Two-step W-methods and peer methods with approximate matrix factorization

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1 Introduction

In this PhD thesis, we consider initial value problems for systems of stiff ordinary differential equations (ODEs) in the form

$$y'(t) = f(t, y(t)), \quad y(t_0) = y_0 \in \mathbb{R}^n, \quad t \in [t_0, t_e]\,, \tag{1.0.1}$$

with right-hand side $f\colon \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}$. Such problems arise from the spatial semi-discretization of time-dependent partial differential equations (PDEs) with the method of lines (MOL). Of special interest is the numerical integration of convection–diffusion–reaction problems with two or more dimensions in space which possess some stiffness from diffusion coefficients or reaction terms. Due to the stiffness, implicit or linearly-implicit methods must be used for the numerical solution of the problem (1.0.1). This requires to solve algebraic equations which leads directly, or by Newton's method, to linear systems. For low and middle dimensions n of the problem (1.0.1), the solution of the linear systems can be computed with direct solvers. But for high dimensional problems ($n \gg 10000$), this can be very costly with respect to computer memory and computation time. Therefore, it requires special approaches for an efficient solution of the systems of linear equations. To this aim, one frequently uses Krylov techniques applied in the well-known integration codes `VODPK` [9], `ROWMAP` [70] and `EXP4` [29]. Another way is to apply an approximate matrix factorization (AMF). This technique was applied in the early papers by D'Yakonov [17] in 1964 and by Beam and Warming [2] in 1976. The AMF approach is related to the class of alternating direction implicit (ADI) methods which was mentioned for the first time by Peaceman and Rachford [45] in 1955. This can be seen as the very first splitting method in the literature. An overview about AMF and related splitting methods is given in the paper of van der Houwen and Sommeijer [31] and in the book of Hundsdorfer and Verwer [32]. The idea of AMF is to split the full Jacobian of the semi-discretized problem (1.0.1) into a sum of several terms with simpler structures, i.e., the split Jacobian matrices are band matrices of small bandwidth. This can be obtained directly or by rearranging components in the semi-discretization of the PDE problems with the method of lines. Instead of computing the LU-decomposition of a matrix with a large bandwidth, a sequence of linear systems of much simpler structure is solved. Especially for high dimensional ODE problems, this is more efficient and reduces the computation time significantly.

AMF methods have been widely studied in the literature. Linearly-implicit Runge–Kutta methods with AMF approach are considered by Calvo and Gerisch [12] and Zhang *et al.* [75]. Particularly, one-step AMF W-methods and Rosenbrock-type methods are

investigated frequently. Besides that, classical Rosenbrock-type methods with AMF are discussed in [32]. A two-stage second-order Rosenbrock AMF method was proposed by Verwer *et al.* [65] in 1999. A two-stage third-order method has been applied by Lanser *et al.* [43] to shallow water equations. In 2002, Gerisch and Verwer [18] suggested a three-stage second-order Rosenbrock AMF method for arbitrary Jacobian matrices. In later investigations, Rosenbrock-type methods and one-step W-methods with AMF were studied intensively by González-Pinto and co-authors, see e.g. [24–26]. More recent research is concerned with parabolic problems and mixed derivatives [21,22] or with the convergence analysis of one-step AMF W-methods [23].

Due to their low stage order, one-step W-methods may suffer from order reduction for very stiff problems. Furthermore, the construction of higher order methods is rather difficult. For these reasons, Podhaisky *et al.* [47] introduced the class of two-step W-methods in 2002. These methods are linearly-implicit and stage values from the previous step are involved in the numerical scheme. Parallel two-step W-methods are investigated in [49, 71] and high order parallel two-step W-methods with favourable stability properties are proposed by Jackiewicz *et al.* [34]. Parallel two-step W-methods also perform well for the solution of large stiff ODE systems in combination with Krylov approximations. In Klinge *et al.* [38], a special class of stiffly accurate two-step W-methods is presented. These methods are constructed with respect to an additional condition leading to higher order methods for variable step size sequences. By this construction principle, stage values can no longer be computed in parallel. In this thesis, results of this kind will be discussed in detail. Two-step W-methods with application of AMF for solving large stiff ODE systems have been treated recently by Klinge *et al.* [37].

Another class of two-step methods are peer methods as introduced by Schmitt and Weiner [53] in 2004. In contrast to two-step W-methods, all stage values have the same stage order, i.e., the stage order is equal to the order of consistency. This is why, these methods are referred to as *peer*. Peer methods are a special class of general linear methods (GLMs) which have been introduced by Butcher [7]. More information on GLMs can be found in Butcher [8] or in the monograph by Jackiewicz [33]. Again, no order reduction occurs for very stiff problems due to the high stage order of peer methods. They are first considered as linearly-implicit methods for parallel computations [53]. Like Rosenbrock–Wanner methods (ROW-methods), linearly-implicit peer methods can be obtained as a result of one step in Newton's method of a fully implicit method. Later investigations are concerned with fully implicit peer methods and up to ten Newton steps [54] and with sequential computations, see e.g. [46, 48].

Peer methods have been considered frequently in the literature. Explicit peer methods are investigated e.g. in [11, 67, 72]. Horváth *et al.* [30] derived explicit peer methods with strong stability preserving (SSP) property. An application of SSP explicit peer methods to discontinuous Galerkin discretizations is considered by Klinge *et al.* [39]. In general, the nodes of peer methods are assumed to be pairwise distinct. In Klinge *et al.* [40], optimally zero-stable explicit peer methods with variable nodes are proposed.

Implicit and linearly-implicit peer methods with applications have been investigated in several papers, see e.g. [19,35,44,48,63]. Implicit two-step peer methods for the solution of large stiff ODE systems are introduced by Beck *et al.* [5]. Here the non-linear stage equations are solved by the inexact Newton's method with the Krylov solver FOM (*full orthogonalization method*). In further investigations, peer methods with approximate matrix factorization are developed and compared with peer methods and Krylov techniques [3, 4]. For stability reasons, a predictor of low order is proposed for the Newton iteration in AMF methods. In numerical tests on problems of convection–diffusion–reaction type, it is shown that AMF peer methods are superior, especially for low accuracy requirements, and are more efficient compared to standard codes from the MATLAB ODE suite. Soleimani and Weiner [59] introduced a more general class of implicit peer methods for stiff systems using in addition function values from the previous step. This allows an increase in the order of the methods and makes the construction of optimally zero-stable methods rather simple. Numerical tests are promising. These peer methods are reliable, accurate and superior compared to existing implicit peer methods from [3]. Exponential peer methods are derived by Weiner and El-Azab [69] and an application of exponential peer methods to stiff ODE systems of high dimension is discussed by Weiner and Bruder [68].

Many initial value problems arising in practice can be split into a stiff and a non-stiff part where the stiff part is integrated with an implicit numerical scheme and the non-stiff part is treated explicitly. For parabolic PDE problems of convection–diffusion–reaction type, the stiff term often originates from spatial discretization of the diffusion and reaction parts and the non-stiff term is obtained from discretized convection parts. With this splitting strategy, one can combine the advantages of implicit and explicit methods which leads to so-called implicit-explicit (IMEX) methods. Such methods are investigated frequently in the literature. IMEX peer methods are recently introduced and studied by Soleimani *et al.* [58, 60], Lang *et al.* [42] and Schneider *et al.* [55, 56]. In contrast to IMEX Runge–Kutta methods, see e.g. [1, 6, 20], there are no additional coupling conditions between the explicit and implicit part for IMEX peer methods. With this and due to the high stage order, the construction of IMEX peer methods is much simpler. Terms of the split Jacobian corresponding to the non-stiff part of the ODE problem should not be considered in AMF schemes. This leads to the concept of an inexact AMF approach which has been applied successfully to Rosenbrock-type methods by González-Pinto *et al.* [24]. Of course, an inexact AMF approach is also desirable when some parts of the Jacobian are difficult to compute, are not needed to ensure stability in AMF schemes, or are challenging for the solution of linear systems.

In this thesis, we will investigate two-step W-methods and two-step peer methods with application of an AMF approach for large stiff ODE systems. We introduce the class of two-step AMF W-methods, make a linear stability analysis and construct appropriate methods. For AMF peer methods, we consider the more general class of implicit peer methods introduced by Soleimani and Weiner [59]. This leads to an extension of AMF

peer methods introduced and treated by Beck *et al.* [3, 4]. A main contribution of this thesis is a comparison of one-step AMF W-methods with two-step AMF methods. Therefore, it is in our interest to investigate AMF peer methods with an arbitrary, but fixed number of steps in the Newton iteration. This allows a more proper stability, consistency and convergence analysis and comparison with linearly-implicit one-step and two-step AMF W-methods. We propose a predictor for the Newton iteration in AMF peer methods which is designed with respect to both accuracy and stability. The influence of an inexact AMF approach is discussed and we consider IMEX peer methods with AMF for large ODE systems. The test set in our numerical experiments with AMF consists of the well-known two-dimensional Brusselator problem [27] which has already been considered in the investigations of AMF peer methods by Beck *et al.* [3, 4]. Furthermore, we choose a diffusion–convection equation, see e.g. [70]. This test example allows an adaption of IMEX methods by solving the convection part explicitly. We completed our test set with a linear diffusion problem which is considered recently with mixed derivatives for PDE-type W-methods [21] and AMF-type W-methods [22]. More recently, this linear model is also treated in a convergence analysis of one-stage AMF W-methods [23] and in general linear methods with ADI techniques [52].

This PhD thesis is organized as follows. In Chapter 2, we recall the formulation of two-step W-methods. Order conditions and stability properties are discussed. We give a new additional condition which allows the construction of s-stage stiffly accurate two-step W-methods of order $p^* = s + 1$ for variable step sizes. We construct new two-step W-methods up to five stages and test their efficiency on standard stiff test problems. A comparison with existing two-step W-methods and the well-known integration codes `RODAS` and `ode23s` is included. It is shown that two-step W-methods do not suffer from order reduction for stiff problems. Chapter 3 deals with two-step W-methods and the application of AMF. We give the idea of an AMF approach and review one-step AMF W-methods. We introduce the class of two-step AMF W-methods and show that the concept of AMF does not influence the order of two-step AMF W-methods. Furthermore, we prove that in contrast to one-step AMF W-methods, the time derivatives do not appear in the numerical scheme for non-autonomous problems. A linear stability analysis is given and we show a stability result for two-step AMF W-methods at infinity. We construct new two-step W-methods which are suitable for an application with AMF. Peer methods with AMF are considered in Chapter 4. We focus on investigations for a fixed number of Newton steps in the AMF peer iteration. Consistency and convergence of AMF peer methods are proved in this case. We also investigate the influence of an inexact AMF approach. Stability properties are discussed for the linear test equation. We construct a new three-stage AMF peer method of order three and propose a corresponding predictor in the Newton iteration. Furthermore, we study the application of AMF in IMEX peer methods and construct an appropriate three-stage AMF IMEX peer method of order three. In Chapter 5, we show the results of our numerical experiments with linearly-implicit one-step and two-step W-methods and two-step peer methods with

application of AMF. The methods are tested on the autonomous 2D Brusselator problem, a linear diffusion problem with homogeneous and time-dependent Dirichlet boundary conditions and a 2D diffusion–convection equation. The influence of different predictors in AMF peer methods in our numerical experiments with constant time step sizes is demonstrated. Moreover, we present numerical tests for AMF IMEX peer methods on the diffusion–convection equation with an inexact AMF approach. Finally, conclusions are drawn and topics of future work are proposed in Chapter 6.

2 Two-step W-methods

In this chapter, we describe two-step W-methods. We give an overview about order conditions and stability. A new additional condition allows the construction of stiffly accurate methods which are convergent of order $p^* = s + 1$ with s stages for variable step size sequences. We construct and optimize new two-step W-methods up to five stages in detail. Numerical tests on standard stiff test problems show the efficiency of the new methods compared to well-known integration methods and existing two-step W-methods. It is also illustrated that two-step W-methods avoid order reduction for stiff problems.

2.1 Formulation of the methods

For the numerical solution of stiff initial value problems

$$y'(t) = f(t, y(t)), \quad y(t_0) = y_0 \in \mathbb{R}^n, \quad t \in [t_0, t_e]\,, \tag{2.1.1}$$

with right-hand side $f\colon \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n$, Rosenbrock–Wanner methods (ROW-methods) are applied frequently. There exist A- and L-stable methods. Due to their linear-implicit structure, these methods are easy to implement. Well-known codes are `GRK4T` [28, 36], `RODAS` [28] and `RODASP` [28, 62]. For more information on ROW-methods, we refer to the review paper by Lang [41] and the references therein. However, due to their low stage order, an order reduction can occur for very stiff problems, see e.g. [46]. Another drawback of ROW-methods is the need to compute the Jacobian in every step. One-step W-methods allow keeping the Jacobian constant for several steps. However, because of additional order conditions, the construction of higher order methods is rather difficult.

To overcome these problems, Podhaisky and co-workers introduced and investigated two-step W-methods [34,47,49,71] which retain the linear-implicit structure. Recently, these methods were applied in combination with approximate matrix factorization (AMF) for the solution of two-dimensional partial differential equations (PDEs) [37]. These methods can be derived from implicit two-step Runge–Kutta methods by applying one

step of Newton's method. An s-stage two-step W-method (TSW-method) is given by

$$\begin{aligned} Y_{m,i} &= u_m + h_m \sum_{j=1}^{s} a_{ij} k_{m-1,j} + h_m \sum_{j=1}^{i-1} \widetilde{a}_{ij} k_{m,j}, \quad i = 1, \ldots, s, \\ (I - h_m \gamma T_m) k_{m,i} &= f(t_{m,i}, Y_{m,i}) + h_m T_m \sum_{j=1}^{s} \gamma_{ij} k_{m-1,j} + h_m T_m \sum_{j=1}^{i-1} \widetilde{\gamma}_{ij} k_{m,j}, \\ & \qquad i = 1, \ldots, s, \\ u_{m+1} &= u_m + h_m \sum_{j=1}^{s} (b_j k_{m,j} + v_j k_{m-1,j}). \end{aligned} \tag{2.1.2}$$

Here u_{m+1} is an approximation to the exact solution $y(t_{m+1})$ at each time step $t_{m+1} = t_m + h_m$. The matrix T_m is arbitrary and the order of the method is independent of the choice of T_m. For stability reasons, it should be an approximation to the Jacobian $f_y(t_m, u_m)$, but it can be kept constant for some steps in practical computations. Note that with $T_m = 0$, the methods reduce to explicit two-step Runge–Kutta methods which are not suited for stiff problems, see e.g. [14]. The s external stage values $Y_{m,i}$ are approximations to $y(t_{m,i})$, where $t_{m,i} = t_m + c_i h_m$ and $k_{m,i}$ represent approximations to the corresponding stage derivatives, i.e., $k_{m,i}$ are approximations to $y'(t_{m,i})$. We always assume that $\gamma > 0$ and the nodes c_i are pairwise distinct with $c_s = 1$. The parameters of the method can be collected in matrices $A = (a_{ij})_{i,j=1}^{s}$, $\widetilde{A} = (\widetilde{a}_{ij})$, $\Gamma = (\gamma_{ij})$, $\widetilde{\Gamma} = (\widetilde{\gamma}_{ij})$ and vectors $b = (b_i)_{i=1}^{s}$, $v = (v_i)$, $c = (c_i)$. The coefficients $\widetilde{A}$ and $\widetilde{\Gamma}$ are strictly lower triangular matrices. Note that some of the coefficients will depend on the step size ratio $\sigma = h_m / h_{m-1}$. The methods are linearly-implicit. For every stage a system of linear equations has to be solved with a coefficient matrix which is constant within the step, i.e., only one LU-decomposition is required per step. Due to the two-step character, the methods require additional starting values $k_{0,i}$, $i = 1, \ldots, s$. For $A = 0$, $\Gamma = 0$ and $v = 0$, we obtain the classical one-step W-methods, cf. Section 3.1. Parallel two-step W-methods with $\widetilde{A} = 0$ and $\widetilde{\Gamma} = 0$ are investigated in [49, 71] and high order parallel two-step W-methods are studied in [34]. Two-step W-methods with $\widetilde{A} \neq 0$ and $\widetilde{\Gamma} = 0$ are considered in [47].

2.2 Order conditions and stability issues

In this section, we review results about order and stability. The results are collected from [47] and [49]. Order conditions can be derived by inserting the exact solution in the numerical scheme and studying the Taylor series expansions of the residuals. The

residual errors can be analyzed with the help of the following simplifying assumptions:

$$C(q): \quad \sigma^l c_i^l/l! = \sigma \sum_{j=1}^{s} a_{ij}(c_j-1)^{l-1}/(l-1)! + \sigma^l \sum_{j=1}^{i-1} \widetilde{a}_{ij} c_j^{l-1}/(l-1)!, \tag{2.2.3}$$
$$l = 1,\dots,q, \quad i = 1,\dots,s,$$

$$\Gamma(q): \quad -\gamma\sigma^l c_i^{l-1}/(l-1)! = \sigma \sum_{j=1}^{s} \gamma_{ij}(c_j-1)^{l-1}/(l-1)! + \sigma^l \sum_{j=1}^{i-1} \widetilde{\gamma}_{ij} c_j^{l-1}/(l-1)!, \tag{2.2.4}$$
$$l = 1,\dots,q, \quad i = 1,\dots,s,$$

$$B(p): \quad \sigma^l/l! = \sigma^l \sum_{i=1}^{s} b_i c_i^{l-1}/(l-1)! + \sigma \sum_{i=1}^{s} v_i (c_i-1)^{l-1}/(l-1)!, \tag{2.2.5}$$
$$l = 1,\dots,p.$$

A two-step W-method (2.1.2) is said to be of stage order q if conditions $C(q)$ and $\Gamma(q)$ are satisfied. In contrast to multistep methods, two-step W-methods are stable for $h_m \to 0$ (zero-stability) by design and hence convergence follows without additional stability conditions. We denote the errors of the starting values by

$$\varepsilon_0 = \|y(t_0) - u_0\|, \quad \nu_0 = \max_{i=1,\dots,s} \|y'(t_0 + c_i h_0) - k_{0,i}\|.$$

Analogously to the class of parallel two-step W-methods [49], one shows the following theorem.

Theorem 2.2.1 ([47]). *Assume that the initial errors satisfy $\varepsilon_0 = \mathcal{O}(h_0^p)$ and $\nu_0 = \mathcal{O}(h_0^q)$ with $p, q \in \mathbb{N}$. Let the coefficients of a two-step W-method (2.1.2) and the step size ratio be bounded, i.e., $\sigma = h_m/h_{m-1} < \sigma_{max}$. If the two-step W-method (2.1.2) satisfies the simplifying assumptions C(q), Γ(q) and B(p), then for arbitrary matrices T_m it is convergent of order $p^* = \min(q+1, p)$ for a sufficiently smooth right-hand side f.* □

The simplifying conditions (2.2.3)–(2.2.5) are linear relations between the coefficient matrices. In the convenient case $p = q = s$, i.e., the method has stage order s, we can satisfy the order conditions by solving for A, Γ and $v^\top$:

$$A = (CV_0D^{-1} - \widetilde{A}V_0)SV_1^{-1}, \tag{2.2.6}$$
$$\Gamma = -(\gamma I + \widetilde{\Gamma})V_0SV_1^{-1}, \tag{2.2.7}$$
$$v^\top = (\mathbb{1}^\top D^{-1} - b^\top V_0)SV_1^{-1}. \tag{2.2.8}$$

Here we use the notations

$$V_0 = \left(c_i^{j-1}\right)_{i,j=1}^{s}, \quad V_1 = \left((c_i-1)^{j-1}\right)_{i,j=1}^{s}, \quad D = \operatorname{diag}(1,\dots,s),$$
$$C = \operatorname{diag}(c_1,\dots,c_s), \quad S = \operatorname{diag}\left(1,\sigma,\dots,\sigma^{s-1}\right), \quad \mathbb{1}^\top = (1,\dots,1) \in \mathbb{R}^s. \tag{2.2.9}$$

Note that the Vandermonde-type matrices V_0 and V_1 are quadratic and non-singular in the case of pairwise distinct nodes, i.e., the coefficients A, Γ and $v^\top$ are uniquely defined by (2.2.6)–(2.2.8). The system (2.2.6)–(2.2.8) also allows the computation of the coefficients when the step size is changed in a step size control implementation.

