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Dedication

To
the memory of my father,
my mother, Mahira,
my sister, Nahed,
my brother, Mostafa,
my wife, Sally
and
my daughter, Marim.

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Abstract

The objectives of this thesis are to design, analyze and numerically investigate easily implementable Exponential Peer Methods (EPMs) for ordinary differential equations (ODEs), where the problem splits into a linear stiff and a nonlinear non-stiff part. The spatial discretization of time-dependent partial differential equations (PDEs) in general leads to such systems.

The thesis consists of two parts. The first part concerns EPMs with constant step size. The first aspect of this part involves an analytical investigation of consistency and zero stability of the methods. We formulate simplifying conditions which guarantee order $p = s-1$, where s is the number of stages. For the non-stiff case the order is $p = s$. A special class of EPMs with only two different arguments for the exponential functions is studied, and by a special choice of the nodes we obtain optimally zero-stable methods. We show that the methods solve linear problems $y' = Ty$ exactly. The second aspect is using the framework of EXPINT to perform a variety of numerical experiments to test the numerical order which confirm the theoretically obtained orders and no order reduction is observed.

The second part of the thesis is concerned with EPMs with variable step size. 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 $\varphi-$functions bounds for the step size ratio are given, which ensure zero-stability. These bounds are fairly large for practical computations. Various 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.

Zusammenfassung

Ziele dieser Arbeit sind die Konstruktion, Analyse und numerische Tests von Exponentiellen Peer-Methoden (EPMs) für gewöhnliche Differentialgleichungen, die einen steifen linearen und einen nichtsteifen nichtlinearen Anteil besitzen. Solche Systeme entstehen i. Allg. bei der Ortsdiskretisierung von zeitabhängigen partiellen Differentialgleichungen (PDEs).

Die Arbeit besteht aus zwei Teilen. Der erste Teil befasst sich mit EPMs mit konstanter Schrittweite. Er beinhaltet Untersuchungen der Konsistenz und Nullstabilität der Methoden. Wir formulieren vereinfachende Bedingungen, um Verfahren der Ordnung $p = s$ für nichtsteife und $p = s - 1$ für steife Probleme zu erhalten, wobei s die Anzahl der Stufen ist.

Eine spezielle Klasse von EPMs mit nur zwei unterschiedlichen Argumenten für die Exponentialfunktionen wird untersucht. Durch eine spezielle Wahl der Knoten erhalten wir optimal nullstabile Verfahren. Wir zeigen, dass die Methoden lineare Probleme $y' = Ty$ exakt lösen. Unter Verwendung des Programmsystems EXPINT werden die Methoden implementiert und eine Vielzahl von numerischen Experimenten durchgeführt. Die numerisch bestimmte Ordnung bestätigt die theoretisch gewonnenen Aussagen, es wird keine Ordnungsreduktion beobachtet.

Der zweite Teil der Arbeit ist EPMs mit variabler Schrittweite gewidmet. Bedingungen für die steife Ordnung p werden abgeleitet. Die Nullstabilität der Methoden wird untersucht. Für eine spezielle Unterklasse von Methoden mit nur zwei unterschiedlichen Argumente der $\varphi-$Funktionen werden Schranken für die Schrittweitenverhältnisse gegeben, die Nullstabilität garantieren. Diese Grenzen sind für praktische Rechnungen hinreichend groß. Verschiedene Strategien zur Fehlerschätzung und Schrittweitensteuerung werden betrachtet. Numerische Untersuchungen zeigen, dass die Schrittweitensteuerung zuverlässig funktioniert und dass für spezielle Problemklassen die Methoden klassischen Integratoren überlegen sind.

Contents

Abbreviations, Symbols, and Notation

BDF	**B**ackward **D**ifferentiation **F**ormula
EPM	**E**xponential **P**eer **M**ethod
IVP	**I**nitial **V**alue **P**roblem
ODE	**O**rdinary **D**ifferential **E**quation
PDE	**P**artial **D**ifferential **E**quation
$\mathbb{R}$	Space of real numbers
$\mathbb{C}$	Space of complex numbers
$\\|.\\|$	Norm
$\mu(.)$	Logarithmic Norm
$\varphi_0(A) = exp(A)$	The matrix exponential
$b_{ij}, A_{ij}, R_{ij}, \alpha_i, c_i$	Coefficients of $s-$stage EPMs (3.6) and (4.1)
B, A, R	Coefficients in matrix notation
T	Approximation to the Jacobian f_y
Δ_{mi}	The local residual errors (3.11)
V_1, V_α, S_m	Matrices in the consistency conditions
$h = h_{peer}$	Time step size for peer methods
h_{start}	Time step size for starting method
h_m, σ_m	Time step size, step size ratio $\sigma_m = \frac{h_m}{h_{m-1}}$ (4.2)
$M(z), \varrho(M(z))$	Stability matrix (3.19), spectral radius
$\mathbb{1}^T = (1, \dots, 1)$	Ones vector
$e_i^T = (\delta_{ij})_{j=1,\dots,s}$	i^{th} unit vector (i.e., vector which is zero everywhere except for the element i where it is one)
$X \otimes Y$	Kronecker product

List of Figures

Chapter 1

Introduction

Mathematical modeling of physical, chemical, and biological systems often leads to one or more ordinary differential equations (ODEs). In general, it is extremely difficult, if not impossible, to get an analytic solution for ODEs, so these equations are usually solved numerically by powerful numerical techniques on fast computers. In particular, the numerical solution of initial value problems (IVPs) for ODEs has been, and is still being, one of the most active field of investigation in numerical analysis. Many of the obtained results for numerical integration of ordinary differential equations have been collected in several books, among which we quote [2, 4, 18, 19, 29, 33]. ODEs can be classified as stiff or non-stiff, and may be stiff for some parts of an interval and non-stiff for others. Stiff differential equations are of great practical importance. For instance, the semi-discretization of time-dependent partial differential equations (PDEs) in general leads to large stiff problems.

Over the years, there was a need to improve the properties of numerical solution. Specifically up to the early fifties, the concern about accuracy properties were considered as the most important for the solution. After that, stability requirements became focal, in particular in connection with the numerical solution of stiff problems.

Stiffness is one major problem associated with the numerical integration of differential equations. Stiffness may be due to the problems characterized by a Jacobian that possesses eigenvalues with large negative real parts. Problems that consist of highly oscillatory solutions with purely imaginary eigenvalues of large modulus also are highly demanding for numerical methods. Stiff systems are requiring the development of special integrators scheme, with increased requirements to the stability. Stiff and highly oscillatory ODE systems are those ODEs whose Jacobians have at least one eigenvalue with a very negative real part or very large imaginary part respectively.

For many years the numerical methods for solving PDEs have been studied. A great deal of the research focuses on the stability problem in the time integration of the systems of ODEs which result from the spatial discretization of PDEs. Numerical methods for solving systems of ordinary differential equations can be divided into two categories, stiff and non-stiff solvers.

For solving stiff ODEs, implicit methods are mandatory to be used, because of the weak stability properties of explicit methods. Approval codes for stiff problems are based on BDF methods (e.g., [21]), implicit Runge-Kutta methods (e.g., [20]), or linearly-implicit Runge-Kutta methods (e.g., [30]). On the other hand, implicit methods require the solution of a nonlinear system of equations, at each integration step, and this is a considerable computational task. In order to overcome this difficulty, some authors in recent years have proposed various alternatives, such as the use of the so called Runge-Kutta-Chebyshev methods (see e.g., [1, 50, 51]) with the aim of creating explicit integrators with extended stability domains [39].

Recently, exponential integrators have been introduced as an alternative to implicit methods for large and stiff or highly oscillatory differential equations. These integrators are based on the computation of the exponential function (or related functions) of the Jacobian or an approximation to it, inside the numerical method (see e.g., [22]).

Exponential integrators have attracted a lot of interest and have been developed rapidly in the past three decades. They have been applied successfully to numerical solutions of PDEs. 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 non-stiff part. Nowadays, they are some of the powerful tools as well as implicit methods, for numerical solutions of partial differential equations. Since the first paper about exponential integrators by Certaine [6], 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., [5, 36, 40].

To solve the stiff semi-linear time-dependent PDE of the form

$$\frac{\partial u}{\partial t} = \mathcal{T}u + \mathcal{G}(u,t), \tag{1.1}$$

where $u \in \mathbb{R}^d$, $\mathcal{T}$ is a linear differential operator (usually of second order) and $\mathcal{G}(u,t)$ is a nonlinear operator, we first discretize the spatial derivatives (the linear operator $\mathcal{T}$) of a PDE with a spatial derivative approximation method (e.g. Finite Difference Formulas and spectral method, Chebyshev polynomials and Fourier spectral methods) to turn the PDE into a system of ODEs

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

where $y = y(t)$, $y : \mathbb{R} \mapsto \mathbb{R}^N$, $g : \mathbb{R} \times \mathbb{R}^N \mapsto \mathbb{R}^N$, N is a discretization parameter equal to the number of spatial grid points. The matrix $T \in \mathbb{R}^{N \times N}$ has in general a large norm for large numbers of grid points. Therefore, the resulting ODE system is stiff.

Exponential integrators had been constructed to solve semi-linear problems of the form (1.2). The goal of the exponential integrators is to treat the linear term exactly and allow the remaining part of the integration to be integrated numerically using an explicit scheme. They have been introduced in the sixties of last century, but have not been considered in practical computations, since they involve the computation of matrix exponential functions. Using modern techniques, such functions can now be computed quite efficiently.

The main distinctive features of the exponential integrators are as follow:

1. If the linear part is vanished (i.e., $T = 0$) then the scheme reduces to a standard explicit scheme and

2. If the nonlinear part is vanished (i.e., $g(t, y(t)) = 0$) then the scheme reduces to the evaluation of the exponential function of the matrix T and reproduces the exact solution of the problem.

Since their introduction in the 1950's, cf. [8], numerical methods for stiff problems have been studied extensively, in particular during the last thirty years. Hundreds of papers, which deal with the construction of efficient integrators and with the theoretical analysis of such integrators have been published. The idea of exponential integrators has been successfully applied to various classes of differential equations. These classes of integrators had been abandoned for a long time due to their excessive computational expense. Recently, there has been a renewed interest in exponential integrators that have emerged as a viable alternative for dealing efficiently with stiffness of ODEs.

The central topic of this thesis is exponential peer methods (EPMs) as a tool for solving time-dependent partial differential equations. Exponential peer methods are based on explicit peer methods, which were introduced by Weiner et al. [52, 53]. The essential property of peer methods is the use of several stages per time step with same accuracy properties.

Exponential peer methods for the numerical integration of stiff ordinary differential equations offer good properties like a high classical order and high stage order and an excellent stability behavior. A subclass of EPMs allows the construction of high-order schemes that possess favorable stability properties (optimal zero-stable for constant step sizes and solves linear problems $y' = Ty$ exactly) and exhibit no order reduction when applied to very stiff problems.

The thesis is organized as follows. Chapter 2 is devoted to give a brief introduction to the concept of stiff problems, the phenomenon of numerical stiffness is explained, and to exponential integrators as alternative numerical methods developed to overcome the phenomenon of stiffness. Mathematical background material that we need later in the thesis is collected. In particular, we introduce Lipschitz condition and the logarithmic norm. Main effort in exponential integrators is the computation of exponential matrices. We restrict in this thesis to problems of not very high dimension and use the methods of the MATLAB package called EXPINT by Berland et al. [3] for the computation of the $\varphi-$functions. We describe EXPINT, which is used as a tool for testing and comparison of exponential integrators for constant step sizes, in particular the definition of some related function to exponential integrators called $\varphi-$function and their computations. For high dimensions the use of Krylov techniques will be necessary and more efficient, e.g., [23, 27, 45], but we will not consider this in this thesis.

Chapter 3 is devoted to give an overview about the derivation, analysis, implementation and evaluation of exponential peer methods for constant step sizes. Consistency and stability of the methods are investigated, and we formulate simplifying conditions which guarantee order $p = s - 1$, where s is the number of stages. For the non-stiff case the order is $p = s$. Due to the two-step character of the methods zero-stability has to be discussed. A special class of EPMs of stiff order $p = s - 1$ with only two different arguments for the exponential functions is studied, and by a special choice of the nodes we obtain optimally zero-stable methods. We show that the methods solve linear problems $y' = Ty$ exactly. Numerical order tests show the theoretically obtained orders.

A generalization for the methods presented in Chapter 3, for variable step sizes, is given in Chapter 4, and the idea of methods with an adaptive step size control is described. Most practical software for solving ODEs does not use a fixed time step but rather adjusts the time step during the integration process to try to achieve some specified error bound. Adaptive step size control is used to control the local errors of the numerical solution. For optimization purposes smoother step size controllers are wanted, such that the errors and step sizes also behave smoothly. Order conditions for the coefficients, which now will depend on the step size ratio, are derived. Due to the variable 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 $\varphi-$functions we prove stiff order $p = s - 1$. For this class we compute bounds on the step size ratio which guarantee zero-stability in the non-stiff case. These bounds are fairly large for practical computations. In the stiff case we show convergence of stiff order $p = s-1$ under mild restrictions of the step size sequence. 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 numerical results obtained using the framework of the EXPINT package for the new methods are reported and analyzed in Chapter 5 for constant and variable step sizes. In particular, for constant step sizes we compare EPMs with other exponential integrators implemented in EXPINT package and the results confirm our theoretical results and show the potential of the new class of exponential integrators.

For variable step sizes, the constructed methods are tested on problems of the EXPINT package and we compare EPMs with the results for the standard MATLAB routines `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. The most expensive part in EPMs is the computation of the $\varphi-$functions. Better numerical methods for this task will highly improve the performance of the methods.

Finally, in Chapter 6 we give conclusions and an outlook for future work.

Chapter 2

Exponential Integrators

Introduction

The main purposes of this chapter are threefold. Firstly, we point out the concept of stiffness of numerical solution of differential equations, which appears often in practical situations, and we summarize some definitions of stiffness. Secondly, a MATLAB package called EXPINT [3], which is designed as a tool for testing and comparison of exponential integrators, is introduced. The definition of some related functions to the exponential integrators called $\varphi-$functions with their computations are shown. Thirdly, a brief history of exponential integrators, which were introduced as an effective alternative to classical implicit methods for solving time-dependent differential equations of stiff or highly oscillatory differential equations, is given.

We start with the review of some mathematical background that is needed later in this thesis.

2.1 Initial value problem

We will consider in this thesis the numerical solution of the initial value problem for a system of ODEs of the form

$$\begin{aligned} \frac{dy}{dt} &= f(t, y(t)) = Ty + g(t, y), \quad t \in [t_0, t_{end}] \\ y(t_0) &= y_0 \in \mathbb{R}^n, \end{aligned} \tag{2.1}$$

where t is the independent variable which represents the time and the dependent variable $y(t)$ which constitute the solution of the problem. $y(t)$ is a vector valued function, i.e.,

$$y : \mathbb{R} \mapsto \mathbb{R}^n \quad \text{and} \quad f : [t_0, t_{end}] \times \mathbb{R}^n \mapsto \mathbb{R}^n.$$

We will always assume that $f : [t_0, t_{end}] \times \mathbb{R}^n \mapsto \mathbb{R}^n$ is well defined and sufficiently smooth, especially it satisfies a Lipschitz condition with respect to $y \in \mathbb{R}^n$ with Lipschitz constant L. These conditions are sufficient to guarantee the existence of a unique solution $y(t)$ of (2.1) in $[t_0, t_{end}]$ (Picard's Theorem).

Definition 2.1 (Lipschitz condition)**.** *The function $f : [t_0, t_{end}] \times \mathbb{R}^n \longrightarrow \mathbb{R}^n$ is said to satisfy a* Lipschitz condition *in its second variable if there exists a constant $L > 0$ such that for any two points (t, Y) and (t, Z) in the solution space $D = \{t_0 \leq t \leq t_{end},\, Y \in \mathbb{R}^n\}$ the relation*

$$\|f(t, Y) - f(t, Z)\| \leq L\|Y - Z\|,$$

holds for all $Y, Z \in \mathbb{R}^n$, $\|.\|$ is a norm in $\mathbb{R}^n$. The constant L is called a Lipschitz constant *for f.*

For stiff problems the concept of logarithmic matrix norm is of major importance,

Definition 2.2 (Logarithmic Norm [9])**.** *Let $A, I \in \mathbb{R}^{n\times n}$, where I is the identity matrix, and $h \in \mathbb{R}^+$ and $\|\cdot\|$ be any matrix norm subordinate to a vector norm. Then the associated logarithmic norm μ of A is defined as*

$$\mu(A) = \lim_{h \to 0^+} \frac{\|I + hA\| - 1}{h}.$$

The matrix norm $\|A\|$ is always positive if $A \neq 0$, but the logarithmic norm $\mu(A)$ may also take negative values, e.g., when A is negative definite. Therefore, the logarithmic norm does not satisfy the axioms of a norm.

Basic properties of the logarithmic norm of a matrix include [12]:

1. $\mu(A) \leq \|A\|$,
2. $\mu(\gamma A) = \gamma\, \mu(A)$ for scalar $\gamma > 0$,
3. $\mu(A + B) \leq \mu(A) + \mu(B)$,
4. $\|e^{tA}\| \leq e^{t\mu(A)}$ for $t \geq 0$,
5. $\mu(A) < 0 \Rightarrow \|A^{-1}\| \leq -1/\mu(A)$,
6. $\alpha(A) \leq \mu(A)$ where $\alpha(A)$ is the maximal real part of the eigenvalues of A.

The importance of the logarithmic norm comes from the following theorem [12]:

Theorem 2.1. *Let $\| \,.\, \|$ be a given norm. Let $\nu : [0, t_{end}] \longrightarrow \mathbb{R}$ be a piecewise continuous function satisfying*

$$\mu(f_\zeta(t, \zeta)) \leq \nu(t), \quad t \in [0, t_{end}], \quad \forall \zeta$$

Then for any two solutions Y and Z of (2.1)

$$\| Z(t_2) - Y(t_2) \| \leq \exp\left(\int_{t_1}^{t_2} \nu(\tau)\, d\tau\right) \| Z(t_1) - Y(t_1) \|,$$

for all t_1, t_2 satisfying $0 \leq t_1 \leq t_2 \leq t_{end}$. $\square$

The theorem shows that for $\mu < 0$ the system will be dissipative.

2.2 Stiff ODEs

Stiff problems are encountered in many fields of science and engineering, e.g., electrical circuits, chemical reaction kinetics, nuclear reactors, electrical networks and automatic control, biochemical systems and so on.

One major source of stiff differential equations is the semi-discretization of partial differential equations. These systems are often stiff and highly expensive to solve due to a huge number of components, in particular for multi-dimensional problems.

Numerical methods in use to solve (2.1) are classified either to explicit or implicit methods. Explicit integrators such as Runge-Kutta and linear multistep methods are usually used for integration of non-stiff problems since these methods are forced to take very small integration steps to maintain numerical stability and significantly the use of adaptive algorithms do not alleviate this problem, and implicit integrators, which require the solution of nonlinear algebraic systems of equations at each integration step, are preferred when ODEs are stiff.

Stiff differential equations and highly oscillatory differential equations seriously defy traditional numerical methods. In the last decade, considerable interest has been generated in the study of classes of numerical methods for partial differential equations, with particular emphasis on the stiffness property.

Despite the great progress which has been made in numerical methods so far, there are still many problems facing them and represent a serious challenge to them. Such problems do not require to be extensive or complex and some of them are very simple. Stiffness is one major problem associated with the numerical integration of differential equations.

C.F. Curtiss and J.O. Hirschfelder [8] were the first to use the term stiff. They attempt to give the first definition of stiff systems as: "stiff equations are equations where certain implicit methods perform better, than using classical explicit ones". They also proposed a numerical procedure to solve this type of ODEs which nowadays are known as backward differentiation formula (BDF).

Stiffness is one of the most ambiguous concepts until now widespread in the numerical solution of initial value ODEs. Some authors propose multiple criteria for stiffness, we summarize some of them:

Shampine and Gear [15, 44] : *By a stiff problem we mean one for which no solution component is unstable (no eigenvalue has a real part which is at all large and positive) and at least some component is very stable (at least one eigenvalue has a real part which is large and negative). Further, we will not call a problem stiff unless its solution is slowly varying with respect to the most negative real part of the eigenvalues. (Roughly, we mean that the derivatives of the solution are small compared to the corresponding derivatives of* e^{Ax}*). Consequently, a problem may be stiff for some intervals of the independent variable and not for others* . Also, *the initial value problem for ODEs is stiff if the Jacobian* $J_{i,j} = \frac{\partial f_i}{\partial y_j}$, $i, j = 1, \ldots, N$

has at least one eigenvalue, for which real part is negative with high modulus, while the solution within the major part of the interval of integration changes slowly.

Dahlquist [11]: *Systems containing very fast components as well as very slow components.*

Hairer and Wanner [19]: *Stiff equations are problems for which explicit methods don't work.*

Each of the previous concepts of stiffness reflects certain aspects of the numerical solution (e.g., impossibility of using explicit methods of integration, large Lipschitz constants or large norms of Jacobian matrices, big difference among eigenvalues of Jacobian matrix, etc.).

2.3 EXPINT package

EXPINT [3] is a MATLAB package designed as a tool to facilitate easy testing and comparison of various exponential integrators, like Runge-Kutta, multistep and general linear type methods. Berland, Skaflestad and Wright published this package with three aims : Firstly, to create a uniform environment which enables the comparison of various integrators; Secondly, to provide tools for easy visualization of numerical behavior; Thirdly, to be easily modified so that users can include problems and integrators of their own. EXPINT contains several semi-discretized PDEs as test problems such as the KdV, Kuramoto-Sivashinsky, Allen-Cahn and Grey-Scott equations and a collection of well-known exponential integrators implemented with constant step size. The most important part of the EXPINT package is the evaluation of the $\varphi-$functions.

Lawson [34] introduced scaling and squaring technique to compute the matrix exponential. In [37] various methods for the computation of the $\varphi-$functions are investigated. For problems of not too large dimensions Padé approximations combined with scaling and squaring has become the standard approach in numerical software like MATLAB for computing the matrix exponential. EXPINT package is relying on Padé approximations combined with scaling-and-squaring for the computation of $\varphi-$functions.

Fourier spectral methods [48, 49] are used for problems with spatially periodic boundary conditions to discretize the spatial derivatives of (1.1), and hence to obtain a stiff system (1.2) of coupled ODEs in time t. The resulting linear part

T of the system is represented by a diagonal matrix, and g represents the action of the nonlinear operator on y on the grid. On the other side for problems where the boundary conditions are not periodic, finite difference formulas [35, 48] or Chebyshev polynomials [48, 49] are used and in this case, the linearized system is represented by a non-diagonal matrix.

2.4 $\varphi-$functions

The most commonly related and associated functions with exponential integrators are $\varphi-$functions, which are defined as follows (e.g., [40]):

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

$$\begin{aligned} \varphi_0(z) &= e^z, \\ \varphi_\ell(z) &= \frac{1}{(\ell-1)!}\int_0^1 \mathrm{e}^{(1-\theta)z}\,\theta^{\ell-1}\,\mathrm{d}\theta, \qquad \ell \geq 1, \end{aligned} \tag{2.2}$$

and the explicit formula

$$\varphi_\ell(z) = \frac{1}{z^\ell}\Big(\mathrm{e}^z - \sum_{i=0}^{\ell-1}\frac{z^i}{i!}\Big).$$

The $\varphi-$functions are related by the recurrence relation

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

For small values of $\ell \neq 0$, with $z \neq 0$, (2.2) gives

$$\varphi_1(z) = \frac{\mathrm{e}^z-1}{z}, \quad \varphi_2(z) = \frac{\mathrm{e}^z-z-1}{z^2}, \quad \varphi_3(z) = \frac{\mathrm{e}^z-z^2/2-z-1}{z^3}.$$

The importance of the $\varphi-$functions comes from the following theorem.

Theorem 2.2. *The exact solution of the non-autonomous linear initial value problem*

$$y'(t) = T\,y(t) + \sum_{l=0}^{p} a_l(t-t_m)^l, \quad y(t_m) = y_m \tag{2.4}$$

is given by

$$y(t) = \varphi_0((t-t_m)\,T)\,y_m + \sum_{l=0}^{p} l!\varphi_{l+1}((t-t_m)T)\,a_l(t-t_m)^{l+1}.$$

Proof. The general solution of the linear differential equation is given by

$$y(t) = (\mu(t))^{-1}\,C + (\mu(t))^{-1}\sum_{l=0}^{p} a_l \int_{t_m}^{t} \mu(\tau)(\tau - t_m)^l \mathrm{d}\tau,$$

where $\mu(t) = \varphi_0(-t\,T)$ is the integrating factor for (2.4) and $C = \varphi_0(-t_m\,T)y_m$. Now for the integrated term with the substitution $\theta = (\tau - t_m)/(t-t_m)$,

$$\begin{aligned}
\int_{t_m}^{t} \mu(\tau)(\tau-t_m)^l d\tau &= \int_{t_m}^{t} \varphi_0(-\tau\,T)(\tau-t_m)^l\,d\tau \\
&= (t-t_m)^{l+1}\int_0^1 \varphi_0\Big(\Big((1-\theta)(t-t_m)-t\Big)\,T\Big)\,\theta^l\,\mathrm{d}\theta \\
&= (t-t_m)^{l+1}\varphi_0(-t\,T)\int_0^1 \varphi_0\Big((1-\theta)(t-t_m)\,T\Big)\,\theta^l\,\mathrm{d}\theta
\end{aligned}$$

and by (2.2) with $z = (t-t_m)\,T$

$$= (t-t_m)^{l+1}\varphi_0(-t\,T)l!\varphi_{l+1}((t-t_m)\,T).$$

So that, we have

$$y(t) = \varphi_0((t-t_m)\,T)\,y_m + \sum_{l=0}^{p} l!\varphi_{l+1}((t-t_m)T)\,a_l(t-t_m)^{l+1}. \qquad \blacksquare$$

2.5 Computation of $\varphi-$functions

The hard part of implementing exponential integrators is the evaluation of (linear combinations of) $\varphi-$functions. The accurate and reliable computation of the matrix exponential function is a long standing problem of numerical analysis. According to Minchev and Wright [36], the main computational challenge in the implementation of any exponential integrator is the need for fast and computationally stable evaluations of the exponential and related $\varphi-$functions.

