests are promising. Of course this can be only a first step, for instance it is necessary to extend the methods for variable stepsizes. A further challenge is the application to higher dimensional problems using Krylov techniques for the computation of the φ-functions multiplied by a vector. This will be the topic of future work.

References

[1] H. Berland, B. Skaflestad, and W. Wright, *Expint—a matlab package for exponential integrators*, ACM Trans. Math. Softw. 33 (2007).

[2] M. Hochbruck, *Exponential integrators*, In: Workshop on Exponential Integrators, Innsbruck, October 20-23 (2004).

[3] M. Hochbruck, Ch. Lubich, and H. Selhofer, *Exponential integrators for large systems of differential equations*, SIAM J. Sci. Comput. 19, 1552–1574 (1998).

[4] M. Hochbruck, A. Ostermann, and J. Schweitzer, *Exponential Rosenbrock-type methods*, SIAM J. Numer. Anal. 47, 786–803 (2009).

[5] W. Hundsdorfer and J. Verwer, *Numerical Solution of Time-Dependent Advection-Diffusion-Reaction Equations*, Springer, 2003.

[6] B.V. Minchev and W.M. Wright, *A review of exponential integrators for first order semi-linear problems*, Technical Report, 2/05, Department of Mathematics, NTNU., April 2005.

[7] C. Moler and Ch. Van Loan, *Nineteen dubious ways to compute the exponential of a matrix, twenty-five years later*, SIAM Rev. 45(1):3–49 (2003).

[8] A. Ostermann, M. Thalhammer, and W.M. Wright, *A class of explicit exponential general linear methods*, BIT Numerical Mathematics 46, 409–431 (2006).

[9] H. Podhaisky, R. Weiner and B.A. Schmitt, *Rosenbrock-type 'Peer' two-step methods*, APNUM 53, 409–420 (2005).

[10] B.A. Schmitt, R. Weiner and K. Erdmann, *Implicit parallel peer methods for stiff initial value problems*, APNUM 53, 457–470 (2005)

[11] B.A. Schmitt and R. Weiner, *Parallel two-step w-methods with peer variables*, SIAM J. Numer. Anal. 42, 265282 (2004).

[12] R. Sidje, *EXPOKIT: Software package for computing matrix exponentials*, ACM Trans. on Math. Soft. 24, 130–156 (1998).

[13] R. Weiner, K. Biermann, B.A. Schmitt, and H. Podhaisky, *Explicit two-step peer methods*, Computers & Mathematics with Applications 55, 609–619 (2008)

[14] R. Weiner, B.A. Schmitt, H. Podhaisky and St. Jebens, *Superconvergent explicit two-step peer methods*, Journal of Computational and Applied Mathematics 223, 753–764 (2009).

Reports of the Institutes 2009

01-09. Jan Prüss, Vicente Vergara, Rico Zacher, *Well-Posedness and Long-Time Behaviour for the Non-Isothermal Cahn-Hilliard Equation with Memory*

02-09. Siegfried Carl, Patrick Winkert, *General comparison principle for variational-hemivariational inequalities*

03-09. Patrick Winkert, *$L^\infty-$Estimates for Nonlinear Elliptic Neumann Boundary Value Problems*

04-09. Wilma Di Palma, *John Neper's rods: Calculations are boring and tiring! Leon Battista Alberti's Cipher Wheel*

05-09. Stefan Sperlich, *An integration calculus for stochastic processes with stationary increments and spectral density with applications to parabolic Volterra equations*

06-09. Stefan Sperlich, *A Regularity Theory for Stochastic Processes with Stationary Increments and Spectral Density with Applications to Anomalous Diffusion*

07-09. Andreas Löhne, Thomas Riedrich, Christiane Tammer, *Festschrift zum 75. Geburtstag von Prof. Dr. Alfred Göpfert*

08-09. Sadaf Manzoor and Salahuddin, *Outliers in Uniform Distribution*

09-09. Gerd Steinebach, Rüdiger Weiner, *Peer methods for the one-dimensional shallow water equations with CWENO space discretization*

10-09. Jan Prüss, Gieri Simonett, *On the two-phase Navier-Stokes equations with surface tension*

11-09. Jan Prüss, Gieri Simonett, *Analytic solutions for the two-phase Navier-Stokes equations with surface tension and gravity*

12-09. Jan Prüss, Gieri Simonett, *On the Rayleigh-Taylor instability for the two-phase Navier-Stokes equations*

13-09. Matthias Köhne, Jan Prüss, Mathias Wilke, *On quasilinear parabolic evolution equations in weighted* L_p*-spaces*

Reports are available via WWW: http://www2.mathematik.uni-halle.de/institut/reports/