For stability investigations, we consider the usual scalar Dahlquist test equation [16]

$$y'(t) = \lambda y(t), \quad \lambda \in \mathbb{C}^-. \tag{2.2.10}$$

We consider $T_m = \lambda$. Then the application of the two-step W-method (2.1.2) to the test problem (2.2.10) leads to the matrix recursion with $z = h_{m-1}\lambda$ in the form

$$\begin{pmatrix} h_m K_m \\ u_{m+1} \end{pmatrix} = M(z) \begin{pmatrix} h_{m-1} K_{m-1} \\ u_m \end{pmatrix}, \tag{2.2.11}$$

where the $(s+1) \times (s+1)$ amplification matrix $M(z)$ is given by

$$M(z) = \begin{pmatrix} \sigma W(z)\beta & W(z)\mathbb{1} \\ \sigma(b^\top W(z)\beta + v^\top) & 1 + b^\top W(z)\mathbb{1} \end{pmatrix} \tag{2.2.12}$$

with $K_m := (k_{m,1}, \ldots, k_{m,s})^\top$, $\beta := A + \Gamma$, $\widetilde{\beta} := \widetilde{A} + \widetilde{\Gamma}$ and $W(z) = \left((1 - z\gamma)I - z\widetilde{\beta}\right)^{-1} z$. Of course, the stability matrix $M(z)$ depends on the step size ratio σ. From the order conditions (2.2.6)–(2.2.8), we can derive

$$\beta = \left(CV_0D^{-1} - \gamma V_0 - \widetilde{\beta}V_0\right) SV_1^{-1} = \left(CV_0D^{-1} + W_\infty^{-1}V_0\right) SV_1^{-1}$$

with $W_\infty := W(\infty) = -\left(\gamma I + \widetilde{\beta}\right)^{-1}$. In the following, we consider constant step sizes, i.e., $\sigma = 1$. Then stability is characterized by the spectral radius of M, which is denoted by $\varrho(M(\cdot))$.

Definition 2.2.2. We call the set $\mathcal{S} = \{z \in \mathbb{C} : \varrho(M(z)) < 1\}$ stability domain of the two-step W-method (2.1.2). The method is called A(α)-stable if $\{z \in \mathbb{C}\colon |\arg(z) - \pi| \leq \alpha\} \subseteq \bar{\mathcal{S}}$. It is said to be A-stable if $\alpha = \frac{\pi}{2}$. We call a method stiffly accurate if for all fixed $u_m, k_{m-1,i},\ i = 1, \ldots, s$, the condition

$$\lim_{|z| \to \infty} u_{m+1} = 0 \tag{2.2.13}$$

holds. A method is called L(α)-stable if it is A(α)-stable and the condition (2.2.13) is fulfilled. It is said to be L-stable if $\alpha = \frac{\pi}{2}$. □

The condition (2.2.13) for stiff accuracy is equivalent to a vanishing last row in the stability matrix $M(z)$ for $|z| \to \infty$, i.e., $e_{s+1}^\top M(\infty) = 0$. This can also be achieved for variable step sizes. We recall the following lemma.

Lemma 2.2.3 ([47]). *Let the two-step W-method* (2.1.2) *satisfy the conditions* $\Gamma(s)$, $C(s)$ *and* $B(s)$. *Then we have* $e_{s+1}^\top M(\infty) = 0$ *if and only if* $c_k = 1$ *for some* k *and*

$$b^\top = -e_k^\top W_\infty^{-1} = e_k^\top \left(\gamma I + \widetilde{A} + \widetilde{\Gamma}\right), \tag{2.2.14}$$

$$v^\top = e_k^\top (A + \Gamma) \tag{2.2.15}$$

hold. □

With $c_s = 1$, i.e., $k = s$, the conditions (2.2.14) and (2.2.15) for stiff accuracy give

$$b^\top = e_s^\top \left(\gamma I + \widetilde{A} + \widetilde{\Gamma}\right), \tag{2.2.16}$$

$$v^\top = e_s^\top (A + \Gamma). \tag{2.2.17}$$

In [47, 49, 71], stiffly accurate methods of order $p^* = s$ with $\widetilde{\Gamma} = 0$ were constructed. However, Theorem 2.2.1 shows that the methods will have order of convergence $p^* = s+1$ if $B(s+1)$ is satisfied for variable step sizes. In the following, we will give a new additional condition which allows the construction of a stiffly accurate two-step W-method which satisfies $B(s+1)$ and thus has order of convergence $p^* = s+1$ for variable step sizes.

2.3 Stiffly accurate methods of order $p^* = s + 1$

In this section, we will prove our main result of this chapter. We assume that the order conditions (2.2.6)–(2.2.8) are satisfied, i.e., the simplifying assumptions $C(s)$, $\Gamma(s)$ and $B(s)$ are fulfilled and therefore we have a two-step W-method of order $p^* = s$ by Theorem 2.2.1. For $B(s+1)$ it remains to satisfy

$$\frac{\sigma^{s+1}}{(s+1)!} = \frac{\sigma^{s+1}}{s!} b^\top c^s + \frac{\sigma}{s!} v^\top (c - \mathbb{1})^s,$$

where $c^s := (c_1^s, \ldots, c_s^s)^\top$. Substituting condition (2.2.8) leads to

$$\sigma^s = (s+1)\sigma^s b^\top c^s + (s+1)(\mathbb{1}^\top D^{-1} - b^\top V_0) S V_1^{-1} (c - \mathbb{1})^s. \tag{2.3.18}$$

Due to the appearance of S, this condition must be satisfied for variable σ. This leads to $s+1$ conditions for the coefficients at powers σ^l, $l = 0, \ldots, s$. It turns out that it is possible to find stiffly accurate two-step W-methods which satisfy in addition to the order conditions (2.2.6)–(2.2.8), also the condition (2.3.18) for all σ.

Theorem 2.3.1. *Let the two-step W-method* (2.1.2) *satisfy the conditions* $\Gamma(s)$, $C(s)$ *and* $B(s)$ *and let* $c_s = 1$. *Then under the conditions*

$$b^\top = \left(\frac{1}{2}, \ldots, \frac{1}{s+1}\right) V_0^{-1} C^{-1}, \tag{2.3.19}$$

$$(\widetilde{\gamma}_{s,1}, \ldots, \widetilde{\gamma}_{s,s-1}, \gamma) = \left(\frac{1}{2}, \ldots, \frac{1}{s+1}\right) V_0^{-1} C^{-1} - e_s^\top \widetilde{A}, \tag{2.3.20}$$

the two-step W-method satisfies $B(s+1)$ and is stiffly accurate.

Proof. For $B(s+1)$ we have to show that condition (2.3.18) is satisfied. We denote $x := V_1^{-1}(c-\mathbb{1})^s$ with $x = (x_1, \ldots, x_s)^\top$. Considering the powers of σ, condition (2.3.18) is equivalent to the $s+1$ conditions

$$\begin{aligned} 0 &= \left(\frac{1}{l} - b^\top c^{l-1}\right) x_l, \quad l = 1, \ldots, s, \\ 0 &= \frac{1}{s+1} - b^\top c^s. \end{aligned} \tag{2.3.21}$$

For $l = 1$, we have by the definition of the matrix V_1 and because of $c_s = 1$

$$x_1 = e_1^\top x = e_1^\top V_1^{-1}(c-\mathbb{1})^s = e_s^\top (c-\mathbb{1})^s = 0.$$

Furthermore, it is

$$CV_0 = (c, c^2, \ldots, c^s)$$

and hence

$$b^\top C V_0 = (b^\top c, \ldots, b^\top c^s).$$

On the other hand, it holds with assumption (2.3.19)

$$b^\top C V_0 = \left(\frac{1}{2}, \ldots, \frac{1}{s+1}\right).$$

It follows that the remaining s conditions of (2.3.21) for all $l = 2, \ldots, s+1$ are fulfilled, i.e., the condition $B(s+1)$ holds.

To prove stiff accuracy, we have to show that (2.2.16) and (2.2.17) are satisfied. It holds

$$\begin{aligned} e_s^\top(\widetilde{A} + \gamma I + \widetilde{\Gamma}) &= e_s^\top \widetilde{A} + (\widetilde{\gamma}_{s,1}, \ldots, \widetilde{\gamma}_{s,s-1}, \gamma) \\ &= e_s^\top \widetilde{A} + \left(\frac{1}{2}, \ldots, \frac{1}{s+1}\right) V_0^{-1} C^{-1} - e_s^\top \widetilde{A} \quad \text{(by (2.3.20))} \\ &= b^\top \quad \text{(by (2.3.19))}, \end{aligned}$$

i.e., (2.2.16) is fulfilled. With (2.2.6) and (2.2.7), it follows

$$\begin{aligned} e_s^\top(A + \Gamma) &= e_s^\top(CV_0 D^{-1} - \widetilde{A} V_0 - \gamma V_0 - \widetilde{\Gamma} V_0) S V_1^{-1} \\ &= (\mathbb{1}^\top D^{-1} - b^\top V_0) S V_1^{-1} \quad \text{(by } e_s^\top C V_0 = e_s^\top V_0 = \mathbb{1}^\top \text{ and (2.2.16))} \\ &= v^\top \quad \text{(by (2.2.8))}, \end{aligned}$$

i.e., (2.2.17) is satisfied, and thus the two-step W-method is stiffly accurate. ■

This theorem allows us to construct stiffly accurate two-step W-methods which are convergent of order $p^* = s+1$ for variable step sizes. Note that the order $p^* = s$ of two-step W-methods is guaranteed by the order conditions (2.2.6)–(2.2.8), i.e., it is not influenced by the additional conditions (2.3.19) and (2.3.20). We summarize this in the following corollary.

Corollary 2.3.2. *Let a two-step W-method* (2.1.2) *be given which satisfies the assumptions of Theorem 2.3.1. If the initial errors satisfy* $\varepsilon_0 = \mathcal{O}(h_0^{s+1})$, $\nu_0 = \mathcal{O}(h_0^s)$ *and the step size ratio is bounded, i.e.,* $\sigma = h_m/h_{m-1} < \sigma_{max}$, *then the two-step W-method is convergent of order* $p^* = s+1$ *for variable step sizes.*

Proof. With Theorem 2.3.1, the condition $B(s+1)$ is satisfied and the two-step W-method is stiffly accurate. Convergence order $p^* = \min(q+1, p) = s+1$ for variable step sizes follows with Theorem 2.2.1 and $q = s$ and $p = s+1$. ■

Remark 2.3.3. *For explicit peer methods, superconvergence for variable step sizes can be proved under certain assumptions and the condition given by*

$$\sum_{i=1}^{s-1} r_{si} c_i^{l-1} = \frac{1}{l}, \quad l = 2, \ldots, s+1, \tag{2.3.22}$$

cf. [72, Theorem 2]. Condition (2.3.19) *can be rewritten with* $CV_0 = (c, c^2, \ldots, c^s)$ *in the form*

$$\sum_{i=1}^{s} b_i c_i^{l-1} = \frac{1}{l}, \quad l = 2, \ldots, s+1,$$

so that (2.3.19) *can be considered as a special case of the condition for superconvergence of peer methods with* $e_s^\top R = b^\top$, *where* R *is a strictly lower triangular matrix. Actually, the proof of Theorem 2.3.1 is based on arguments which are also used for the proof of the superconvergence of explicit peer methods. Peer methods are discussed in detail in Chapter 4.* □

Remark 2.3.4. *For peer methods, condition* (2.3.22) *is an overdetermined system for the non-trivial elements of the last row of the matrix* R. *In contrast to that, the weights* b *are uniquely defined by* (2.3.19) *and the pairwise distinct nodes* c. *Furthermore, the coefficients* b *are independent of the step size ratio* σ. □

Remark 2.3.5. *By condition* (2.3.20), *the coefficients* $\widetilde{A}$ *and* $\widetilde{\Gamma}$ *can not be chosen as zeros simultaneously since*

$$\gamma e_s^\top C V_0 = \gamma e_s^\top V_0 = \gamma \mathbb{1}^\top \neq \left(\frac{1}{2}, \ldots, \frac{1}{s+1}\right) \quad \text{for all } \gamma > 0,$$

i.e., it is not possible to construct stiffly accurate parallel two-step W-methods which satisfy $B(s+1)$ *for variable step sizes. Of course, one can obtain stiffly accurate two-step W-methods with* $\widetilde{\Gamma} = 0$ *and* $\widetilde{A} \neq 0$ *which satisfy* $B(s+1)$ *for variable step sizes, e.g.* `TSW2B` *from [47].* □

Despite the additional conditions (2.3.19) and (2.3.20), there are free parameters left, namely $c_1, \ldots, c_{s-1}$, $\widetilde{A}$ and $\widetilde{\Gamma}$ (except the last row). In the next section, we describe the construction of stiffly accurate two-step W-methods of convergence order $p^* = s + 1$ for variable step sizes with good stability properties and small error constants.

2.4 Construction of methods with $B(s+1)$

In this section, the construction of two-step W-methods is discussed which satisfies the order conditions (2.2.6)–(2.2.8) and the conditions for $B(s+1)$ and stiff accuracy (2.3.19) and (2.3.20), i.e., the methods are stiffly accurate and have the properties

$$C(s),\ \Gamma(s),\ B(s+1) \text{ and } c_s = 1.$$

In this case, the parameters A, Γ, $v^\top$, $b^\top$, $\widetilde{\gamma}_{s,1}, \ldots, \widetilde{\gamma}_{s,s-1}$ and γ are determined. The remaining free $s(s-1)$ parameters are $\widetilde{A}$, $\widetilde{\gamma}_{ij}$, $i = 1, \ldots, s-1$, $j = 1, \ldots, i-1$ and $c_1, \ldots, c_{s-1}$ and should not depend on the step size ratio σ. Then $\widetilde{\gamma}_{s,1}, \ldots, \widetilde{\gamma}_{s,s-1}$ and γ are also uniquely defined by (2.3.20) with pairwise distinct nodes c and independent of the step size ratio. We search for suitable two-step W-methods with a large angle α of L(α)-stability, small error constants and small spectral radius at infinity $\varrho(M(\infty))$ for $\sigma = 1$. For stiffly accurate two-step W-methods, this is equivalent to $\varrho(G_\infty)$, cf. [47, Sect. 3], where $G_\infty := W_\infty \beta$. We consider as error constant *ferr* the sum of the magnitude of the residual errors in $C(s+1)$, $\Gamma(s+1)$ and $B(s+2)$. It is also our aim to have small coefficients for the methods. The optimization is done for constant step sizes, i.e., for $\sigma = 1$. We use `fmincon` from the optimization toolbox in MATLAB and the computer algebra system MAXIMA for algebraic computations. In the following, we discuss the construction of two-step W-methods for different numbers of stages s in detail.

2.4.1 Methods with $s = 2$ stages

In this case, we have only two free parameters, namely, c_1 and $\widetilde{a}_{21}$. One can determine c_1 with respect to the angle α of L(α)-stability and the spectral radius $\varrho(G_\infty)$ for $\sigma = 1$. Figure 2.4.1 shows the angle α and $\varrho(G_\infty)$ as functions of the node c_1. Note that one can find methods with $\alpha = 90°$ only for $c_1 > 1$ and there is also a method with significant minimal $\varrho(G_\infty)$, cf. Figure 2.4.1 (*right*). We denote this L-stable two-step W-method with `2c`. For $c_1 < 1$, we find a method `2a` with maximal angle α and sufficiently small spectral radius $\varrho(G_\infty)$, see Figure 2.4.1 (*left*). Furthermore, we obtain a method `2b` with minimal spectral radius and sufficiently large angle α. Anyway, the conditions $\varrho(G_\infty) = 0$ and $B(3)$ cannot be satisfied simultaneously. With fixed c_1, we determine $\widetilde{a}_{21}$ of corresponding two-step W-methods to have small error constants and coefficients, cf. Figure 2.4.2.

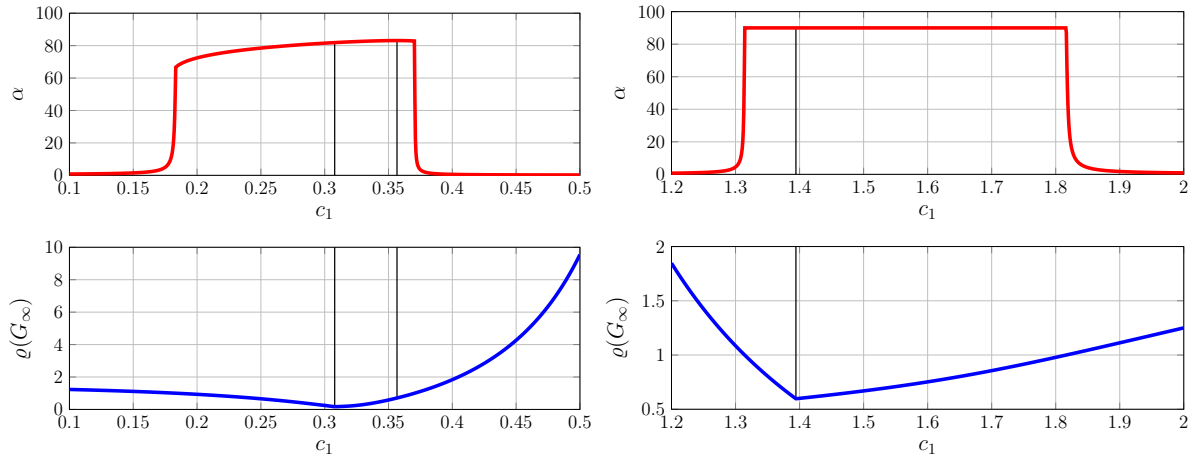

Figure 2.4.1: Angle α of L(α)-stability vs. c_1 (*top*) and $\varrho(G_\infty)$ vs. c_1 (*bottom*), with $c_1 < 1$ (*left*) and $c_1 > 1$ (*right*).

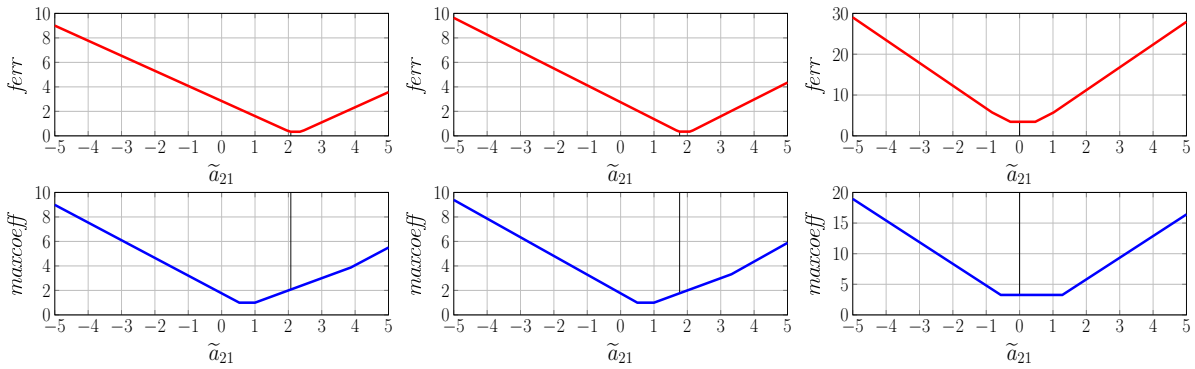

Figure 2.4.2: Error constant *ferr* vs. $\widetilde{a}_{21}$ (*top*) and maximal magnitude of the coefficients *maxcoeff* vs. $\widetilde{a}_{21}$ (*bottom*), for method `2a` (*left*), for method `2b` (*middle*) and for method `2c` (*right*).