The efficiency of exponential integrators strongly depends on the numerical linear algebra used to compute the approximations of the $\varphi-$function.

Several methods have been proposed for evaluating these functions [37].

In EXPINT package $\varphi-$functions for matrices of not too large dimensions are calculated using Padé approximations combined with scaling and squaring. In this case the norm of the arguments $z = hT$ is reduced firstly by scaling

$$\tilde{z} = z/2^{max(0,r+1)},$$

where r is the smallest integer number with $2^r \geq \| z \|_\infty$. Then $\varphi_\ell(\tilde{z})$ will be calculated using Padé approximation and taking the inverse transform.

The functions $\varphi_\ell(\tilde{z})$ are evaluated using diagonal $(d,d)-$Padé approximants,

$$\varphi_\ell(\tilde{z}) = \frac{N_d^\ell(\tilde{z})}{D_d^\ell(\tilde{z})} + \mathcal{O}(\tilde{z}^{2d+1}),$$

where the unique polynomials N_d^ℓ and D_d^ℓ are

$$\begin{aligned} N_d^\ell(\tilde{z}) &= \frac{d!}{(2d+\ell)!} \sum_{i=0}^{d} \left[\sum_{j=0}^{i} \frac{(2d+\ell-j)!(-1)^j}{j!(d-j)!(\ell+i-j)!} \right] \tilde{z}^i, \\ D_d^\ell(\tilde{z}) &= \frac{d!}{(2d+\ell)!} \sum_{i=0}^{d} \frac{(2d+\ell-i)!}{i!(d-i)!} (-\tilde{z})^i. \end{aligned}$$

For $\ell = 0$, these reduce to the well known diagonal Padé approximations of the exponential function $(\mathrm{e}^{\tilde{z}})$. In EXPINT $d = 6$ is used.

For small norms of $\tilde{z}$, the approximation of Padé approximation is very accurate and will be considered as exact function $\varphi_\ell(\tilde{z})$. To reverse the scaling for $\ell > 0$ is not trivial. It is done by using the relations [3]

$$\begin{aligned} \varphi_\ell(2z) &= \frac{1}{2^{2\ell}} \left[\varphi_\ell(z)\varphi_\ell(z) + \sum_{j=\ell+1}^{2\ell} \frac{2}{(2\ell-j)!} \varphi_j(z) \right], \\ \varphi_{2\ell+1}(2z) &= \frac{1}{2^{2\ell+1}} \left[\varphi_\ell(z)\varphi_{\ell+1}(z) + \sum_{j=\ell+2}^{2\ell+1} \frac{2}{(2\ell+1-j)!} \varphi_j(z) + \frac{1}{\ell!}\varphi_{\ell+1}(z) \right]. \end{aligned}$$

2.6 An overview on exponential integrators

Exponential integrators are a well-known class of numerical integration methods for stiff or highly oscillatory systems of ordinary differential equations, which involve exponential functions e^{hT} (or related functions), where T is the Jacobian of the right hand side f (or an approximation to it) and h is the step size. One advantage of exponential methods is that they usually have good stability properties, which make them suitable for solving stiff problems.

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 non-stiff part.

They require the evaluation of matrix functions $P(T)$ or matrix-vector products $P(T)b$, where T is a negative semi-definite matrix and P is the exponential function or one of the related "$\varphi-$functions".

For problems of moderate size these functions are computed with the methods of Section 2.4. For very large dimensions Krylov techniques for the computation of $P(T)b$ are more efficient and frequently used, cf. [23, 27, 45].

2.6.1 A brief history of exponential integrators

Although exponential integrators have a long history in numerical analysis, they did not play a prominent role in applications for quite a long time because they depend on explicit use of the exponential and related functions of (large) matrices. However, in recent years a wide range of results for this problem had been emerged, although of course much remains to be done.

The historical roots of exponential integrators are easy to identify. In 1967 Lawson [34] proposed the generalized Runge-Kutta processes. The novelty of his idea was to solve the linear part ($y'(t) = T\,y(t)$) of (2.1) exactly then making a change of variables, $v(t) = e^{(t_m - t)\,T}y(t)$ (also known as Lawson transformation).

By differentiation we get

$$v'(t) = e^{(t_m - t)\,T}g(t, e^{(t-t_m)\,T}v(t))$$

Apply a numerical method (e.g., Explicit Euler method) to the transformed equation

$$v_{m+1} = v_m + hg(t_m, v_m), \quad v_m = v(t_m)$$

Transform the approximate solution to the original variable with $v_m = y_m$ and $v_{m+1} = e^{(t_m - t_{m+1})\,T} y_{m+1}$

$$\begin{aligned} e^{(t_m - t_{m+1})\,T} y_{m+1} &= y_m + hg(t_m, y_m) \\ e^{-h\,T} y_{m+1} &= y_m + h\,g(t_m, y_m) \end{aligned}$$

Finally, we get Lawson-Euler method (see Example 2.1)

$$y_{m+1} = e^{h\,T} y_m + he^{h\,T} g(t_m, y_m).$$

These methods have been known later as Integrating Factor (IF) methods. The same result can be obtained by multiplying the original problem by the integrating factor $e^{(t_m - t)\,T} y(t)$, and the methods are represented many times with different names, e.g., Linearly Exact Runge-Kutta (LERK). The purpose of transforming the differential equation in this way is to remove the explicit dependence in the differential equation on the operator T, except inside the exponential. The exponential function will damp the behavior of T removing the stiffness or highly oscillatory nature of the problem. Generalized Integrating Factor (GIF) methods [32] were recently constructed by Krogstad as a means of overcoming some of the undesirable properties of the Lawson schemes. This class of schemes uses approximations of the nonlinear term from previous steps, resulting in an exponential general linear method.

It is more than half a century ago since the publication of the paper by Certaine [6] on exponential integrators who constructed the first exponential multistep methods, Exponential Time Differencing (ETD) methods.

IF and ETD methods treat the linear part exactly (and so are necessarily $A-$stable), but differ in the assumptions used when handling the nonlinear part. ETD is based on the variation of constants formula, which is the integral form of

$$(e^{(t_m - t)\,T}\, y(t))' = e^{(t_m - t)\,T}\, g(t, y(t))$$

Then

$$y(t_m + h) = e^{h\,T} y_m + e^{h\,T} \int_0^h e^{-\tau\,T}\, g(t_m + \tau, y(t_m + \tau))\,\mathrm{d}\tau$$

Various schemes can be obtained by approximating the integral with different quadrature formulas. The simplest method is obtained by approximating the nonlinearity g over one timestep by its value at the known point (t_m, y_m) and solving the rest of the integral explicitly. With the same notation as before the exponential Euler method (see Example 2.2) becomes

$$y_{m+1} = e^{hT} y_m + h\varphi_1(hT) g(t_m, y_m).$$

Certaine constructed two exponential integrators based on the Adams-Moulton methods of order two and three by finding approximations to the integral in the variation of constants formula, using an algebraic polynomial approximation to the nonlinear term. In 1969, Nørsett [38] constructed ETD based on Adams-Bashforth methods. ETD schemes based on Runge-Kutta schemes were independently discovered by several authors, e.g., [13, 46]. Calvo and Palencia [5] constructed and analyzed a related class of k-step methods, where the variation of constants formula is taken over an interval of length kh instead of h. In contrast to exponential Adams methods, their methods have all parasitic roots on the unit circle. In 2002, Cox and Matthews [7] derived ETDRK methods as a class of ETD methods based on the Runge-Kutta time stepping. ETDRK4 suffers from numerical instability when T has eigenvalues close to zero. Kassam and Trefethen [31] modified the ETDRK4 method and studied their instabilities and have found that they can be removed by evaluating a certain integral on a contour that is separated from zero.

In 1999, Munthe-Kaas [17] used the affine Lie group to solve semi-linear problems using Lie group schemes. Unfortunately, the RKMK schemes were shown to exhibit instabilities due to the use of commutators [3].

Recently, exponential Rosenbrock-type methods were considered by Hochbruck et al. [27], and a class of explicit exponential general linear methods has been studied by Ostermann et al. [40].

A historical survey is given by Minchev and Wright [36], an actual survey on exponential integrators can be found in Hochbruck and Ostermann [26].

2.6.2 Exponential Runge-Kuta methods

For an $s-$stage exponential integrator of Runge-Kutta type for (1.2), we define the internal stages and output approximation [3]:

$$\begin{aligned} Y_i &= h \sum_{j=1}^{s} a_{ij}(hT)\, g(t_{n-1} + c_j h, Y_j) + u_{i1}(hT)\, y_{n-1}, \quad i = 1, \ldots, s, \\ y_n &= h \sum_{i=1}^{s} b_i(hT)\, g(t_{n-1} + c_i h, Y_i) + v_1(hT)\, y_{n-1}, \end{aligned} \tag{2.5}$$

where $g(t, y) = f(t, y) - T\, y$. This method is $A-$ and $L-$stable, because it gives the exact solution of linear problem $y'(t) = T\, y(t)$ with the exact starting values. By setting $T = 0$ we obtain an explicit Runge-Kutta method with the coefficients

$$u_{i1}(0) = 1, \quad a_{ij}(0) = a_{ij}, \quad v_1(0) = 1 \quad \text{and} \quad b_i(0) = b_i.$$

The matrix functions $a_{ij}(h\,T)$ and $b_j(h\,T)$ are linear combinations of the well known $\varphi-$functions. The coefficients are defined to give a high order of the method.

The functions used in (2.5) are conveniently represented in an extended Butcher tableau

$$\begin{array}{c|ccc|c} c_1 & a_{11}(z) & \cdots & a_{1s}(z) & u_{11}(z) \\ \vdots & \vdots & & \vdots & \vdots \\ c_s & a_{s1}(z) & \cdots & a_{ss}(z) & u_{s1}(z) \\ \hline & b_1(z) & \cdots & b_s(z) & v_1(z) \end{array}$$

Definition 2.3. *The exponential Runge-Kutta method* (2.5) *has in the* i^{th} *stage the stiff stage order* q_i *for* (1.2)*, if with* $y_n = y(t_n)$

$$\| \, y(t_n + c_i h) - Y_i \, \| \leq D_i h^{q_i + 1}, \quad \textit{for} \quad h \leq h_0$$

is satisfied.

It is consistent of stiff order q*, if*

$$\| \, y(t_n + h) - y_{n+1} \, \| \leq D h^{q+1}, \quad \textit{for} \quad h \leq h_0$$

holds.

Here the constants D_i, D and h_0 are independent of $\| T \|$. It has non-stiff order and stage order q, if the constants are allowed to depend on $\| T \|$.

2.6.3 Exponential general linear methods

The extension to general linear schemes is carried out as follows. A step of length h in an exponential general linear scheme, requires to import r approximations into the step, denoted as $y_i^{[n-1]}$, $i = 1, \ldots, r$. The internal stages (as in the Runge-Kutta case) are written as Y_i, $i = 1, \ldots, s$. After the step is completed, r updated approximations are computed. These are then used in the next step. Each step in an exponential general linear scheme can be written as [3]

$$
\begin{aligned}
Y_i &= h \sum_{j=1}^{s} a_{ij}(hT)\, g(t_{n-1} + c_j h, Y_j) + \sum_{j=1}^{r} u_{ij}(hT)\, y_j^{[n-1]}, \quad i = 1, \ldots, s, \\
y_i^{[n]} &= h \sum_{j=1}^{s} b_{ij}(hT)\, g(t_{n-1} + c_j h, Y_j) + \sum_{j=1}^{r} v_{ij}(hT)\, y_j^{[n-1]}, \quad i = 1, \ldots, r.
\end{aligned}
$$

The exponential integrators of Runge-Kutta type are easily seen to be a special case when $r = 1$ with $u_{i1}(z) = a_{i0}(z)$, $v_{11}(z) = b_0(z)$ and $b_{1j}(z) = b_j(z)$.

The coefficient functions are grouped into matrices,

$$
\begin{array}{c|ccc|ccc}
c_1 & a_{11}(z) & \cdots & a_{1s}(z) & u_{11}(z) & \cdots & u_{1r}(z) \\
\vdots & \vdots & & \vdots & \vdots & & \vdots \\
c_s & a_{s1}(z) & \cdots & a_{ss}(z) & u_{s1}(z) & \cdots & u_{sr}(z) \\
\hline
 & b_{11}(z) & \cdots & b_{1s}(z) & v_{11}(z) & \cdots & v_{1r}(z) \\
 & \vdots & & \vdots & \vdots & & \vdots \\
 & b_{s1}(z) & \cdots & b_{ss}(z) & v_{r1}(z) & \cdots & v_{rr}(z)
\end{array}
$$

To implement the exponential general linear schemes, the EXPINT package assumes a special structure of the vector $y^{[n-1]}$, the quantities of which are passed from step to step:

$$
y^{[n-1]} = [y_{n-1},\, hg_{n-2},\, hg_{n-3},\, \cdots,\, hg_{n-r}]^T,
$$

where $g_{n-i} = g(y_{n-i}, t_{n-i})$. This choice enables both the ETD Adams-Bashforth and generalized Lawson schemes to be conveniently represented in a single framework [3]. Exponential integrators that do not fit into this framework are the methods developed in Calvo and Palencia [5].

The extension from a traditional integrator to an exponential integrator is not unique. The two simplest choices of exponential integrators of Runge-Kutta type are the Lawson-Euler and Nørsett-Euler methods.

We give here some examples of exponential integrators implemented in EXPINT [3] and which we will use for comparison in our numerical tests.

Example 2.1. Lawson-Euler

$$y_n = \varphi_0(hL)y_{n-1} + h\varphi_0(hL)g(y_{n-1}, t_{n-1}), \qquad \begin{array}{c|c|c} 0 & 0 & 1 \\ \hline & \varphi_0(hL) & \varphi_0(hL) \end{array}$$

Example 2.2. Nørsett-Euler

$$y_n = \varphi_0(hL)y_{n-1} + h\varphi_1(hL)g(y_{n-1}, t_{n-1}), \qquad \begin{array}{c|c|c} 0 & 0 & 1 \\ \hline & \varphi_1(hL) & \varphi_0(hL) \end{array}$$

Example 2.3. ABLawson4

This scheme bases on the Adams-Bashforth scheme of order four. It has stiff order one and non-stiff order four. Its coefficients are given by

$$\begin{array}{c|cc|cccc} 0 & & & 1 & 0 & 0 & 0 \\ 1 & \frac{55}{12}\varphi_0(z) & & \varphi_0(z) & -\frac{59}{24}\varphi_0^2(z) & \frac{37}{24}\varphi_0^3(z) & -\frac{3}{8}\varphi_0^4(z) \\ \hline & \frac{55}{12}\varphi_0(z) & 0 & \varphi_0(z) & -\frac{59}{24}\varphi_0^2(z) & \frac{37}{24}\varphi_0^3(z) & -\frac{3}{8}\varphi_0^4(z) \\ & 1 & 0 & 0 & 0 & 0 & 0 \\ & 0 & 0 & 0 & 1 & 0 & 0 \\ & 0 & 0 & 0 & 0 & 1 & 0 \end{array}$$

Example 2.4. Lawson4

Lawson exponential integrator based on Kutta's classical fourth order method. The coefficients of Lawson4 are given by

$$\begin{array}{c|cccc|c} 0 & & & & & 1 \\ \frac{1}{2} & \frac{1}{2}\varphi_0(\frac{z}{2}) & & & & \varphi_0(\frac{z}{2}) \\ \frac{1}{2} & 0 & \frac{1}{2} & & & \varphi_0(\frac{z}{2}) \\ 1 & 0 & 0 & \varphi_0(\frac{z}{2}) & & \varphi_0(z) \\ \hline & \frac{1}{6}\varphi_0(z) & \frac{1}{3}\varphi_0(\frac{z}{2}) & \frac{1}{3}\varphi_0(\frac{z}{2}) & \frac{1}{6} & \varphi_0(z) \end{array}$$

Example 2.5. ETD4RK

The fourth order ETD scheme, ETD4RK, due to Cox and Matthews [7]. The coefficients of ETD4RK are given by

$$
\begin{array}{c|cccc|c}
0 & & & & & 1 \\
\frac{1}{2} & \frac{1}{2}\varphi_1(\frac{z}{2}) & & & & \varphi_0(\frac{z}{2}) \\
\frac{1}{2} & 0 & \frac{1}{2}\varphi_1(\frac{z}{2}) & & & \varphi_0(\frac{z}{2}) \\
1 & \varphi_1(\frac{z}{2})\big(\varphi_0(\frac{z}{2})-1\big) & 0 & \varphi_1(\frac{z}{2}) & & \varphi_0(z) \\
\hline
 & \varphi_1(z)-3\varphi_2(z)+4\varphi_3(z) & b_2(z) & b_3(z) & 4\varphi_3(z)-\varphi_2(z) & \varphi_0(z)
\end{array}
$$

where $b_2(z) = b_3(z) = 2\varphi_2(z) - 4\varphi_3(z)$.

Example 2.6. Strehmel-Weiner

One of the earliest exponential Runge-Kutta methods with 4−*stages, it has stiff order three. Its coefficients are given by*

$$
\begin{array}{c|cccc|c}
0 & & & & & 1 \\
\frac{1}{2} & \frac{1}{2}\varphi_1(\frac{z}{2}) & & & & \varphi_0(\frac{z}{2}) \\
\frac{1}{2} & \frac{1}{2}\varphi_1(\frac{z}{2})-\frac{1}{2}\varphi_2(\frac{z}{2}) & \frac{1}{2}\varphi_2(\frac{z}{2}) & & & \varphi_0(\frac{z}{2}) \\
1 & \varphi_1(z)-2\varphi_2(z) & -2\varphi_2(z) & 4\varphi_2(z) & & \varphi_0(z) \\
\hline
 & b_1(z) & 0 & 4\varphi_2(z)-8\varphi_3(z) & 4\varphi_3(z)-\varphi_2(z) & \varphi_0(z)
\end{array}
$$

where $b_1(z) = \varphi_1(z) - 3\varphi_2(z) + 4\varphi_3(z)$.

Example 2.7. Hochbruck-Ostermann

This scheme developed by Hochbruck and Ostermann , with five-stages is the only known exponential Runge-Kutta method with stiff order four. Its coefficients are given by

$$
\begin{array}{c|ccccc|c}
0 & & & & & & 1 \\
\frac{1}{2} & \frac{1}{2}\varphi_1(\frac{z}{2}) & & & & & \varphi_0(\frac{z}{2}) \\
\frac{1}{2} & \frac{1}{2}\varphi_1(\frac{z}{2})-\varphi_2(\frac{z}{2}) & \varphi_2(\frac{z}{2}) & & & & \varphi_0(\frac{z}{2}) \\
1 & \varphi_1(z)-2\varphi_2(z) & \varphi_2(z) & \varphi_2(z) & & & \varphi_0(z) \\
\frac{1}{2} & \frac{1}{2}\varphi_1(\frac{z}{2})-2a_{52}-a_{54} & a_{52} & a_{52} & a_{54} & & \varphi_0(\frac{z}{2}) \\
\hline
 & b_1(z) & 0 & 0 & 4\varphi_3(z)-\varphi_2(z) & 4\varphi_2(z)-8\varphi_3(z) & \varphi_0(z)
\end{array}
$$

where

$$
\begin{aligned}
b_1(z) &= \varphi_1(z) - 3\varphi_2(z) + 4\varphi_3(z) \\
a_{52} &= \frac{1}{2}\varphi_2(\frac{z}{2}) - \varphi_3(z) + \frac{1}{2}\varphi_2(z) - \frac{1}{2}\varphi_3(\frac{z}{2}) \\
a_{54} &= \frac{1}{4}\varphi_2(\frac{z}{2}) - a_{52}.
\end{aligned}
$$

Example 2.8. RKMK4t

This scheme was developed by Munthe-Kaas [17] using a suitable truncation of the dexp^{-1} operator. It is of non-stiff order four and stiff order two but suffers from instabilities, especially when non-periodic boundary conditions are used. Its coefficients are given by

$$\begin{array}{c|cccc|c}
0 & & & & & 1 \\
\frac{1}{2} & \frac{1}{2}\varphi_1(\frac{z}{2}) & & & & \varphi_0(\frac{z}{2}) \\
\frac{1}{2} & \frac{z}{2}\varphi_1(\frac{z}{2}) & \frac{1}{2}(1-\frac{z}{4})\varphi_1(\frac{z}{2}) & & & \varphi_0(\frac{z}{2}) \\
1 & 0 & 0 & \varphi_1(z) & & \varphi_0(z) \\
\hline
 & \frac{1}{6}\varphi_1(z)(1+\frac{z}{2}) & \frac{1}{3}\varphi_1(z) & \frac{1}{3}\varphi_1(z) & \frac{1}{6}\varphi_1(z)(1-\frac{z}{2}) & \varphi_0(z)
\end{array}$$

Chapter 3

Exponential Peer Methods

In this chapter, we will be concerned with the construction, implementation and numerical analysis of a new class of exponential integrators, exponential peer methods (EPMs).

The first Section 3.1 will be devoted to give an overview on peer methods. The definition of the new methods and the basic properties of their coefficients are given in Section 3.2. Consistency and zero-stability of the methods will be investigated in Section 3.2.2, and we formulate simplifying conditions which guarantee order $p = s - 1$, where s is the number of stages. For the non-stiff case the order is $p = s$. Due to the two-step character of the methods, zero-stability has to be discussed. Finally, in Section 3.3 we consider a special class of EPMs of stiff order $p = s - 1$ with only two 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.

3.1 Peer methods

Two-step peer methods are a class of time integration schemes for the numerical solution of non-stiff and stiff IVPs either for sequential or parallel computers, which were introduced by B. A. Schmitt and R. Weiner [43]. This class has a two-step character and propagates s different "peer" solution variables with essentially identical characteristics from step to step. All s stage solutions are peers sharing essentially the same accuracy and stability properties. Linearly-implicit peer methods have been studied for parallel and sequential implementation e.g., in [41–43]. They are characterized by a high stage order what makes them attractive for very stiff systems.

The new feature of peer methods is that they possess several stages like Runge-Kutta-type methods, but all these stages have the same properties and no extraordinary solution variable is used. These methods combine positive features of both Runge-Kutta and multistep methods having good stability properties and no order reduction for very stiff systems. In particular, several explicit peer methods [52, 53] have been proved to be competitive with standard Runge-Kutta methods in a wide selection of non-stiff test problems.

We consider the numerical solution of initial value problems for systems of ODEs of the form,

$$\begin{aligned} \frac{dy}{dt} &= f(t,y), \quad t \in [t_0, t_{end}] \\ y(t_0) &= y_0 \in \mathbb{R}^n, \end{aligned} \tag{3.1}$$

where $y = y(t)$, $y : \mathbb{R} \mapsto \mathbb{R}^n$ and $f : \mathbb{R} \times \mathbb{R}^n \mapsto \mathbb{R}^n$.

The form of the explicit two-step peer methods is as follows. In each time step from t_m to $t_{m+1} = t_m + h_m$ solutions $Y_{mi} \cong y(t_{mi})$, $i = 1, \dots, s$, are computed as approximations at the points $t_{mi} = t_m + c_i\, h_m$. The time step consists of s stages,

$$\begin{aligned} Y_{mi} = \sum_{j=1}^{s} b_{ij}\, Y_{m-1,j} &+ h_m \sum_{j=1}^{s} a_{ij}\, f\left(t_{m-1,j}, Y_{m-1,j}\right) \\ &+ h_m \sum_{j=1}^{i-1} r_{ij}\, f\left(t_{mj}, Y_{mj}\right), \quad i = 1, \dots, s. \end{aligned} \tag{3.2}$$

We point out that the right-hand side in (3.2) depends on the stages $Y_{m-1,j}$ of the previous time step with the contribution from actual stages. Because of $r_{ij} = 0$ for

$j \geq i$ the methods are explicit. We store the stage vectors Y_{mi} and also $f\left(t_{mj},\, Y_{mj}\right)$ in vectors.

$$Y_m = \begin{pmatrix} Y_{m1} \\ Y_{m2} \\ \vdots \\ Y_{ms} \end{pmatrix} \in \mathbb{R}^{ns}, \qquad F\left(t_m, Y_m\right) = \begin{pmatrix} f(t_m + c_1\, h_m,\, Y_{m1}) \\ f(t_m + c_2\, h_m,\, Y_{m2}) \\ \vdots \\ f(t_m + c_s\, h_m,\, Y_{ms}) \end{pmatrix} \tag{3.3}$$

Explicit peer methods yield high order approximations $Y_{mi} - y(t_{mi}) = \mathcal{O}(h_m^s)$, $i = 1, \ldots, s$, uniformly in all stages. So, dense output is available cheaply.

For stiff problems in [41] linearly-implicit peer methods are considered. They are given by

$$\begin{aligned}(I - h_m \gamma T_m) Y_{mi} = {} & \sum_{j=1}^{s} b_{ij}\, Y_{m-1,j} + h_m \sum_{j=1}^{s} a_{ij} \left[F_{m-1,j} - T\, Y_{m-1,j}\right] \\ & + h_m T_m \sum_{j=1}^{i-1} g_{ij}\, Y_{mj}, \qquad\qquad i = 1, 2, \ldots, s. \end{aligned} \tag{3.4}$$

Note that for peer methods all stage values are of order p, i.e., the order of consistency is equal to the stage order. A consequence is that in implicit peer methods no order reduction for stiff problems occurs.

3.2 Exponential peer methods

3.2.1 Definition of exponential peer methods

We consider the initial value problem (3.1). For the formulation of exponential peer methods we assume as usual in exponential integrators a linearization of the form

$$\begin{aligned} \frac{dy}{dt} &= f(t, y) = T\, y \;+\; g(t, y), \quad t \in [t_0, t_{end}] \\ y(t_0) &= y_0 \in \mathbb{R}^n, \end{aligned} \tag{3.5}$$

where $g(t, y) = f(t, y) - Ty$. Here $T \in \mathbb{R}^{n \times n}$ is an arbitrary matrix, which is supposed to carry the stiffness of the system, and which should approximate the Jacobian f_y for stability reasons. In our tests with the EXPINT package [3] 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 and assume a constant step size h. In this method, a numerical solution Y_{mi}, $i = 1, 2, \dots, s$ will be calculated for the system (3.5) by an $s-$stage scheme with step size h of the form

$$\begin{aligned} Y_{mi} = \varphi_0(\alpha_i hT) \sum_{j=1}^{s} b_{ij}\, Y_{m-1,j} + h \sum_{j=1}^{s} A_{ij}(\alpha_i hT) \big[f_{m-1,j} - T\, Y_{m-1,j} \big] \\ + h \sum_{j=1}^{i-1} R_{ij}(\alpha_i hT) \big[f_{mj} - T\, Y_{mj} \big], \qquad i = 1, 2, \dots, s. \end{aligned} \tag{3.6}$$

The coefficients

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

are free parameters of the scheme. The idea is to determine the parameters in such a way that the method is of high order and has good stability properties. In this chapter we will assume constant step sizes.

The coefficients b_{ij}, c_i and α_i are constant and we assume $\alpha_i \geq 0$. The matrix functions $A_{ij}\,(hT)$ and $R_{ij}\,(hT)$ are linear combinations of $\varphi-$functions, see Section 2.4. Parallel methods are obtained by the choice $R = 0$ eliminating any reference to the stages Y_{mi} of the actual step.

The values Y_{mi} approximate the exact solution $y(t_m + c_i\, h)$ at points $t_{mi} = t_m + c_i\, h$, where the nodes c_i are assumed to be pairwise distinct. They are chosen such that $c_s = 1$ and the other nodes satisfy $0 \leq c_i < 1$, $i = 1, \dots, s-1$. Further we denote $f_{mj} = f(t_{mj}, Y_{mj})$. The s stage values Y_{mi} have the same characteristics so we call them "peer" [43]. By setting $T = 0$, we obtain explicit peer methods (3.2).

The compact notation for EPMs is obtained by storing the stages Y_{mi} into Y_m and, accordingly, $G(Y_m) := F(Y_m) - TY_m$ with (3.3) then (3.6) corresponds to

$$Y = \Phi(B \otimes I)Y_{m-1} + h(A \otimes I)G\,(Y_{m-1}) + h(R \otimes I)G\,(Y_m)\,,$$

where $\otimes$ is the Kronecker product, and

$$\Phi = \operatorname{diag}(\varphi_0(\alpha_1 hT), \dots, \varphi_0(\alpha_s hT)). \tag{3.7}$$

3.2.2 Consistency and convergence

In this section we will derive order conditions for EPMs when applied to stiff semi-linear problems (3.5). Essential in choosing a numerical method is its order of consistency and its numerical stability.

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

$$\|g(t,u) - g(t,v)\| \leq L_g \|u - v\|, \tag{3.8}$$

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

$$\mu(T) \leq \omega. \tag{3.9}$$

If we use different matrices T in different steps, then we will assume (3.9) for all steps. If the system (3.5) comes from semi-discretization of parabolic equations then this condition is usually satisfied. Assumption (3.9) implies

$$\begin{aligned} \|\varphi_0(hT)\| = \|e^{hT}\| &\leq e^{h\mu(T)} \\ &\leq e^{h\omega}, \end{aligned} \tag{3.10}$$

see e.g., [28].

Remark 3.1. *A consequence of* (3.9) *is that* $\|\varphi_l(hT)\|$ *and* $\|hT\varphi_l(hT)\|$ *are uniformly bounded for* $l \geq 1$. *This also holds for the matrix coefficients* $A_{ij}(\alpha_i hT)$ *and* $R_{ij}(\alpha_i hT)$ *which are linear combinations of the* $\varphi_l(\alpha_i hT)$, $l \geq 1$.

We are interested in error estimates, which may depend on bounds of derivatives of the exact solution, on ω and L_g, but do not depend on the norm of T. For our investigations of the order of consistency we always assume that the right hand side is sufficiently smooth.

The order conditions for exponential peer methods can be derived by replacing the numerical solutions Y_{mi} and $Y_{m-1,i}$ in (3.6) by values of the exact solution $y(t)$ in the numerical method where $f(t_{mi}, y(t_{mi})) = y'(t_{mi})$. Then the local residual errors Δ_{mi} are

$$\Delta_{mi} = y(t_{mi}) - \varphi_0(\alpha_i hT) \sum_{j=1}^{s} b_{ij} y(t_{m-1,j}) - h \sum_{j=1}^{s} A_{ij}(\alpha_i hT) \Big[y'(t_{m-1,j})$$

$$- Ty(t_{m-1,j})\Big] - h\sum_{j=1}^{i-1} R_{ij}(\alpha_i hT)\Big[y'(t_{mj}) - Ty(t_{mj})\Big], \quad i = 1, \dots, s. \quad (3.11)$$

By Taylor expansion of the exact solution $y(t)$ and $y'(t)$ at the point t_m, we have

$$\begin{aligned}
y\big(t_{mi}\big) &= y\big(t_m + c_i h\big) = \sum_{r=0}^{q} \frac{h^r c_i^r}{r!} y^{(r)}(t_m) + \mathcal{O}(h^{q+1}),\\
y\big(t_{m-1,j}\big) &= y\big(t_{m-1} + c_j\, h\big) = y\big(t_m + (c_j - 1)\, h\big)\\
&= \sum_{r=0}^{q} \frac{h^r (c_j-1)^r}{r!} y^{(r)}(t_m) + \mathcal{O}(h^{q+1}),\\
y'\big(t_m + c_j\, h\big) &= \sum_{r=0}^{q} \frac{h^r c_j^r}{r!} y^{(r+1)}(t_m) + \mathcal{O}(h^{q+1}),\\
y'\big(t_{m-1,j}\big) &= y'\big(t_{m-1} + c_j\, h\big) = y'\big(t_m + (c_j - 1)\, h\big)\\
&= \sum_{r=0}^{q} \frac{h^r\, (c_j-1)^r}{r!} y^{(r+1)}(t_m) + \mathcal{O}(h^{q+1}),
\end{aligned}$$

where the $\mathcal{O}$-term is uniformly bounded due to the smoothness assumption on the solution.

Substitution into (3.11) yields

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

By collecting the coefficients of $\dfrac{h^r}{r!} y^{(r)}(t_m)$ we get

$$\begin{aligned}
\Delta_{mi} = &\sum_{r=0}^{q} \Bigg\{ c_i^r I - \varphi_0(\alpha_i\, h\, T) \sum_{j=1}^{s} b_{ij} (c_j-1)^r - r \sum_{j=1}^{s} A_{ij}(\alpha_i\, h\, T)(c_j-1)^{r-1}\\
&+ hT\sum_{j=1}^{s} A_{ij}(\alpha_i\, h\, T)(c_j-1)^r - r\sum_{j=1}^{i-1} R_{ij}(\alpha_i\, h\, T) c_j^{r-1}\\
&+ hT\sum_{j=1}^{i-1} R_{ij}(\alpha_i\, h\, T) c_j^r \Bigg\} \frac{h^r}{r!} y^{(r)}(t_m) + \mathcal{O}(h^{q+1}) \qquad (3.12)
\end{aligned}$$

Here the remainder results from products of the coefficients of the method with the $\mathcal{O}(h^{q+1})$-terms of the Taylor expansion of the solution. Due to Remark 3.1 the remainder is bounded independent of $\|T\|$.

Definition 3.1. *The exponential peer method* (3.6) *is consistent of non-stiff order p if there are constants $h_0, C > 0$ such that*

$$\|\Delta_{mi}\| \leq Ch^{p+1} \quad \textit{for all } h \leq h_0, \textit{ and for all } 1 \leq i \leq s.$$

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 exponential peer methods stage order and order are equal. To determine the coefficients of the method, B, A, R, c, and α, such that the method has high order, it is advantageous to consider the linear case $y' = Ty$ first.

Theorem 3.1. *If the exponential peer method satisfies the conditions*

$$\sum_{j=1}^{s} b_{ij}(c_j - 1)^l = (c_i - \alpha_i)^l, \quad l = 0, 1, \ldots, q, \tag{3.13}$$

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

Proof. From (3.11), for the equation $y' = Ty$ the local residual errors will be

$$\begin{aligned}\Delta_{mi} &= y(t_m + c_i h) - \varphi_0(\alpha_i hT) \sum_{j=1}^{s} b_{ij} y(t_m + (c_j - 1)h) \\ &= \varphi_0(c_i hT) y(t_m) - \varphi_0(\alpha_i hT) \sum_{j=1}^{s} b_{ij} \varphi_0((c_j - 1)hT) y(t_m)\end{aligned}$$

Using the relation

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

which follows from (2.3), we obtain

$$\begin{aligned}\Delta_{mi} = \sum_{l=0}^{q} \left[c_i^l - \sum_{j=1}^{s} b_{ij}(\alpha_i + c_j - 1)^l \right] \frac{h^l T^l}{l!} y(t_m) + h^{q+1} \Big\{ c_i^{q+1} \varphi_{q+1}(c_i hT) \\ - \sum_{j=1}^{s} b_{ij}(\alpha_i + c_j - 1)^{q+1} \varphi_{q+1}\Big((\alpha_i + c_j - 1)hT \Big) \Big\} T^{q+1} y(t_m)\end{aligned}$$

With $T^{q+1}y(t_m) = y^{(q+1)}(t_m)$ the second term is $\mathcal{O}(h^{q+1})$, where the constants are independent of $\|T\|$.

For the coefficients of $\dfrac{h^l T^l}{l!} y(t_m)$ for $l = 0, \dots, q$ we have

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

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

If we write the equations (3.13) in matrix form for $l = 0, \dots, s-1$, we obtain immediately

Corollary 3.1. *Let*

$$B = V_\alpha V_1^{-1}, \tag{3.14}$$

where

$$V_\alpha = \left(\mathbb{1}, c - \alpha, \dots, (c - \alpha)^{s-1}\right) = \begin{pmatrix} 1 & c_1 - \alpha_1 & (c_1 - \alpha_1)^2 & \dots & (c_1 - \alpha_1)^{s-1} \\ 1 & c_2 - \alpha_2 & (c_2 - \alpha_2)^2 & \dots & (c_2 - \alpha_2)^{s-1} \\ \vdots & \vdots & \dots & \dots & \vdots \\ 1 & c_s - \alpha_s & (c_s - \alpha_s)^2 & \dots & (c_s - \alpha_s)^{s-1} \end{pmatrix},$$

$$V_1 = \left(\mathbb{1}, c - \mathbb{1}, \dots, (c - \mathbb{1})^{s-1}\right) = \begin{pmatrix} 1 & c_1 - 1 & (c_1 - 1)^2 & \dots & (c_1 - 1)^{s-1} \\ 1 & c_2 - 1 & (c_2 - 1)^2 & \dots & (c_2 - 1)^{s-1} \\ \vdots & \vdots & \dots & \vdots & \vdots \\ 1 & c_s - 1 & (c_s - \alpha_s)^2 & \dots & (c_s - 1)^{s-1} \end{pmatrix},$$

$$c = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_s \end{pmatrix}, \qquad \alpha = \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_s \end{pmatrix}, \qquad \textit{and} \qquad \mathbb{1} = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}.$$

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

For $\alpha = c$ we have $V_\alpha = \mathbb{1}e_1^T$, where $e_1 = (1, 0, \dots, 0)^T$. If furthermore $c_s = 1$ then $e_s^T V_1 = e_1^T$ i.e., $e_1^T V_1^{-1} = e_s^T$, where $e_s = (0, 0, \dots, 1)^T$. Therefore we have

Corollary 3.2. *Let $\alpha = c$, $c_s = 1$. Then with (3.14) we have $B = \mathbb{1}e_s^T$, and*

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

Therefore (3.13) is satisfied for all l, the exponential peer method solves the system $y' = Ty$ with exact starting values exactly. $\square$

If $q = s - 1$, then the general solution of (3.13) will be

$$b_{ij} = \prod_{\substack{k=1\\k\neq j}}^{s} \frac{c_k + \alpha_i - c_i - 1}{c_k - c_j}.$$

We consider the following two examples for the choice of c and α.

Case 1 (*Corollary* 3.2) Let

$$c_i = \alpha_i$$

Then

$$B = \begin{pmatrix} 0 & 0 & 0 & \dots & 0 & 1 \\ 0 & 0 & 0 & \dots & 0 & 1 \\ \vdots & \vdots & \dots & \dots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & 1 \\ 0 & 0 & 0 & \dots & 0 & 1 \\ 0 & 0 & 0 & \dots & 0 & 1 \end{pmatrix} = \mathbb{1}e_s^T.$$

A disadvantage of this choice is that $\varphi-$functions of s different arguments have to be calculated. This leads to a high computational effort. To minimize the number of $\varphi-$function evaluations, we choose to set the parameter α to have only two different arguments.

Case 2 Let

$$\begin{aligned} &\alpha_s = 1, \qquad \alpha_i = \alpha^*, \quad i = 1, \dots, s-1, \\ &c_1 = \frac{(s-1)(\alpha^* - 1) + 1 - \beta}{1 - \beta}, \qquad c_i = (s-i)(\alpha^* - 1) + 1, \quad i = 2, \dots, s. \end{aligned} \tag{3.15}$$

Then

$$B = \begin{pmatrix} \beta & g_1(\beta) & \beta g_2(\beta) & \dots & \beta g_{s-1}(\beta) & \beta g_s(\beta) \\ 0 & 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \dots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 1 & 0 \\ 0 & 0 & 0 & \dots & 0 & 1 \\ 0 & 0 & 0 & \dots & 0 & 1 \end{pmatrix},$$

where $g_1(0) = 1$.

The coefficients b_{ij} are determined by Theorem 3.1 for given α and c. We now will consider the general case (3.5) to obtain conditions for the matrix coefficients $A_{ij}(\alpha_i hT)$ and $R_{ij}(\alpha_i hT)$.

From (3.12) with (3.13) we need to show that the coefficients of $\frac{h^r T^r}{r!} y(t_m)$ for $r = 0, \dots, q$ are zeros.

Theorem 3.2. *Let the conditions (3.13) be satisfied for $l = 0, \dots, q$. Let further $A_{ij}(\alpha_i hT)$ and $R_{ij}(\alpha_i hT)$ be linear combinations of $\varphi_1(\alpha_i hT), \dots, \varphi_{q+1}(\alpha_i hT)$ satisfying the condition*

$$\sum_{j=1}^{s} A_{ij}(\alpha_i hT)\,(c_j - 1)^r + \sum_{j=1}^{i-1} R_{ij}(\alpha_i hT) c_j^r = \sum_{l=0}^{r} \binom{r}{l} l! \alpha_i^{l+1} (c_i - \alpha_i)^{r-l} \varphi_{l+1}(\alpha_i hT) \tag{3.16}$$

for $r = 0, \dots, q$. Then the exponential peer method is at least of stiff order of consistency $p = q$ for (3.5).

Proof. For order q the coefficients of $y^{(r)}(t_m)$ in (3.12) should be equal to zero for $r = 0, \dots, q$.

For $r = 0$ using (3.13) and (3.16) we obtain

$$I - \varphi_0(\alpha_i hT) \sum_{j=1}^{s} b_{ij} + hT \sum_{j=1}^{s} A_{ij}(\alpha_i hT) + hT \sum_{j=1}^{i-1} R_{ij}(\alpha_i hT) = I - \varphi_0(\alpha_i hT) + \alpha_i hT \varphi_1(\alpha_i hT) = 0 \quad \text{by (2.3).}$$

For $r = 1, \ldots, q$ holds for the coefficients

$$
\begin{aligned}
&c_i^r I - \varphi_0(\alpha_i hT) \sum_{j=1}^{s} b_{ij}(c_j - 1)^r - r \sum_{j=1}^{s} A_{ij}(\alpha_i hT)(c_j - 1)^{r-1} \\
&\quad + hT \sum_{j=1}^{s} A_{ij}(\alpha_i hT)(c_j - 1)^r - r \sum_{j=1}^{i-1} R_{ij}(\alpha_i hT) c_j^{r-1} + hT \sum_{j=1}^{i-1} R_{ij}(\alpha_i hT) c_j^r \\
&= c_i^r I - \varphi_0(\alpha_i hT)(c_i - \alpha_i)^r - r \sum_{l=0}^{r-1} \binom{r-1}{l} \alpha_i^{l+1} (c_i - \alpha_i)^{r-1-l} l! \varphi_{l+1}(\alpha_i hT) \\
&\quad + hT \sum_{l=0}^{r} \binom{r}{l} \alpha_i^{l+1} (c_i - \alpha_i)^{r-l} l! \varphi_{l+1}(\alpha_i hT) \quad \text{by (3.16)} \\
&= c_i^r I - \varphi_0(\alpha_i hT)(c_i - \alpha_i)^r - r \sum_{l=1}^{r} \binom{r-1}{l-1} \alpha_i^{l} (c_i - \alpha_i)^{r-l} (l-1)! \varphi_{l}(\alpha_i hT) \\
&\quad + \sum_{l=0}^{r} \binom{r}{l} \alpha_i^{l} (c_i - \alpha_i)^{r-l} (l! \varphi_{l}(\alpha_i hT) - I) \quad \text{by (2.3)}
\end{aligned}
$$

Using the fact $l\binom{r}{l} = r\binom{r-1}{l-1}$

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

Corollary 3.3. *Let $\alpha = c$, $c_s = 1$ and $B = \mathbb{1} e_s^T$. Let*

$$
\begin{aligned}
\sum_{j=1}^{s} A_{ij}(c_i hT)(c_j - 1)^r + &\sum_{j=1}^{i-1} R_{ij}(c_i hT) c_j^r \\
&= r! c_i^{r+1} \varphi_{r+1}(c_i hT) \quad \text{for } r = 0, \ldots, q. \qquad (3.17)
\end{aligned}
$$

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 (3.16) for A, due to the regularity of V_1. Therefore we can construct exponential peer methods of any order by increasing the number of stages.

If we allow the bounds to depend on $T\,y^{(q+1)}$ (non-stiff order), then the order of the methods will be $p = q + 1$,

Theorem 3.3. *Let the solution $y(t)$ be $(q+2)$-times continuously differentiable. Let the conditions (3.13) be satisfied for $l = 0, \dots, q+1$, and (3.16) for $l = 0, \dots, q$. Then the method is of non-stiff order $p = q+1$.*

Proof. The beginning of the proof is identical to the proof of Theorem 3.2. Considering now one more term in (3.16) gives for the term with h^{q+1}

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

Using the fact $\binom{q+1}{l+1} = \frac{q+1}{l+1}\binom{q}{l}$

$$\begin{aligned}
= &\Bigg\{ c_i^{q+1} I - \varphi_0(\alpha_i hT)(c_i - \alpha_i)^{q+1} \\
&\quad - \sum_{l=1}^{q+1} \binom{q+1}{l} l! \alpha_i^{l} (c_i - \alpha_i)^{q+1-l} \varphi_{l}(\alpha_i hT) \Bigg\} \frac{h^{q+1}}{(q+1)!} y^{(q+1)}(t_m) \\
&\quad + \mathcal{O}\left(h^{q+2}\right) \\
= &\Bigg\{ c_i^{q+1} I - \sum_{l=0}^{q+1} \binom{q+1}{l} l! \alpha_i^{l} (c_i - \alpha_i)^{q+1-l} \varphi_{l}(\alpha_i hT) \Bigg\} \frac{h^{q+1}}{(q+1)!} y^{(q+1)}(t_m) \\
&\quad + \mathcal{O}\left(h^{q+2}\right),
\end{aligned}$$

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

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

So $\Delta_{mi} = \mathcal{O}\left(h^{q+2}\right)$ and the method is of non-stiff order $p = q + 1$. ■

Remark 3.2. *Note that $\|Ty^{(q+1)}\|$ can be of moderate size although $\|T\|$ is very large, for instance for linear problem $y' = Ty$ or for special semi-discretized partial differential equations with homogeneous Dirichlet boundary conditions.*

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

3.2.3 Linear stability analysis

We now focus our attention on the basic linear stability requirements that any numerical method for ODEs has to accomplish. The definition of such properties we present in this section are formulated according to the formalism of EPMs. To study stability of a formula, it is often useful to analyze its performance on the following test problem (Dahlquist test equation [10]):

$$y'(t) = \lambda y, \quad y(t_0) = y_0, \tag{3.18}$$

where $\lambda \in \mathbb{C}^- := \{z \in \mathbb{C} : \operatorname{Re}(z) \leq 0\}$.

The solution of this simple problem remains bounded when time goes to infinity and we need to require that the numerical solution possesses an analogous stability property to that displayed by the exact solution (see e.g., [33]). Let us analyze the conditions to be imposed on the numerical method in order to reproduce the same behavior of the exact solution.

By applying the EPM (3.6) to the linear test equation (3.18), we obtain the following recurrence relation

$$Y_m = M(z)\, Y_{m-1} = (M(z))^m\, Y_0, \qquad z = hT, \tag{3.19}$$

Here, $Y_m = \left(Y_{mi}\right)_{i=1}^{s}$ and $M(z)$ is the stability matrix, which takes the form, cf. (3.7)

$$M(z) = \Phi(B \otimes I).$$

For zero-stability we consider $z = 0$.

In 1963, Dahlquist [10] introduced the concept of $A-$stability. The concept of $A-$stability is based on the linear test equation (3.17). When a numerical method is $A-$stable, there are no stability restriction on the step size in the implementation, which is a desirable property for the integration of stiff systems.

Definition 3.2. *The exponential peer method* (3.6) *is zero-stable if the spectral radius of the stability matrix at $z = 0$ is one (i.e., $\varrho(M(0)) = 1$) and all eigenvalues on the unit circle are simple.* $\square$

From (3.19) we have $M(0) = B$. from (3.13) for $l = 0$ we have $B\mathbb{1} = \mathbb{1}$ i.e., B has always one eigenvalue $\lambda_1 = 1$.

Analogously to Adams methods we will consider methods where all other eigenvalues are zero, i.e., the matrix B has the eigenvalues

$$\lambda_1 = 1, \qquad \lambda_2 = \lambda_3 = \cdots = \lambda_s = 0. \tag{3.20}$$

The parasitic roots are zero, a property also shared by the exponential general linear methods of Ostermann et al. [40]. We call such methods optimally zero-stable. Since the matrix B is constant, zero-stability implies that powers of B are uniformly bounded.

For the methods of Case 1 and Case 2 obviously hold:

Theorem 3.4. *The methods* (3.15) *with $\mid \beta \mid < 1$ are zero-stable. With $\beta = 0$ they are optimally zero-stable.* $\square$

For convergence consider first the non-stiff case. Then we have

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

for $h \to 0$. By standard arguments (e.g., [52]) follows

Theorem 3.5. *Let the exponential peer method be consistent of non-stiff 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 non-stiff order p.* $\square$

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

Theorem 3.6. *Let the exponential peer method be consistent of stiff 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

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

From (3.13) we have for $l = 0$ the relation $\sum_{j=1}^{s} b_{ij} = 1$. By Remark 3.1 the norms of the matrix coefficients A_{ij} and R_{ij} are bounded by some constants C_A and C_R. With (3.10) we have for $h \le h_0$, where h_0 is independent of $\|T\|$

$$\|\varphi_0(\alpha_i hT)\| \le e^{\alpha_i h\omega} \le 1 + C^* h,$$

C^* independent of $\|T\|$. With the assumptions on b_{ij}, with the Lipschitz constant L_g of g (3.8) and with $\|\varepsilon_{m-1}\| = \max_i \|\varepsilon_{m-1,i}\|$ we arrive at

$$\|\varepsilon_{mi}\| \le (1 + C^* h)\|\varepsilon_{m-1}\| + hC_A L_g\|\varepsilon_{m-1}\| + hC_R L_g \sum_{j=1}^{i-1}\|\varepsilon_{mj}\| + Ch^{p+1}.$$

Here the constants are independent of $\|T\|$.

For ε_{mi} on the right hand side only quantities $\varepsilon_{m1}, \ldots, \varepsilon_{m,i-1}$ from lower stages appear (R is strictly lower triangular). By induction over the stages we will prove the relation

$$\|\varepsilon_{mi}\| \le (1 + h\gamma_i)\|\varepsilon_{m-1}\| + \delta_i h^{p+1},$$

where γ_i and δ_i are independent of $\|T\|$.

For $i = 1$:

$$\|\varepsilon_{m1}\| \le (1 + h(\alpha_1 C^* + C_A L_g))\|\varepsilon_{m-1}\| + Ch^{p+1},$$

i.e., The recurrence relation is satisfied with $\gamma_1 = \alpha_1 C^* + C_A L_g$, $\delta_1 = C$.