The coefficients of the methods are given by:

`2a`:

$$c_1 = 3.0782143245063232e{-}1, \quad c_2 = 1.0000000000000000e{+}0, \quad \widetilde{a}_{21} = 2.0690788660374544e{+}0,$$
$$\widetilde{\gamma}_{21} = -1.2868537668693829e{+}0, \quad \gamma = 2.5921434947524624e{-}1.$$

`2b`:

$$c_1 = 3.4450201538310682e{-}1, \quad c_2 = 1.0000000000000000e{+}0, \quad \widetilde{a}_{21} = 1.7664815214862395e{+}0,$$
$$\widetilde{\gamma}_{21} = -1.0284317978823534e{+}0, \quad \gamma = 2.4574038276551641e{-}1.$$

2c:

$$c_1 = 1.3943190448038838e{+}0, \quad c_2 = 1.0000000000000000e{+}0, \quad \widetilde{a}_{21} = 0.0000000000000000e{+}0,$$
$$\widetilde{\gamma}_{21} = -3.0313692240435608e{-}1, \quad \gamma = 9.2266958409163080e{-}1.$$

2.4.2 Methods with $s = 3$ stages

In the case of three stages, we have six free parameters: $\widetilde{a}_{21}$, $\widetilde{a}_{31}$, $\widetilde{a}_{32}$, $\widetilde{\gamma}_{21}$, c_1 and c_2. Analogous to [47], we want to have methods with $\varrho(G_\infty) = 0$ for $\sigma = 1$. The characteristic polynomial is given by $\det(xI - G_\infty) = x^3 + p_2x^2 + p_1x + p_0$. We compute $\widetilde{a}_{21}, \widetilde{a}_{31}$ and $\widetilde{a}_{32}$ so that $p_2 = p_1 = p_0 = 0$ are satisfied. Note that $p_2 = p_1 = 0$ is a linear system in $\widetilde{a}_{31}$ and $\widetilde{a}_{32}$. Inserting this into $p_0 = 0$ yields a condition for $\widetilde{a}_{21}$. These calculations are done with the computer algebra system MAXIMA. Note that we have to add a further constraint in the optimization process to satisfy condition (2.3.20). Then we optimize $\widetilde{\gamma}_{21}$, c_1 and c_2 with respect to the angle α of L(α)-stability, error constant and the magnitude of the coefficients, whereby we apply different heuristics to find appropriate methods. The following method `3b` has been found in this way:

3b:

$$c_1 = 4.2451803798618165e{-}1, \quad c_2 = 1.2555618550820942e{+}0, \quad c_3 = 1.0000000000000000e{+}0,$$
$$\widetilde{a}_{21} = 5.1774789773658938e{+}0, \quad \widetilde{a}_{31} = 6.3391015556851371e{-}1, \quad \widetilde{a}_{32} = -4.0773189037882983e{-}2,$$
$$\widetilde{\gamma}_{21} = -4.3034644907058750e{+}0, \quad \widetilde{\gamma}_{31} = -1.3659849627611041e{-}2, \quad \widetilde{\gamma}_{32} = -6.4041956977805674e{-}3,$$
$$\gamma = 2.9592668175830239e{-}1.$$

Additionally, we present a method, for which $\varrho(G_\infty) = 0$ does not hold, but with larger angle α than `3b`, see Table 2.4.1. This method is obtained by numerical search with `fmincon` and with respect to the described properties above. The coefficients of the method `3a` are given by:

3a:

$$c_1 = 2.7585435173749423e{-}1, \quad c_2 = 1.2974145641639010e{+}0, \quad c_3 = 1.0000000000000000e{+}0,$$
$$\widetilde{a}_{21} = 4.6146103121913240e{-}1, \quad \widetilde{a}_{31} = -6.3013501027799779e{-}1, \quad \widetilde{a}_{32} = 3.3481277271620247e{-}1,$$
$$\widetilde{\gamma}_{21} = 1.0038467404049227e{+}0, \quad \widetilde{\gamma}_{31} = 1.2814081673484539e{+}0, \quad \widetilde{\gamma}_{32} = -4.2958347323894375e{-}1,$$
$$\gamma = 4.4330035256651801e{-}1.$$

2.4.3 Methods with $s = 4$ and $s = 5$ stages

In the case of four and five stages, we perform the numerical optimization with different strategies to find good parameter sets for the two-step W-methods. Here, we have no explicit conditions for $\varrho(G_\infty) = 0$, but we want to satisfy $\varrho(G_\infty) < 1$ for $\sigma = 1$. Again, we optimize with respect to the angle α for L(α)-stability, error constants and coefficients.

The optimization process is done by `fmincon` from the optimization toolbox in MATLAB. The following methods `4a`, `4b` and `5a` are obtained:

`4a`:

$$
\begin{aligned}
c_1 &= 3.4475069518575380e{-}1, & c_2 &= -3.0199601869781884e{-}1, & c_3 &= 1.2715954631040773e{+}0,\\
c_4 &= 1.0000000000000000e{+}0,\\
\widetilde{a}_{21} &= -1.3807276352109585e{-}1, & \widetilde{a}_{31} &= 4.0288429533730259e{+}0, & \widetilde{a}_{32} &= -1.6608358550657365e{+}0,\\
\widetilde{a}_{41} &= 5.5395665635891145e{-}1, & \widetilde{a}_{42} &= 5.7259556650406740e{-}1, & \widetilde{a}_{43} &= 1.7058748218129905e{-}2,\\
\widetilde{\gamma}_{21} &= -1.3109542641248575e{-}1, & \widetilde{\gamma}_{31} &= -2.7740318778345143e{+}0, & \widetilde{\gamma}_{32} &= 1.1944608079043511e{+}0,\\
\widetilde{\gamma}_{41} &= 1.4615607370092432e{-}1, & \widetilde{\gamma}_{42} &= -5.4352839808888898e{-}1, & \widetilde{\gamma}_{43} &= -7.4801424301146488e{-}2,\\
\gamma &= 3.4083914367433077e{-}1.
\end{aligned}
$$

`4b`:

$$
\begin{aligned}
c_1 &= 2.4902046482054652e{-}1, & c_2 &= 1.8463585014782384e{+}0, & c_3 &= 1.2904402196609168e{+}0,\\
c_4 &= 1.0000000000000000e{+}0,\\
\widetilde{a}_{21} &= 1.2369099563404959e{+}0, & \widetilde{a}_{31} &= 4.6203540002585880e{-}1, & \widetilde{a}_{32} &= -9.1462206621367961e{-}2,\\
\widetilde{a}_{41} &= -2.7636893446018787e{-}2, & \widetilde{a}_{42} &= -1.6369452680547052e{-}2, & \widetilde{a}_{43} &= -6.4152678919227064e{-}3,\\
\widetilde{\gamma}_{21} &= 1.2850995505590568e{+}0, & \widetilde{\gamma}_{31} &= 5.3577018410535193e{-}1, & \widetilde{\gamma}_{32} &= -3.9108197137041377e{-}3,\\
\widetilde{\gamma}_{41} &= 6.2457914347561516e{-}1, & \widetilde{\gamma}_{42} &= 3.4191540363782635e{-}2, & \widetilde{\gamma}_{43} &= -2.1472697867924981e{-}1,\\
\gamma &= 6.0381404956018603e{-}1.
\end{aligned}
$$

`5a`:

$$
\begin{aligned}
c_1 &= 3.2465871853888723e{-}1, & c_2 &= -5.7205917060903488e{-}1, & c_3 &= -1.1099213511352013e{-}1,\\
c_4 &= 1.3004743005526314e{+}0, & c_5 &= 1.0000000000000000e{+}0,\\
\widetilde{a}_{21} &= 5.9748351460406468e{-}1, & \widetilde{a}_{31} &= 8.4900192603721406e{-}2, & \widetilde{a}_{32} &= 5.3094512231111113e{-}1,\\
\widetilde{a}_{41} &= 8.8827878595016430e{-}1, & \widetilde{a}_{42} &= 4.9147902177027525e{-}1, & \widetilde{a}_{43} &= 1.2679272894751348e{-}2,\\
\widetilde{a}_{51} &= 5.6153469017790658e{-}1, & \widetilde{a}_{52} &= 6.2974213872145413e{-}1, & \widetilde{a}_{53} &= -6.1893110194158951e{-}1,\\
\widetilde{a}_{54} &= -1.3411914475329847e{-}1,\\
\widetilde{\gamma}_{21} &= -1.4281493182994098e{-}1, & \widetilde{\gamma}_{31} &= -1.3877813480227719e{-}1, & \widetilde{\gamma}_{32} &= -5.7036440762831186e{-}1,\\
\widetilde{\gamma}_{41} &= 1.0635092143559879e{+}0, & \widetilde{\gamma}_{42} &= -3.0330420318920742e{-}1, & \widetilde{\gamma}_{43} &= 7.0492608165871473e{-}1,\\
\widetilde{\gamma}_{51} &= 3.9600375095807683e{-}1, & \widetilde{\gamma}_{52} &= -6.5043986251488239e{-}1, & \widetilde{\gamma}_{53} &= 1.2297356798131087e{+}0,\\
\widetilde{\gamma}_{54} &= 9.9758762294221981e{-}2,\\
\gamma &= 2.8976577262256498e{-}1.
\end{aligned}
$$

2.4.4 Properties of the methods

We want to summarize the results of our numerical optimization. Some properties of the optimized two-step W-methods are listed in Table 2.4.1. For comparison, we include the two-step W-methods `TSW2B`, `TSW3A` and `TSW3B` with $\widetilde{\Gamma} = 0$ from [47]. For the new two-step W-methods, we have convergence order $p^* = s + 1$. We have tried different

strategies and heuristics in our numerical search. Of course, we cannot claim that our new methods are optimal.

label	s	p^*	α	$\varrho(G_\infty)$	*ferr*	*maxcoeff*
2a	2	3	81.85	0.1699	0.3354	2.0690
2b	2	3	83.00	0.4907	0.3459	1.7664
2c	2	3	90.00	0.5969	3.4435	3.2625
3a	3	4	88.68	0.1746	4.6259	4.7382
3b	3	4	76.81	0.0000	1.7578	5.3985
4a	4	5	86.09	0.4832	10.8643	4.8077
4b	4	5	89.87	0.4690	15.6969	16.0839
5a	5	6	74.27	0.5842	33.2437	12.4194
TSW2B	2	3	82.75	0.3333	1.7778	1.0000
TSW3A	3	3	90.00	0.0000	5.3590	3.2000
TSW3B	3	3	83.49	0.0000	2.7344	3.5000

Table 2.4.1: Some properties of two-step W-methods: stages s, order p^*, angle α of $\mathrm{L}(\alpha)$-stability, spectral radius $\varrho(G_\infty)$, error constant *ferr* and maximal magnitude of the coefficients *maxcoeff*, new methods (*top*) and two-step W-methods from [47] (*bottom*).

Our numerical optimization is done for constant step sizes, i.e., $\sigma = 1$. It is interesting to see how the properties of the obtained methods behave by changing step sizes. Therefore, we illustrate for the methods 3a and 3b the error constant *ferr*, spectral radius $\varrho(G_\infty)$ and the maximal magnitude of the coefficients *maxcoeff* as functions of σ with $0.2 \leq \sigma \leq 1.6$ which is the crucial range for practical computations, cf. Figure 2.4.3. For method 3b, we observe $\varrho(G_\infty) < 1$ for all $0.2 \leq \sigma \leq 1.6$. Furthermore, we have smaller error constants compared to method 3a, but the coefficients are slightly larger.

Note that $c_i < 0$ holds for some optimized two-step W-methods. In our following numerical experiments, we use an appropriate starting process to avoid that t-values move outside the interval of the time integration, see e.g. [64, p. 176]. Furthermore, we have $c_i > 1$ for some methods. In these cases, a special choice of the step size in the last time step guarantees that t-values do not exceed the endpoint t_e.

2.5 Numerical tests

In this section, we test the constructed two-step W-methods from Section 2.4 and compare them with two-step W-methods from [47]. All numerical experiments are implemented in MATLAB. Furthermore, we include numerical tests with the standard codes ode23s and RODAS. The code ode23s from the MATLAB ODE-suite [57] is based on a

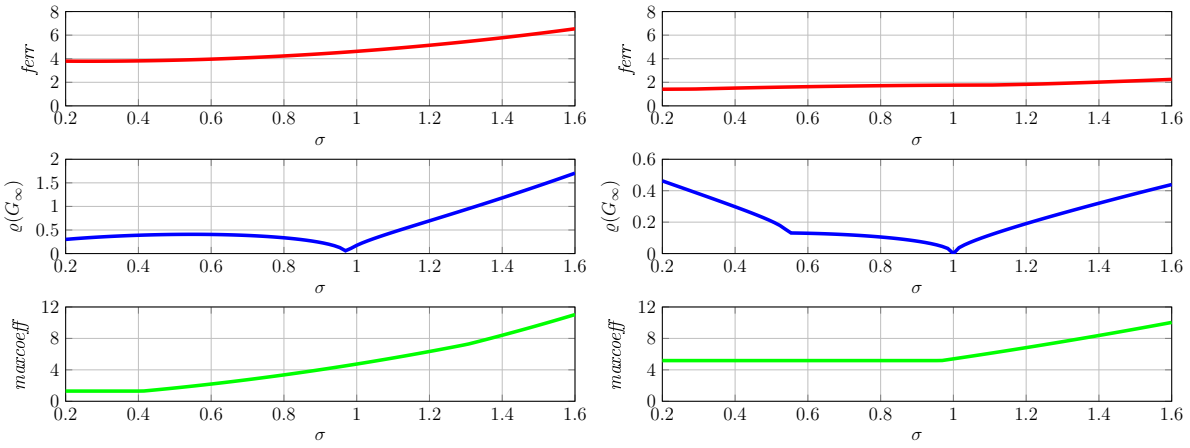

Figure 2.4.3: Error constant *ferr* (*top*), spectral radius $\varrho(G_\infty)$ (*middle*), maximal magnitude of the coefficients *maxcoeff* (*bottom*) vs. step size ratio σ, for method `3a` (*left*) and for method `3b` (*right*).

Rosenbrock formula of order two and uses a third order method for error estimation and step size control. The code `RODAS` is based on an L-stable ROW-method of order four with an embedded method of order three [28].

2.5.1 Test case 1: Test of order reduction

First, we want to illustrate the effect of order reduction in ROW-methods. For that, we consider the van der Pol equation from [28, 64]

$$\begin{aligned} y' &= z, \\ \varepsilon z' &= (1-y^2)z - y, \quad \varepsilon = 10^{-5}, \quad t \in [0, 0.5]\,, \\ y(0) &= 2, \quad z(0) = 0. \end{aligned}$$

We test our new two-step W-methods `2a`, `3a`, `4a` and `5a`, cf. Section 2.4, and compare them with `RODAS`. We have implemented the methods with constant step sizes. The additional starting values for the two-step W-methods are computed with `RODAS` and high accuracy. The exact Jacobian is used in each step and a reference solution y_{ref} with high accuracy is computed with `ode15s` from the MATLAB ODE-suite [57]. The errors are computed at the endpoint t_e in a weighted maximum norm

$$err = \max_{i=1,\ldots,n} \frac{|u_{m+1,i} - y_{\text{ref},i}|}{1 + |y_{\text{ref},i}|}. \tag{2.5.23}$$

In Figure 2.5.1, we present the logarithm of the obtained errors at the endpoint $t_e = 0.5$ versus the constant step size h. The order reduction of `RODAS` can be clearly observed. It behaves as a second order method numerically. As opposed to this, all two-step W-methods show the expected orders which can be explained with their high stage order.

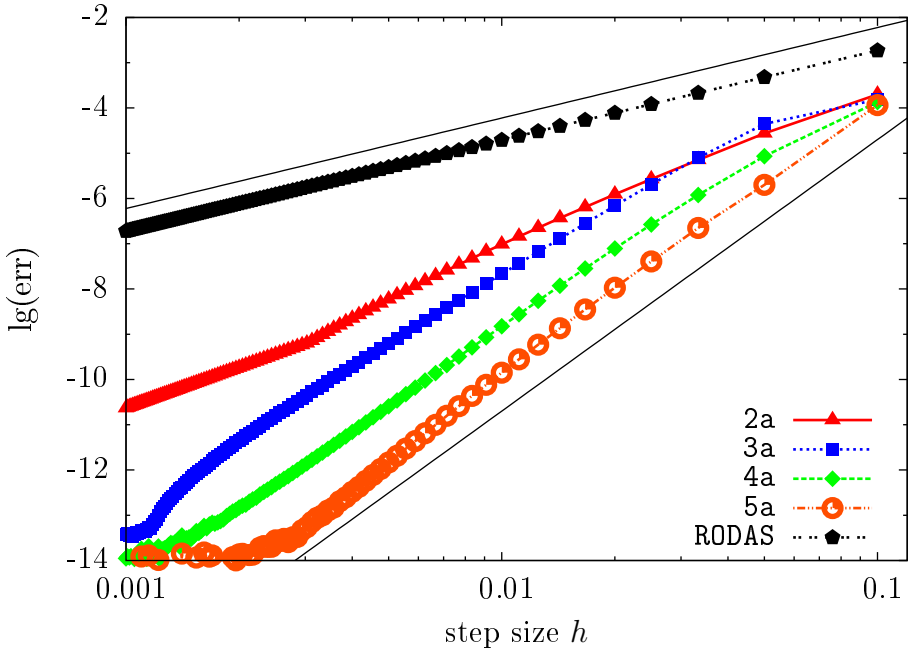

Figure 2.5.1: Illustration of order reduction for ROW-method `RODAS`: Errors vs. time step size h.

2.5.2 Test case 2: Small dimensional problems with step size control

Instead of (2.1.2), we use a transformed formulation for the numerical tests with step size control given by

$$\begin{aligned}(I - h_m\gamma T_m)(k_{m,i} + \xi_{m,i}) &= f(t_{m,i}, Y_{m,i}) + \xi_{m,i},\\ \xi_{m,i} &= \frac{1}{\gamma}\left(\sum_{j=1}^{s}\gamma_{ij}k_{m-1,j} + \sum_{j=1}^{i-1}\widetilde{\gamma}_{ij}k_{m,j}\right).\end{aligned} \tag{2.5.24}$$

This formulation avoids matrix-vector multiplications and is already used in [47]. Furthermore, this transformation allows the application of an approximate matrix factorization, cf. Section 3.2. In all cases, the Jacobian $f_y(t_m, u_m)$ is computed numerically in each step and we use LU-decomposition for the solution of the linear systems. Again, the additional starting values are computed with the ROW-method `RODAS` and high accuracy. We follow [47] for the error estimation. We calculate the weights of an embedded method by

$$b_e^\top := 0.5b^\top, \quad v_e^\top := \left(\left(\mathbb{1}^\top + 0.2e_s^\top\right) SD^{-1} - b_e^\top V_0 S\right) V_1^{-1} \tag{2.5.25}$$

and obtain an embedded solution

$$\widetilde{u}_{m+1} = u_m + h_m \sum_{j=1}^{s} (b_{e,j} k_{m,j} + v_{e,j} k_{m-1,j}). \tag{2.5.26}$$

Because of the term $0.2e_s^\top$ in (2.5.25) for v_e, condition $B(s)$ is not satisfied, i.e., the embedded method is of order $p_e^* = s - 1$. Then the local error err_{emb} is estimated by

$$err_{\text{emb}} = \max_{i=1,\ldots,n} \frac{|u_{m+1,i} - \widetilde{u}_{m+1,i}|}{atol + rtol\,|u_{m,i}|}, \tag{2.5.27}$$

where *atol* and *rtol* denote the absolute and relative tolerances. In our tests, we used the tolerances $atol = rtol = 10^{-2}, \ldots, 10^{-10}$. We compute a new step size h_{new} by

$$h_{\text{new}} = h_m \min\left(a_{\max}, \max\left(a_{\min}, a_{\text{save}} err_{\text{emb}}^{-1/s}\right)\right) \tag{2.5.28}$$

with $a_{\text{save}} = 0.7$, $a_{\min} = 0.2$, and $a_{\max} = 1.5$ for all $s \leq 4$ and $a_{\max} = 1.1$ for all $s > 4$. If $err_{\text{emb}} \leq 1$, we set $h_{m+1} := h_{\text{new}}$. Otherwise, we put $h_m := h_{\text{new}}$ and the last time step is repeated. We test our new two-step W-methods, the two-step W-methods from [47] and compare them with `ode23s` and `RODAS`. Note that for `ode23s` and the two-stage two-step W-methods, the tolerance 10^{-10} is omitted for some problems because of high computing time. Reference solutions for all problems are computed with high accuracy with `ode15s` and the errors are computed at the endpoint t_e in the weighted maximum norm (2.5.23). We used the following standard stiff test problems which can be found in [28]:

- **HIRES:** a stiff system of eight non-linear ordinary differential equations given by

$$\begin{aligned}
y_1' &= -1.71y_1 + 0.43y_2 + 8.32y_3 + 0.0007,\\
y_2' &= 1.71y_1 - 8.75y_2,\\
y_3' &= -10.03y_3 + 0.43y_4 + 0.035y_5,\\
y_4' &= 8.32y_2 + 1.71y_3 - 1.12y_4,\\
y_5' &= -1.745y_5 + 0.43y_6 + 0.43y_7,\\
y_6' &= -280y_6y_8 + 0.69y_4 + 1.71y_5 - 0.43y_6 + 0.69y_7,\\
y_7' &= 280y_6y_8 - 1.81y_7,\\
y_8' &= -280y_6y_8 + 1.81y_7
\end{aligned}$$

  with initial value $y_1(0) = 1,\ y_2(0) = y_3(0) = \ldots = y_7(0) = 0,\ y_8(0) = 0.0057$ and endpoint $t_e = 321.8122$.

- **OREGO:** a stiff system of three non-linear ordinary differential equations in the form

$$\begin{aligned}
y_1' &= 77.27\left(y_2 + y_1\left(1 - 8.375 \cdot 10^{-6} y_1 - y_2\right)\right),\\
y_2' &= \frac{1}{77.27}\left(y_3 - (1 + y_1)\, y_2\right),\\
y_3' &= 0.161\,(y_1 - y_3)
\end{aligned}$$

with initial value $y_1(0) = 1,\ y_2(0) = 2,\ y_3(0) = 3$ and endpoint $t_e = 360$.

- **VDPOL:** the van der Pol oscillator of two ordinary differential equations given by

$$\begin{aligned} y_1' &= y_2, \\ y_2' &= \left(\left(1 - y_1^2\right) y_2 - y_1\right) / \varepsilon \end{aligned}$$

with $\varepsilon = 10^{-6}$ and with initial value $y_1(0) = 2$ and $y_2(0) = 0$. We consider two different endpoints $t_e = 2$ and $t_e = 11$.