Let the relation be satisfied for $j = 1, \ldots, l-1$

$$\| \varepsilon_{mj}\| \le (1 + h\gamma_j)\|\varepsilon_{m-1}\| + \delta_j h^{p+1}.$$

Then for $i = l$:

$$\begin{aligned}\|\varepsilon_{m-1,l}\| \le\ & (1 + h(\alpha_l C^* + C_A L_g))\|\varepsilon_{m-1}\| + hC_R L_g \sum_{j=1}^{l-1} \big((1 + h\gamma_j)\|\varepsilon_{m-1}\| + \delta_j h^{p+1}\big) \\ & + Ch^{p+1} \\ & \le (1 + h\gamma_l)\|\varepsilon_{m-1}\| + \delta_l h^{p+1} \quad \text{for } h \le h_0.\end{aligned}$$

The constants γ_l, δ_l in the stages depend on the logarithmic norm ω, on C_A, C_R and L_g, but are independent of $\|T\|$ and therefore uniformly bounded. We finally arrive at the recursion

$$\|\varepsilon_m\| = \max_i \|\varepsilon_{mi}\| \le (1 + \widehat{C}h)\|\varepsilon_{m-1}\| + \widetilde{C}h^{p+1}$$

with constants $\widehat{C}$ and $\widetilde{C}$ not depending on $\|T\|$. Stiff order of convergence p follows by standard techniques. ■

3.3 A special class of methods

In our numerical tests we will use the framework of EXPINT. Although there exist relations among $\varphi-$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. We consider the methods of Case 2 with $\alpha_s = 1$, cf. Section 3.2.2.

For zero-stability the choice $\beta = 0$ in (3.15) is optimal. We have

$$\alpha = \begin{pmatrix} \alpha^* \\ \vdots \\ \alpha^* \\ 1 \end{pmatrix}, \quad c_i = (s-i)(\alpha_i - 1) + 1. \tag{3.21}$$

Furthermore, we will always assume that B is defined by (3.14). By Corollary 3.1 the conditions (3.13) are fulfilled up to $s-1$. For this choice we immediately obtain

Theorem 3.7. *For*

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

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

With (3.14) and (3.21) the methods are also optimally zero-stable.

Theorem 3.8. *The methods defined by (3.14), (3.21) are optimally zero-stable, the matrix B is given by*

$$B = \begin{pmatrix} 0 & 1 & 0 & \dots & 0 & 0 \\ 0 & 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 1 & 0 \\ 0 & 0 & 0 & \dots & 0 & 1 \\ 0 & 0 & 0 & \dots & 0 & 1 \end{pmatrix}. \tag{3.22}$$

Proof. We have with $c_s = 1$

$$V_\alpha = \begin{pmatrix} 1 & c_1 - \alpha_1 & (c_1-\alpha_1)^2 & \dots & (c_1-\alpha_1)^{s-1} \\ 1 & c_2 - \alpha_2 & (c_2-\alpha_2)^2 & \dots & (c_2-\alpha_2)^{s-1} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & c_{s-1} - \alpha_{s-1} & (c_{s-1}-\alpha_{s-1})^2 & \dots & (c_{s-1}-\alpha_{s-1})^{s-1} \\ 1 & 0 & 0 & \dots & 0 \end{pmatrix}.$$

(3.22) is equivalent to

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

This is equal to V_α iff

$$\begin{aligned} c_{s-1} &= \alpha_{s-1}, \\ c_{i+1} - 1 &= c_i - \alpha_i, \quad i = 1, \dots, s-1. \end{aligned} \tag{3.23}$$

Inserting (3.21) immediately proves the statement. ■

Corollary 3.4. *The methods* (3.22) *are convergent of stiff order* $p = s - 1$.

Proof. Because of $b_{i,j} \geq 0 \quad \forall\, i, j = 1, \ldots, s$ and by using Theorem 3.6 so the methods are convergent of stiff order $p = s - 1$. ■

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 shown in Corollary 3.2. Here we will prove this property also for the choice (3.21).

Theorem 3.9. *Let* (3.21) *be satisfied and let the starting values* Y_{0i} *be exact. Then* $Y_{1i} = e^{(1+c_i)hT} y(t_0)$, *i.e., we have the exact solution of* $y' = Ty$.

Proof. By (3.6) 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 $i = 1, \ldots, s-1$ this simplifies to

$$\begin{aligned} Y_{1i} &= e^{(c_{i+1}h + \alpha_i h)T} y(t_0) \\ &= e^{(c_i h + h)T} y(t_0) \quad \text{(by (3.21))} \\ &= e^{(1+c_i)hT} y(t_0), \end{aligned}$$

i.e., Y_{1i} is exact. For the last stage ($c_s = 1$) 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 (3.16) for $r = 0, \ldots, s-1$ using MAPLE. There remain $\dfrac{s(s-1)}{2}$ free parameters. For simplicity, to get a uniquely defined method, we set free parameters to zero to obtain an upper triangular matrix A and a strictly lower triangular matrix R. For this very special choice each stage of the resulting exponential peer method can be interpreted as an exponential multistep method [5], however with different methods in different stages. Our choice is arbitrary and may be not the best. For instance it is possible to set $R = 0$ to obtain parallel methods.

With (3.21) and $\alpha^* = \dfrac{(s-1)}{s}$ we have computed methods for $s = 3, 4, 5, 6, 7$ in this way. They are called `epm3`–`epm7`. By Theorem 3.2 the methods are of stiff order and stage order $p \geq s-1$, and by Theorem 3.3 of non-stiff order $p = s$.

Remark 3.3. *Another choice for α and c with also two different arguments is given in Appendix C.*

As example we present the coefficients of `epm4` and `epm5`. The other methods′ coefficients are found in Appendix A.

Example 3.1. *Method `epm4` with 4 stages of stiff order $p \geq 3$:*

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

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

where

$$\begin{aligned} A_{11} &= -\frac{3}{4}\varphi_2 + \frac{27}{4}\varphi_3 - \frac{81}{4}\varphi_4, & A_{12} &= \frac{3}{4}\varphi_1 - \frac{9}{8}\varphi_2 - \frac{27}{2}\varphi_3 + \frac{243}{4}\varphi_4, \\ A_{13} &= \frac{9}{4}\varphi_2 + \frac{27}{4}\varphi_3 - \frac{243}{4}\varphi_4, & A_{14} &= -\frac{3}{8}\varphi_2 + \frac{81}{4}\varphi_4, \\ A_{44} &= \varphi_1 - \frac{22}{3}\varphi_2 + 32\varphi_3 - 64\varphi_4, & R_{41} &= 12\varphi_2 - 80\varphi_3 + 192\varphi_4, \\ R_{42} &= -6\varphi_2 + 64\varphi_3 - 192\varphi_4, & R_{43} &= \frac{4}{3}\varphi_2 - 16\varphi_3 + 64\varphi_4. \end{aligned}$$

Example 3.2. *Method `epm5` with 5 stages of stiff order $p \geq 4$:*

$$\alpha = \left[\frac{4}{5}, \frac{4}{5}, \frac{4}{5}, \frac{4}{5}, 1\right]^T, \quad C = \left[\frac{1}{5}, \frac{2}{5}, \frac{3}{5}, \frac{4}{5}, 1\right]^T, \quad B = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$A = \begin{pmatrix} A_{11} & A_{12} & A_{13} & A_{14} & A_{15} \\ 0 & A_{11} & A_{12} & A_{13} & A_{14} \\ 0 & 0 & A_{11} & A_{12} & A_{13} \\ 0 & 0 & 0 & A_{11} & A_{12} \\ 0 & 0 & 0 & 0 & A_{55}, \end{pmatrix} \qquad R = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ A_{15} & 0 & 0 & 0 & 0 \\ A_{14} & A_{15} & 0 & 0 & 0 \\ A_{13} & A_{14} & A_{15} & 0 & 0 \\ R_{51} & R_{52} & R_{53} & R_{54} & 0 \end{pmatrix}$$

where

$$\begin{aligned}
A_{11} &= -\frac{4}{5}\varphi_2 + \frac{176}{15}\varphi_3 - \frac{384}{5}\varphi_4 + \frac{1024}{5}\varphi_5, \\
A_{12} &= \frac{4}{5}\varphi_1 - \frac{8}{3}\varphi_2 - \frac{64}{3}\varphi_3 + 256\varphi_4 - \frac{4096}{5}\varphi_5, \\
A_{13} &= \frac{24}{5}\varphi_2 + \frac{32}{5}\varphi_3 - \frac{1536}{5}\varphi_4 + \frac{6144}{5}\varphi_5, \\
A_{14} &= -\frac{8}{5}\varphi_2 + \frac{64}{15}\varphi_3 + \frac{768}{5}\varphi_4 - \frac{4096}{5}\varphi_5, \\
A_{15} &= \frac{4}{15}\varphi_2 - \frac{16}{15}\varphi_3 - \frac{128}{5}\varphi_4 + \frac{1024}{5}\varphi_5, \\
A_{55} &= \varphi_1 - \frac{125}{12}\varphi_2 + \frac{875}{12}\varphi_3 - \frac{625}{2}\varphi_4 + 625\varphi_5, \\
R_{51} &= 20\varphi_2 - \frac{650}{3}\varphi_3 + 1125\varphi_4 - 2500\varphi_5, \\
R_{52} &= -15\varphi_2 + \frac{475}{2}\varphi_3 - 1500\varphi_4 + 3750\varphi_5, \\
R_{53} &= \frac{20}{3}\varphi_2 - \frac{350}{3}\varphi_3 + 875\varphi_4 - 2500\varphi_5, \\
R_{54} &= -\frac{5}{4}\varphi_2 + \frac{275}{12}\varphi_3 - \frac{375}{2}\varphi_4 + 625\varphi_5.
\end{aligned}$$

Here, in A_{ij}, R_{ij} the argument of the $\varphi-$functions is $\alpha_i hT$.

3.4 Numerical experiments

In this section, we illustrate the theoretical results given on the convergence behavior of exponential peer methods for constant step sizes.

3.4.1 Starting procedure

Due to the two-step structure with s stages all peer methods require s initial values Y_{0i}, $i = 1, \ldots, s$ at the beginning. We need to know the s approximations $Y_{0i} \approx y(t_1 + (c_i - 1)h_{peer})$. So far these starting values have been computed by one-step methods.

In order to obtain the required approximations, we perform one time step of size $h_{start} > 0$ of a suitable one-step method with continuous output using the initial data y_0 of the problem at time $t = t_0$. This gives access to a numerical solution $\tilde{y}(t)$ in the interval $[t_0, t_0 + h_{start}]$ [16].

The s starting values for the exponential peer methods are computed by using MATLAB routine `ode15s`.

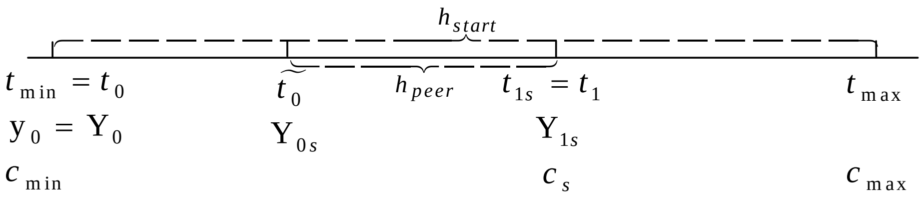

FIGURE 3.1: A simplified diagram to illustrate h_{peer} and h_{start}.

To avoid computations with negative step sizes we proceed as follows assuming $c_{\max} = \max_i(c_i)$ and $c_{\min} = \min_i(c)$.

From Fig. 3.1 we have

$$
\begin{aligned}
t_{\max} &= \tilde{t}_0 + c_{\max}\, h_{peer} \qquad \& \qquad t_{\max} = t_0 + h_{start} \\
\tilde{t}_0 + c_{\max}\, h_{peer} &= t_0 + \ h_{start} \\
\text{But} \quad t_0 &= \tilde{t}_0 + c_{\min}\, h_{peer} \\
t_0 - c_{\min} h_{peer} + c_{\max} h_{peer} &= t_0 + h_{start} \\
h_{peer} &= \frac{1}{c_{\max} - c_{\min}} h_{start}.
\end{aligned}
$$

Also

$$
\begin{aligned}
t_{0i} &= \tilde{t}_0 + c_i\, h_{peer} \\
t_{0i} &= t_0 + (c_i - c_{\min})\ h_{peer} \\
t_{0i} &= t_0 + \frac{c_i - c_{\min}}{c_{\max} - c_{\min}}\ h_{start}.
\end{aligned}
$$

To perform n_{steps} with the peer method to reach t_{end} we define,

$$
\begin{aligned}
Y_{0i} &:= \tilde{y}(t_1 + (c_i - 1)h_{peer}) = \tilde{y}\left(t_0 + \frac{c_i - c_{\min}}{c_{\max} - c_{\min}}\, h_{start}\right) \\
h_{peer} &= \frac{t_{end} - t_1}{n_{steps}} \\
t_0 &= t_1 + c_{\min} h_{peer} - h_{peer} \\
t_1 &= t_0 + (1 - c_{\min})\, h_{peer}
\end{aligned}
$$

Therefore

$$
\begin{aligned}
h_{peer} &= \frac{t_{end} - t_0 - (1 - c_{\min})\, h_{peer}}{n_{steps}} \\
h_{peer} &= \frac{t_{end} - t_0}{n_{steps} + 1 - c_{\min}}.
\end{aligned}
$$

For the methods in our numerical tests $c_{\min} = c_1$ so

$$
h_{peer} = \frac{t_{end} - t_0}{n_{steps} + 1 - c_1}, \qquad t_{0i} = t_0 + (c_i - c_1)h_{start}, \quad i = 1, \ldots, s. \quad \square
$$

As test problems, we choose a one-dimensional semi-linear parabolic initial-boundary value problem, a Schrödinger type equation, the 1D Gray-Scott equation [3] and the Prothero-Robinson equation.

Problem 3.1. Parabolic test equation [40]

We consider the following parabolic differential equation

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

Problem 3.2. Schrödinger type equation

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

In the Problems 3.1 and 3.2 $\phi(t, x)$ is chosen to give the exact solution $u(t, x) = x(1 - x)e^{-t}$. Standard finite differences with $N = 200$, Dirichlet boundary conditions and exact initial conditions are used. T is defined by the space discretization of u_{xx}.

Problem 3.3. 1D Gray-Scott equation

The Gray-Scott equation is a reaction-diffusion equation, here in 1D,

$$
\begin{aligned}
u_t &= D_1 u_{xx} - uv^2 + a(1 - u), \\
v_t &= D_2 v_{xx} + uv^2 - (a + b)v, \\
a &= 0.035, \quad b = 0.065, \quad D_1 = 2.10^{-5}, \quad D_2 = 1.10^{-5},
\end{aligned}
$$

with periodic boundary conditions and scaled Gauss curves as initial conditions, see [3]. Fourier space discretization gives a diagonal matrix T of dimension 128.

Problem 3.4. Prothero-Robinson equation

This problem usually serves as model problem for stiff equations

$$u' = T(u - g(t)) + g'(t).$$

As an example we consider

$$g(t) = \begin{pmatrix} \cos(t) \\ \cos(2t) \end{pmatrix}, \quad T = \begin{pmatrix} 1 & 0 \\ a & a \end{pmatrix}, \quad a = -10^4.$$

The exact solution is $u(t) = \Big(\cos(t), \cos(2t)\Big)^T$. *The initial condition is* $u(0) = (1, 1)^T$. *This problem is very stiff,* $\| T \| \simeq 10^4$.

In the following figures we present the accuracy of the numerical solution Y at $t_{end} = 1$ versus the time step h varying from 10^{-3} to 10^0. The error is computed by the formula

$$Error = \frac{\|Y - Y_{ref}\|_\infty}{\|Y_{ref}\|_\infty},$$

where Y_{ref} is a reference solution which is computed with MATLAB routine `ode15s` and high accuracy. For comparison we included lines with slopes corresponding to orders $p = 3, \ldots, 7$ into Figures 3.2–3.5.

The results show that the exponential peer methods in general give very accurate results, and for the four test problems compare with order $p = s$, i.e., with the non-stiff order. There is no order reduction as in some other methods, cf. Section 5.1.

Although we were only able to prove theoretically stiff order $p = s - 1$ for the considered stiff problems the observed order is $p = s$. An explanation of this fact can be given by the following two remarks.

Remark 3.4. *For* $\omega < 0$ *and sufficiently small Lipschitz constant* L*, we obtain for constant step sizes in the recursion for the global error*

$$\| \varepsilon_{m+1} \| \leq \gamma \| \varepsilon_m \| + C\, h^{q+1}$$

with $\gamma = e^{\omega\alpha^* h} + h\, D < 1$. *With* $\varepsilon_0 = 0$ *this gives*

$$\| \varepsilon_{m+1} \| \leq \frac{C}{1-\gamma} h^{q+1}.$$

The method behaves for sufficiently small γ *as a method of order* $p = q + 1$, *an effect which is commonly observed in tests with constant step size.*

Remark 3.5. *Our theorems about the stiff-consistency order regarding* (3.5) *are based on the premise* (3.9). *The systems resulting from the semi-discretization of PDEs often show special boundedness properties, e.g., for homogeneous or periodic boundary conditions. Therefore in numerical tests on semi-discretized PDEs with constant step size in general a higher order of convergence of the methods is observed [3]. A detailed discussion of the exponential Runge-Kutta method for semi-discretized parabolic equation can be found in Hochbruck-Ostermann [24]. In [27] exponential Rosenbrock methods are investigated for autonomous systems, where* $T_m = f_y(y_m)$ *is used. Implicit exponential Runge-Kutta methods of collocation type are found in [25].*

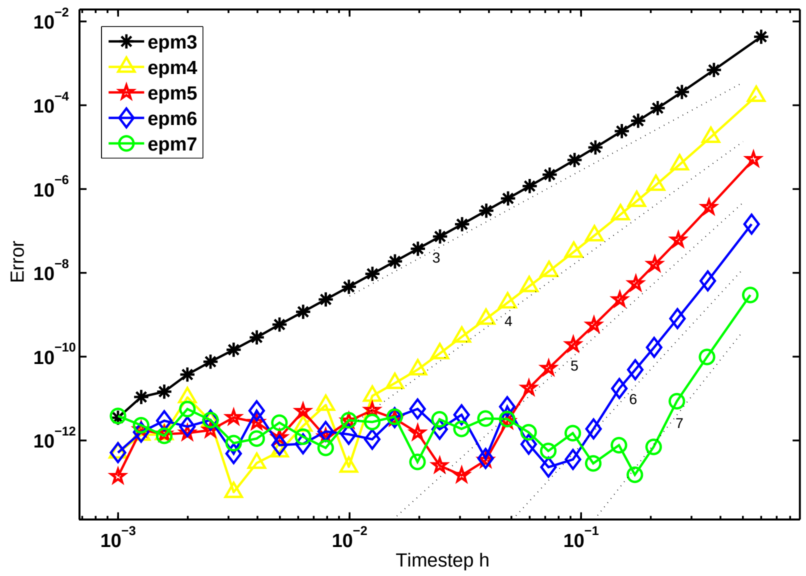

Figure 3.2: Order plot for the EPMs applied to Parabolic test equation (Prob. 3.1).

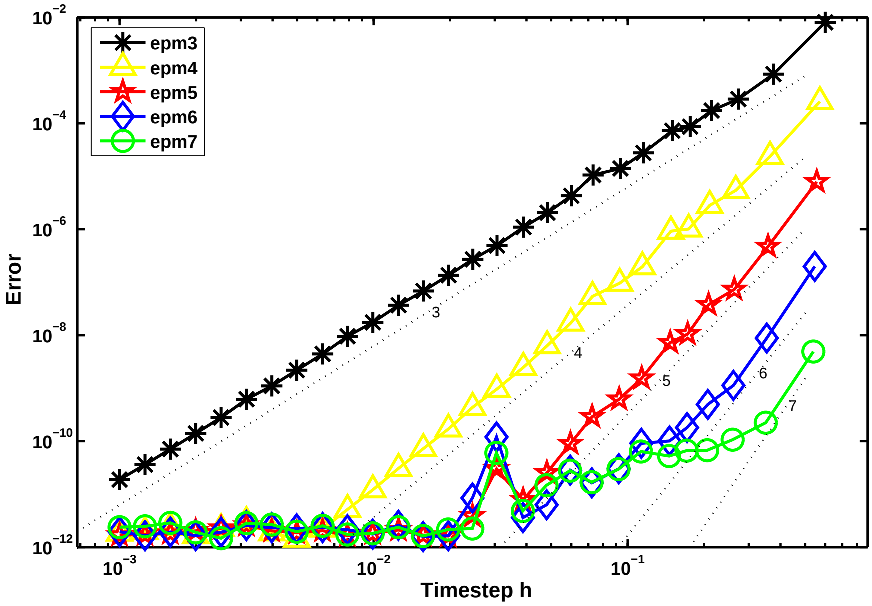

Figure 3.3: Order plot for the EPMs applied to Schrödinger type equation (Prob. 3.2).

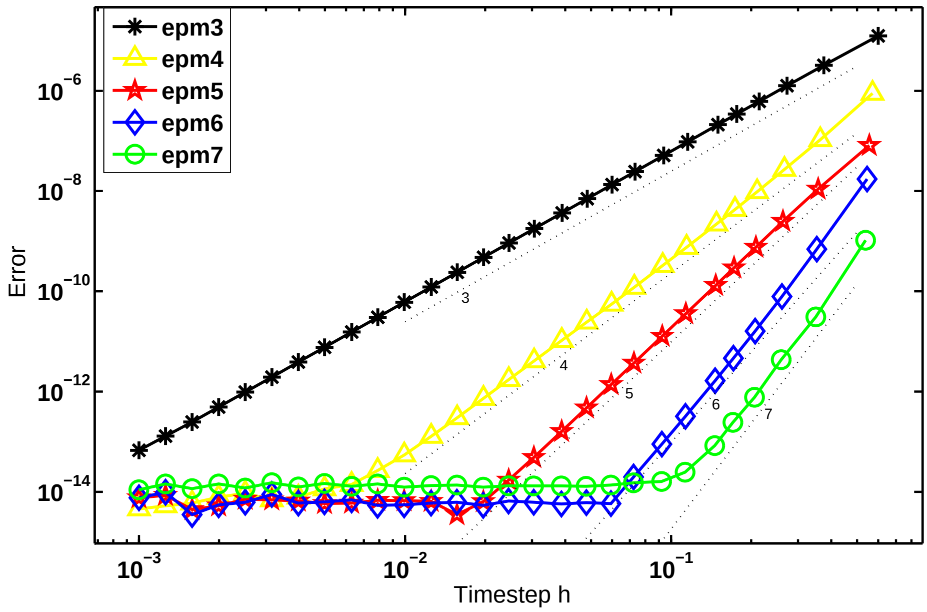

FIGURE 3.4: Order plot for the EPMs applied to Gray-Scott (Prob. 3.3).

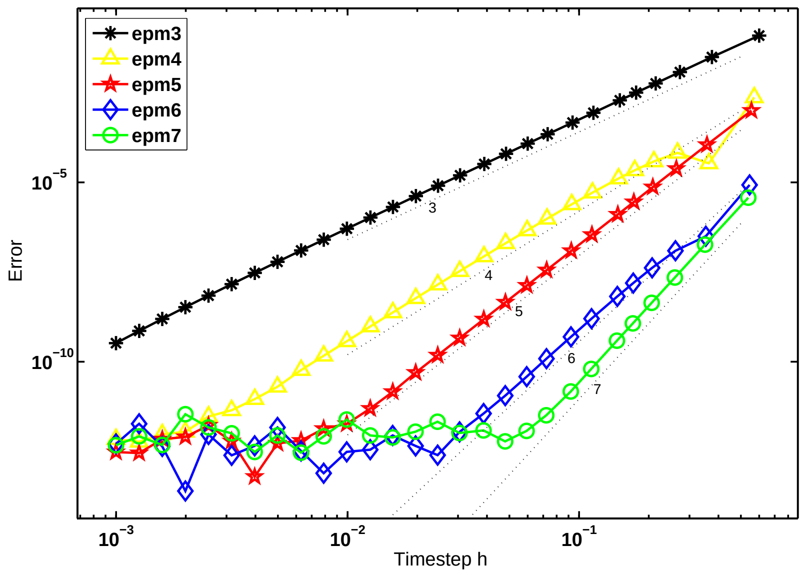

FIGURE 3.5: Order plot for the EPMs applied to Prothero-Robinson equation (Prob. 3.4).

Chapter 4

Exponential Peer Methods with Variable Step Sizes

Methods with step size control are currently the default methods for solving ODEs in major computing software. These methods, which can adapt the step size to the conditions of the problem, are most useful when the coefficients in the problem change very rapidly over some time intervals and smoothly otherwise. In this chapter, we generalize the investigations in Chapter 3 for variable step sizes. In Section 4.1.1 the formulation for variable step sizes are given. In Section 4.1.2 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 in Section 4.1.3. For a class with only two different arguments in the $\varphi-$functions bounds for the step size ratio are derived which guarantee zero-stability. These bounds are sufficiently large for practical computations. In Section 4.2 various aspects of the implementation are discussed, especially possibilities of error estimation and step size control.

4.1 Exponential peer methods with variable step sizes

4.1.1 Definition of EPMs with variable step sizes

In this section we generalize the numerical methods presented in Chapter 3 for variable step sizes for the numerical solution of the initial value problem (3.5).

We consider the class of exponential peer methods with variable step sizes

$$\begin{aligned} Y_{mi} &= \varphi_0(\alpha_i h_m T_m) \sum_{j=1}^{s} b_{ij}\, Y_{m-1,j} + h_m \sum_{j=1}^{s} A_{ij}(\alpha_i h_m T_m)[f_{m-1,j} - T_m\, Y_{m-1,j}] \\ &+ h_m \sum_{j=1}^{i-1} R_{ij}(\alpha_i h_m T_m)[f_{m,j} - T_m\, Y_{mj}], \qquad i = 1, 2, \ldots, s. \end{aligned} \tag{4.1}$$

Here the coefficients c_i and α_i are constant and we assume $\alpha_i \geq 0$, and the coefficients $b_{ij} \in \mathbb{R}$ will depend on the step size ratio

$$\sigma_m = \frac{h_m}{h_{m-1}}. \tag{4.2}$$

The matrix functions $A_{ij}\,(h_m T_m)$ and $R_{ij}\,(h_m T_m)$ are linear combinations of the well known $\varphi-$functions, see Section 2.4. They depend on the step size ratio too. Parallel methods are obtained by the choice $R = 0$ eliminating any reference to the stages Y_{mi} of the actual step.

As in Chapter 3, 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 $f_{m,j} = f(t_{mj}, Y_{mj})$. By setting $T_m = 0$ we obtain explicit peer methods. In this chapter we will consider $T_m = T$.

4.1.2 Consistency

In this section we will derive order conditions for EPMs (4.1) with variable step sizes when applied to stiff semi-linear problems (3.5).

Again we will assume that the stiffness in (3.5) is due to the linear part Ty and that the nonlinear part satisfies a global Lipschitz condition (3.8) with Lipschitz constant L_g of moderate size. We assume that T has a bounded logarithmic norm ω (3.9).

In the case of variable step sizes the local residual errors Δ_{mi} are

$$\begin{aligned}\Delta_{mi} = y(t_{mi}) - \varphi_0(\alpha_i h_m T_m) \sum_{j=1}^{s} b_{ij}\, y(t_{m-1,j}) \\ -h_m \sum_{j=1}^{s} A_{ij}(\alpha_i h_m T_m)\Big[y'(t_{m-1,j}) - T_m\, y(t_{m-1,j})\Big] \\ -h_m \sum_{j=1}^{i-1} R_{ij}(\alpha_i h_m T_m)\Big[y'(t_{mj}) - T_m\, y(t_{mj})\Big], \quad i = 1, \dots, s. \end{aligned} \tag{4.3}$$

By Taylor expansion of the exact solution $y(t)$ and $y'(t)$ at the point t_m, we have

$$\begin{aligned} y\big(t_{mi}\big) &= y\big(t_m + c_i h_m\big) = \sum_{r=0}^{q} \frac{h_m^r c_i^r}{r!} y^{(r)}(t_m) + \mathcal{O}(h_m^{q+1}), \\ y\big(t_{m-1,j}\big) &= y\big(t_{m-1} + c_j\, h_{m-1}\big) = y\big(t_m + (c_j - 1)\, h_{m-1}\big) \\ &= y\Big(t_m + \frac{(c_j - 1)\, h_m}{\sigma_m}\Big) \quad \text{by}(4.2) \\ &= \sum_{r=0}^{q} \frac{(c_j - 1)^r\, h_m^r}{\sigma_m^r r!} y^{(r)}(t_m) + \mathcal{O}(h_m^{q+1}), \\ y'\big(t_m + c_j\, h_m\big) &= \sum_{r=0}^{q} \frac{h_m^r c_j^r}{r!} y^{(r+1)}(t_m) + \mathcal{O}(h_m^{q+1}), \\ y'\big(t_{m-1,j}\big) &= y'\big(t_{m-1} + c_j\, h_{m-1}\big) = y'\big(t_m + (c_j - 1)\, h_{m-1}\big) \\ &= y'\Big(t_m + \frac{(c_j - 1)\, h_m}{\sigma_m}\Big) \quad \text{by}(4.2) \\ &= \sum_{r=0}^{q} \frac{(c_j - 1)^r\, h_m^r}{\sigma_m^r r!} y^{(r+1)}(t_m) + \mathcal{O}(h_m^{q+1}), \end{aligned}$$

where the $\mathcal{O}$-term is uniformly bounded due to the smoothness assumption on the solution.

Substitution into (4.3) yields

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

$$- h_m \sum_{j=1}^{i-1} R_{ij}\left(\alpha_i h_m T_m\right) \sum_{r=0}^{q} \left\{ c_j^r \, y^{(r+1)}(t_m) - T_m c_j^r \, y^{(r)}(t_m) \right\} \frac{h_m^r}{r!} + \mathcal{O}(h_m^{q+1})$$

By collecting the coefficients of $\dfrac{h_m^r}{r!} y^{(r)}(t_m)$we get

$$\begin{aligned}
\Delta_{mi} = \sum_{r=0}^{q} \Bigg\{ & c_i^r I - \varphi_0(\alpha_i h_m T_m) \sum_{j=1}^{s} b_{ij} \Big(\frac{c_j - 1}{\sigma_m}\Big)^r - r \sum_{j=1}^{s} A_{ij}(\alpha_i h_m T_m)(c_j - 1)^{r-1} \\
& + h_m T_m \sum_{j=1}^{s} A_{ij}(\alpha_i h_m T_m) \Big(\frac{c_j - 1}{\sigma_m}\Big)^r - r \sum_{j=1}^{i-1} R_{ij}(\alpha_i h_m T_m) c_j^{r-1} \\
& + h_m T_m \sum_{j=1}^{i-1} R_{ij}(\alpha_i \, h_m \, T_m) c_j^r \Bigg\} \frac{h_m^r}{r!} y^{(r)}(t_m) + \mathcal{O}(h_m^{q+1})
\end{aligned} \tag{4.4}$$

Here the remainder results from products of the coefficients of the method with the $\mathcal{O}(h_m^{q+1})$-terms of the Taylor expansion of the solution. Due to Remark 3.1 the remainder is bounded independent of $\|T_m\|$.

Again we consider the linear case $y' = Ty$ first.

Theorem 4.1. *If the exponential peer method satisfies the conditions*

$$\sum_{j=1}^{s} b_{ij} \left(\frac{c_j - 1}{\sigma_m}\right)^l = (c_i - \alpha_i)^l, \quad l = 0, 1, \ldots, q, \tag{4.5}$$

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

Proof. From (4.3), for the equation $y' = Ty$ the local residual errors will be

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

Using the relation

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

we obtain

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

$$-\sum_{j=1}^{s} b_{ij}\left(\alpha_i+\frac{c_j-1}{\sigma_m}\right)^{q+1}\varphi_{q+1}\left(\left(\alpha_i+\frac{c_j-1}{\sigma_m}\right)h_mT_m\right)\Bigg\}T_m^{q+1}y(t_m).$$

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 $\dfrac{h_m^lT_m^l}{l!}y(t_m)$ for $l=0,\dots,q$, 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 (4.5) for $q=s-1$ as matrix equation and solving for B we obtain

Corollary 4.1. *Let*

$$B_m=V_\alpha S_m V_1^{-1}, \tag{4.6}$$

where

$$S_m=diag(1,\sigma_m,\dots,\sigma_m^{s-1})=\begin{pmatrix}1&0&0&\dots&0\\0&\sigma_m&0&\dots&0\\0&0&\sigma_m^2&\dots&0\\\vdots&\vdots&\vdots&\ddots&\vdots\\0&0&0&\dots&\sigma_m^{s-1}\end{pmatrix}.$$

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

Corollary 4.2. *Let $\alpha=c$, $c_s=1$. Then with (4.6) we have $B=\mathbb{1}e_s^T$, and*

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

Therefore (4.5) is satisfied for all l, the exponential peer method solves the system $y'=Ty$ with exact starting values exactly. □

If $q = s-1$, then the general solution of (4.5) will be

$$b_{ij} = \prod_{\substack{k=1\\k\neq j}}^{s} \frac{c_k + (\alpha_i - c_i)\sigma_m - 1}{c_k - c_j}$$

For special choices of the nodes c_i and the values of α_i, we consider the following two examples for the choice of c and α.

Case 1 (*Corollary* 4.2) Let $c = \alpha$. This gives $V_\alpha = \mathbb{1}e_1^T$ and with $e_1^T S_m = e_1^T$ we have

$$B = \begin{pmatrix} 0 & 0 & \dots & 0 & 1 \\ 0 & 0 & \dots & 0 & 1 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 0 & 1 \\ 0 & 0 & \dots & 0 & 1 \end{pmatrix} = \mathbb{1}e_s^T,$$

where $e_1 = (1, 0, \dots, 0)^T$.

An advantage of this choice is that the matrix B will not depend on the step size ratio σ, so the method will be zero-stable for all step size sequences (see Theorem 4.4) and a disadvantage of this choice is that $\varphi-$functions of s different arguments have to be calculated. This leads to a high computational effort.

To minimize the number of φ-function evaluations, as in Chapter 3 we choose to set the parameter α to have only two different arguments.

Case 2 Let

$$\begin{aligned} \alpha_s = 1, \qquad \alpha_i = \alpha^*, \quad i = 1, \dots, s-1, \\ c_i = (s-i)(\alpha^* - 1) + 1, \quad i = 1, \dots, s. \end{aligned} \tag{4.7}$$

Then

$$B_m = \begin{pmatrix} b_{11}(\sigma_m) & b_{12}(\sigma_m) & \dots & b_{1,s-1}(\sigma_m) & b_{1s}(\sigma_m) \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ b_{s-2,1}(\sigma_m) & b_{s-2,2}(\sigma_m) & \dots & b_{s-2,s-1}(\sigma_m) & b_{s-2,s}(\sigma_m) \\ 0 & 0 & \dots & 0 & 1 \\ 0 & 0 & \dots & 0 & 1 \end{pmatrix}$$

In the following we will always assume B to be defined by (4.6).

We now will consider the general case (3.5) to obtain conditions for the matrix coefficients $A_{ij}(\alpha_i hT)$ and $R_{ij}(\alpha_i hT)$.

From (4.4) with (4.5) we need to show that the coefficients of $\frac{h_m^r T_m^r}{r!} y(t_m)$ for $r = 0, \ldots, q$ are zeros.

In general we have the following theorem:

Theorem 4.2. *Let the conditions* (4.5) *be satisfied for* $l = 0, \ldots, q$. *Let further*

$$\sum_{j=1}^{s} A_{ij}(\alpha_i h_m T_m) \left(\frac{c_j - 1}{\sigma_m} \right)^r + \sum_{j=1}^{i-1} R_{ij}(\alpha_i h_m T_m) c_j^r = \sum_{l=0}^{r} \binom{r}{l} l! \alpha_i^{l+1} (c_i - \alpha_i)^{r-l} \varphi_{l+1}(\alpha_i h_m T_m) \tag{4.8}$$

for $r = 0, \ldots, q$. *Then the exponential peer method is at least of stiff order* $p = q$ *for* (3.5).

Proof. For order q the coefficients of $y^{(r)}(t_m)$ in (4.4) should be equal to zero for $r = 0, \ldots, q$.

For $r = 0$ using (4.5) and (4.8) we obtain

$$\begin{aligned} I - \varphi_0(\alpha_i h_m T_m) \sum_{j=1}^{s} b_{ij} + h_m T_m \sum_{j=1}^{s} A_{ij}(\alpha_i h_m T_m) + h_m T_m \sum_{j=1}^{i-1} R_{ij}(\alpha_i h_m T_m) \\ = I - \varphi_0(\alpha_i h_m T_m) + \alpha_i h_m T_m \varphi_1(\alpha_i h_m T_m) = 0 \quad \text{by (2.3)}. \end{aligned}$$

For $r = 1, \ldots, q$ holds for the coefficients

$$\begin{aligned} & c_i^r I - \varphi_0(\alpha_i h_m T_m) \sum_{j=1}^{s} b_{ij} \left(\frac{c_j - 1}{\sigma_m} \right)^r - r \sum_{j=1}^{s} A_{ij}(\alpha_i h_m T_m) \left(\frac{c_j - 1}{\sigma_m} \right)^{r-1} \\ & \quad + h_m T_m \sum_{j=1}^{s} A_{ij}(\alpha_i h_m T_m) \left(\frac{c_j - 1}{\sigma_m} \right)^r - r \sum_{j=1}^{i-1} R_{ij}(\alpha_i h_m T_m) c_j^{r-1} \\ & +h_m T_m \sum_{j=1}^{i-1} R_{ij}(\alpha_i h_m T_m) c_j^r \\ & = c_i^r I - \varphi_0(\alpha_i h_m T_m)(c_i - \alpha_i)^r - r \sum_{l=0}^{r-1} \binom{r-1}{l} \alpha_i^{l+1} (c_i - \alpha_i)^{r-1-l} l! \varphi_{l+1}(\alpha_i h_m T_m) \\ & \quad + h_m T_m \sum_{l=0}^{r} \binom{r}{l} \alpha_i^{l+1} (c_i - \alpha_i)^{r-l} l! \varphi_{l+1}(\alpha_i h_m T_m) \quad \text{by (4.8)} \end{aligned}$$

$$=c_i^r I - \varphi_0(\alpha_i h_m T_m)(c_i-\alpha_i)^r - r\sum_{l=1}^{r}\binom{r-1}{l-1}\alpha_i^l(c_i-\alpha_i)^{r-l}(l-1)!\varphi_l(\alpha_i h_m T_m)$$
$$+\sum_{l=0}^{r}\binom{r}{l}\alpha_i^l(c_i-\alpha_i)^{r-l}(l!\varphi_l(\alpha_i h_m T_m)-I) \quad \text{by (2.3)}$$

Using the fact $l\binom{r}{l} = r\binom{r-1}{l-1}$

$$=c_i^r I - \varphi_0(\alpha_i h_m T_m)(c_i-\alpha_i)^r - \sum_{l=1}^{r}\binom{r}{l}\alpha_i^l(c_i-\alpha_i)^{r-l}l!\varphi_l(\alpha_i h_m T_m)$$
$$+\sum_{l=0}^{r}\binom{r}{l}\alpha_i^l(c_i-\alpha_i)^{r-l}l!\varphi_l(\alpha_i h_m T_m) - c_i^r I = 0. \qquad \blacksquare$$

Corollary 4.3. *Let $\alpha = c$, $c_s = 1$ and B given by (4.6). Let*

$$\sum_{j=1}^{s} A_{ij}(c_i h_m T_m)\left(\frac{c_j-1}{\sigma_m}\right)^r + \sum_{j=1}^{i-1} R_{ij}(c_i h_m T_m)c_j^r = r!c_i^{r+1}\varphi_{r+1}(c_i h_m T_m) \tag{4.9}$$

for $r = 0, \dots, q$. 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 (4.8) 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 $T_m y^{(q+1)}$ (non-stiff order), then the order of the methods will be $p = q+1$,

Theorem 4.3. *Let the solution $y(t)$ be $(q+2)$-times continuously differentiable. Let the conditions (4.5) be satisfied for $l = 0, \dots, q+1$, and (4.8) for $l = 0, \dots, q$. Then the method is of non-stiff order $p = q+1$.*

Proof. The beginning of the proof is identical to the proof of Theorem 4.2. Considering one more term in (4.8) gives for the term with h_m^{q+1}

$$\Bigg\{c_i^{q+1}I - \varphi_0(\alpha_i h_m T_m)\sum_{j=1}^{s} b_{ij}\left(\frac{c_j-1}{\sigma_m}\right)^{q+1} - (q+1)\sum_{j=1}^{s} A_{ij}(\alpha_i h_m T_m)\left(\frac{c_j-1}{\sigma_m}\right)^{q}$$
$$-(q+1)\sum_{j=1}^{i-1} R_{ij}(\alpha_i h_m T_m)c_j^q + h_m T_m\sum_{j=1}^{i-1} R_{ij}(\alpha_i h_m T_m)c_j^{q+1}$$

$$+h_m T_m \sum_{j=1}^{s} A_{ij}(\alpha_i h_m T_m) \left(\frac{c_j - 1}{\sigma_m}\right)^{q+1} \Bigg\} \frac{h_m^{q+1}}{(q+1)!} y^{(q+1)}(t_m)$$

$$= \Bigg\{ c_i^{q+1} I - \varphi_0(\alpha_i h_m T_m)(c_i - \alpha_i)^{q+1}$$

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

Using the fact $\binom{q+1}{l+1} = \frac{q+1}{l+1} \binom{q}{l}$

$$= \Bigg\{ c_i^{q+1} I - \varphi_0(\alpha_i h_m T_m)(c_i - \alpha_i)^{q+1}$$

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

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

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

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

$$= \mathcal{O}\left(h_m^{q+2}\right).$$

So $\Delta_{mi} = \mathcal{O}\left(h_m^{q+2}\right)$ and the method is of non-stiff order $p = q + 1$. ■

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

4.1.3 Stability and convergence

Due to the variable step size, zero-stability now leads to restrictions of the step size ratio in general. The methods of Case 1 are zero-stable for all step size sequences. For Case 2, we compute bounds on the step size ratio which guarantee zero-stability. These bounds are fairly large for practical computations.

Definition 4.1. *The exponential peer method* (4.1) *is called stable (zero-stable) if*

$$\|B_{m+l} B_{m+l-1} \dots B_m\| \leq K \quad \textit{for all } m, l \geq 0. \tag{4.10}$$

In general B_m depends on the step ratio σ_m (i.e. $B_m = B(\sigma_m)$). Therefore, condition (4.10) 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 multi-step and general linear methods. Here we will consider two special classes of exponential peer methods. The first is given with the choice of Corollary 4.2.

Theorem 4.4. *Let $\alpha = c$, $c_s = 1$ and B given by (4.6). Then the exponential peer method is stable for all step size sequences.*

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

The choice $\alpha = c$ is optimal with respect to stability. However, this class of methods requires the computation of $\varphi-$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 Section 3.3 for constant step sizes. We will consider here the stability of this class for variable step sizes.

Theorem 4.5. *Let $\alpha = (\alpha^*, \ldots, \alpha^*, 1)^T$ and $c_i = (s-i)(\alpha_i - 1) + 1$, $i = 1, \ldots, s$. Let B given by (4.6). 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 Section 3.3 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 $F_0 = (\delta_{i-1,j})_{i,j=1}^s$. $B(1)$ 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 $\Lambda = \mathrm{diag}(0, 1, \varepsilon, \ldots, \varepsilon^{s-2})$, with a parameter $0 < \varepsilon < 1$, transforms $B(1)$ to Jordan canonical form [12]

$$Q^{-1}B(1)Q = \psi = \begin{pmatrix} 1 & 0 & 0 & \ldots & 0 & 0 \\ 0 & 0 & \epsilon & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \ldots & 0 & \epsilon \\ 0 & 0 & 0 & \ldots & 0 & 0 \end{pmatrix} =: \begin{pmatrix} 1 & 0 & \ldots & 0 \\ 0 & & & \\ \vdots & & \widehat{\psi} & \\ 0 & & & \end{pmatrix}. \tag{4.11}$$

This follows from

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

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

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

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

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

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

For $s = 3, 4, 5$ we have computed the following bounds with Maple:

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

These bounds are sufficiently large for practical computations. Note that $\sigma_{min} = 0$ what is a necessary property for practical use of the method.

Remark 4.1. *By considering the special case of increasing h in each step by a constant factor σ we found numerically $\sigma_{max} = \dfrac{s-1}{s-2}$. So we suppose that there exists some norm such that*

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

Remark 4.2. *If we perform $s-1$ consecutive steps with constant step size, then $\Big(B(1)\Big)^{s-1} = \mathbb{1}e_s^T$, 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.*

We now consider convergence. We denote

$$\Phi_m = \operatorname{diag}\left(\varphi_0(\alpha_i h_m T_m)\right)_{i=1}^{s}.$$

To prove convergence of our methods in addition to consistency we have to show

$$\|\prod_{j=m+l}^{m} \Phi_j(B_j \otimes I)\| \leq K \quad \text{for all} \quad 0 \leq m < m+l \leq N-1, \quad t_N = t_{end}. \tag{4.12}$$

For simplicity of notation in the following we consider scalar equations. In the non-stiff case we can exploit the property

$$\Phi_m = I + \mathcal{O}(h_m).$$

Then zero-stability ensures convergence. Denote the global error by

$$\varepsilon_m = Y(t_m) - Y_m.$$

Theorem 4.6. *Let the method be consistent of non-stiff order p and zero-stable for $0 < \sigma_m \leq \sigma_{max}$ with $\sigma_{max} > 1$. Let the starting values be of order p and let the coefficients of the method be bounded for $\sigma \leq \sigma_{max}$. Then the method is convergent of non-stiff order p.*

Proof. With the mean value theorem for vector functions and with (3.9) we have

$$\varepsilon_m = B_m\varepsilon_{m-1} + \mathcal{O}(h_m)\varepsilon_{m-1} + \mathcal{O}(h_m)\varepsilon_m + \Delta_m.$$

For $h_m \to 0$ follows

$$\begin{aligned}
\varepsilon_m &= B_m\varepsilon_{m-1} + \mathcal{O}(h_m)\varepsilon_{m-1} + (1 + \mathcal{O}(h_m))\Delta_m \\
&= \cdots \\
&= (B_m \cdots B_1)\varepsilon_0 + \sum_{j=0}^{m-1} \mathcal{O}(h_{j+1})(B_m \cdots B_{j+2})\varepsilon_j \\
&+ \sum_{j=0}^{m-1} (B_m \cdots B_{j+2})(1 + \mathcal{O}(h_{j+1}))\Delta_{j+1}.
\end{aligned}$$

With the assumptions on the starting values, by zero-stability and order of consistency p follows

$$\|\varepsilon_m\| \leq C_1 h_{max}^p + C_2 \sum_{j=0}^{m-1} h_{j+1}\|\varepsilon_j\|,$$

where $h_{\max} = \max\limits_m h_m$.

From this recursion analogously to the proof of Theorem 5.8, p. 408 in [18] convergence of order p follows. ■

Corollary 4.4. *The methods of Theorem 4.4 are convergent of non-stiff order p for all step size sequences. The methods of Theorem 4.5 are convergent of non-stiff order p with the values of σ_{max} given above.* □

In the stiff case the situation is more complicated. For the methods of Theorem 4.4 we have the special structure

$$\Phi_j B_j = \begin{pmatrix} 0 & \ldots & 0 & \varphi_0(\alpha^* h_j T_j) \\ \vdots & & \vdots & \vdots \\ 0 & \ldots & 0 & \varphi_0(\alpha^* h_j T_j) \\ 0 & \ldots & 0 & \varphi_0(h_j T_j) \end{pmatrix}$$

Relation (4.12) follows here immediately from (3.10). We obtain in standard way

Theorem 4.7. *Let the methods in Theorem 4.4 be consistent of stiff order p. Let the starting values be of order p and let the coefficients of the method be bounded for $\sigma \leq \sigma^*$ with $\sigma^* > 1$. Then the method is convergent of stiff order p.* $\square$

For the methods considered in Theorem 4.5 we need an additional assumption for the step size sequences, which is frequently considered for multistep methods with variable step sizes, cf. [18]:

$$\sum_{j=1}^{N-1} |\sigma_j - 1| \leq K_1, \quad t_N = t_{end}. \tag{4.13}$$

Then we can prove

Theorem 4.8. *Let the methods in Theorem 4.5 be consistent of stiff order p. Let the starting values be of order p. Let the coefficients $b_{ij}(\sigma)$ be continuously differentiable and let the coefficients of the method be bounded for $\sigma \leq \sigma^*$. Let (4.13) be satisfied, then the method is convergent of stiff order p.*

Proof. From the mean value theorem we have

$$|b_{ij}(\sigma) - b_{ij}(1)| \leq \gamma |\sigma - 1|$$

for all $0 < \sigma \leq \sigma^*$ with some constant γ. This yields for the ∞-norm

$$\|B_m\| = \|B(1) + B(\sigma_m) - B(1)\| \leq 1 + s\gamma|\sigma_m - 1|.$$

Then we have with $\gamma_1 = s\gamma$, $\beta = \max(\alpha^*\omega, \omega)$

$$\begin{aligned}
\|\prod_{j=m+l}^{m} \Phi_j(B_j \otimes I)\| &\leq \prod_{j=m+l}^{m} \|\Phi_j\|\|B_j\| \\
&\leq \prod_{j=m+l}^{m} e^{\beta h_j}\Big(1 + \gamma_1|\sigma_j - 1|\Big) \leq e^{\beta\left(t_{m+l}-t_m\right)} e^{\gamma_1 \sum_{j=m}^{m+l} |\sigma_j - 1|} \\
&\leq K.
\end{aligned}$$

With this stability result convergence follows in standard way. ■

4.2 Implementation issues

Variable step size codes adjust the step size in such a way, that the global error increment is kept below a certain tolerance threshold TOL. This requires a good estimation of this quantity. The error can be estimated by comparing two different methods.

We constructed exponential peer methods with variable step size due to Theorems 4.1 and 4.2 with $s-$stage of stiff order $p = s-1$. The nodes c_i are determined by Theorem 4.5 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 Chapter 3.

For error estimation we consider two possibilities

Interpolation

The main idea of this method is to interpolate values Y_{mi}, $i = 1, \ldots, s-1$, by an interpolation polynomial $P(t)$ of degree $s-2$. We compute a solution $\widetilde{Y}_{ms} = P(t_{m+1})$ of order $p = s-2$. For implementation purposes using interpolation, we will use the Newton form of the interpolation polynomial.

Embedding

The main idea of this method is to use two exponential peer schemes of different order. Basically, one estimates the error by computing the difference between a solution calculated with a given scheme and the one obtained using a scheme with a different order of accuracy.

For the time-step control, we use exponential peer methods of order $p-1$ and p. 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 $c = (c_2, \ldots, c_s)$ to compute $\widetilde{Y}_{ms}$ of order $s-2$.

(b) We solve the equations (4.8) for $i = s$ up to $r = s$. Because for $i = s$ (4.5) is also satisfied for $l = 0, \dots, s$, we have $\widetilde{Y}_{ms}$ of local order $p = s$. We use $\widetilde{Y}_{ms}$ for error estimation and continue with $Y_{m1}, \dots, Y_{m,s-1}, \widetilde{Y}_{ms}$.

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, respectively.

The error is estimated by

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

where $atol$ and $rtol$ are the absolute and relative error tolerances respectively.