- **PLATE:** a linear and non-autonomous problem, which is obtained by spatial discretization of the PDE problem

$$u_{tt} + \omega u_t + \eta \Delta^2 u = f(x, y, t), \quad (x, y) \in \Omega = [0, 2] \times [0, 4/3]\,, \tag{2.5.29}$$

where Δ^2 denotes the biharmonic operator and with the parameters $\omega = 1000$ and $\eta = 100$. The initial conditions are given by

$$u(x, y, 0) = 0 \quad \text{and} \quad u_t(x, y, 0) = 0$$

and we consider the endpoint $t_e = 7$. The boundary conditions are given by

$$u(x, y, t) = 0 \quad \text{and} \quad \Delta u(x, y, t) = 0 \quad \text{for all } (x, y) \in \partial\Omega.$$

The partial differential equation (2.5.29) is discretized on a uniform mesh grid in space

$$(x_i, y_j) = (i\Delta x, j\Delta x), \quad \Delta x = 2/9, \quad i = 1, 2, \ldots, 8, \quad j = 1, 2, \ldots, 5.$$

The right-hand side f of (2.5.29) is idealized by the sum of two Gaussian curves, which move in x-direction, and is given by

$$f(x, y, t) = \begin{cases} 200\left(e^{-5(t-x-2)^2} + e^{-5(t-x-5)^2}\right), & \text{if } y = y_2 \text{ or } y = y_4, \\ 0, & \text{for all other } y. \end{cases}$$

Transformation of the obtained second-order system of ordinary differential equations results in a system of first-order differential equations of dimension $n = 80$.

Furthermore, we used a PDE problem in one space dimension from [10] which leads to an ODE system of higher dimension.

- **BURGERS:** a stiff system of 2500 ordinary differential equations obtained by semi-discretization of Burgers' equation

$$u_t = \nu u_{xx} + u u_x + \varphi(x, t), \quad \nu = 0.1, \quad x \in [-1, 1]$$

with source term given by

$$\varphi(x,t) = r(x)\sin(t), \quad r(x) = \begin{cases} 0, & -1 \le x \le -1/3, \\ 3(x+1/3), & -1/3 \le x \le 0, \\ 3(2/3-x)/2, & 0 \le x \le 2/3, \\ 0, & 2/3 \le x \le 1 \end{cases}$$

and with initial condition $u(x,0) = \sin(\pi(x+1))$ and homogeneous Dirichlet boundary conditions. We consider the endpoint $t_e = 2$. Central differences of second order with $\Delta x = 1/2500$ are used for the spatial discretization. For the two-step W-methods, we used as the constant Jacobian the discretization of the diffusion part. As opposed to this, the code `RODAS` needs the exact Jacobian in each time step. We computed the Jacobian using `numjac` from MATLAB where we exploited the band structure by providing `JPattern`.

The results are presented in Figures 2.5.2–2.5.7. We show the computation time in seconds versus the logarithm of the obtained errors at the endpoint t_e. Our numerical tests show the potential of the two-step W-methods. The step size control in two-step W-methods works well. The methods of order three are clearly superior to `ode23s` and the higher order methods are more efficient than `RODAS` for more stringent tolerances, especially for PLATE. We observe that `RODAS` is the best method for crude tolerances where it requires a small number of steps. Furthermore, `RODAS` can quickly adjust the step size to the dynamics of the solution as the step size can be enlarged by a factor 5 in a single step. For the two-step W-methods, we need to be more conservative and restrict this factor to 1.5 (for the five-stage method even to 1.1) to avoid large changes in the coefficients A and Γ. Except for method `2c`, the new two-step W-methods with two stages are comparable to the two-step W-methods `TSW2B`, `TSW3A` and `TSW3B` from [47]. Despite the fact that method `2c` is L-stable, this method has a larger error constant and also a slightly larger spectral radius at infinity, cf. Table 2.4.1. Also $c_1 > 1$ may be a disadvantage of this method. The new higher order methods become superior compared to the methods `TSW2B`, `TSW3A` and `TSW3B`. In general, we can also observe the expected orders for the two-step W-methods for variable step sizes. The achieved accuracy is for most problems in much better accordance with the prescribed tolerance than for `RODAS`. For the higher dimensional problem BURGERS, the possibility to use a constant Jacobian for the two-step W-methods clearly pays off. Note that for non-autonomous problems, the codes `RODAS` and `ode23s` also incorporate the time derivatives in contrast to two-step W-methods.

Except for BURGERS problem, we computed in our numerical experiments for all two-step W-methods, `RODAS` and `ode23s` the exact Jacobian at each time step. This is necessary for `RODAS` and `ode23s`, but not for two-step W-methods due to the fact that their order is independent of the choice of the matrix T_m. This drawback for `RODAS` and `ode23s` can be clearly seen in Figure 2.5.7.

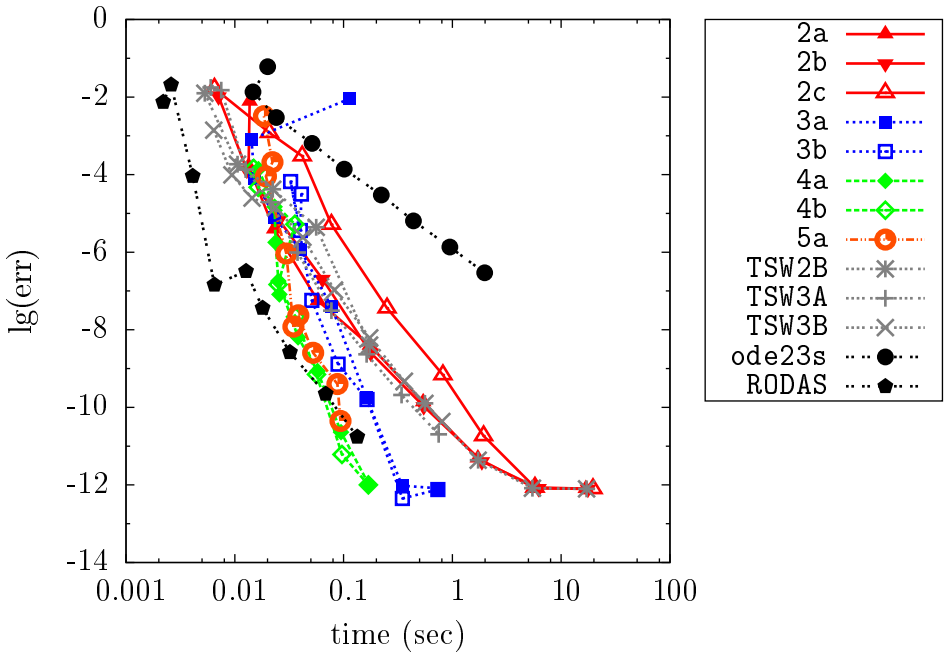

Figure 2.5.2: Results for HIRES: Errors vs. computing time in seconds.

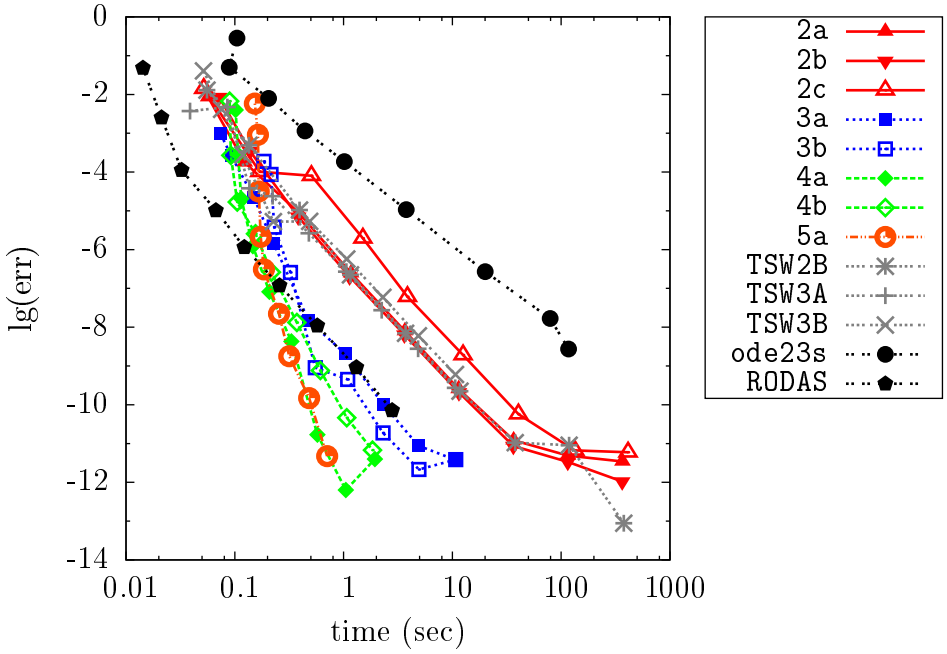

Figure 2.5.3: Results for OREGO: Errors vs. computing time in seconds.

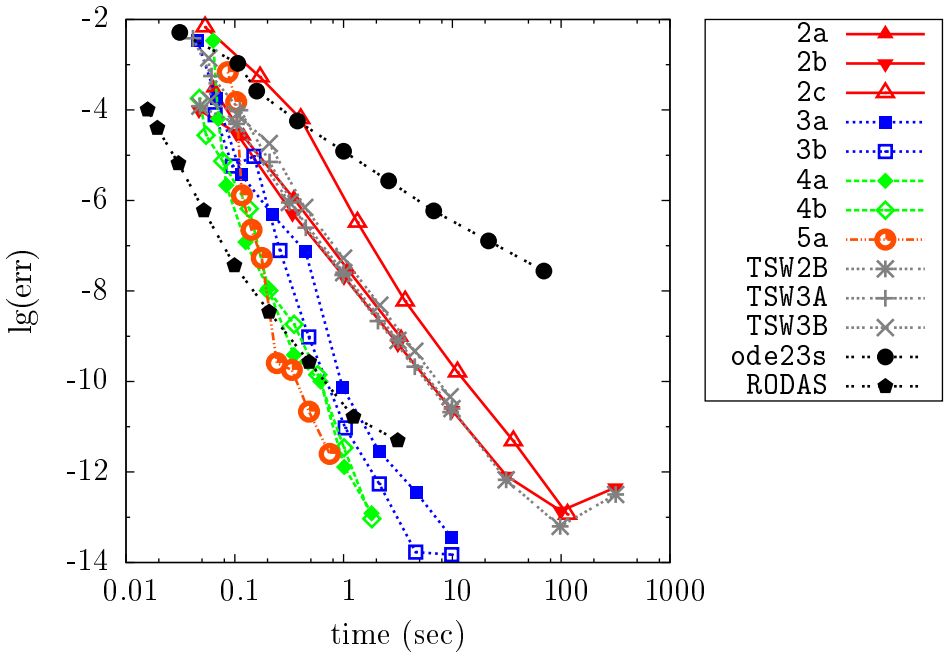

Figure 2.5.4: Results for VDPOL with $t_e = 2$: Errors vs. computing time in seconds.

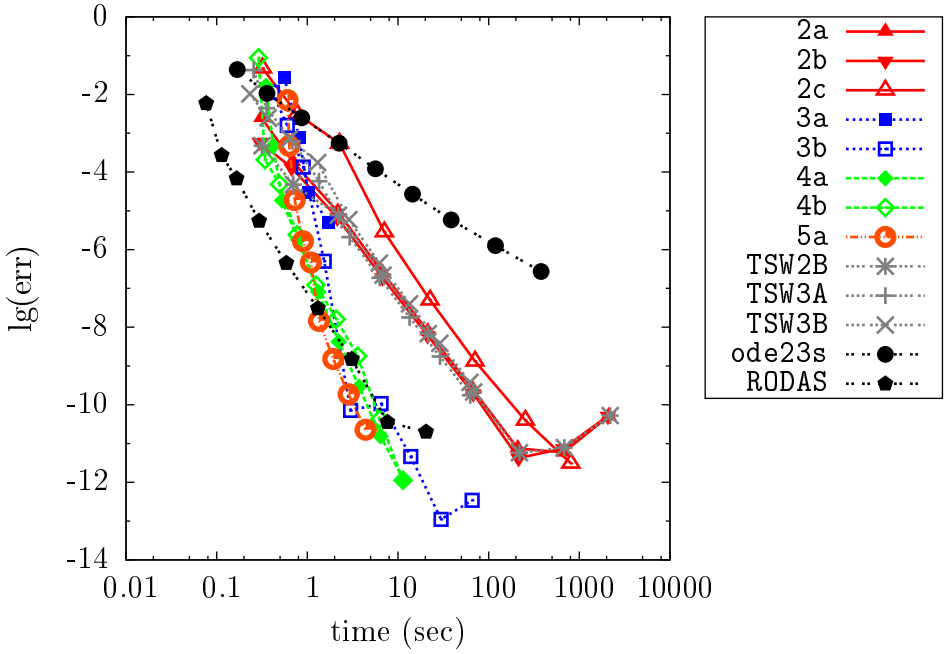

Figure 2.5.5: Results for VDPOL with $t_e = 11$: Errors vs. computing time in seconds.

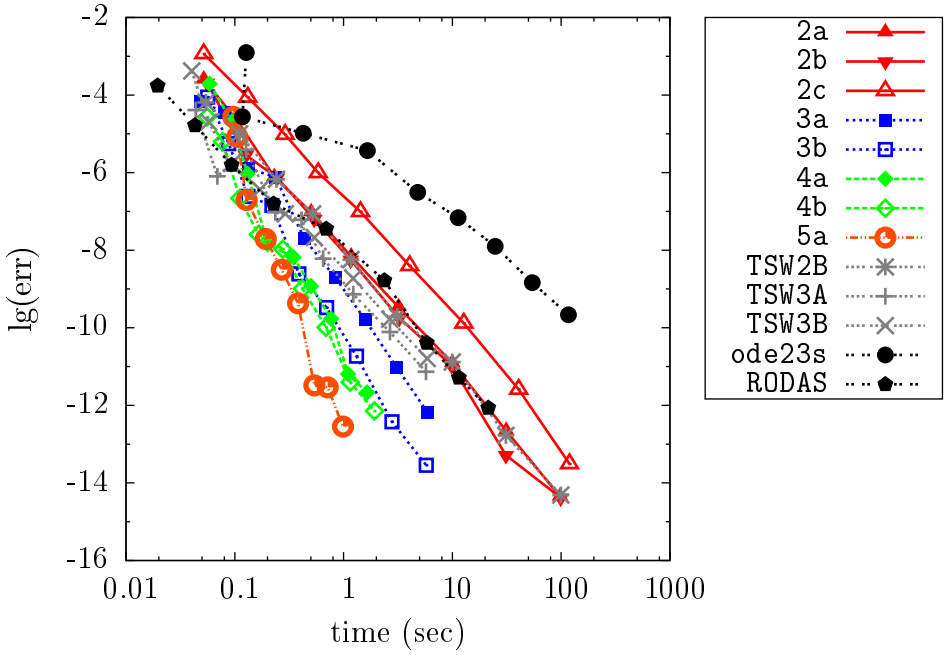

Figure 2.5.6: Results for PLATE: Errors vs. computing time in seconds.

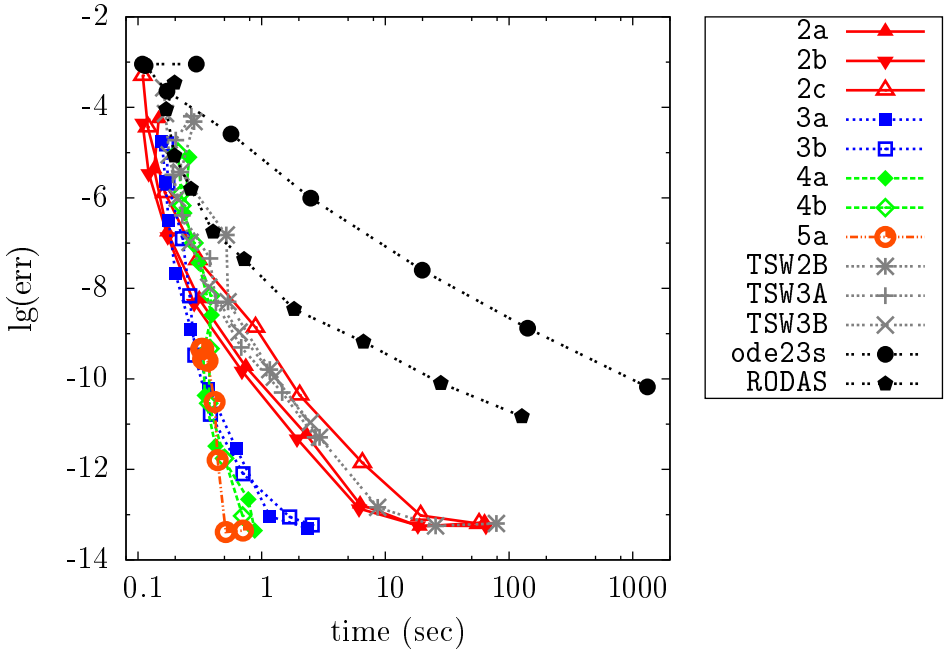

Figure 2.5.7: Results for BURGERS: Errors vs. computing time in seconds.

For BURGERS problem, we used a constant Jacobian for the two-step W-methods. We can also hold the Jacobian constant for several time steps to reduce the computing time. This is illustrated for the two-step W-methods `2a`, `3a`, `4a` and `5a` in Figure 2.5.8. We show the results for the VDPOL problem with endpoint $t_e = 11$ when the Jacobian is computed at each time step and when the Jacobian is computed only every second step. We can clearly observe this potential advantage of saving computing time. But we want to mention that a strategy for recomputation of the Jacobian requires further investigations.

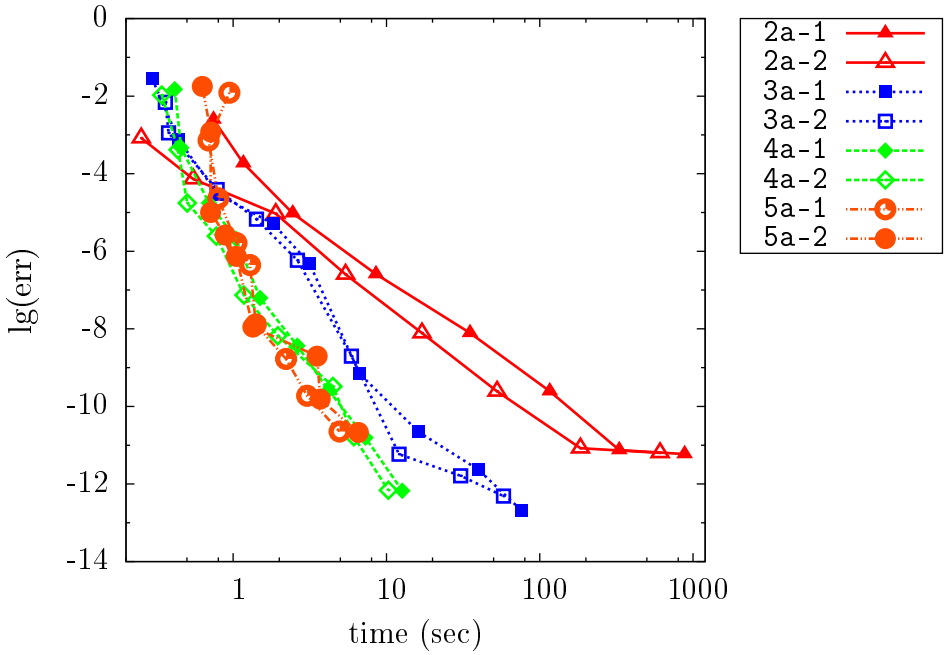

Figure 2.5.8: Results for VDPOL with $t_e = 11$: Errors vs. computing time in seconds. For two-step W-methods, denoted with suffix `-1`, the Jacobian is computed at each step, for methods with suffix `-2`, the Jacobian is computed only every second time step.

3 Two-step W-methods with approximate matrix factorization

In this chapter, we recall the concept of approximate matrix factorization (AMF), the formulation of one-step AMF W-methods and summarize some results. We introduce the class of two-step AMF W-methods. We show that in contrast to one-step AMF W-methods, the time derivatives are not involved in the numerical scheme. Furthermore, we prove a stability result at infinity and describe the construction of appropriate two-step AMF W-methods.