We then compute $fac = err^{-1/(s-1)}$. With respect to Remark 4.2 the new step size is computed as follows

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

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

Coefficients for special methods are given in Appendix B.

Chapter 5

Numerical Results

In this section we use the framework of EXPINT [3] to test our methods. We have adapted our methods to the structure required and we use the computation of the $\varphi-$functions implemented in EXPINT.

For the calculation of $\varphi_\ell(z)$ all $\varphi_\jmath(z)$ with $\jmath < \ell$ are needed. This complicated calculation must be run again if T or the step size h changes. EXPINT is therefore kept the matrix T and the step size h over the entire integration constant, a typical approach in implementations of exponential integrators.

EXPINT contains several semidiscretized PDEs as test problems and a collection of well-known exponential integrators implemented with constant step size. By N the number of Fourier nodes or the number of inner points in a finite difference discretization is denoted.

Here we give only a short overview about the problems and for more detailed information we refer to [3] and the description in the package.

Problem 5.1. Allen-Cahn equation

The Allen-Cahn equation is a parabolic problem, which reads

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

The Dirichlet boundary conditions are chosen to be $u(t,-1) = -1$ *and* $u(t,1) = 1$. *The linear part* λu_{xx} *is discretized using a Chebyshev differentiation matrix resulting in a full matrix* T *of dimension* 64.

Problem 5.2. Kuramoto-Sivashinsky equation

The Kuramoto-Sivashinsky equation has been used to study many reaction-diffusion systems, in 1D it is written as

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

Spectral discretization with periodic boundary conditions and dimension $N = 128$ *is used. Various choices of initial condition are supported, the choice of smooth initial condition is*

$$u(x,0) = \cos\left(\frac{x}{16}\right)\left(1 + \sin\left(\frac{x}{16}\right)\right).$$

Problem 5.3. Nonlinear Schrödinger equation

The 1D nonlinear Schrödinger equation is

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

Periodic boundary conditions and the initial condition $u(0,x) = e^{\sin(2x)}$ *are considered. We used* $\lambda = 1$, $V(x) = \dfrac{1}{1+\sin^2 x}$ *and a spectral semi-discretization with* $N = 256$.

Problem 5.4. Hochbruck-Ostermann equation

A semi-linear parabolic problem with homogeneous Dirichlet boundary conditions from [24]

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

Problem 5.5. Hyperbolic test equation (cf. [40])

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

In the Problems 5.4 and 5.5 $\phi(t,x)$ *is chosen to give the exact solution* $u(t,x) = x(1-x)e^t$ *for problem 5.4, and* $u(t,x) = x(1-x)e^{-t}$ *for 5.5. Standard finite differences with* $N = 200$*, Dirichlet boundary conditions and exact initial conditions are used.* T *is defined by the space discretization of* u_{xx}.

Furthermore we use the Problems 3.1–3.4 of Section 3.4.

5.1 Numerical results for constant step sizes

In this section we compare our exponential peer methods with some of the exponential integrators included in EXPINT at these test problems. All calculations are performed with constant step sizes.

In what follows, we briefly describe the numerical schemes defining the exponential integrators that have been used in our comparative study. All these integrators belong to the EXPINT package. See [3] for more information about these methods.

- `ABLawson4` scheme has stiff order one and non-stiff order four and is based on the Adams-Bashforth scheme of order four (see Example 2.3).
- `Lawson4` scheme was developed by Lawson. It is based on the classical fourth order scheme of Rung-Kutta and this scheme has stiff order one and non-stiff order four (see Example 2.4).
- `ETD4RK` scheme was developed by Cox and Matthews [7]. It has four-stages and it has only stiff order two and non-stiff order four (see Example 2.5).
- `Strehmelweiner` scheme was developed by Strehmel and Weiner [47]. It is one of the earliest exponential Runge-Kutta methods with four stages, it has stiff order three (see Example 2.6).
- `hochost4` scheme was developed by Hochbruck and Ostermann [24]. It has five-stages and is the only known exponential Runge-Kutta method with stiff and non-stiff order four [3] (see Example 2.7).
- `RKMK4t` scheme uses a convenient truncation of the $dexp^{-1}$ operator, leading to the method of Munthe-Kaas [17], which again is of stiff order two but suffers from instabilities, especially when non-periodic boundary conditions are used (see Example 2.8).
- `ETD5RKF` scheme based on the six stage fifth order scheme of Fehlberg [14]. It has non-stiff order five and stiff order one. It usually performs worse than other order four schemes presented here due to bad error constant.

In our figures we will use the same names for the integrators and problems as in EXPINT.

In EXPINT package some schemes need some starting values. An exponential Runge-Kutta scheme can be used for the first $r-1$ steps. In our tests the scheme `hochost4` is used for the first $r-1$ steps e.g., For `ABLawson4` scheme the incoming approximation has the form $y^{[n-1]} = [y_{n-1}, hg_{n-2}, hg_{n-3}, hg_{n-4}]^T$.

The s starting values for the exponential peer methods are computed by using MATLAB routine `ode15s`. To avoid computations with negative step sizes we proceed as follows:

$$h_{peer} = \frac{t_{end} - t_0}{n_{steps} + 1 - c_1}, \qquad t_{0i} = t_0 + (c_i - c_1)h_{start}, \quad i = 1, \ldots, s.$$

In the following figures we present the accuracy of the numerical solution Y at $t_{end} = 1$ versus the timestep h. The error is computed by

$$Error = \frac{\|Y - Y_{ref}\|_\infty}{\|Y_{ref}\|_\infty},$$

where Y_{ref} is a reference solution which is computed with MATLAB routine `ode15s` and high accuracy. For comparison we included lines with slopes corresponding to orders $p = 4, 5$ in the figures.

In Figures 5.1–5.10 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` and `etd5rkf`, suffer from order reduction when applied to some test problems (see Fig. 3.2–5.10), but for exponential peer methods no order reduction is observed.

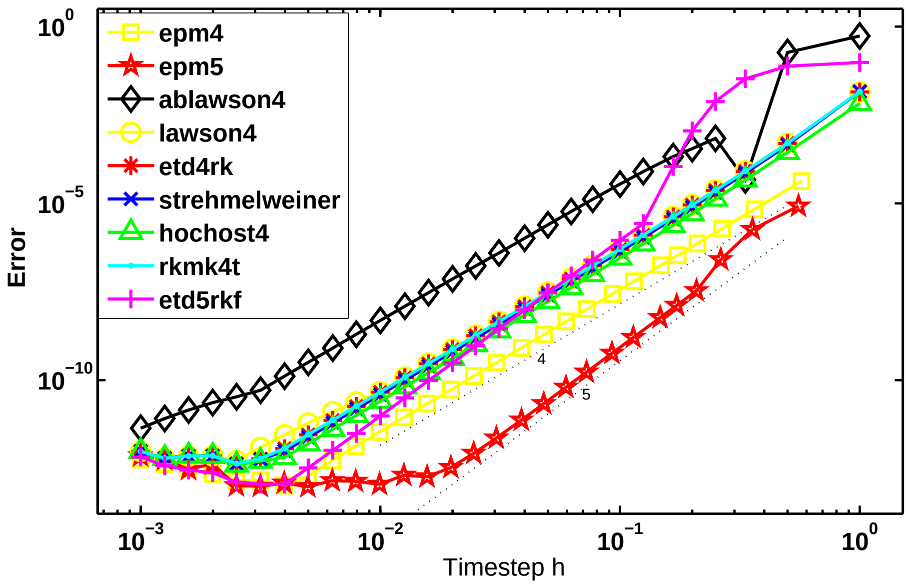

FIGURE 5.1: Results for Gray-Scott (Prob. 3.3).

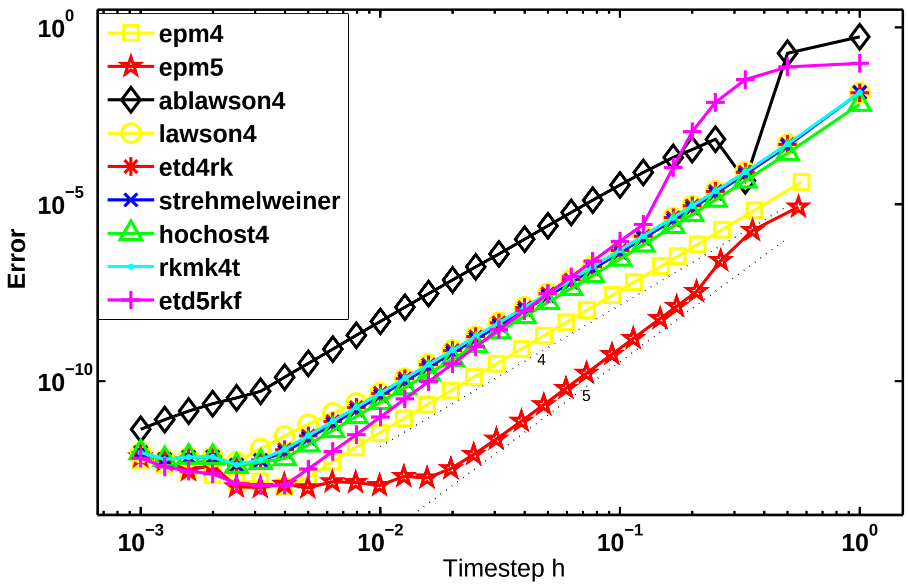

FIGURE 5.2: Results for the Allen-Cahn equation (Prob. 5.1).

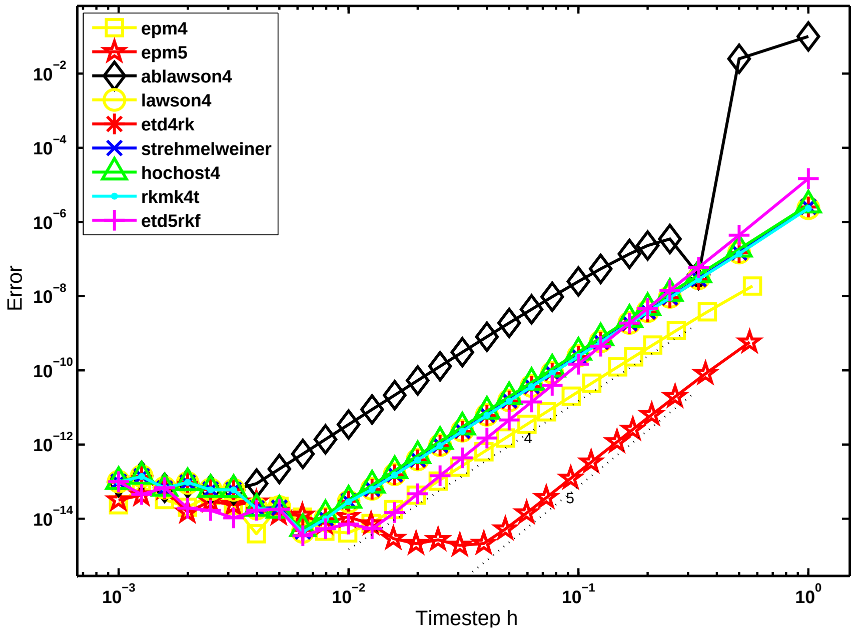

FIGURE 5.3: Results for the Kuramoto-Sivashinsky equation (Prob. 5.2).

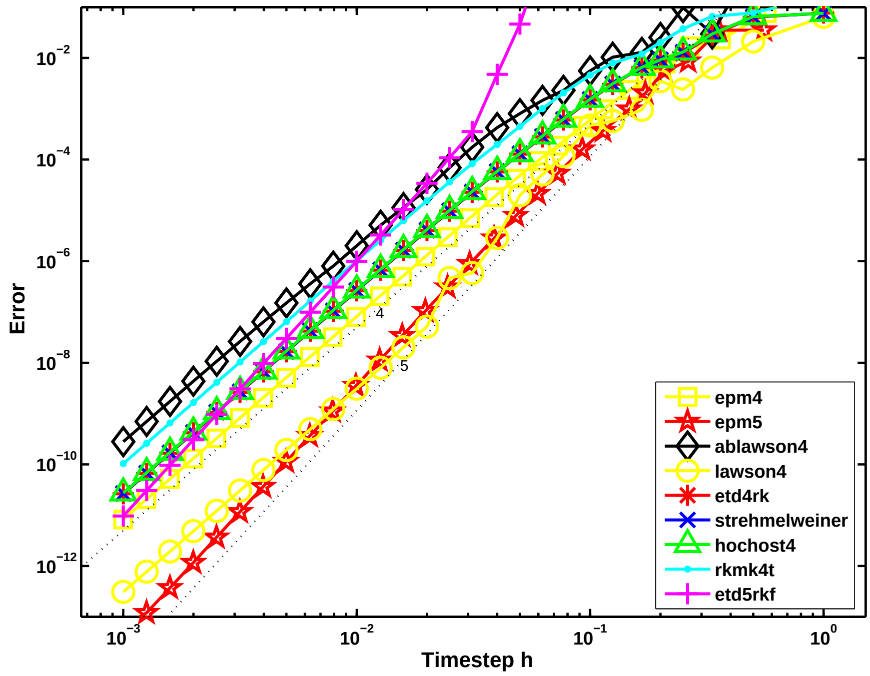

FIGURE 5.4: Results for the Nonlinear Schrödinger equation (Prob. 5.3).

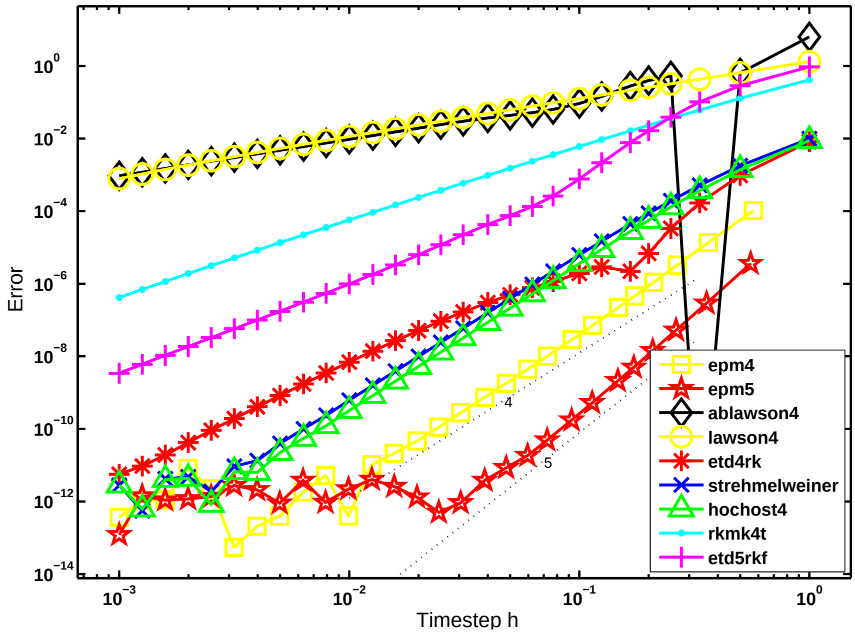

FIGURE 5.5: Results for the Hochbruck-Ostermann equation (Prob. 5.4).

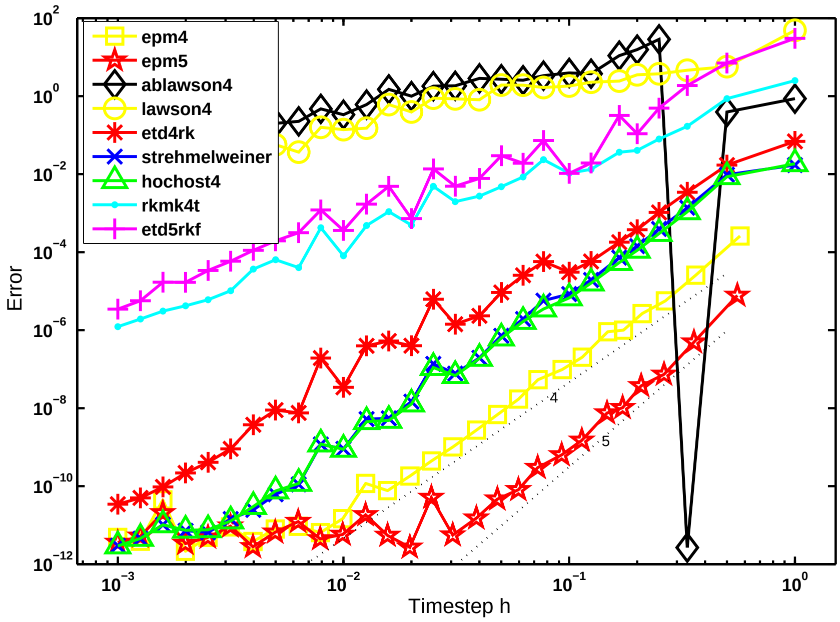

FIGURE 5.6: Results for the hyperbolic test equation (Prob. 5.5).

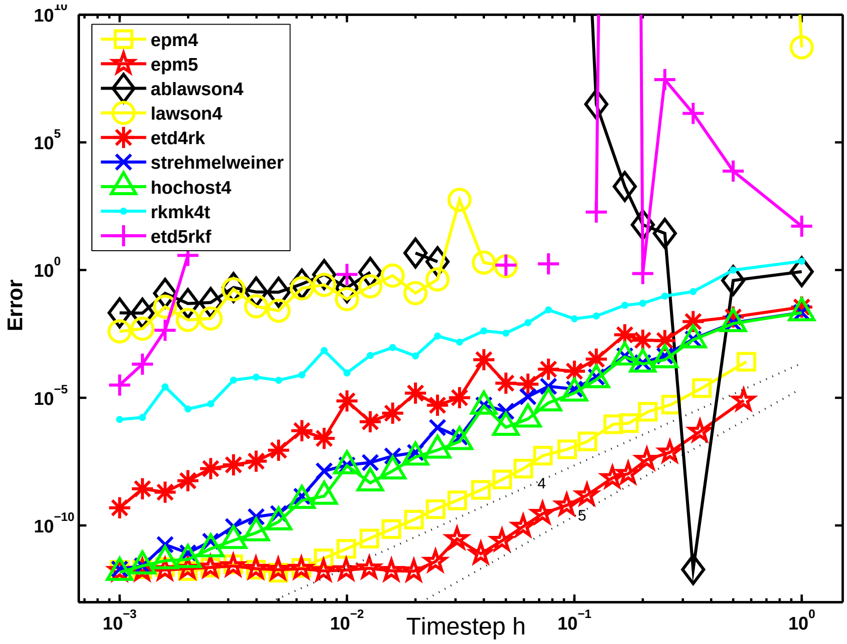

FIGURE 5.7: Results for the Schrödinger type equation (Prob. 3.2).

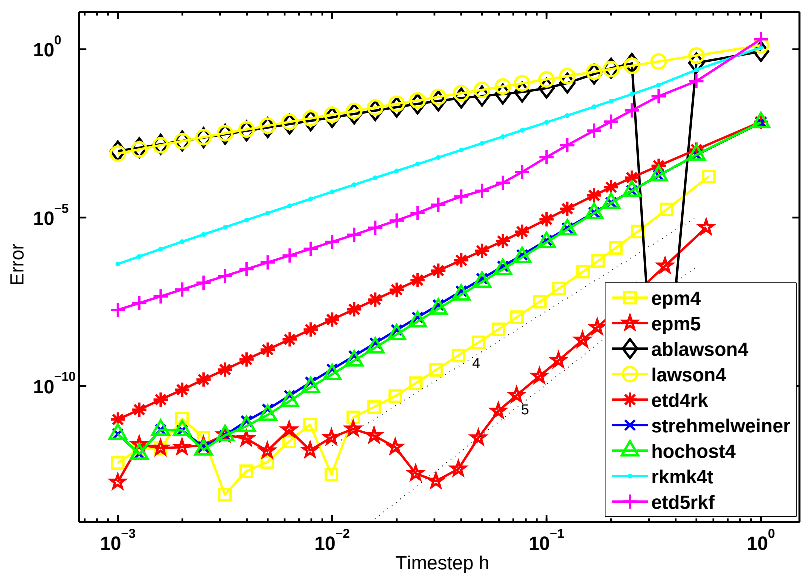

FIGURE 5.8: Results for the Parabolic test equation equation (Prob. 3.1).

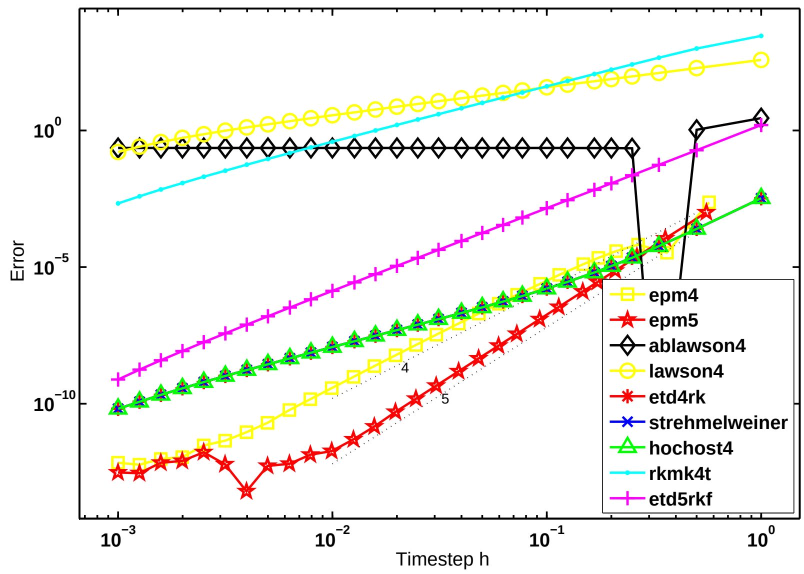

FIGURE 5.9: Results for Prothero-Robinson equation (Prob. 3.4).

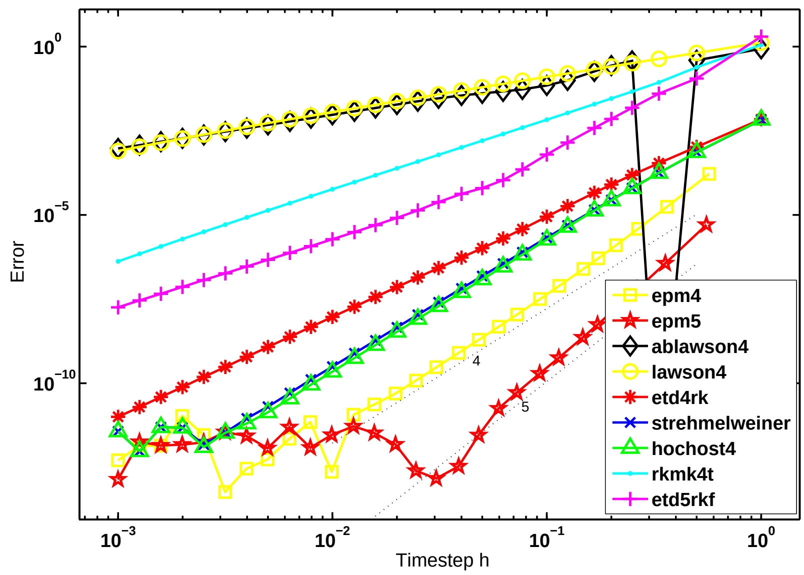

FIGURE 5.10: Results for Parabolic test equation (Prob. 3.1).

5.2 Numerical results for variable step sizes

In this section we test exponential peer methods for variable step sizes. The integrators in EXPINT are implemented with constant step size only. Therefore, we compare our exponential peer methods with MATLAB routines `ode15s` and `ode45` now at these test problems.

We constructed EPMs with variable step size due to Theorems 4.1 and 4.2 with $s = 3, 4, 5$ stages of stiff order $p = s - 1$. The nodes c_i are determined by Theorem 4.5 with $\alpha^* = \frac{s-1}{s}$.

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

In the following figures we present the accuracy of the numerical solution Y at $t_{end} = 10$ 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 MATLAB routine `ode15s` and high accuracy. We computed numerical solutions for the tolerances $atol = rtol = 10^{-1} - 10^{-10}$.

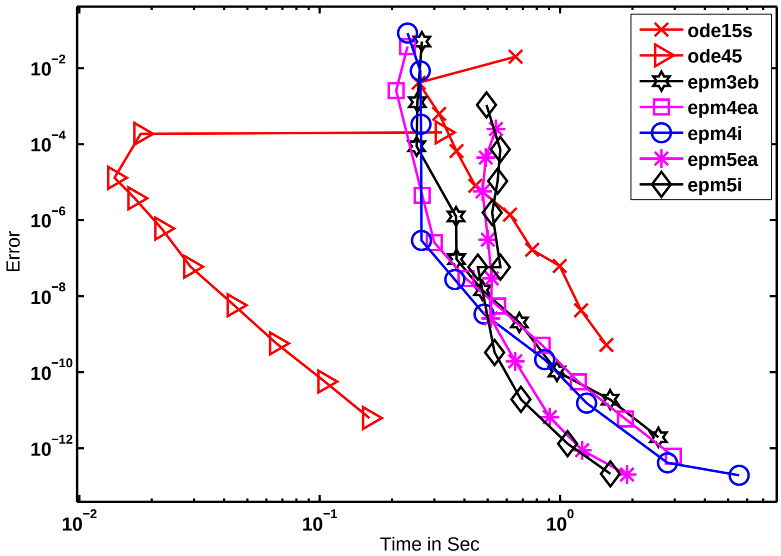

FIGURE 5.11: Results for Gray-Scott Prob. (Prob. 3.3).

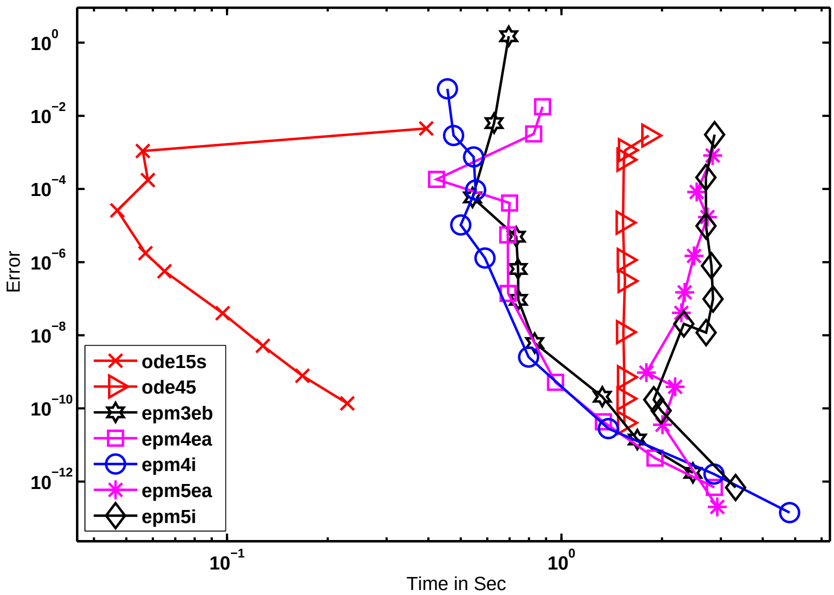

FIGURE 5.12: Results for the Allen-Cahn equation (Prob. 5.1).

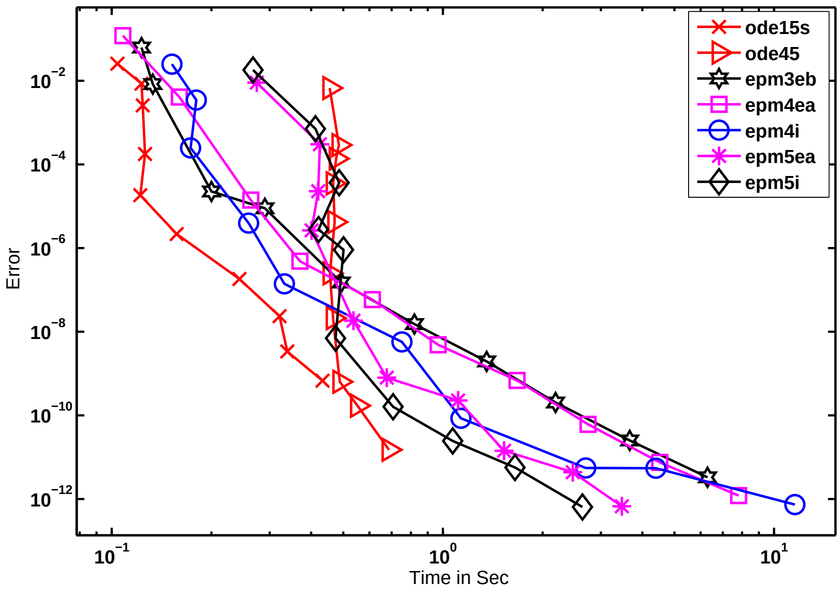

FIGURE 5.13: Results for the Kuramoto-Sivashinsky equation (Prob. 5.2).

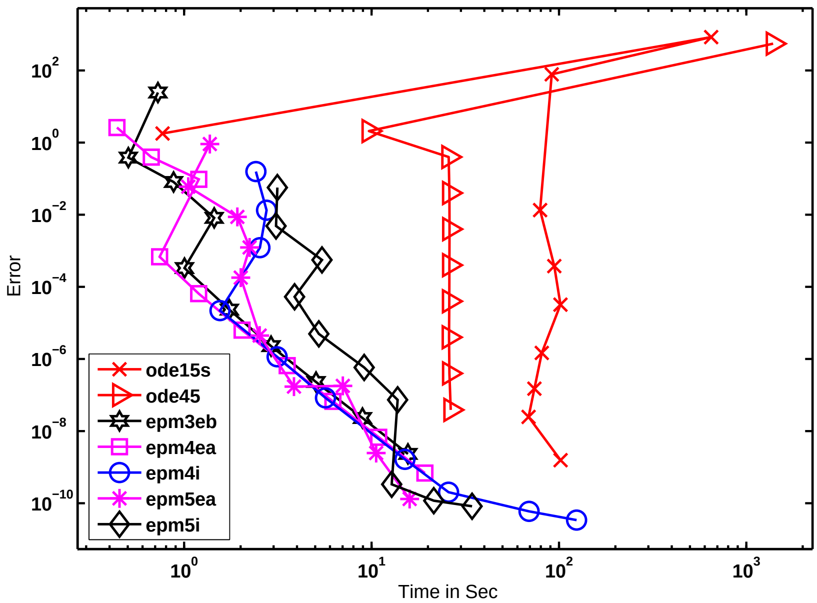

FIGURE 5.14: Results for the Nonlinear Schrödinger equation (Prob. 5.3).

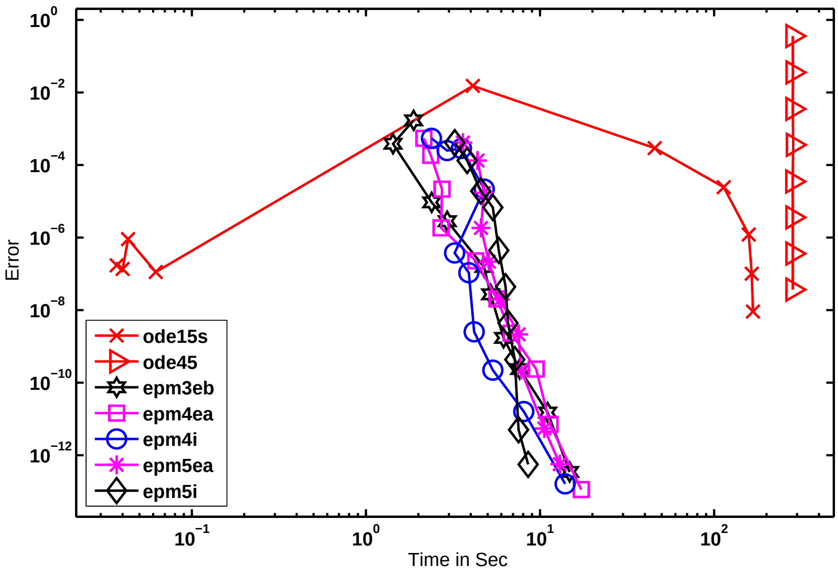

FIGURE 5.15: Results for the Schrödinger type equation (Prob. 3.2).

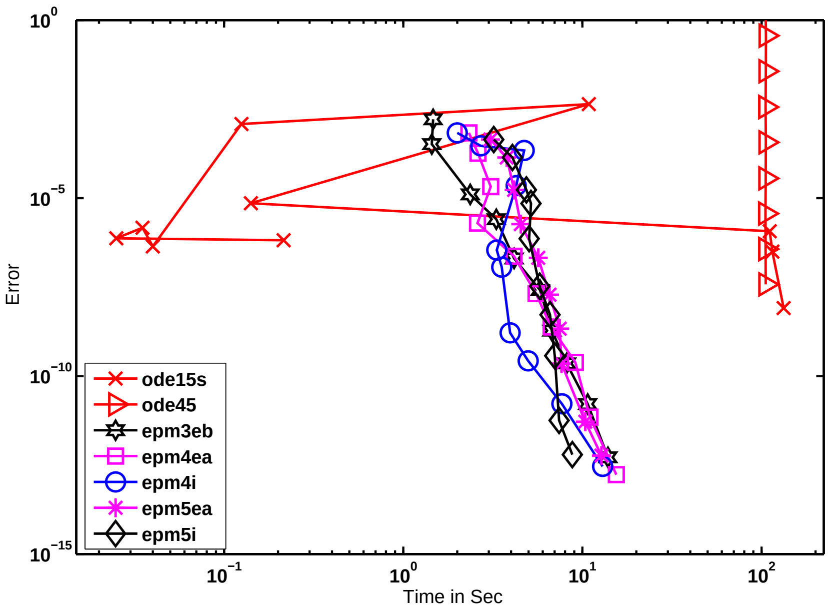

FIGURE 5.16: Results for the hyperbolic test equation (Prob. 5.5).

5.3 Discussion

The tests with constant step size show that the exponential peer methods in general give more accurate results than the other methods of EXPINT. On the other hand they require more computations of the $\varphi-$functions leading to higher expense.

We did not observe an order reduction for EPMs in contrast to most of the other methods, for instance for the Schrödinger type equation and the Prothero-Robinson example.

Surprisingly, also the method `hochost4` shows an order reduction for the Prothero-Robinson example.

The numerical tests with step size control show that all our strategies of step size control work reliably. As expected, with more strict tolerances the error decreases.

For crude tolerances the 3- and 4-stage methods are more efficient than the 5-stage methods which may be due to the larger value of σ_{max}. MATLAB routine `ode45` is the most efficient code for the non-stiff Gray-Scott problem, for Allen-Cahn `ode15s` is superior.

All methods are comparable for the Kuramoto-Sivashinski equation. Significant advantage of the exponential peer methods can be observed for problems with large imaginary parts of the eigenvalues of T as Schrödinger and hyperbolic problems. This is mainly due to the fact that `ode15s` is only $A-$stable for $p \leq 2$.

In general the results with step size control show the potential of the new class of methods. This efficiency depends strongly on the efficient computation of the $\varphi-$functions.

Chapter 6

Conclusions

We have constructed and analyzed exponential peer methods with constant and variable step size. We have derived order conditions, which allow to construct methods of arbitrary high order, in this thesis we have considered methods up to 7 stages and it is easy to construct methods with more stages.

We have proved that for a wide class of stiff problems an $s-$stage method is of stiff order and stage order $p \geq s-1$. These results are confirmed by our numerical tests. In general we observe the non-stiff order $p = s$ for the test problems. A possible explanation for this can be Remarks 3.4 and 3.5.

We have identified a special class of methods with only two different arguments in $\varphi-$functions, which is optimally zero-stable for constant step sizes and solves linear problems $y' = Ty$ exactly.

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 for these methods are promising. They indicate that exponential peer methods are a suitable class especially for problems with large imaginary eigenvalues. In contrast to many other exponential integrators we did not observe an order reduction.

The results of the exponential peer methods with variable step sizes show that the proposed kinds of error estimation and step size control work reliably.

The computing time of the exponential peer methods is in general determined by the computation of the $\varphi-$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 resulting for instance by semi-discretization of 3-dimensional PDEs. Here the use of Krylov methods for the approximation of products of $\varphi-$functions times a vector is advantageous. This will be the topic of future research.

Appendix A

Coefficients for EPMs with constant step sizes

We constructed EPMs with constant step sizes due to Theorems 3.1 and 3.2 with $s = 3, 4, 5, 6, 7$ stages of stiff order $p = s - 1$. The nodes c_i are determined by Theorem 3.8 with $\alpha^* = \dfrac{s-1}{s}$.

In the numerical tests for EPM for constant step size we set the free $\dfrac{s(s-1)}{2}$ coefficients $A_{ij} \quad \forall\, i > j$ to be zeros. So the general structure of the matrix A and R will be in the form

$$\mathcal{A} = \begin{pmatrix} A_{11} & A_{12} & A_{13} & \dots & A_{1s} \\ A_{21} & A_{22} & A_{23} & \dots & A_{2s} \\ \vdots & \vdots & \dots & \dots & \vdots \\ A_{s1} & A_{s2} & \dots & \dots & A_{ss} \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & A_{13} & A_{14} & \dots & A_{1,s-1} & A_{1s} \\ 0 & A_{11} & A_{12} & A_{13} & \dots & A_{1,s-2} & A_{1,s-1} \\ 0 & 0 & A_{11} & A_{12} & \dots & A_{1,s-3} & A_{1,s-2} \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & A_{11} & A_{12} & A_{13} \\ 0 & 0 & 0 & 0 & 0 & A_{11} & A_{12} \\ 0 & 0 & 0 & 0 & 0 & 0 & A_{ss} \end{pmatrix},$$

$$\mathcal{R} = \begin{pmatrix} R_{11} & R_{12} & R_{13} & \dots & R_{1s} \\ R_{21} & R_{22} & R_{23} & \dots & R_{2s} \\ \vdots & \vdots & \dots & \dots & \vdots \\ R_{s1} & R_{s2} & \dots & \dots & R_{ss} \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 & \dots & 0 & 0 \\ A_{1s} & 0 & 0 & 0 & \dots & 0 & 0 \\ A_{1,s-1} & A_{1s} & 0 & 0 & \dots & 0 & 0 \\ A_{1,s-2} & A_{1,s-1} & A_{1s} & 0 & \dots & 0 & 0 \\ \vdots & \vdots\ddots & \ddots & \ddots & \vdots & \vdots & \\ A_{13} & A_{14} & \dots & A_{1,s-1} & A_{1s} & 0 & 0 \\ R_{s1} & R_{s2} & \dots & R_{s,s-3} & R_{s,s-2} & R_{s,s-1} & 0 \end{pmatrix}.$$

3−**stage:** Method `epm3` with 3 stages of stiff order $p \geq 2$:

$$\alpha = \begin{pmatrix} \frac{2}{3} \\ \frac{2}{3} \\ 1 \end{pmatrix}, \qquad C = \begin{pmatrix} \frac{1}{3} \\ \frac{2}{3} \\ 1 \end{pmatrix} \quad \text{then} \quad B = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{pmatrix},$$

$$A = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ 0 & A_{11} & A_{12} \\ 0 & 0 & A_{33} \end{pmatrix}, \qquad R = \begin{pmatrix} 0 & 0 & 0 \\ A_{13} & 0 & 0 \\ R_{31} & R_{32} & 0 \end{pmatrix},$$

where

$$\begin{aligned} A_{11} &= -\frac{2}{3}\varphi_2 + \frac{8}{3}\varphi_3, & A_{12} &= -\frac{16}{3}\varphi_3 + \frac{2}{3}\varphi_1, \\ A_{13} &= \frac{2}{3}\varphi_2 + \frac{8}{3}\varphi_3, & A_{33} &= -\frac{9}{2}\varphi_2 + \varphi_1 + 9\varphi_3, \\ R_{31} &= 6\varphi_2 - 18\varphi_3, & R_{32} &= -\frac{3}{2}\varphi_2 + 9\varphi_3. \end{aligned}$$

4−**stage:** Method `epm4` with 4 stages of stiff order $p \geq 3$:

$$\alpha = \begin{pmatrix} \frac{3}{4} \\ \frac{3}{4} \\ \frac{3}{4} \\ 1 \end{pmatrix}, \qquad C = \begin{pmatrix} \frac{1}{4} \\ \frac{2}{4} \\ \frac{3}{4} \\ 1 \end{pmatrix} \quad \text{then} \quad B = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

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

where

$$\begin{aligned} A_{11} &= -\frac{3}{4}\varphi_2 + \frac{27}{4}\varphi_3 - \frac{81}{4}\varphi_4, & A_{12} &= \frac{3}{4}\varphi_1 - \frac{9}{8}\varphi_2 - \frac{27}{2}\varphi_3 + \frac{243}{4}\varphi_4, \\ A_{13} &= \frac{9}{4}\varphi_2 + \frac{27}{4}\varphi_3 - \frac{243}{4}\varphi_4, & A_{14} &= -\frac{3}{8}\varphi_2 + \frac{81}{4}\varphi_4, \\ A_{44} &= \varphi_1 - \frac{22}{3}\varphi_2 + 32\varphi_3 - 64\varphi_4, & R_{41} &= 12\varphi_2 - 80\varphi_3 + 192\varphi_4, \\ R_{42} &= 6\varphi_2 + 64\varphi_3 - 192\varphi_4, & R_{43} &= \frac{4}{3}\varphi_2 - 16\varphi_3 + 64\varphi_4. \end{aligned}$$

5−**stage:** Method `epm5` with 5 stages of stiff order $p \geq 4$:

$$\alpha = \begin{pmatrix} \frac{4}{5} \\ \frac{4}{5} \\ \frac{4}{5} \\ \frac{4}{5} \\ 1 \end{pmatrix}, \qquad C = \begin{pmatrix} \frac{1}{5} \\ \frac{2}{5} \\ \frac{3}{5} \\ \frac{4}{5} \\ 1 \end{pmatrix} \quad \text{then} \quad B = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix},$$

$$A = \begin{pmatrix} A_{11} & A_{12} & A_{13} & A_{14} & A_{15} \\ 0 & A_{11} & A_{12} & A_{13} & A_{14} \\ 0 & 0 & A_{11} & A_{12} & A_{13} \\ 0 & 0 & 0 & A_{11} & A_{12} \\ 0 & 0 & 0 & 0 & A_{55} \end{pmatrix}, \qquad R = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ A_{15} & 0 & 0 & 0 & 0 \\ A_{14} & A_{15} & 0 & 0 & 0 \\ A_{13} & A_{14} & A_{15} & 0 & 0 \\ R_{51} & R_{52} & R_{53} & R_{54} & 0 \end{pmatrix},$$

where

$$\begin{aligned}
A_{11} &= -\frac{4}{5}\varphi_2 + \frac{176}{15}\varphi_3 - \frac{384}{5}\varphi_4 + \frac{1024}{5}\varphi_5, \\
A_{12} &= \frac{4}{5}\varphi_1 - \frac{8}{3}\varphi_2 - \frac{64}{3}\varphi_3 + 256\varphi_4 - \frac{4096}{5}\varphi_5, \\
A_{13} &= \frac{24}{5}\varphi_2 + \frac{32}{5}\varphi_3 - \frac{1536}{5}\varphi_4 + \frac{6144}{5}\varphi_5, \\
A_{14} &= -\frac{8}{5}\varphi_2 + \frac{64}{15}\varphi_3 + \frac{768}{5}\varphi_4 - \frac{4096}{5}\varphi_5, \\
A_{15} &= \frac{4}{15}\varphi_2 - \frac{16}{15}\varphi_3 - \frac{128}{5}\varphi_4 + \frac{1024}{5}\varphi_5, \\
A_{55} &= \varphi_1 - \frac{125}{12}\varphi_2 + \frac{875}{12}\varphi_3 - \frac{625}{2}\varphi_4 + 625\varphi_5, \\
R_{51} &= 20\varphi_2 - \frac{650}{3}\varphi_3 + 1125\varphi_4 - 2500\varphi_5, \\
R_{52} &= -15\varphi_2 + \frac{475}{2}\varphi_3 - 1500\varphi_4 + 3750\varphi_5, \\
R_{53} &= \frac{20}{3}\varphi_2 - \frac{350}{3}\varphi_3 + 875\varphi_4 - 2500\varphi_5, \\
R_{54} &= -\frac{5}{4}\varphi_2 + \frac{275}{12}\varphi_3 - \frac{375}{2}\varphi_4 + 625\varphi_5.
\end{aligned}$$

6−**stage:** Method `epm6` with 6 stages of stiff order $p \geq 5$:

$$\alpha = \begin{pmatrix} \frac{5}{6} \\ \frac{5}{6} \\ \frac{5}{6} \\ \frac{5}{6} \\ \frac{5}{6} \\ 1 \end{pmatrix}, \qquad C = \begin{pmatrix} \frac{1}{6} \\ \frac{2}{6} \\ \frac{3}{6} \\ \frac{4}{6} \\ \frac{5}{6} \\ 1 \end{pmatrix} \quad \text{then} \quad B = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix},$$

$$A = \begin{pmatrix} A_{11} & A_{12} & A_{13} & A_{14} & A_{15} & A_{16} \\ 0 & A_{11} & A_{12} & A_{13} & A_{14} & A_{15} \\ 0 & 0 & A_{11} & A_{12} & A_{35} & A_{14} \\ 0 & 0 & 0 & A_{11} & A_{12} & A_{13} \\ 0 & 0 & 0 & 0 & A_{11} & A_{12} \\ 0 & 0 & 0 & 0 & 0 & A_{66} \end{pmatrix}, \quad R = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ A_{16} & 0 & 0 & 0 & 0 & 0 \\ A_{15} & A_{16} & 0 & 0 & 0 & 0 \\ A_{14} & A_{15} & A_{16} & 0 & 0 & 0 \\ A_{15} & A_{14} & A_{15} & A_{16} & 0 & 0 \\ R_{61} & R_{62} & R_{63} & R_{64} & R_{65} & 0 \end{pmatrix},$$

where

$$\begin{aligned}
A_{11} &= -\frac{5}{6}\varphi_2 + \frac{625}{36}\varphi_3 - \frac{4375}{24}\varphi_4 + \frac{3125}{3}\varphi_5 - \frac{15625}{6}\varphi_6, \\
A_{12} &= \frac{5}{6}\varphi_1 - \frac{325}{72}\varphi_2 - \frac{625}{24}\varphi_3 + \frac{15625}{24}\varphi_4 - \frac{9375}{2}\varphi_5 + \frac{78125}{6}\varphi_6, \\
A_{13} &= \frac{25}{3}\varphi_2 - \frac{125}{18}\varphi_3 - \frac{10625}{12}\varphi_4\frac{25000}{3}\varphi_5 - \frac{78125}{3}\varphi_6, \\
A_{14} &= -\frac{25}{6}\varphi_2 + \frac{875}{36}\varphi_3 + \frac{6875}{12}\varphi_4 - \frac{21875}{3}\varphi_5 + \frac{78125}{3}\varphi_6, \\
A_{15} &= \frac{25}{18}\varphi_2 - \frac{125}{12}\varphi_3 - \frac{4375}{24}\varphi_4 + 3125\varphi_5 - \frac{78125}{6}\varphi_6 \\
A_{16} &= -\frac{5}{24}\varphi_2 + \frac{125}{72}\varphi_3 + \frac{625}{24}\varphi_4 - \frac{3125}{6}\varphi_5 + \frac{15625}{6}\varphi_6, \\
A_{66} &= \varphi_1 - \frac{137}{10}\varphi_2 + 135\varphi_3 - 918\varphi_4 + 3888\varphi_5 - 7776\varphi_6, \\
R_{61} &= 30\varphi_2 - 462\varphi_3 + 3834\varphi_4 - 18144\varphi_5 + 38880\varphi_6, \\
R_{62} &= -30\varphi_2 + 642\varphi_3 - 6372\varphi_4 + 33696\varphi_5 - 77760\varphi_6, \\
R_{63} &= 20\varphi_2 - 468\varphi_3 - 31104\varphi_5 + 5292\varphi_4 + 77760\varphi_6, \\
R_{64} &= -\frac{15}{2}\varphi_2 + 183\varphi_3 - 2214\varphi_4 + 14256\varphi_5 - 38880\varphi_6, \\
R_{65} &= \frac{6}{5}\varphi_2 - 30\varphi_3 + 378\varphi_4 - 2592\varphi_5 + 7776\varphi_6.
\end{aligned}$$

$7-$**stage:** Method `epm6` with 7 stages of stiff order $p \geq 6$:

$$\alpha = \begin{pmatrix} \frac{6}{7} \\ \frac{6}{7} \\ \frac{6}{7} \\ \frac{6}{7} \\ \frac{6}{7} \\ \frac{6}{7} \\ 1 \end{pmatrix} \quad \& \quad C = \begin{pmatrix} \frac{1}{7} \\ \frac{2}{7} \\ \frac{3}{7} \\ \frac{4}{7} \\ \frac{5}{7} \\ \frac{6}{7} \\ 1 \end{pmatrix} \quad \text{then} \quad B = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix},$$

$$A = \begin{pmatrix} A_{11} & A_{12} & A_{13} & A_{14} & A_{15} & A_{16} & A_{17} \\ 0 & A_{11} & A_{12} & A_{13} & A_{14} & A_{15} & A_{16} \\ 0 & 0 & A_{11} & A_{12} & A_{13} & A_{14} & A_{15} \\ 0 & 0 & 0 & A_{11} & A_{12} & A_{13} & A_{14} \\ 0 & 0 & 0 & 0 & A_{11} & A_{12} & A_{13} \\ 0 & 0 & 0 & 0 & 0 & A_{11} & A_{12} \\ 0 & 0 & 0 & 0 & 0 & 0 & A_{77} \end{pmatrix},$$

$$R = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ A_{17} & 0 & 0 & 0 & 0 & 0 & 0 \\ A_{16} & A_{17} & 0 & 0 & 0 & 0 & 0 \\ A_{15} & A_{16} & A_{17} & 0 & 0 & 0 & 0 \\ A_{13} & A_{14} & A_{15} & A_{16} & A_{17} & 0 & 0 \\ R_{71} & R_{72} & R_{73} & R_{74} & R_{75} & R_{76} & 0 \end{pmatrix},$$

where

$$\begin{aligned}
A_{11} &= -\frac{6}{7}\varphi_2 + \frac{822}{35}\varphi_3 - \frac{2430}{7}\varphi_4 + \frac{22032}{7}\varphi_5 - \frac{116640}{7}\varphi_6 + \frac{279936}{7}\varphi_7, \\
A_{12} &= \frac{6}{7}\varphi_1 - \frac{33}{5}\varphi_2 - \frac{126}{5}\varphi_3 + 1296\varphi_4 - 15552\varphi_5 + 93312\varphi_6 - \frac{1679616}{7}\varphi_7, \\
A_{13} &= \frac{4199040}{7}\varphi_7 - \frac{1516320}{7}\varphi_6 + \frac{221616}{7}\varphi_5 - \frac{13446}{7}\varphi_4 - \frac{306}{7}\varphi_3 + \frac{90}{7}\varphi_2, \\
A_{14} &= \frac{10368}{7}\varphi_4 - \frac{238464}{7}\varphi_5 - \frac{60}{7}\varphi_2 + \frac{564}{7}\varphi_3 + \frac{1866240}{7}\varphi_6 - \frac{5598720}{7}\varphi_7, \\
A_{15} &= -\frac{4698}{7}\varphi_4 + \frac{143856}{7}\varphi_5 + \frac{30}{7}\varphi_2 - \frac{342}{7}\varphi_3 - \frac{1283040}{7}\varphi_6 + \frac{4199040}{7}\varphi_7, \\
A_{16} &= -\frac{46656}{7}\varphi_5 - \frac{9}{7}\varphi_2 + \frac{558}{35}\varphi_3 + \frac{1296}{7}\varphi_4 + \frac{466560}{7}\varphi_6 - \frac{1679616}{7}\varphi_7, \\
A_{17} &= \frac{6}{35}\varphi_2 - \frac{78}{35}\varphi_3 - \frac{162}{7}\varphi_4 + \frac{6480}{7}\varphi_5 - \frac{69984}{7}\varphi_6 + \frac{279936}{7}\varphi_7, \\
A_{77} &= \varphi_1 - \frac{343}{20}\varphi_2 + \frac{9947}{45}\varphi_3 - \frac{16807}{8}\varphi_4 + \frac{84035}{6}\varphi_5 - \frac{117649}{2}\varphi_6 + 117649\varphi_7, \\
R_{71} &= 42\varphi_2 - \frac{4263}{5}\varphi_3 + 9947\varphi_4 - 74431\varphi_5 + 336140\varphi_6 - 705894\varphi_7, \\
R_{72} &= -\frac{105}{2}\varphi_2 + \frac{5733}{4}\varphi_3 - \frac{158123}{8}\varphi_4 + \frac{328937}{2}\varphi_5 - \frac{1596665}{2}\varphi_6 + 1764735\varphi_7, \\
R_{73} &= \frac{140}{3}\varphi_2 - \frac{12446}{9}\varphi_3 + 21266\varphi_4 - \frac{581042}{3}\varphi_5 + 1008420\varphi_6 - 2352980\varphi_7, \\
R_{74} &= -\frac{105}{4}\varphi_2 + \frac{1617}{2}\varphi_3 - \frac{105301}{8}\varphi_4 + \frac{256907}{2}\varphi_5 - \frac{1428595}{2}\varphi_6 + 1764735\varphi_7, \\
R_{75} &= \frac{42}{5}\varphi_2 - \frac{1323}{5}\varphi_3 + 4459\varphi_4 - 45619\varphi_5 + 268912\varphi_6 - 705894\varphi_7, \\
R_{76} &= -\frac{7}{6}\varphi_2 + \frac{6713}{180}\varphi_3 - \frac{5145}{8}\varphi_4 + \frac{40817}{6}\varphi_5 - \frac{84035}{2}\varphi_6 + 117649\varphi_7.
\end{aligned}$$