3.1 One-step AMF W-methods

We first consider an autonomous initial value problem

$$y'(t) = f(y(t)), \quad y(t_0) = y_0 \in \mathbb{R}^n, \quad t \in [t_0, t_e]. \tag{3.1.1}$$

An s-stage one-step W-method for the solution of problem (3.1.1) is given by Steihaug and Wolfbrandt [61]

$$\begin{aligned} (I - h_m\gamma T_m)k_{m,i} &= h_m f\left(u_m + \sum_{j=1}^{i-1} a_{ij}k_{m,j}\right) + \sum_{j=1}^{i-1} l_{ij}k_{m,j}, \quad i = 1, \ldots, s, \\ u_{m+1} &= u_m + \sum_{j=1}^{s} b_j k_{m,j}, \end{aligned} \tag{3.1.2}$$

where T_m is an arbitrary matrix. Here u_{m+1} is an approximation to the exact solution $y(t_{m+1})$ at each time step $t_{m+1} = t_m + h_m$. In formulation (3.1.2), $A = (a_{ij})_{i,j=1}^s$, $L = (l_{ij})_{i,j=1}^s$, $b = (b_i)_{i=1}^s$ and γ are the parameters of the method, where A and L are strictly lower triangular matrices. W-methods are linearly-implicit and only one LU-decomposition is required per time step. In contrast to two-step W-methods, one-step W-methods do not need additional starting values. For $T_m = J_m = \partial_y f(u_m)$, the family of Rosenbrock–Wanner methods (ROW-methods) is obtained [51, 66]. Although T_m can be arbitrary, a reduced number of order conditions and better stability properties are obtained when T_m is an approximation to the exact Jacobian J_m. Furthermore, the construction of higher order methods is rather difficult for arbitrary matrix T_m.

Implicit integration methods require the solution of algebraic equations, which leads directly, or by Newton's method, to linear systems with matrix $(I - h_m\gamma T_m)$, where T_m is usually an approximation to the Jacobian. For low and middle dimensions of the problem (3.1.1) this can be done with direct solvers and LU-decomposition. But for high dimensional problems ($n \gg 10000$), the solution of the linear systems can be very expensive. Therefore, special approaches for the efficient solution of the algebraic equations are necessary. One possibility is to apply Krylov techniques. Krylov methods have been investigated and implemented in the well-known codes `VODPK` [9], `ROWMAP` [70] and `EXP4` [29]. Another approach is the use of an approximate matrix factorization (AMF). For this purpose, we consider a general non-autonomous system of stiff ordinary differential equations with a $(d+1)$-term-splitting in the form

$$y'(t) = f(t, y(t)) = f_0(t, y(t)) + \sum_{j=1}^{d} f_j(t, y(t)), \quad y(t_0) = y_0 \in \mathbb{R}^n, \quad t \in [t_0, t_e] \quad (3.1.3)$$

and a corresponding splitting for the Jacobian matrices into $d+1$ addends at the current point (t_m, u_m)

$$J_m = J_{m,0} + \sum_{j=1}^{d} J_{m,j}, \quad J_{m,j} = \partial_y f_j(t_m, u_m), \quad (3.1.4)$$

where the matrices $J_{m,j}$, $j = 1, \ldots, d$, have simple structures or can be brought to band matrices of small bandwidth. Problems of this structure arise, in general, when solving time-dependent partial differential equations with the method of lines (MOL). The matrix $J_{m,0}$ stands for the term of the split Jacobian which is not considered in the AMF approach, i.e., $J_{m,0}$ collects parts of the Jacobian which are difficult to compute, or are not important to ensure stability in AMF schemes. This is typical for PDE problems where convection terms should be treated explicitly. If $J_{m,0} = 0$, then the AMF approach will be called *exact*. Otherwise, it will be said to be *inexact*, cf. [24, Definition 1]. Inexact AMF will be considered for peer methods in Section 4.2. The idea of AMF is now to replace the matrix $(I - h_m\gamma T_m)$ by the approximation

$$(I - h_m\gamma T_m) \approx \prod_{j=1}^{d} (I - h_m\gamma J_{m,j}) =: \Pi_d \quad (3.1.5)$$

to exploit the special structure of the matrices $J_{m,j}$, $j = 1, \ldots, d$. The matrix Π_d is called AMF matrix and d is the dimension of the AMF splitting. We obtain the following relations between the AMF matrix and the Jacobian

$$\Pi_d = \prod_{j=1}^{d} (I - h_m\gamma J_{m,j}) =: (I - h_m\gamma \widetilde{J}_m)$$

with

$$\widetilde{J}_m = \sum_{j=1}^{d} J_{m,j} + (-h_m\gamma) \sum_{1\le i<j\le d} J_{m,i}J_{m,j} + (-h_m\gamma)^2 \sum_{1\le i<j<k\le d} J_{m,i}J_{m,j}J_{m,k} + \cdots + (-h_m\gamma)^{d-1} J_{m,1}J_{m,2}\cdots J_{m,d}.$$

In the case of an exact AMF, i.e., $J_{m,0} = 0$, we observe $\widetilde{J}_m = J_m + \mathcal{O}(h_m)$ and hence

$$(I - h_m\gamma\widetilde{J}_m) = (I - h_m\gamma J_m) + \mathcal{O}(h_m^2).$$

On the other hand, in the case of an inexact AMF with $J_{m,0} \neq 0$, we have $\widetilde{J}_m = J_m - J_{m,0} + \mathcal{O}(h_m)$ and thus

$$(I - h_m\gamma\widetilde{J}_m) = (I - h_m\gamma J_m) + \mathcal{O}(h_m).$$

Of course, the replacement (3.1.5) in the AMF approach has influence on the accuracy and stability of the numerical methods. AMF methods have been considered frequently in the literature. The classical alternating direction implicit (ADI) methods first proposed by Peaceman and Rachford [45] can be already interpreted as AMF methods. An overview about basic strategies can be found in the paper of van der Houwen and Sommeijer [31] and in the book of Hundsdorfer and Verwer [32]. One-step AMF W-methods have been intensively studied by González-Pinto and co-workers, e.g. [4, 21–26]. The application of AMF to linearly-implicit Runge–Kutta methods is considered in [12, 75]. In [75], a correction procedure is proposed to obtain higher order methods.

In this chapter, we always assume an exact AMF approach, i.e., $f_0(t, y(t)) = 0$ in (3.1.3) and $J_{m,0} = 0$. With this, the matrices T_m fulfil

$$J_m - T_m = \mathcal{O}(h_m), \quad h_m \to 0. \tag{3.1.6}$$

This assumption is frequently considered in the literature, e.g. [25, 32, 50]. Observe that the formulation (3.1.2) allows the application of the AMF approach (3.1.5) directly. One-step AMF W-methods for non-autonomous problems (3.1.3) are usually obtained by application of a one-step W-method (3.1.2) to the equivalent autonomous problem via the transformation $z(t) = (y(t)^\top, t)^\top$

$$z'(t) = \begin{bmatrix} f(t, y(t)) \\ 1 \end{bmatrix} = g(z(t)). \tag{3.1.7}$$

By considering the corresponding Jacobian splitting, the Jacobians for the associated autonomous problem (3.1.1) are given by

$$\widehat{J}_m = \sum_{j=1}^{d} \widehat{J}_{m,j}, \quad \widehat{J}_{m,j} = \begin{bmatrix} \partial_y f_j(t_m, u_m) & \partial_t f_j(t_m, u_m) \\ 0^\top & 0 \end{bmatrix}. \tag{3.1.8}$$

For exact Jacobians, the AMF matrix is then obtained from

$$(I - h_m\gamma T_m) \approx \prod_{j=1}^{d}(I - h_m\gamma \widehat{J}_{m,j}). \tag{3.1.9}$$

We observe that in this case $T_m = \widehat{J}_m + \mathcal{O}(h_m)$. This approach with AMF technique leads to one-step AMF W-methods for non-autonomous problems (3.1.3) in the form [22, 25]

$$\begin{aligned} K_i^{(0)} &= h_m f\left(t_{m,i}, u_m + \sum_{j=1}^{i-1} a_{ij}k_{m,j}\right) + \sum_{j=1}^{i-1} l_{ij}k_{m,j}, \\ \big(I - h_m\gamma\partial_y f_j(t_m, u_m)\big)K_i^{(j)} &= K_i^{(j-1)} + \gamma\rho_i h_m^2 \partial_t f_j(t_m, u_m), \quad j = 1, \dots, d, \\ k_{m,i} &= K_i^{(d)}, \quad i = 1, \dots, s, \\ u_{m+1} &= u_m + \sum_{j=1}^{s} b_j k_{m,j}. \end{aligned} \tag{3.1.10}$$

Here are $(\rho_i)_{i=1}^s = (I - L)^{-1}\mathbb{1}$, $(c_i)_{i=1}^s = \alpha\mathbb{1}$ with $\alpha = A(I - L)^{-1}$ and $t_{m,i} = t_m + c_i h_m$. We observe that the time derivatives $\partial_t f_j$ are incorporated for non-autonomous problems in the numerical scheme.

We indicate the following three one-step W-methods. For more details, we refer to the references given below.

(i) The well-known one-stage W-method with $\gamma = \frac{1}{2}$, see [32, p. 153], which we denote by `W1`, reaches order $p = 2$ whenever T_m fulfils (3.1.6).

(ii) The two-stage W-method from [32, p. 400] is of order $p = 3$ if (3.1.6) is satisfied. We indicate this method with `W2`.

(iii) The three-stage W-method from [25, Eq. (37)] is also considered. This method, denoted by `W3`, is of order $p = 3$ if (3.1.6) is fulfilled.

The corresponding methods `W1` and `W2` with AMF are A-stable when $d = 2$, cf. [32, pp. 400–403]. For the method `W3` with AMF, A(α)-stability for $d = 2$ is obtained with $\alpha \approx 0.5659 \cdot \frac{\pi}{2}$, see [25, p. 571]. For one-step AMF W-methods, which are stable at infinity, the maximal angle α for linear stability on a d-term-splitting, $d \geq 2$, fulfils $(d-1)\alpha \leq \frac{\pi}{2}$, cf. [32, pp. 402–403]. Moreover, if $z_i, z_j \to \infty$, for at least two indices $1 \leq i < j \leq d$, then the corresponding linear stability function $R_d = R_d(z_1, \dots, z_d)$ of a one-step AMF W-method becomes $|R_d| = 1$, i.e.,

$$\lim_{\substack{z_i, z_j \to \infty \\ i \neq j}} |R_d(z_1, \dots, z_d)| = 1. \tag{3.1.11}$$

For comparison, these methods are used in our numerical experiments, see Chapter 5.

3.2 Two-step AMF W-methods

We recall the formulation of an s-stage two-step W-method as considered in Chapter 2, Equation (2.1.2)

$$\begin{aligned} Y_{m,i} &= u_m + h_m \sum_{j=1}^{s} a_{ij} k_{m-1,j} + h_m \sum_{j=1}^{i-1} \widetilde{a}_{ij} k_{m,j}, \quad i = 1, \ldots, s, \\ (I - h_m \gamma T_m) k_{m,i} &= f(t_{m,i}, Y_{m,i}) + h_m T_m \sum_{j=1}^{s} \gamma_{ij} k_{m-1,j} + h_m T_m \sum_{j=1}^{i-1} \widetilde{\gamma}_{ij} k_{m,j}, \\ & \qquad i = 1, \ldots, s, \\ u_{m+1} &= u_m + h_m \sum_{j=1}^{s} (b_j k_{m,j} + v_j k_{m-1,j}). \end{aligned} \tag{3.2.12}$$

For the application of an AMF approach, we have to avoid products of the matrix T_m in the right-hand side of (3.2.12). Therefore, we consider the transformation

$$\xi_{m,i} = \frac{1}{\gamma} \left(\sum_{j=1}^{s} \gamma_{ij} k_{m-1,j} + \sum_{j=1}^{i-1} \widetilde{\gamma}_{ij} k_{m,j} \right), \tag{3.2.13}$$

which is already introduced in [47] and is also applied in our numerical tests of two-step W-methods, cf. Section 2.5. This leads to a formulation of two-step W-methods in the alternative form

$$\begin{aligned} Y_{m,i} &= u_m + h_m \sum_{j=1}^{s} a_{ij} k_{m-1,j} + h_m \sum_{j=1}^{i-1} \widetilde{a}_{ij} k_{m,j}, \\ (I - h_m \gamma T_m)(k_{m,i} + \xi_{m,i}) &= f(t_{m,i}, Y_{m,i}) + \xi_{m,i}, \quad i = 1, \ldots, s, \\ u_{m+1} &= u_m + h_m \sum_{j=1}^{s} (b_j k_{m,j} + v_j k_{m-1,j}). \end{aligned} \tag{3.2.14}$$

For the application of AMF, the matrix $(I - h_m \gamma T_m)$ is then replaced by the AMF matrix

$$\Pi_d = \prod_{j=1}^{d} (I - h_m \gamma J_{m,j}), \quad J_{m,j} = \partial_y f_j(t_m, u_m). \tag{3.2.15}$$

The order of two-step W-methods is independent of the matrix T_m. Due to this, the replacement (3.2.15) does not influence the order of two-step AMF W-methods. This leads to the following theorem.

Theorem 3.2.1. *Let a two-step W-method* (3.2.12) *satisfy the simplifying conditions* $C(s)$, $\Gamma(s)$ *and* $B(s)$, *i.e., the order conditions* (2.2.6)–(2.2.8) *are fulfilled. Then the corresponding two-step AMF W-method* (3.2.14) *with AMF matrix* (3.2.15) *fulfils the conditions* $C(s)$, $\Gamma(s)$ *and* $B(s)$.

Proof. The formulations for $Y_{m,i}$ and u_{m+1} in (3.2.12) and (3.2.14) are equal, i.e., the conditions $C(s)$ and $B(s)$ are obviously satisfied for the two-step AMF W-method. With the AMF matrix (3.2.15), we get from the second equation of (3.2.14)

$$\Pi_d(k_{m,i} + \xi_{m,i}) = f(t_{m,i}, Y_{m,i}) + \xi_{m,i}, \quad i = 1, \ldots, s.$$

Inserting the exact values $y(t_{m,i})$ for $Y_{m,i}$ and $y'(t_{m,i})$ for $k_{m,i}$, then one has

$$\begin{aligned} 0 &= y'(t_{m,i}) + \xi_{m,i} - \Pi_d \left(y'(t_{m,i}) + \xi_{m,i} \right), \\ 0 &= (I - \Pi_d) \left(y'(t_{m,i}) + \xi_{m,i} \right), \\ 0 &= y'(t_{m,i}) + \xi_{m,i}, \quad i = 1, \ldots, s. \end{aligned}$$

With (3.2.13), the statement for two-step AMF W-methods follows by Taylor series expansion with the assumption $\Gamma(s)$ for the two-step W-method (3.2.12). ■

In contrast to one-step AMF W-methods as considered in Section 3.1, the time derivatives of $f(t, y(t))$ for non-autonomous problems are not incorporated in the numerical scheme of two-step AMF W-methods. To this aim, we consider a non-autonomous system with a d-term-splitting in the form (3.1.3). We have the following theorem.

Theorem 3.2.2. *Let a two-step W-method* (3.2.14) *fulfilling the simplifying conditions* $C(1)$, $\Gamma(1)$ *and* $B(1)$ *be applied with the AMF* (3.1.8) *and* (3.1.9) *to a non-autonomous system of stiff ordinary differential equations with a d-term-splitting* (3.1.3). *Then the numerical scheme takes the form*

$$\begin{aligned} Y_{m,i} &= u_m + h_m \sum_{j=1}^{s} a_{ij} k_{m-1,j} + h_m \sum_{j=1}^{i-1} \widetilde{a}_{ij} k_{m,j}, \\ \xi_{m,i} &= \frac{1}{\gamma} \left(\sum_{j=1}^{s} \gamma_{ij} k_{m-1,j} + \sum_{j=1}^{i-1} \widetilde{\gamma}_{ij} k_{m,j} \right), \\ k_{m,i}^{(0)} &= f(t_{m,i}, Y_{m,i}) + \xi_{m,i}, \\ (I - h_m \gamma \partial_y f_j(t_m, u_m))\, k_{m,i}^{(j)} &= k_{m,i}^{(j-1)}, \quad j = 1, \ldots, d, \\ k_{m,i} &= k_{m,i}^{(d)} - \xi_{m,i}, \quad i = 1, \ldots, s, \\ u_{m+1} &= u_m + h_m \sum_{j=1}^{s} (b_j k_{m,j} + v_j k_{m-1,j}). \end{aligned} \tag{3.2.16}$$

Proof. The application of the two-step W-method (3.2.14) with transformation (3.2.13) to the equivalent autonomous problem (3.1.7) gives

$$\begin{aligned}
\widehat{Y}_{m,i} &= \widehat{u}_m + h_m \sum_{j=1}^{s} a_{ij}\widehat{k}_{m-1,j} + h_m \sum_{j=1}^{i-1} \widetilde{a}_{ij}\widehat{k}_{m,j},\\
\widehat{\xi}_{m,i} &= \frac{1}{\gamma}\left(\sum_{j=1}^{s} \gamma_{ij}\widehat{k}_{m-1,j} + \sum_{j=1}^{i-1} \widetilde{\gamma}_{ij}\widehat{k}_{m,j}\right),\\
(I - h_m\gamma T_m)(\widehat{k}_{m,i} + \widehat{\xi}_{m,i}) &= g(\widehat{Y}_{m,i}) + \widehat{\xi}_{m,i},\\
\widehat{u}_{m+1} &= \widehat{u}_m + h_m \sum_{j=1}^{s} (v_j\widehat{k}_{m-1,j} + b_j\widehat{k}_{m,j}),
\end{aligned} \tag{3.2.17}$$

with T_m given by (3.1.8) and (3.1.9), and with $\widehat{Y}_{m,i} := (Y_{m,i}^\top, \tau_{m,i})^\top$, $\widehat{\xi}_{m,i} := (\xi_{m,i}^\top, \phi_i)^\top$, $\widehat{k}_{m-j,i} := (k_{m-j,i}^\top, 1)^\top$, $\widehat{u}_{m+j} := (u_{m+j}^\top, t_{m+j})^\top$, for all $j = 0, 1$, and $i = 1, \ldots, s$. The last component in the equations for $\widehat{Y}_{m,i}$, $\widehat{\xi}_{m,i}$ and $\widehat{u}_{m+1}$ in (3.2.17) gives, respectively,

$$\begin{aligned}
\tau_{m,i} &= t_m + h_m\left(\sum_{j=1}^{s} a_{ij} + \sum_{j=1}^{i-1} \widetilde{a}_{ij}\right), \quad \phi_i = \frac{1}{\gamma}\left(\sum_{j=1}^{s} \gamma_{ij} + \sum_{j=1}^{i-1} \widetilde{\gamma}_{ij}\right),\\
t_{m+1} &= t_m + h_m \sum_{j=1}^{s} (v_j + b_j).
\end{aligned}$$

From $C(1)$, $\Gamma(1)$ and $B(1)$ we get, respectively, that $\tau_{m,i} = t_m + c_i h_m = t_{m,i}$, $\phi_i = -1$, $i = 1, \ldots, s$, and $t_{m+1} = t_m + h_m$. With the matrix T_m in (3.1.8) and (3.1.9), the first n components in each equation of (3.2.17) give

$$\begin{aligned}
Y_{m,i} &= u_m + h_m \sum_{j=1}^{s} a_{ij}k_{m-1,j} + h_m \sum_{j=1}^{i-1} \widetilde{a}_{ij}k_{m,j},\\
\xi_{m,i} &= \frac{1}{\gamma}\left(\sum_{j=1}^{s} \gamma_{ij}k_{m-1,j} + \sum_{j=1}^{i-1} \widetilde{\gamma}_{ij}k_{m,j}\right),\\
k_{m,i}^{(0)} &= f(t_{m,i}, Y_{m,i}) + \xi_{m,i},\\
(I - h_m\gamma\partial_y f_j(t_m, u_m))\, k_{m,i}^{(j)} &= k_{m,i}^{(j-1)} + h_m\gamma\partial_t f_j(t_m, u_m)(1 + \phi_i),\\
& \qquad j = 1, \ldots, d,\\
k_{m,i} &= k_{m,i}^{(d)} - \xi_{m,i}, \quad i = 1, \ldots, s,\\
u_{m+1} &= u_m + h_m \sum_{j=1}^{s} (b_j k_{m,j} + v_j k_{m-1,j}).
\end{aligned} \tag{3.2.18}$$

This concludes the proof since $1 + \phi_i = 0,\ i = 1, \ldots, s$. ■

Remark 3.2.3. *For a general two-step W-method* (3.2.18)*, the time-derivatives of the split terms* $f_j(t, y(t))$ *are multiplied by* $1 + \phi_i$*. These quantities vanish for two-step W-methods fulfilling the simplifying condition* $\Gamma(1)$*. However, for one-step W-methods, i.e., two-step W-methods with* $A = 0$*,* $\Gamma = 0$ *and* $v = 0$*, condition* $\Gamma(1)$ *cannot hold. To see this, observe that for one-step W-methods*

$$\Gamma(1) \Longleftrightarrow (\gamma I + \widetilde{\Gamma})\mathbb{1} = 0,$$

and this cannot hold since $\gamma > 0$ *and* $\widetilde{\Gamma}$ *is strictly lower triangular. Furthermore, comparing* (3.1.2)*,* (3.2.13) *and* (3.2.14)*, it is readily checked that the matrices* L *in* (3.1.2) *and* $\widetilde{\Gamma}$ *in* (3.2.13) *are related by* $\gamma(I - L)^{-1} = (\gamma I + \widetilde{\Gamma})$*. From here, the quantities* $(1 + \phi_i)_{i=1}^s$ *appearing in* (3.2.18) *are just given by*

$$(1 + \phi_i)_{i=1}^s = \left(I + \frac{1}{\gamma}\widetilde{\Gamma}\right)\mathbb{1} = (I - L)^{-1}\mathbb{1} = (\rho_i)_{i=1}^s$$

as presented in the non-autonomous formulation for one-step W-methods (3.1.10)*.* □

3.2.1 Stability investigations

For the stability analysis of two-step AMF W-methods, we consider the linear scalar Dahlquist test equation, see e.g. [31, 32]

$$y'(t) = \lambda y(t), \quad \lambda = \sum_{j=1}^{d} \lambda_j, \quad \mathrm{Re}(\lambda_j) \leq 0, \quad j = 1, \ldots, d, \tag{3.2.19}$$

where d denotes the dimension of the AMF splitting. Here is $T_m = \lambda$. We then apply the two-step W-method (3.2.14) with constant step sizes $h_m = h$ to the test problem (3.2.19) and obtain with

$$z_j = h\lambda_j, \quad j = 1, \ldots, d, \quad z = \sum_{j=1}^{d} z_j \tag{3.2.20}$$

and $K_m = (k_{m,1}, \ldots, k_{m,s})^\top$ the following recursion for the numerical solution

$$\begin{pmatrix} hK_m \\ u_{m+1} \end{pmatrix} = M_d \begin{pmatrix} hK_{m-1} \\ u_m \end{pmatrix}.$$

Here the stability matrix $M_d := M_d(z_1, \ldots, z_d)$ of dimension $(s+1) \times (s+1)$ is given by

$$M_d(z_1, \ldots, z_d) = \begin{pmatrix} W_d\left(\frac{1}{\gamma}(1 - \Pi_d)\Gamma + zA\right) & zW_d\mathbb{1} \\ b^\top W_d\left(\frac{1}{\gamma}(1 - \Pi_d)\Gamma + zA\right) + v^\top & 1 + zb^\top W_d\mathbb{1} \end{pmatrix} \tag{3.2.21}$$

with $W_d := \left(\Pi_d I - \frac{1}{\gamma}(1-\Pi_d)\widetilde{\Gamma} - z\widetilde{A}\right)^{-1}$ and AMF factor Π_d, which is defined as

$$\Pi_d := \prod_{j=1}^{d}(1-\gamma z_j). \tag{3.2.22}$$

In particular, for the special case $d = 1$ in (3.2.21), we get the usual stability matrix $M(z)$ of a two-step W-method (2.1.2), cf. [47]. Analogously to [47, Definition 1], we introduce the concepts of A- and L-stability for two-step AMF W-methods. Again, the spectral radius of a matrix is denoted by $\varrho(\cdot)$.