Appendix B

Coefficients for EPMs with variable step sizes

3−**stage:** Method `epm3` with 3 stages of stiff order $p \geq 2$:

$$\alpha = \begin{pmatrix} \frac{2}{3} \\ \frac{2}{3} \\ 1 \end{pmatrix} \quad \& \quad c = \begin{pmatrix} \frac{1}{3} \\ \frac{2}{3} \\ 1 \end{pmatrix} \quad \text{then}$$

$$B = \begin{pmatrix} \dfrac{1}{2}\sigma(\sigma-1) & \sigma(2-\sigma) & \frac{1}{2}(\sigma-1)(\sigma-2) \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{pmatrix},$$

$$A = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ 0 & \dfrac{4}{3}\dfrac{\sigma^2\left(4\varphi_3-\varphi_2\right)}{1+\sigma} & \dfrac{2}{3}\varphi_1+\dfrac{4}{3}\left(\sigma-1\right)\varphi_2-\dfrac{16}{3}\sigma\varphi_3 \\ 0 & 0 & \varphi_1-\dfrac{9}{2}\varphi_2+9\varphi_3 \end{pmatrix},$$

$$R = \begin{pmatrix} 0 & 0 & 0 \\ \dfrac{4}{3}\dfrac{4\sigma\varphi_3+\varphi_2}{1+\sigma} & 0 & 0 \\ -18\varphi_3+6\varphi_2 & 9\varphi_3-\frac{3}{2}\varphi_2 & 0 \end{pmatrix}$$

where

$$\begin{aligned}
A_{11} &= \frac{1}{3}\sigma\left(\sigma-1\right)\varphi_1-\frac{2}{3}\sigma\left(2\sigma-1\right)\varphi_2+\frac{8}{3}\sigma^2\varphi_3 \\
A_{12} &= \frac{2}{3}\sigma\left(2-\sigma\right)\varphi_1+\frac{8}{3}\sigma\left(\sigma-1\right)\varphi_2-\frac{16}{3}\sigma^2\varphi_3 \\
A_{13} &= \frac{1}{3}\left(\sigma-1\right)\left(\sigma-2\right)\varphi_1-\frac{2}{3}\sigma\left(2\sigma-3\right)\varphi_2+\frac{8}{3}\sigma^2\varphi_3.
\end{aligned}$$

4−**stage:** Method `epm4` with 4 stages of stiff order $p \geq 3$:

$$\alpha = \begin{pmatrix} \frac{3}{4} \\ \frac{3}{4} \\ \frac{3}{4} \\ 1 \end{pmatrix} \quad \& \quad C = \begin{pmatrix} \frac{1}{4} \\ \frac{2}{4} \\ \frac{3}{4} \\ 1 \end{pmatrix} \quad \text{then}$$

$$B = \begin{pmatrix} \frac{2}{3}\sigma(2\sigma-1)(\sigma-1) & -\sigma(2\sigma-1)(2\sigma-3) & 2\sigma(\sigma-1)(2\sigma-3) & b_{14} \\ \frac{1}{6}\sigma(\sigma-1)(\sigma-2) & -\frac{1}{2}\sigma(\sigma-1)(\sigma-3) & \frac{1}{2}\sigma(\sigma-2)(\sigma-3) & b_{24} \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

$$A = \begin{pmatrix} A_{11} & A_{12} & A_{13} & A_{14} \\ 0 & A_{22} & A_{23} & A_{24} \\ 0 & 0 & -\frac{9}{2}\frac{\sigma^3(\varphi_2 - 9\varphi_3 + 27\varphi_4)}{(\sigma+1)(2\sigma+1)} & A_{34} \\ 0 & 0 & 0 & \varphi_1 - \frac{22}{3}\varphi_2 + 32\varphi_3 - 64\varphi_4 \end{pmatrix},$$

$$R = \begin{pmatrix} 0 & 0 & 0 & 0 \\ R_{21} & 0 & 0 & 0 \\ \frac{9}{2}\frac{(6\sigma-3)\varphi_3 + \varphi_2 - 27\sigma\varphi_4}{\sigma+1} & -\frac{9}{8}\frac{(6\sigma-6)\varphi_3 + \varphi_2 - 54\sigma\varphi_4}{2\sigma+1} & 0 & 0 \\ 12\varphi_2 - 80\varphi_3 + 192\varphi_4 & -6\varphi_2 + 64\varphi_3 - 192\varphi_4 & R_{43} & 0 \end{pmatrix},$$

where

$$\begin{aligned}
b_{14} &= -\frac{1}{3}(\sigma-1)(2\sigma-1)(2\sigma-3), \\
b_{24} &= -\frac{1}{6}(\sigma-1)(\sigma-2)(\sigma-3), \\
A_{11} &= \frac{1}{2}\sigma(2\sigma-1)(\sigma-1)\varphi_1 - \frac{3}{4}\sigma\left(-6\sigma+1+6\sigma^2\right)\varphi_2 + \frac{27}{4}\sigma^2(2\sigma-1)\varphi_3 \\
&\quad - \frac{81}{4}\sigma^3\varphi_4, \\
A_{12} &= -\frac{3}{4}\sigma(2\sigma-1)(2\sigma-3)\varphi_1 + \frac{9}{8}\sigma\left(3+12\sigma^2-16\sigma\right)\varphi_2 - \frac{27}{2}\sigma^2(3\sigma-2)\varphi_3 \\
&\quad + \frac{243}{4}\sigma^3\varphi_4, \\
A_{13} &= \frac{3}{2}\sigma(\sigma-1)(2\sigma-3)\varphi_1 - \frac{9}{4}\sigma\left(6\sigma^2-10\sigma+3\right)\varphi_2 + \frac{27}{4}\sigma^2(6\sigma-5)\varphi_3 \\
&\quad - \frac{243}{4}\varphi_4\sigma^3, \\
A_{14} &= -\frac{1}{4}(\sigma-1)(2\sigma-1)(2\sigma-3)\varphi_1 + \frac{3}{8}\sigma\left(11-24\sigma+12\sigma^2\right)\varphi_2 \\
&\quad - \frac{27}{2}\sigma^2(\sigma-1)\varphi_3 + \frac{81}{4}\sigma^3\varphi_4,
\end{aligned}$$

$$
\begin{aligned}
A_{22} &= \frac{3}{8}\frac{\sigma^2\left((2\sigma-2)\,\varphi_1+(9-15\sigma)\,\varphi_2+(72\sigma-18)\,\varphi_3-162\sigma\varphi_4\right)}{2+\sigma},\\
A_{23} &= -\frac{3}{4}\frac{\sigma^2\left((2\sigma-4)\,\varphi_1+(18-15\sigma)\,\varphi_2+(72\sigma-36)\,\varphi_3-162\sigma\varphi_4\right)}{\sigma+1},\\
A_{24} &= \frac{3}{4}\left(\sigma-1\right)\left(\sigma-2\right)\varphi_1+\frac{9}{8}\left(-5\sigma^2+9\sigma-2\right)\varphi_2+\frac{27}{4}\sigma\left(4\sigma-3\right)\varphi_3-\frac{243}{4}\sigma^2\varphi_4,\\
A_{34} &= \frac{3}{4}\varphi_1+\frac{9}{8}\left(2\sigma-3\right)\varphi_2+\frac{27}{4}\left(1-3\sigma\right)\varphi_3+\frac{243}{4}\sigma\varphi_4,\\
R_{21} &= -\frac{3}{4}\frac{(\sigma-1)\,(\sigma-2)\,\varphi_1+\left(-6+18\sigma-9\sigma^2\right)\varphi_2+54\sigma\,(\sigma-1)\,\varphi_3-162\sigma^2\varphi_4}{(\sigma+2)\,(\sigma+1)},\\
R_{43} &= \frac{4}{3}\varphi_2-16\varphi_3+64\varphi_4.
\end{aligned}
$$

5−**stage:** Method `epm5` with 5 stages of stiff order $p \geq 4$:

$$
\alpha=\begin{pmatrix}\frac{4}{5}\\ \frac{4}{5}\\ \frac{4}{5}\\ \frac{4}{5}\\ 1\end{pmatrix},\qquad C=\begin{pmatrix}\frac{1}{5}\\ \frac{2}{5}\\ \frac{3}{5}\\ \frac{4}{5}\\ 1\end{pmatrix}\quad\text{then}\quad B=\begin{pmatrix}b_{11}&b_{12}&b_{13}&b_{14}&b_{15}\\ b_{21}&b_{22}&b_{23}&b_{24}&b_{25}\\ b_{31}&b_{32}&b_{33}&b_{34}&b_{35}\\ 0&0&0&0&1\\ 0&0&0&0&1\end{pmatrix},
$$

$$
A=\begin{pmatrix}A_{11}&A_{12}&A_{13}&A_{14}&A_{15}\\ 0&A_{22}&A_{23}&A_{24}&A_{25}\\ 0&0&A_{33}&A_{34}&A_{35}\\ 0&0&0&A_{44}&A_{45}\\ 0&0&0&0&A_{55}\end{pmatrix},\qquad R=\begin{pmatrix}0&0&0&0&0\\ R_{21}&0&0&0&0\\ R_{31}&R_{32}&0&0&0\\ R_{41}&R_{42}&R_{43}&0&0\\ R_{51}&R_{52}&R_{53}&R_{54}&0\end{pmatrix},
$$

where

$$
\begin{aligned}
b_{11} &= \frac{3}{8}\sigma\left(\sigma-1\right)\left(3\sigma-1\right)\left(3\sigma-2\right), & b_{22} &= -\frac{4}{3}\sigma\left(\sigma-1\right)\left(\sigma-2\right)\left(2\sigma-1\right),\\
b_{13} &= \frac{9}{4}\sigma\left(\sigma-1\right)\left(3\sigma-1\right)\left(3\sigma-4\right), & b_{14} &= -\frac{3}{2}\sigma\left(\sigma-1\right)\left(3\sigma-4\right)\left(3\sigma-2\right),\\
b_{15} &= \frac{1}{8}\left(\sigma-1\right)\left(3\sigma-1\right)\left(3\sigma-4\right)\left(3\sigma-2\right), & b_{21} &= \frac{1}{6}\sigma\left(\sigma-1\right)\left(2\sigma-1\right)\left(2\sigma-3\right),\\
b_{12} &= -\frac{1}{2}\sigma\left(3\sigma-1\right)\left(3\sigma-4\right)\left(3\sigma-2\right), & b_{23} &= \sigma\left(\sigma-2\right)\left(2\sigma-1\right)\left(2\sigma-3\right),\\
b_{25} &= \frac{1}{6}\left(\sigma-1\right)\left(\sigma-2\right)\left(2\sigma-1\right)\left(2\sigma-3\right), & b_{24} &= -\frac{4}{3}\sigma\left(\sigma-1\right)\left(\sigma-2\right)\left(2\sigma-3\right),\\
b_{31} &= \frac{1}{2}4\sigma\left(\sigma-1\right)\left(\sigma-2\right)\left(\sigma-3\right), & b_{32} &= -\frac{1}{6}\sigma\left(\sigma-1\right)\left(\sigma-2\right)\left(\sigma-4\right),\\
b_{33} &= \frac{1}{4}\sigma\left(\sigma-1\right)\left(\sigma-3\right)\left(\sigma-4\right), & b_{34} &= -\frac{1}{6}\sigma\left(\sigma-2\right)\left(\sigma-3\right)\left(\sigma-4\right),\\
b_{35} &= \frac{1}{2}4\left(\sigma-1\right)\left(\sigma-2\right)\left(\sigma-3\right)\left(\sigma-4\right), & &
\end{aligned}
$$

$$
\begin{aligned}
A_{11} &= \frac{3}{10}\sigma\left(\sigma-1\right)\left(3\sigma-1\right)\left(3\sigma-2\right)\varphi_1 - \frac{4}{5}\sigma\left(2\sigma-1\right)\left(9\sigma^2-9\sigma+1\right)\varphi_2 \\
&+ \frac{16}{15}\sigma^2\left(-54\sigma+11+54\sigma^2\right)\varphi_3 - \frac{384}{5}\sigma^3\left(2\sigma-1\right)\varphi_4 + \frac{1024}{5}\sigma^4\varphi_5, \\
A_{12} &= -\frac{2}{5}\sigma\left(3\sigma-1\right)\left(3\sigma-4\right)\left(3\sigma-2\right)\varphi_1 + \frac{8}{15}\sigma\left(-189\sigma^2+84\sigma+108\sigma^3-8\right)\varphi_2 \\
&- \frac{64}{15}\sigma^2\left(-63\sigma+14+54\sigma^2\right)\varphi_3 + \frac{256}{5}\sigma^3\left(12\sigma-7\right)\varphi_4 - \frac{4096}{5}\sigma^4\varphi_5, \\
A_{13} &= \frac{9}{5}\sigma\left(\sigma-1\right)\left(3\sigma-1\right)\left(3\sigma-4\right)\varphi_1 - \frac{24}{5}\sigma\left(3\sigma-2\right)\left(6\sigma^2-8\sigma+1\right)\varphi_2 \\
&+ \frac{32}{5}\sigma^2\left(-72\sigma+19+54\sigma^2\right)\varphi_3 - \frac{1536}{5}\sigma^3\left(3\sigma-2\right)\varphi_4 + \frac{6144}{5}\sigma^4\varphi_5, \\
A_{14} &= -\frac{6}{5}\sigma\left(\sigma-1\right)\left(3\sigma-4\right)\left(3\sigma-2\right)\varphi_1 + \frac{8}{5}\sigma\left(-81\sigma^2+52\sigma+36\sigma^3-8\right)\varphi_2 \\
&- \frac{64}{15}\sigma^2\left(-81\sigma+26+54\sigma^2\right)\varphi_3 + \frac{768}{5}\sigma^3\left(4\sigma-3\right)\varphi_4 - \frac{4096}{5}\sigma^4\varphi_5, \\
A_{15} &= \frac{1}{10}\left(\sigma-1\right)\left(3\sigma-1\right)\left(3\sigma-4\right)\left(3\sigma-2\right)\varphi_1 - \frac{4}{15}\sigma\left(6\sigma-5\right)\left(9\sigma^2-15\sigma+5\right)\varphi_2 \\
&+ \frac{16}{15}\sigma^2\left(-90\sigma+54\sigma^2+35\right)\varphi_3 - \frac{128}{5}\sigma^3\left(6\sigma-5\right)\varphi_4 + \frac{1024}{5}\sigma^4\varphi_5, \\
A_{22} &= \frac{8\sigma^2}{15}\left\{\frac{3\left(2\sigma-1\right)\left(\sigma-1\right)\varphi_1 - 2\left(5-24\sigma+22\sigma^2\right)\varphi_2 + 8\left(2-21\sigma+30\sigma^2\right)\varphi_3}{3+\sigma}\right. \\
&\left. + \frac{-288\sigma\left(3\sigma-1\right)\varphi_4 + 1536\sigma^2\varphi_5}{3+\sigma}\right\}, \\
A_{23} &= \frac{4}{5}\left\{\frac{192\,\sigma^3\left(9\,\sigma-2\right)\varphi_4 - 3072\sigma^4\varphi_5 - 16\,\sigma^2\left(3-28\,\sigma-15\,\sigma^2\right)\varphi_3}{\sigma+2}\right. \\
&\left. + \frac{2\,\sigma^2\left(15-64\,\sigma+22\,\sigma^2\right)\phi_2 - 3\,\sigma^2\left(2\,\sigma-1\right)\left(2\,\sigma-3\right)\varphi_1}{\sigma+2}\right\} \\
A_{24} &= \frac{8\sigma^2}{5}\left\{\frac{3\left(\sigma-1\right)\left(2\sigma-3\right)\varphi_1 - 2\left(15-40\sigma+22\sigma^2\right)\varphi_2 + 1536\sigma^2\varphi_5}{\sigma+1}\right. \\
&\left. + \frac{8\left(6-35\sigma+30\sigma^2\right)\varphi_3 - 96\sigma\left(-5+9\sigma\right)\varphi_4}{\sigma+1}\right\}, \\
A_{25} &= \frac{4}{15}\left\{-3\left(\sigma-1\right)\left(2\sigma-1\right)\left(2\sigma-3\right)\varphi_1 + 2\left(-6+55\sigma+44\sigma^3-96\sigma^2\right)\varphi_2\right. \\
&\left. - 16\sigma\left(-42\sigma+11+30\sigma^2\right)\varphi_3 + 1152\sigma^2\left(3\sigma-2\right)\varphi_4 - 6144\sigma^3\varphi_5\right\}, \\
A_{33} &= \frac{2\sigma^3}{5}\left\{\frac{3\left(\sigma-1\right)\varphi_1 - 2\left(17\sigma-11\right)\varphi_2 + 16\left(-6+17\sigma\right)\varphi_3}{\left(\sigma+1\right)\left(\sigma+2\right)}\right. \\
&\left. + \frac{-192\left(7\sigma-1\right)\varphi_4 + 3072\sigma\varphi_5}{\left(\sigma+1\right)\left(\sigma+2\right)}\right\},
\end{aligned}
$$

$$A_{34} = \frac{8\sigma^3}{5}\left\{\frac{-3\left(\sigma-2\right)\varphi_1+2\left(17\sigma-22\right)\varphi_2-16\left(17\sigma-12\right)\varphi_3}{\left(\sigma+1\right)\left(2\sigma+1\right)}\right.$$
$$\left.+\frac{192\left(7\sigma-2\right)\varphi_4-3072\sigma\varphi_5}{\left(\sigma+1\right)\left(2\sigma+1\right)}\right\},$$

$$A_{35} = \frac{2}{5}\left\{3\left(\sigma-1\right)\left(\sigma-2\right)\varphi_1-2\left(-33\sigma+10+17\sigma^2\right)\varphi_2-192\sigma\left(-3+7\sigma\right)\varphi_4\right.$$
$$\left.+16\left(2+17\sigma^2-18\sigma\right)\varphi_3+3072\sigma^2\varphi_5\right\},$$

$$A_{44} = \frac{\sigma^4}{5}\left\{\frac{-96\varphi_2+1408\varphi_3-9216\varphi_4+24576\varphi_5}{\left(2\sigma+1\right)\left(3\sigma+1\right)\left(\sigma+1\right)}\right\},$$

$$A_{45} = \frac{12\varphi_1+8\left(6\sigma-11\right)\varphi_2-64\left(11\sigma-6\right)\varphi_3+768\left(6\sigma-1\right)\varphi_4-12288\sigma\varphi_5}{15},$$

$$A_{55} = \varphi_1-\frac{125}{12}\varphi_2+\frac{875}{12}\varphi_3-\frac{625}{2}\varphi_4+625\varphi_5,$$

$$R_{21} = \frac{16\left(\sigma-1\right)\left(2\sigma-1\right)\left(2\sigma-3\right)\varphi_1-32\left(4\sigma-3\right)\left(4\sigma^2-6\sigma+1\right)\varphi_2}{5\left(3+\sigma\right)\left(\sigma+2\right)\left(\sigma+1\right)}$$
$$+\frac{128\sigma\left(-36\sigma+11+24\sigma^2\right)\varphi_3-3072\sigma^2\left(4\sigma-3\right)\varphi_4+24576\sigma^3\varphi_5}{5\left(3+\sigma\right)\left(\sigma+2\right)\left(\sigma+1\right)},$$

$$R_{31} = \frac{-12\left(\sigma-1\right)\left(\sigma-2\right)\varphi_1+16\left(2\sigma-1\right)\left(5\sigma-8\right)\varphi_2-128\left(12\sigma^2-15\sigma+2\right)\varphi_3}{5\left(\sigma+1\right)\left(\sigma+2\right)}$$
$$+\frac{4608\sigma\left(2\sigma-1\right)\varphi_4-24576\sigma^4\varphi_5}{5\left(\sigma+1\right)\left(\sigma+2\right)},$$

$$R_{32} = \frac{2\sigma^2\left(\sigma-1\right)\left(\sigma-2\right)\varphi_1-4\left(7\sigma^2-15\sigma+6\right)\varphi_2+32\left(9\sigma^2-12\sigma+2\right)\varphi_3}{5\left(\sigma+1\right)\left(2\sigma+1\right)}$$
$$+\frac{-384\sigma\left(5\sigma-3\right)\varphi_4+6144\sigma^2\varphi_5}{5\left(\sigma+1\right)\left(2\sigma+1\right)},$$

$$R_{41} = \frac{48\varphi_2+64\left(6\sigma-5\right)\varphi_3-768\left(5\sigma-1\right)\varphi_4+12288\sigma\varphi_5}{5\left(\sigma+1\right)},$$

$$R_{42} = \frac{-24\varphi_2-64\left(3\sigma-4\right)\varphi_3+768\left(4\sigma-1\right)\varphi_4-12288\sigma\varphi_5}{5\left(2\sigma+1\right)},$$

$$R_{43} = \frac{16\varphi_2+64\left(2\sigma-3\right)\varphi_3-768\left(3\sigma-1\right)\varphi_4+12288\sigma\varphi_5}{15\left(3\sigma+1\right)},$$

$$R_{51} = 20\varphi_2-\frac{650}{3}\varphi_3+1125\varphi_4-2500\varphi_5,$$

$$R_{52} = -15\varphi_2+\frac{475}{2}\varphi_3-1500\varphi_4+3750\varphi_5,$$

$$R_{53} = \frac{20}{3}\varphi_2-\frac{350}{3}\varphi_3+875\varphi_4-2500\varphi_5,$$

$$R_{54} = -\frac{15}{12}\varphi_2+\frac{275}{12}\varphi_3-\frac{375}{2}\varphi_4+625\varphi_5.$$

Appendix C

Another special class of methods

In this section we give another special class of methods, where the vector α has only two different arguments.

$$\begin{aligned} &\alpha_1 = 1, \qquad \alpha_i = \alpha^*,\ i = 2, \dots, s, \\ &c_1 = \frac{(s-1)(1-\alpha^*) + 1 - \beta}{1-\beta}, \qquad c_i = (s-i)(1-\alpha^*) + 1,\ i = 2, \dots, s, \end{aligned} \tag{1}$$

Then

$$B = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ g_1(\beta) & \beta g_2(\beta) & \beta g_3(\beta) & \dots & \beta g_{s-1}(\beta) & \beta \\ \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & \ddots & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix},$$

where $\quad g_1(0) = 1$.

For zero-stability the choice $\beta = 0$ in (1) is optimal and we have

$$\alpha = \begin{pmatrix} 1 \\ \alpha^* \\ \vdots \\ \alpha^* \end{pmatrix}, \quad c_i = (s-i)(1-\alpha_i) + 1. \tag{2}$$

In similar manner to Section 3.3 we mention some theorems, where their proofs are similar to Theorems 3.7-3.9.

Theorem .1. *For*

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

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 stiff order $p \geq s-1$ for $y' = Ty$.

Theorem .2. *The methods defined by (3.14), (2) are optimally zero-stable, the matrix B is given by*

$$B = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & \dots & 0 & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & \ddots & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}. \tag{3}$$

Corollary .1. *The methods (3) are convergent of stiff order $p = s - 1$.*

Theorem .3. *Let (2) be satisfied and 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 $y' = Ty$.*

We tested this class of methods using the framework of EXPINT [3] with $\alpha^* = \frac{s+1}{s}$ and the results are similar to the class discussed in Section 3.3.

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