Definition 3.2.4. The stability domain of the two-step AMF W-method (3.2.16) is the set $\mathcal{S} = \{(z_1,\ldots,z_d) \in \mathbb{C}^d \mid \varrho(M_d) < 1\}$. The method is called $A(\alpha)$-stable if $\{(z_1,\ldots,z_d) \in \mathbb{C}^d \mid |\arg(z_i)-\pi| \le \alpha,\ i = 1,\ldots,d\} \subseteq \bar{\mathcal{S}}$. We call a method stiffly accurate if for all fixed u_m, $k_{m-1,i}$, $i = 1,\ldots,s$, and for at least two variables z_i, z_j, $i \neq j$, the condition

$$\lim_{\substack{z_i,z_j\to\infty \\ i\neq j}} u_{m+1} = 0 \tag{3.2.23}$$

holds. A two-step AMF W-method is called L(α)-stable if it is A(α)-stable and the condition (3.2.23) is fulfilled. The method is said to be A-stable if $\alpha = \frac{\pi}{2}$ and L-stable if $\alpha = \frac{\pi}{2}$ and (3.2.23) is fulfilled. □

In order to check linear stability, it is useful to consider a transformation $Q^{-1}M_dQ$ instead of the stability matrix M_d directly, cf. [47]. We obtain with

$$Q = \begin{pmatrix} I & 0 \\ b^\top & 1 \end{pmatrix}$$

the transformed stability matrix M_d^{trans}

$$M_d^{\text{trans}} = \begin{pmatrix} W_d\left(\frac{1}{\gamma}(1-\Pi_d)\Gamma + zA\right) + zW_d\mathbb{1}b^\top & zW_d\mathbb{1} \\ v^\top + b^\top & 1 \end{pmatrix}. \tag{3.2.24}$$

In general, the computation of the eigenvalues of M_d^{trans} for arbitrary z_j is a difficult task. Our next result indicates that two-step AMF W-methods cannot be L-stable for a d-term-splitting with $d \ge 2$. Indeed, all the eigenvalues of M_d tend to be equal to one whenever two variables z_i, z_j, $i \neq j$, tend to infinity. This property is shared with one-step AMF W-methods, see e.g. [32].

Theorem 3.2.5. *Let $M_d = M_d(z_1,\ldots,z_d)$ be the stability matrix (3.2.21) of an s-stage two-step AMF W-method (3.2.16) of stage order $p = s$ with arbitrary $d \ge 2$. If $z_i, z_j \to \infty$, for at least two indices $1 \le i < j \le d$, then the eigenvalues of M_d tend to $\xi_1 = \xi_2 = \ldots = \xi_{s+1} = 1$.*

Proof. The eigenvalues of M_d are the same as those of the transformed stability matrix M_d^{trans} in (3.2.24). Since

$$\lim_{\substack{z_i, z_j \to \infty \\ i \neq j}} \frac{z}{\Pi_d} = 0 \quad \text{and} \quad \lim_{\substack{z_i, z_j \to \infty \\ i \neq j}} \frac{1 - \Pi_d}{\Pi_d} = -1,$$

we obtain that $\lim\limits_{\substack{z_i, z_j \to \infty \\ i \neq j}} z W_d \mathbb{1} = 0$ and

$$\lim_{\substack{z_i, z_j \to \infty \\ i \neq j}} W_d \left(\frac{1}{\gamma}(1 - \Pi_d)\Gamma + zA \right) = \left(I + \frac{1}{\gamma}\widetilde{\Gamma} \right)^{-1} \left(-\frac{1}{\gamma}\Gamma \right).$$

With notations (2.2.9), $S = I$ and

$$P = \left(\binom{j-1}{i-1} \right)_{i,j=1}^{s}, \quad V_1 = V_0 P^{-1}, \tag{3.2.25}$$

the order condition $\Gamma(s)$ in (2.2.7) gives

$$\left(I + \frac{1}{\gamma}\widetilde{\Gamma} \right)^{-1} \left(-\frac{1}{\gamma}\Gamma \right) = V_0 V_1^{-1} = V_0 P V_0^{-1}.$$

Hence

$$\lim_{\substack{z_i, z_j \to \infty \\ i \neq j}} M_d^{\text{trans}} = \begin{pmatrix} V_0 P V_0^{-1} & 0 \\ v^\top + b^\top & 1 \end{pmatrix},$$

whose eigenvalues are those of P in (3.2.25) and one additional eigenvalue 1. By the definition of P, we have the eigenvalues $\xi_1 = \xi_2 = \ldots = \xi_{s+1} = 1$. ■

Remark 3.2.6. *With Theorem 3.2.5, the condition* (3.2.23) *for stiff accuracy cannot be satisfied for two-step W-methods with arbitrary $d \geq 2$. By this, two-step AMF W-methods cannot be L-stable for $d \geq 2$.*

Remark 3.2.7. *From Theorem 3.2.5, it follows that the eigenvalue $\xi = 1$ of the stability matrix M_d has multiplicity $s + 1$ and there is only one eigenvector associated to it.*

3.2.2 Construction of two-step AMF W-methods

In Section 2.4, we have presented s-stage stiffly accurate two-step W-methods of order $p^* = s + 1$ for variable step sizes. These methods are optimized with respect to the usual scalar Dahlquist test equation (2.2.10) and have performed well on standard stiff test problems, cf. Section 2.5. Unfortunately, the stability of these two-step W-methods becomes worse in the AMF case. Furthermore, numerical experiments with application

of AMF have been far from satisfactory. Therefore, it is necessary to optimize new coefficients of two-step W-methods with respect to AMF-stability and test equation (3.2.19). In the following, we describe the construction of a three-stage two-step AMF W-method of order three. Note that we have dropped the property $B(4)$ to have more degrees of freedom in the optimization process. The construction is done for constant step sizes and with `fmincon` from the optimization toolbox in MATLAB. The nodes c_1 and c_2 with $c_3 = 1$ and the matrices $\widetilde{A}$ and $\widetilde{\Gamma}$ and γ are chosen randomly. The coefficients A, Γ, $v^\top$ and $b^\top$ are computed for these values by the conditions (2.2.6)–(2.2.8) and (2.2.16). By this, the method has stage order three and is stiffly accurate when $d = 1$. For stability, we restrict to the case $d = 2$ and $z_1 = z_2 \in \mathbb{C}^-$, i.e., $z = 2z_1$. For the computation of the boundary of the stability domain, we vary the eigenvalues $\xi = \mathrm{e}^{\mathrm{i}\varphi}$, $\varphi \in [0, 2\pi)$ on the unit circle for the eigenvalue problem

$$M_2^{\text{trans}} \begin{pmatrix} x \\ y \end{pmatrix} = \xi \begin{pmatrix} x \\ y \end{pmatrix}, \quad x \in \mathbb{C}^s, \quad y \in \mathbb{C},$$

where $M_2^{\text{trans}} := M_2^{\text{trans}}(z_1)$ is the transformed stability matrix (3.2.24) for $d = 2$ with $z_1 = z_2$. This can be formulated with the substitution $w = z_1 x$ as generalized eigenvalue problem for each z_1 in the form

$$\begin{pmatrix} 0 & I \\ L_0 - \xi N_0 & L_1 - \xi N_1 \end{pmatrix} \begin{pmatrix} x \\ w \end{pmatrix} = z_1 \begin{pmatrix} I & 0 \\ 0 & \xi N_2 - L_2 \end{pmatrix} \begin{pmatrix} x \\ w \end{pmatrix},$$

where

$$L_0 = 0, \quad L_1 = 2\Gamma + 2A + 2\mathbb{1}b^\top + \frac{2}{\xi - 1}\mathbb{1}\left(v^\top + b^\top\right), \quad L_2 = -\gamma\Gamma,$$
$$N_0 = I, \quad N_1 = -2\gamma I - 2\widetilde{\Gamma} - 2\widetilde{A}, \quad N_2 = \gamma^2 I + \gamma\widetilde{\Gamma}.$$

The set of eigenvalues z_1 contains the boundary of the stability region. We perform our numerical search with different strategies to find good parameter sets with respect to stability. The coefficients of the method are given by:

`TSW-3a`:

$$\begin{aligned}
c_1 &= 2.4997279273105810e{-}1, & c_2 &= 7.4989349830789720e{-}1, & c_3 &= 1.0000000000000000e{+}0,\\
b_1 &= 5.9372545075163241e{-}1, & b_2 &= 1.5605376922224856e{-}1, & b_3 &= 2.4970691193052155e{-}1,\\
v_1 &= -1.2005929847406374e{-}1, & v_2 &= 4.2059509659324684e{-}1, & v_3 &= -3.0002193002358563e{-}1,\\
a_{11} &= 3.4726274738993569e{-}2, & a_{12} &= -2.2905781747629211e{-}1, & a_{13} &= 4.4430433546835663e{-}1,\\
a_{21} &= 3.9573123773204316e{-}1, & a_{22} &= -1.8111728838297050e{+}0, & a_{23} &= 1.6653078847681164e{+}0,\\
a_{31} &= 7.1201967896131857e{-}1, & a_{32} &= -3.0723662165046051e{+}0, & a_{33} &= 2.6102911309612242e{+}0,\\
\widetilde{a}_{21} &= 5.0002725963744266e{-}1, & \widetilde{a}_{31} &= 5.9378678348426617e{-}1, & \widetilde{a}_{32} &= 1.5626862309779524e{-}1,\\
\gamma_{11} &= -8.3357876160813221e{-}2, & \gamma_{12} &= 4.9987314306737002e{-}1, & \gamma_{13} &= -6.6654586967257279e{-}1,\\
\gamma_{21} &= -5.0005232008426348e{-}1, & \gamma_{22} &= 2.2492413581097495e{+}0, & \gamma_{23} &= -1.9992225172030529e{+}0,\\
\gamma_{31} &= -8.3360772658061766e{-}1, & \gamma_{32} &= 3.4995486993682254e{+}0, & \gamma_{33} &= -2.9159781249186900e{+}0,
\end{aligned}$$

$$\widetilde{\gamma}_{21} = \ 2.8764115509315574e{-}6,\ \widetilde{\gamma}_{31} = \ 8.2143371708270889e{-}6,\ \widetilde{\gamma}_{32} = -1.6649721048770168e{-}6,$$
$$\gamma = \ 2.5003060276601602e{-}1.$$

For comparison, we also give the coefficients for the one-stage two-step W-method of order $p^* = 2$, which are obtained with $c_1 = 1$ from the order conditions $\Gamma(1)$, $C(1)$ and $B(1)$ in (2.2.6)–(2.2.8) and with the conditions (2.3.19) and (2.3.20) for b_1 and γ. The one-stage two-step method is also stiffly accurate when $d = 1$ and convergent of order $p^* = 2$ for variable step sizes, cf. Theorem 2.3.1 and Corollary 2.3.2. In contrast to the one-stage one-step W-method with $\gamma = \frac{1}{2}$, see e.g. [32, p. 153], the order for the two-step W-method is independent of the matrix T_m. The following method is obtained:

`TSW-1a`:

$$c_1 = \ 1.0000000000000000e{+}0,\ \ b_1 = \ 5.0000000000000000e{-}1,\ v_1 = \ 5.0000000000000000e{-}1,$$
$$\gamma_{11} = -5.0000000000000000e{-}1,\ a_{11} = \ 1.0000000000000000e{+}0,\ \ \gamma = \ 5.0000000000000000e{-}1.$$

Note that the methods `TSW-1a` and `TSW-3a` are L-stable when $d = 1$. The stability regions of the corresponding two-step AMF W-methods `TSW-1a` (*left*) and `TSW-3a` (*right*) for $d = 2$ when $z_1 = z_2 \in \mathbb{C}^-$ are displayed in Figure 3.2.1. In particular, stability is at least observed when $z_1, z_2 \in \mathbb{R}^-$.

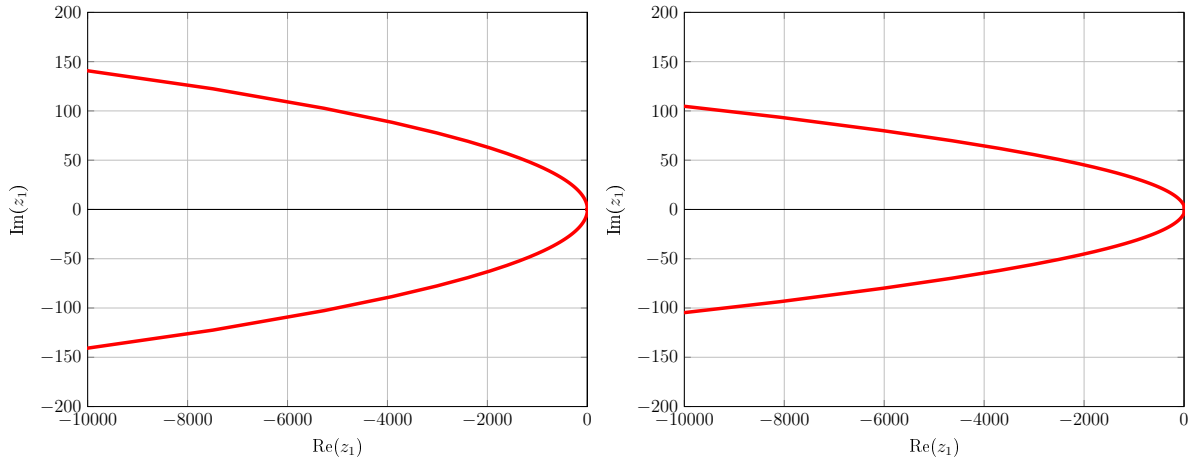

Figure 3.2.1: Stability region $\varrho(M_2(z_1, z_2)) < 1$ when $z_1 = z_2 \in \mathbb{C}^-$ of `TSW-1a` (*left*) and `TSW-3a` (*right*).

If $z_i, z_j \to \infty$, for at least two indices $1 \le i < j \le d$, then the stability matrix M_d has an eigenvalue $\xi = 1$ with multiplicity $s+1$, cf. Remark 3.2.7. This can lead to problems with respect to stability and accuracy. In our numerical tests for the two-step AMF W-methods `TSW-1a` and `TSW-3a`, no stability problems occur and there is no reduction in the convergence order, see Chapter 5. For illustration, we compute the maximum norm

of the n-th power of $M_2(z_1, z_2)$ for $z_1 = z_2$ with $z_1 = -10^2, -10^3, -10^4$ as function of n, cf. Figure 3.2.2. For the two-step AMF W-methods `TSW-1a` and `TSW-3a`, we observe that $\|M_2^n(z_1, z_2)\|_\infty$ tends to zero with an increasing number of steps n. This can be explained by the fact that for larger n the time step size is smaller and $z_1 = z_2$ will be far from infinity. Note, that for methods with more stages s, the stability matrix can cause more problems to guarantee stability.

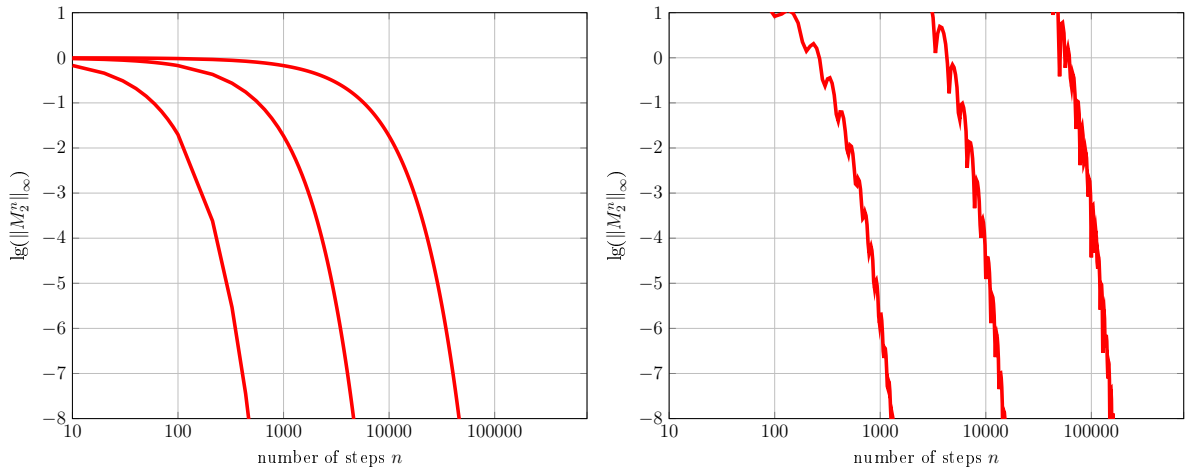

Figure 3.2.2: $\|M_2^n(z_1, z_2)\|_\infty$ for $z_1 = z_2$ with $z_1 = -10^2, -10^3, -10^4$ as function of n for `TSW-1a` (*left*) and `TSW-3a` (*right*).

4 Peer methods with approximate matrix factorization

In this chapter, we consider a class of implicit peer methods which uses additionally function values from the previous step. Therefore, we introduce the application of an approximate matrix factorization (AMF) and obtain a more general class of AMF peer methods as developed by Beck *et al.* (2014). We investigate consistency, convergence and stability properties for a fixed number of Newton steps in the AMF peer iteration. The influence of an inexact AMF approach is also elaborated. We construct a new AMF peer method of order three and give a proposal for the predictor in the Newton iteration. Furthermore, we discuss IMEX peer methods with AMF.

4.1 Implicit peer methods

In this section, we recall the formulation of implicit peer methods, order conditions and stability issues. An implicit peer method with s stages for the solution of an initial value problem (2.1.1) as introduced in Soleimani and Weiner [59] is given by

$$\begin{aligned} U_{m,i} &= \sum_{j=1}^{s} b_{ij} U_{m-1,j} + h_m \sum_{j=1}^{s} a_{ij} f(t_{m-1,j}, U_{m-1,j}) + h_m \sum_{j=1}^{i} g_{ij} f(t_{m,j}, U_{m,j}), \\ & i = 1, \ldots, s. \end{aligned} \tag{4.1.1}$$

Here $B = (b_{ij})_{i,j=1}^{s}$, $A = (a_{ij})_{i,j=1}^{s}$, $G = (g_{ij})_{i,j=1}^{s}$ and $c = (c_1, \ldots, c_s)^\top$ are the parameters of the method, where G is a lower triangular matrix with $g_{ii} = \gamma > 0$. In the case of a strictly lower triangular matrix G, one obtains an explicit peer method which is suitable for the solution of non-stiff initial value problems. The nodes c_i are assumed to be pairwise distinct with $c_s = 1$. In general, the coefficients of the method depend on the step size ratio $\sigma = h_m/h_{m-1}$. In contrast to two-step W-methods, s stage values $U_{m,i},\ i = 1, \ldots, s$, are computed at each time step. Here $U_{m,i}$ is an approximation to the exact solution $y(t_{m,i})$ where $t_{m,i} = t_m + c_i h_m$. Peer methods are a special class of general linear methods (GLMs), see e.g. [7,8,33], in which the approximations in all stages have the same order. Using the vectors $U_m = (U_{m,i})_{i=1}^{s} \in \mathbb{R}^{sn}$ and $F_m = (f(t_{m,i}, U_{m,i}))_{i=1}^{s}$ leads to a compact representation of the method

$$U_m = (B \otimes I) U_{m-1} + h_m (A \otimes I) F_{m-1} + h_m (G \otimes I) F_m,$$

where $\otimes$ stands for the usual Kronecker product of matrices. Like multistep methods and two-step W-methods, peer methods also need s starting values $U_{0,i},\ i = 1, \ldots, s$. Implicit and explicit peer methods have been investigated in several papers, e.g. [11, 19, 39, 40, 44, 48, 59, 67, 72].

We summarize some results for order conditions and stability from [59]. Conditions for the order of consistency can be derived by considering the residuals $\Delta_{m,i}$ obtained when the exact solution $y(t_{m,i})$ is put into the method (4.1.1)

$$\begin{aligned}\Delta_{m,i} := y(t_{m,i}) - \sum_{j=1}^{s} b_{ij} y(t_{m-1,j}) - h_m \sum_{j=1}^{s} a_{ij} y'(t_{m-1,j}) - h_m \sum_{j=1}^{i} g_{ij} y'(t_{m,j}),\\ i = 1, \ldots, s.\end{aligned} \tag{4.1.2}$$

We have the following definition.

Definition 4.1.1. The peer method (4.1.1) is consistent of order p if

$$\Delta_{m,i} = \mathcal{O}(h_m^{p+1}), \quad i = 1, \ldots, s. \qquad \square$$

Note that the stage order of the methods is equal to the order of consistency. By making a Taylor expansion of the sufficiently smooth exact solution and putting these expansions into the residuals $\Delta_{m,i}$, we obtain

$$\begin{aligned}\Delta_{m,i} = \left(1 - \sum_{j=1}^{s} b_{ij}\right) y(t_m) + \sum_{l=1}^{p} \left\{ c_i^l - \sum_{j=1}^{s} b_{ij} \frac{(c_j - 1)^l}{\sigma^l} - l \sum_{j=1}^{s} a_{ij} \frac{(c_j - 1)^{l-1}}{\sigma^{l-1}} \right.\\ \left. - l \sum_{j=1}^{i} g_{ij} c_j^{l-1} \right\} \frac{h_m^l}{l!} y^{(l)}(t_m) + \mathcal{O}(h_m^{p+1}).\end{aligned} \tag{4.1.3}$$

Theorem 4.1.2 ([59]). *A peer method* (4.1.1) *is consistent of order* p *if and only if*

$$\mathbb{AB}(l) = (\mathbb{AB}_i(l))_{i=1}^{s} = 0, \quad \textit{for all } l = 0, 1, \ldots, p, \tag{4.1.4}$$

where

$$\mathbb{AB}_i(l) := c_i^l - \sum_{j=1}^{s} b_{ij} \frac{(c_j - 1)^l}{\sigma^l} - l \sum_{j=1}^{s} a_{ij} \frac{(c_j - 1)^{l-1}}{\sigma^{l-1}} - l \sum_{j=1}^{i} g_{ij} c_j^{l-1}. \qquad \square$$

Like for multistep methods, zero-stability and order of consistency p are required for order of convergence p.

Definition 4.1.3. A peer method (4.1.1) is zero-stable if there is a constant $K > 0$ so that for all $m, k \geq 0$ holds

$$\|B_{m+k} \cdots B_{m+1} B_m\| \leq K. \qquad \square$$

We have the following theorem, see e.g. [46, 59].

Theorem 4.1.4. *A zero-stable peer method* (4.1.1) *with order of consistency p is convergent of order p, i.e.,*

$$U_{m,i} - y(t_{m,i}) = \mathcal{O}(h_{max}^p), \quad i = 1, \ldots, s, \quad h_{max} \to 0$$

with $h_{max} := \max_m h_m$. □

The condition (4.1.4) for $l = 0$ is referred to as preconsistency and yields $B\mathbb{1} = \mathbb{1}$. For arbitrary coefficients B and G, we can characterize methods of order of consistency $p = s$. With the notations (2.2.9), the following theorem can be shown.

Theorem 4.1.5 ([59])**.** *A peer method* (4.1.1) *is consistent of order* $p = s$ *if* $B\mathbb{1} = \mathbb{1}$ *and*

$$A = (CV_0 - GV_0D)D^{-1}SV_1^{-1} - \frac{1}{\sigma}B(C - I)V_1D^{-1}V_1^{-1}. \qquad \square$$

Note that for pairwise distinct nodes c, the Vandermonde-type matrix V_1 is regular and hence the matrix A is uniquely defined. Under certain assumptions, one can construct superconvergent peer methods of order of convergence $p = s + 1$. In [72] and [59], the concept of superconvergence for explicit and implicit peer methods is explained in more detail.

For stability investigations, the peer method (4.1.1) is applied to the usual Dahlquist test equation (2.2.10) with constant step size $h_m = h$. This yields a numerical recursion in the form

$$U_m = M(z)U_{m-1}, \quad M(z) = (I - zG)^{-1}(B + zA), \quad z = \lambda h, \tag{4.1.5}$$

where $M(z)$ denotes the stability matrix. It holds $M(\infty) = -G^{-1}A$. For peer methods with $A = 0$, we have $M(\infty) = 0$, i.e., L(α)-stability is implied for A(α)-stable methods.

Definition 4.1.6. A peer method (4.1.1) is optimally zero-stable if the eigenvalues of B satisfy

$$\xi_1 = 1, \quad \xi_2 = \cdots = \xi_s = 0. \qquad \square$$

For implicit peer methods with $A = 0$, the application of an approximate matrix factorization (AMF) and comparisons with implementation using Krylov techniques have been studied in [4] and in the PhD thesis [3]. In the following, we introduce and consider the more general case $A \neq 0$, i.e., using in addition the function values from the previous step, and the application of AMF.

4.2 AMF peer methods

In this section, we give the formulation of AMF peer methods. We prove a convergence result for AMF peer methods with fixed number of steps in the Newton iteration. We investigate the stability of AMF peer methods and describe the construction of a new three-stage method of order three.

4.2.1 Formulation of the methods

In contrast to one-step and two-step W-methods, for the computation of stage values $U_{m,i},\ i = 1, \ldots, s$, in (4.1.1), one has to solve a system of non-linear equations

$$\begin{aligned} U_{m,i} - h_m\gamma f(t_{m,i}, U_{m,i}) &= w_i, \quad i = 1, \ldots, s, \\ w_i := \sum_{j=1}^{s} b_{ij} U_{m-1,j} + h_m \sum_{j=1}^{s} a_{ij} f(t_{m-1,j}, U_{m-1,j}) &+ h_m \sum_{j=1}^{i-1} g_{ij} f(t_{m,j}, U_{m,j}). \end{aligned} \tag{4.2.6}$$

Here w_i summarizes already known stage and function values. Typically, the simplified Newton's method is applied, which leads to a recursion in the form

$$\begin{aligned} (I - h_m\gamma T_m)\Delta U_{m,i}^k &= w_i - U_{m,i}^k + h_m\gamma f(t_{m,i}, U_{m,i}^k), \\ U_{m,i}^{k+1} &= U_{m,i}^k + \Delta U_{m,i}^k, \quad k = 0, 1, 2, \ldots, \end{aligned} \tag{4.2.7}$$

where T_m is an approximation to the Jacobian $\partial_y f(t_{m-1,s}, U_{m-1,s})$. We denote the maximal number of steps in the Newton iteration by $kmax \geq 1$. Although only one LU-decomposition is required per step, this can be still very expensive for high dimensional linear systems (4.2.7). Therefore, we consider the application of AMF again. In this chapter, we consider a non-autonomous system of stiff ordinary differential equations with a splitting in $d + 1$ terms in the form

$$y'(t) = f(t, y(t)) = f_0(t, y(t)) + \sum_{j=1}^{d} f_j(t, y(t)), \quad y(t_0) = y_0 \in \mathbb{R}^n, \quad t \in [t_0, t_e] \tag{4.2.8}$$

with a corresponding splitting for the Jacobians into $d + 1$ addends

$$J_m = J_{m,0} + \sum_{j=1}^{d} J_{m,j}, \quad J_{m,j} = \partial_y f_j(t_{m-1,s}, U_{m-1,s}), \tag{4.2.9}$$

and with the AMF matrix Π_d

$$\Pi_d = \prod_{j=1}^{d} (I - h_m\gamma J_{m,j}), \tag{4.2.10}$$

see also Section 3.1. Again, $J_{m,0}$ stands for the term of the split Jacobian which is not considered in the AMF approach, i.e., $J_{m,0}$ collects parts of the Jacobian which are difficult to compute or are of no use in AMF schemes. This is typical for PDE problems where convection terms should be treated explicitly. If $J_{m,0} = 0$, then the AMF approach will be called *exact*. Otherwise, it will be said to be *inexact*, cf. [24, Definition 1]. Substituting the matrix $(I - h_m\gamma T_m)$ in (4.2.7) by the AMF matrix (4.2.10) leads to the formulation of AMF peer methods for the dimension of the AMF-splitting $d \geq 2$ in the form

$$\begin{aligned} \Pi_d \Delta U^k_{m,i} &= w_i - U^k_{m,i} + h_m\gamma f(t_{m,i}, U^k_{m,i}), \\ U^{k+1}_{m,i} &= U^k_{m,i} + \Delta U^k_{m,i}, \quad k = 0, 1, \ldots, kmax - 1, \\ U_{m,i} &= U^{kmax}_{m,i}, \quad i = 1, \ldots, s. \end{aligned} \tag{4.2.11}$$

For a fixed number of Newton steps $kmax \geq 1$, the choice of the predictor $U^0_{m,i}$ in (4.2.11) influences accuracy and stability. In the next section, we describe the order of convergence of an AMF peer method (4.2.11) in terms of the order of the underlying peer method (4.2.6), the accuracy of the predictor and the number of Newton steps.

4.2.2 Order of consistency and convergence of the methods

In the case that the Newton iteration has performed until convergence, the order of consistency of the fully implicit peer method (4.2.6) is independent of the matrix T_m. Therefore, it is clear that in this case the AMF approach does not influence the order of consistency.

Theorem 4.2.1 ([3])**.** *Let a peer method* (4.2.6) *be consistent of order* $p \geq 1$*. Then the corresponding AMF peer method* (4.2.11) *is also consistent of order* $p \geq 1$ *if the Newton iteration* (4.2.11) *converges.* □

One-step AMF W-methods and two-step AMF W-methods are linearly-implicit. For comparison, we are interested in AMF peer methods which only need a small number of Newton steps. Therefore, we investigate consistency and convergence of AMF peer methods for a fixed number of Newton steps $kmax$. The following result shows that the order of consistency of an AMF peer method (4.2.11) depends on the order of the underlying peer method (4.2.6), the accuracy of the predictor $U^0_{m,i}$ and the number of Newton steps $kmax$.

Theorem 4.2.2. *Let an AMF peer method* (4.2.11) *be associated to a peer method* (4.2.6) *of order* $p \geq 1$*. We consider an exact AMF approach, i.e.,* $J_{m,0} = 0$*. If* $U^0_{m,i} - y(t_{m,i}) = \mathcal{O}(h^q_m)$*,* $i = 1, \ldots, s$ *with* $0 \leq q \leq p+1$*, then the AMF peer method* (4.2.11) *is consistent of order* p *for arbitrary* d*, i.e.,*

$$U_{m,i} - y(t_{m,i}) = \mathcal{O}(h^{p+1}_m), \quad i = 1, \ldots, s,$$

whenever $U_{m-1,i} = y(t_{m-1,i})$, $i = 1, \dots, s$, *and*

$$kmax \geq \begin{cases} (p+1-q)/2, & \text{if } q \geq 1, \\ (p+2)/2, & \text{if } q = 0. \end{cases} \tag{4.2.12}$$

Proof. We denote the exact solution of (4.2.6) with $U^*_{m,i}$. Then, the exact solution $U^*_{m,i}$ with $U^*_{m-1,i} = y(t_{m-1,i}) = U_{m-1,i}$ fulfils

$$\begin{aligned} U^*_{m,i} - h_m \gamma f(t_{m,i}, U^*_{m,i}) &= w^*_i, \quad i = 1, \dots, s, \\ w^*_i = \sum_{j=1}^{s} b_{ij} U^*_{m-1,j} + h_m \sum_{j=1}^{s} a_{ij} f(t_{m-1,j}, U^*_{m-1,j}) &+ h_m \sum_{j=1}^{i-1} g_{ij} f(t_{m,j}, U^*_{m,j}). \end{aligned} \tag{4.2.13}$$

From (4.2.11), we get

$$\begin{aligned} \Pi_d \left(U^{k+1}_{m,i} - U^*_{m,i} \right) &= \Pi_d \left(\Delta U^k_{m,i} + (U^k_{m,i} - U^*_{m,i}) \right) \\ &= w_i - U^k_{m,i} + h_m \gamma f(t_{m,i}, U^k_{m,i}) + \Pi_d (U^k_{m,i} - U^*_{m,i}) \\ &= w^*_i - U^k_{m,i} + h_m \gamma f(t_{m,i}, U^k_{m,i}) + \Pi_d (U^k_{m,i} - U^*_{m,i}) + (w_i - w^*_i). \end{aligned}$$

Using the first equation of (4.2.13), it holds that

$$\begin{aligned} \Pi_d \left(U^{k+1}_{m,i} - U^*_{m,i} \right) = (\Pi_d - I)(U^k_{m,i} - U^*_{m,i}) &+ h_m \gamma \left(f(t_{m,i}, U^k_{m,i}) - f(t_{m,i}, U^*_{m,i}) \right) \\ &+ (w_i - w^*_i). \end{aligned}$$

Due to the exact AMF approach, the matrices T_m fulfil the assumption $J_m - T_m = \mathcal{O}(h_m)$ for $h_m \to 0$. With (4.2.10), it follows $\Pi_d = I + \mathcal{O}(h_m)$. Since $U^*_{m,i} = y(t_{m,i}) + \mathcal{O}(h_m^{p+1})$, it then follows that

$$\begin{aligned} \Pi_d \left(U^{k+1}_{m,i} - y(t_{m,i}) \right) = (\Pi_d - I)(U^k_{m,i} - y(t_{m,i})) &+ h_m \gamma (f(t_{m,i}, U^k_{m,i}) \\ &- f(t_{m,i}, y(t_{m,i}))) + (w_i - w^*_i) + \mathcal{O}(h_m^{p+1}). \end{aligned} \tag{4.2.14}$$

Furthermore, we have

$$\begin{aligned} f(t_{m,i}, U^k_{m,i}) - f(t_{m,i}, y(t_{m,i})) = \partial_y f(t_{m,i}, y(t_{m,i})) &\left(U^k_{m,i} - y(t_{m,i}) \right) \\ &+ \mathcal{O}\left(\left\| U^k_{m,i} - y(t_{m,i}) \right\|^2 \right). \end{aligned} \tag{4.2.15}$$

Inserting this into (4.2.14) leads for all $k = 0, \dots, kmax - 1$ to

$$\begin{aligned} \Pi_d (U^{k+1}_{m,i} - y(t_{m,i})) = (\Pi_d - I + h_m \gamma \partial_y f(t_{m,i}, y(t_{m,i})))(U^k_{m,i} - y(t_{m,i})) &\\ + (w_i - w^*_i) + \mathcal{O}\left(h_m \left\| U^k_{m,i} - y(t_{m,i}) \right\|^2 \right) + \mathcal{O}(h_m^{p+1}), & \end{aligned} \tag{4.2.16}$$

where $\Pi_d - I + h_m \gamma \partial_y f(t_{m,i}, y(t_{m,i})) = \mathcal{O}(h_m^2)$ for $h_m \to 0$ holds with (4.2.10) and $J_m - T_m = \mathcal{O}(h_m)$ for $h_m \to 0$.

We now prove the statement by induction on s. First, for $i = 1$, from (4.2.6), (4.2.13) and with $U^*_{m-1,j} = y(t_{m-1,j}) = U_{m-1,j}$, $1 \le j \le s$, we have that $w_1 = w^*_1$. Since $U^0_{m,1} - y(t_{m,1}) = \mathcal{O}(h^q_m)$, we get from (4.2.16) that $U_{m,1} - y(t_{m,1}) = \mathcal{O}(h^{p+1}_m)$ whenever (4.2.12) holds.

For the induction step, we assume that $U_{m,j} - y(t_{m,j}) = \mathcal{O}(h^{p+1}_m)$, $j = 1, \dots, i-1$. This implies from (4.2.6) and (4.2.13) that $w_i - w^*_i = \mathcal{O}(h^{p+2}_m)$ and inserting this in (4.2.16) concludes the proof in a similar way as for $i = 1$. ■

With Equation (4.2.16) in the proof of the previous theorem, the accuracy of an AMF peer method (4.2.11) can be characterized after each Newton step. For example, if $U^0_{m,i} - y(t_{m,i}) = \mathcal{O}(h^q_m)$ for all $i = 1, \dots, s$ with $0 \le q \le p+1$, then we have after one Newton step, i.e., for $k = 0$

$$\begin{aligned}(I + \mathcal{O}(h_m))(U^1_{m,i} - y(t_{m,i})) &= \mathcal{O}(h^2_m)\mathcal{O}(h^q_m) + \mathcal{O}(h^{p+2}_m) + \mathcal{O}(h^{2q+1}_m) + \mathcal{O}(h^{p+1}_m) \\ &= \mathcal{O}(h^{q+2}_m) + \mathcal{O}(h^{2q+1}_m) + \mathcal{O}(h^{p+1}_m),\end{aligned}$$

and hence, we obtain

$$U^1_{m,i} - y(t_{m,i}) = \begin{cases} \mathcal{O}(h^{q+2}_m) + \mathcal{O}(h^{p+1}_m), & \text{if } q \ge 1, \\ \mathcal{O}(h_m) + \mathcal{O}(h^{p+1}_m), & \text{if } q = 0. \end{cases}$$

This can be generalized and is summarized in the following corollary.

Corollary 4.2.3. *Let an AMF peer method* (4.2.11) *be associated to a peer method* (4.2.6) *of order* $p \ge 1$. *We consider an exact AMF approach. If* $U^0_{m,i} - y(t_{m,i}) = \mathcal{O}(h^q_m)$ *for all* $i = 1, \dots, s$ *with* $0 \le q \le p+1$, *then for an AMF peer method* (4.2.11) *with* $U_{m-1,i} = y(t_{m-1,i})$, $i = 1, \dots, s$ *and arbitrary* d *it holds*

$$U^k_{m,i} - y(t_{m,i}) = \begin{cases} \mathcal{O}(h^{q+2k}_m) + \mathcal{O}(h^{p+1}_m), & \text{if } q \ge 1, \\ \mathcal{O}(h^{2k-1}_m) + \mathcal{O}(h^{p+1}_m), & \text{if } q = 0. \end{cases}, \quad i = 1, \dots, s, \quad k = 1, 2, \dots$$

whenever $U_{m,j} - y(t_{m,j}) = \mathcal{O}(h^{p+1}_m)$, $j = 1, \dots, i-1$. □

In Theorem 4.2.2, we consider an exact AMF approach, i.e., $J_{m,0} = 0$. Therefore, it holds $J_m - T_m = \mathcal{O}(h_m)$ for $h_m \to 0$ and we obtain $\Pi_d - I + h_m\gamma\partial_y f(t_{m,i}, y(t_{m,i})) = \mathcal{O}(h^2_m)$ for $h_m \to 0$ in the proof above. In the case of an inexact AMF, i.e., $J_{m,0} \neq 0$, we have $J_m - J_{m,0} - T_m = \mathcal{O}(h_m)$ for $h_m \to 0$ and hence

$$\begin{aligned}\Pi_d - I + h_m\gamma\partial_y f(t_{m,i}, y(t_{m,i})) &= h_m\gamma J_{m,0} - h_m\gamma J_m + h_m\gamma\partial_y f(t_{m,i}, y(t_{m,i})) \\ &= \mathcal{O}(h_m), \quad h_m \to 0.\end{aligned} \tag{4.2.17}$$

We observe in this situation a different bound for the necessary number of Newton steps to obtain order p in the AMF peer method. We summarize this in following theorem.

Theorem 4.2.4. *Let an AMF peer method* (4.2.11) *be associated to a peer method* (4.2.6) *of order* $p \geq 1$. *We consider an inexact AMF approach, i.e.,* $J_{m,0} \neq 0$. *If* $U^0_{m,i} - y(t_{m,i}) = \mathcal{O}(h_m^q),\ i = 1, \ldots, s$ *with* $0 \leq q \leq p+1$, *then the AMF peer method* (4.2.11) *is consistent of order* p *for arbitrary* d, *i.e.,*

$$U_{m,i} - y(t_{m,i}) = \mathcal{O}(h_m^{p+1}), \quad i = 1, \ldots, s,$$

whenever $U_{m-1,i} = y(t_{m-1,i}),\ i = 1, \ldots, s$, *and*

$$kmax \geq p + 1 - q, \quad q \geq 0. \tag{4.2.18}$$

Proof. The statement follows for an inexact AMF approach and with (4.2.17) analogously to the proof of Theorem 4.2.2. ■

Analogous to Corollary 4.2.3, the next corollary follows immediately.

Corollary 4.2.5. *Let an AMF peer method* (4.2.11) *be associated to a peer method* (4.2.6) *of order* $p \geq 1$. *We consider an inexact AMF approach. If* $U^0_{m,i} - y(t_{m,i}) = \mathcal{O}(h_m^q)$ *for all* $i = 1, \ldots, s$ *with* $0 \leq q \leq p+1$, *then for an AMF peer method* (4.2.11) *with* $U_{m-1,i} = y(t_{m-1,i}),\ i = 1, \ldots, s$ *and arbitrary* d *it holds*

$$U^k_{m,i} - y(t_{m,i}) = \mathcal{O}(h_m^{q+k}) + \mathcal{O}(h_m^{p+1}), \quad q \geq 0, \quad i = 1, \ldots, s, \quad k = 1, 2, \ldots$$

whenever $U_{m,j} - y(t_{m,j}) = \mathcal{O}(h_m^{p+1}),\ j = 1, \ldots, i-1$. □

In the following, we will show the convergence of AMF peer methods with a fixed number of Newton steps. Therefore, we denote by $\widetilde{U}_m$ the numerical solution after one step of an AMF peer method (4.2.11) obtained with exact starting values, i.e., $\widetilde{U}_{m-1,i} = y(t_{m-1,i}),\ i = 1, \ldots, s$, cf. Theorem 4.2.2. We also use the notation

$$Y(t_m) = \begin{pmatrix} y(t_m + c_1 h_m) \\ \vdots \\ y(t_m + c_s h_m) \end{pmatrix}$$

for the exact solution at time t_m and the global error is defined by

$$\varepsilon_m := U_m - Y(t_m).$$

For simplicity, we suppose in the following theorem that all stage values $U_{m,i},\ i = 1, \ldots, s$, are computed simultaneously by Newton's method. This is not a restriction but allows a more compact proof of the statement. Furthermore, we assume the same upper bound $kmax$ for all stages. Of course, this can be different in practical computations.

Theorem 4.2.6. *Let U_m be the numerical solution of a zero-stable AMF peer method (4.2.11) and let $\widetilde{U}_m$ be the numerical solution after one step of the AMF peer method obtained with exact starting values, i.e., $\widetilde{U}_{m-1,i} = y(t_{m-1,i})$, $i = 1, \dots, s$, with $\widetilde{T}_m = T_m$. Furthermore, we suppose that the coefficient matrices B and G are constant and A is computed by Theorem 4.1.5. Then it holds*

$$\left\| U_m^k - \widetilde{U}_m^k \right\| \leq (1 + \mathcal{O}(h_m)) \left\| \varepsilon_{m-1} \right\|, \quad k = 0, \dots, kmax. \tag{4.2.19}$$

Proof. For simpler notation, we consider scalar and autonomous initial value problems. We get from (4.2.11) for $U_{m,i}^{k+1}$ and $\widetilde{U}_{m,i}^{k+1}$, $i = 1, \dots, s$, with $\widetilde{T}_m = T_m$

$$\begin{aligned} \Pi_d(U_{m,1}^{k+1} - U_{m,1}^k) &= w_1^k - U_{m,1}^k + h_m \gamma f(U_{m,1}^k), \\ &\vdots \\ \Pi_d(U_{m,s}^{k+1} - U_{m,s}^k) &= w_s^k - U_{m,s}^k + h_m \gamma f(U_{m,s}^k) \end{aligned} \tag{4.2.20}$$

and

$$\begin{aligned} \Pi_d(\widetilde{U}_{m,1}^{k+1} - \widetilde{U}_{m,1}^k) &= \widetilde{w}_1^k - \widetilde{U}_{m,1}^k + h_m \gamma f(\widetilde{U}_{m,1}^k), \\ &\vdots \\ \Pi_d(\widetilde{U}_{m,s}^{k+1} - \widetilde{U}_{m,s}^k) &= \widetilde{w}_s^k - \widetilde{U}_{m,s}^k + h_m \gamma f(\widetilde{U}_{m,s}^k). \end{aligned} \tag{4.2.21}$$

Using the vectors $U_m^k = \left(U_{m,i}^k\right)_{i=1}^s \in \mathbb{R}^s$, $\widetilde{U}_m^k = \left(\widetilde{U}_{m,i}^k\right)$, $F(U_m^k) = \left(f(U_{m,i}^k)\right)_{i=1}^s \in \mathbb{R}^s$, $F(\widetilde{U}_m^k) = \left(f(\widetilde{U}_{m,i}^k)\right)_{i=1}^s$, $w^k = (w_i^k)_{i=1}^s \in \mathbb{R}^s$ and $\widetilde{w}^k = (\widetilde{w}_i^k)$ with

$$\begin{aligned} w_i^k &= \sum_{j=1}^s b_{ij} U_{m-1,j} + h_m \sum_{j=1}^s a_{ij} f(U_{m-1,j}) + h_m \sum_{j=1}^{i-1} g_{ij} f(U_{m,j}^k), \\ \widetilde{w}_i^k &= \sum_{j=1}^s b_{ij} \widetilde{U}_{m-1,j} + h_m \sum_{j=1}^s a_{ij} f(\widetilde{U}_{m-1,j}) + h_m \sum_{j=1}^{i-1} g_{ij} f(\widetilde{U}_{m,j}^k), \end{aligned}$$

we obtain from (4.2.20) and (4.2.21) for U_m^{k+1} and $\widetilde{U}_m^{k+1}$, respectively,

$$\begin{aligned} \Pi_d(U_m^{k+1} - U_m^k) &= w^{k+1} - U_m^k + h_m \gamma F(U_m^k), \\ \Pi_d(\widetilde{U}_m^{k+1} - \widetilde{U}_m^k) &= \widetilde{w}^{k+1} - \widetilde{U}_m^k + h_m \gamma F(\widetilde{U}_m^k). \end{aligned} \tag{4.2.22}$$

Note that by collecting all stage values, w^{k+1} and $\widetilde{w}^{k+1}$ depend on the Newton iterates U_m^{k+1} and $\widetilde{U}_m^{k+1}$, respectively. Formally, this looks implicitly in terms of U_m^{k+1} and $\widetilde{U}_m^{k+1}$, but it can be solved successively via the stages. Subtracting the equations in (4.2.22) leads to

$$\begin{aligned} \Pi_d \left(U_m^{k+1} - \widetilde{U}_m^{k+1} \right) = (w^{k+1} - \widetilde{w}^{k+1}) + (\Pi_d - 1) \left(U_m^k - \widetilde{U}_m^k \right) \\ + h_m \gamma \left(F(U_m^k) - F(\widetilde{U}_m^k) \right). \end{aligned} \tag{4.2.23}$$

We consider the case $k = 0$ and use the notation $G = \widetilde{G} + \gamma I$, i.e., $\widetilde{G}$ is a strictly lower triangular matrix. From (4.2.6), and with the assumption $\widetilde{U}_{m-1} = Y(t_{m-1})$ for $\widetilde{w}^1$, we have

$$w^1 - \widetilde{w}^1 = B\varepsilon_{m-1} + h_m A(F(U_{m-1}) - F(Y(t_{m-1}))) + h_m \widetilde{G}(F(U_m^1) - F(\widetilde{U}_m^1)).$$

With the mean value theorem for vector-valued functions, we have

$$\begin{aligned} &F(U_{m-1}) - F(Y(t_{m-1})) = H_{m-1}\varepsilon_{m-1}, \quad \text{with } H_{m-1} = \operatorname{diag}(\xi_{m-1,i}), \\ &\xi_{m-1,i} = \int_0^1 \partial_y f(y(t_{m-1,i}) + \theta(U_{m-1,i} - y(t_{m-1,i}))) \,\mathrm{d}\theta \end{aligned} \tag{4.2.24}$$

and analogous to this also

$$F(U_m^1) - F(\widetilde{U}_m^1) = J_m^1(U_m^1 - \widetilde{U}_m^1). \tag{4.2.25}$$

We have with (4.2.24) and (4.2.25)

$$w^1 - \widetilde{w}^1 = B\varepsilon_{m-1} + h_m A H_{m-1}\varepsilon_{m-1} + h_m \widetilde{G} J_m^1(U_m^1 - \widetilde{U}_m^1). \tag{4.2.26}$$

With predictors in the form $U_m^0 = \widehat{B}U_{m-1} + h_m \widehat{A}F(U_{m-1})$ and with $\widetilde{U}_{m-1} = Y(t_{m-1})$ for $\widetilde{U}_m^0$, we obtain

$$\begin{aligned} U_m^0 - \widetilde{U}_m^0 &= \widehat{B}(U_{m-1} - Y(t_{m-1})) + h_m \widehat{A}(F(U_{m-1}) - F(Y(t_{m-1}))) \\ &= \widehat{B}\varepsilon_{m-1} + h_m \widehat{A} K_{m-1}\varepsilon_{m-1} \end{aligned} \tag{4.2.27}$$

and

$$h_m\gamma(F(U_m^0) - F(\widetilde{U}_m^0)) = h_m\gamma L_m^0(U_m^0 - \widetilde{U}_m^0). \tag{4.2.28}$$

Again, K_{m-1} and L_m^0 are obtained by the mean value theorem as described above. Inserting (4.2.26) and (4.2.28) into (4.2.23) leads to

$$\begin{aligned} \Pi_d \left(U_m^1 - \widetilde{U}_m^1\right) = {} & B\varepsilon_{m-1} + h_m A H_{m-1}\varepsilon_{m-1} + h_m \widetilde{G} J_m^1(U_m^1 - \widetilde{U}_m^1) \\ & + (\Pi_d - 1)(U_m^0 - \widetilde{U}_m^0) + h_m\gamma L_m^0(U_m^0 - \widetilde{U}_m^0) \end{aligned} \tag{4.2.29}$$

and hence, we obtain

$$\begin{aligned} (\Pi_d I - h_m \widetilde{G} J_m^1)\left(U_m^1 - \widetilde{U}_m^1\right) = {} & B\varepsilon_{m-1} + h_m A H_{m-1}\varepsilon_{m-1} \\ & + ((\Pi_d - 1)I + h_m\gamma L_m^0)(U_m^0 - \widetilde{U}_m^0). \end{aligned} \tag{4.2.30}$$

With $\Pi_d = 1 + \mathcal{O}(h_m)$, we have

$$(I + \mathcal{O}(h_m))\left(U_m^1 - \widetilde{U}_m^1\right) = B\varepsilon_{m-1} + h_m A H_{m-1}\varepsilon_{m-1} + \mathcal{O}(h_m)(U_m^0 - \widetilde{U}_m^0).$$

The coefficient matrix G is constant and hence the matrices A are uniformly bounded for $\sigma \leq \sigma_{\max}$. With

$$U_m^0 - \widetilde{U}_m^0 = \widehat{B}\varepsilon_{m-1} + h_m \widehat{A} K_{m-1}\varepsilon_{m-1} = \mathcal{O}(1)\varepsilon_{m-1},$$

we then get

$$\begin{aligned}(I + \mathcal{O}(h_m))\left(U_m^1 - \widetilde{U}_m^1\right) &= B\varepsilon_{m-1} + \mathcal{O}(h_m)\varepsilon_{m-1},\\ U_m^1 - \widetilde{U}_m^1 &= B\varepsilon_{m-1} + \mathcal{O}(h_m)\varepsilon_{m-1}.\end{aligned}$$

Due to the zero-stability, there exists a norm $\|\cdot\|$ such that $\|B\| = 1$ holds for the constant matrix B. Then, it follows in this norm

$$\left\|U_m^1 - \widetilde{U}_m^1\right\| \leq \|B\| \|\varepsilon_{m-1}\| + \mathcal{O}(h_m) \|\varepsilon_{m-1}\| = (1 + \mathcal{O}(h_m)) \|\varepsilon_{m-1}\|.$$

Now, the statement follows recursively, i.e., we have

$$\left\|U_m^k - \widetilde{U}_m^k\right\| \leq (1 + \mathcal{O}(h_m)) \|\varepsilon_{m-1}\|, \quad k = 0, \ldots, kmax.$$

■

We now prove our convergence results.

Theorem 4.2.7. *Let the assumptions of Theorem 4.2.6 be satisfied. Let an AMF peer method* (4.2.11) *with an exact AMF approach be associated to a peer method* (4.2.6)*, which is consistent of order $p \geq 1$.*

(a) If the predictor satisfies $U_{m,i}^0 - y(t_{m,i}) = \mathcal{O}(h_m^q)$, $i = 1, \ldots, s$ with $0 \leq q \leq p+1$, then we have

$$\left\|\varepsilon_m^k\right\| \leq \begin{cases}(1 + \mathcal{O}(h_m)) \|\varepsilon_{m-1}\| + \mathcal{O}(h_m^{q+2k}) + \mathcal{O}(h_m^{p+1}), & \text{if } q \geq 1,\\ (1 + \mathcal{O}(h_m)) \|\varepsilon_{m-1}\| + \mathcal{O}(h_m^{2k-1}) + \mathcal{O}(h_m^{p+1}), & \text{if } q = 0.\end{cases} \tag{4.2.31}$$

(b) Additionally, if the starting values satisfy $U_{0,i} - y(t_{0,i}) = \mathcal{O}(h_0^p)$, $i = 1, \ldots, s$, and whenever

$$kmax \geq \begin{cases}(p + 1 - q)/2, & \text{if } q \geq 1,\\ (p+2)/2, & \text{if } q = 0\end{cases}$$

holds, then an AMF peer method (4.2.11) *is convergent of order p for arbitrary d, i.e.,*

$$\|\varepsilon_m\| = \|U_m - Y(t_m)\| = \mathcal{O}(h_{max}^p), \quad h_{max} \to 0 \tag{4.2.32}$$

with $h_{max} := \max_m h_m$.

Proof.

(a) With

$$\varepsilon_m^k = U_m^k - Y(t_m) = U_m^k - \widetilde{U}_m^k + \widetilde{U}_m^k - Y(t_m)$$

and Theorem 4.2.6, it follows

$$\left\|\varepsilon_m^k\right\| \leq \left\|U_m^k - \widetilde{U}_m^k\right\| + \left\|\widetilde{U}_m^k - Y(t_m)\right\| \leq (1 + \mathcal{O}(h_m)) \left\|\varepsilon_{m-1}\right\| + \left\|\widetilde{U}_m^k - Y(t_m)\right\|.$$

With Corollary 4.2.3, the proof is complete.

(b) With the global error $\varepsilon_m = U_m - Y(t_m)$, $U_m = U_m^{kmax}$ and a fixed number of Newton iterations $kmax \geq 1$, we have with (a) and Theorem 4.2.2 the recursion for the global error

$$\|\varepsilon_m\| = \|U_m - Y(t_m)\| = \left\|U_m^{kmax} - Y(t_m)\right\| \leq (1 + \mathcal{O}(h_m)) \|\varepsilon_{m-1}\| + \mathcal{O}(h_m^{p+1}).$$

Taking into account that $h_m = \sigma h_{m-1}$, the statement now follows with the assumption for the starting values by standard arguments, cf. e.g. the proof of Theorem 5.2.1 in [64].

■

Analogously, the following theorem is obtained for an inexact AMF approach.

Theorem 4.2.8. *Let the assumptions of Theorem 4.2.6 be satisfied. Let an AMF peer method* (4.2.11) *with an inexact AMF approach be associated to a peer method* (4.2.6)*, which is consistent of order $p \geq 1$.*

(a) If the predictor satisfies $U_{m,i}^0 - y(t_{m,i}) = \mathcal{O}(h_m^q)$, $i = 1, \ldots, s$ with $0 \leq q \leq p+1$, then we have

$$\left\|\varepsilon_m^k\right\| \leq (1 + \mathcal{O}(h_m)) \left\|\varepsilon_{m-1}\right\| + \mathcal{O}(h_m^{q+k}) + \mathcal{O}(h_m^{p+1}), \quad q \geq 0. \tag{4.2.33}$$

(b) Additionally, if the starting values satisfy $U_{0,i} - y(t_{0,i}) = \mathcal{O}(h_0^p)$, $i = 1, \ldots, s$, and whenever

$$kmax \geq p + 1 - q, \quad r \geq 0$$

holds, then an AMF peer method (4.2.11) *is convergent of order p for arbitrary d, i.e.,*

$$\|\varepsilon_m\| = \|U_m - Y(t_m)\| = \mathcal{O}(h_{max}^p), \quad h_{max} \to 0 \tag{4.2.34}$$

with $h_{max} := \max_m h_m$. □

Remark 4.2.9. *Note that zero-stability is an essential assumption of Theorem 4.2.6. Hence, convergence of AMF peer methods for a fixed number of Newton steps follows by consistency and zero-stability, which is typical for multistep methods or peer methods, see e.g. [15, 64].* □

4.2.3 Stability investigations of the methods

For stability investigations of AMF peer methods, we again consider the linear scalar test equation, cf. also Section 3.2.1

$$y'(t) = \lambda y(t), \quad \lambda = \sum_{j=1}^{d} \lambda_j, \quad \mathrm{Re}(\lambda_j) \leq 0, \quad j = 1, \ldots, d, \tag{4.2.35}$$

where d denotes the dimension of the AMF splitting. In [3], it is shown that AMF peer methods with $A = 0$ are at most A(α)-stable with

$$\alpha \leq \frac{\pi}{2(d-1)}.$$

The same upper bound for the maximal angle α of A(α)-stability is proved for AMF Rosenbrock methods and even one-step AMF schemes, in general, cf. [32]. We also show this for AMF peer methods with $A \neq 0$. Therefore, we apply a peer method (4.2.6) with constant step sizes $h_m = h$ to the scalar test equation (4.2.35) and obtain with notations (3.2.20)

$$U_m = BU_{m-1} + zAU_{m-1} + zGU_m. \tag{4.2.36}$$

We denote the exact solution of (4.2.36) by U_m^* and then get

$$0 = U_m^* - zGU_m^* - (B + zA)U_{m-1}. \tag{4.2.37}$$

The application of Newton's method to (4.2.36) leads to a recursion in the form

$$(I - zG)\left(U_m^{k+1} - U_m^k\right) = (B + zA)U_{m-1} + zGU_m^k - U_m^k, \quad k = 0, 1, 2, \ldots. \tag{4.2.38}$$

We apply the AMF approach and substituting the matrix $(I - zG)$ in (4.2.38) by the corresponding AMF matrix Π_d yields

$$\begin{aligned} \Pi_d\left(U_m^{k+1} - U_m^k\right) &= (B + zA)U_{m-1} + zGU_m^k - U_m^k, \\ \Pi_d U_m^{k+1} &= \Pi_d U_m^k + (B + zA)U_{m-1} + zGU_m^k - U_m^k. \end{aligned} \tag{4.2.39}$$

We define the error of U_m^k to the exact solution by $\Delta_k := U_m^k - U_m^*$ and obtain with (4.2.37) and (4.2.39) the following recursion for the error

$$\begin{aligned} \Pi_d\Delta_{k+1} &= \Pi_d U_m^{k+1} - \Pi_d U_m^* \\ &= \Pi_d U_m^k - \Pi_d U_m^* + (B + zA)U_{m-1} + zGU_m^k - U_m^k \\ &= \Pi_d U_m^k - \Pi_d U_m^* + (B + zA)U_{m-1} + zGU_m^k - U_m^k \\ &\quad + U_m^* - zGU_m^* - (B + zA)U_{m-1} \\ &= \Pi_d(U_m^k - U_m^*) + zG(U_m^k - U_m^*) - (U_m^k - U_m^*) \\ &= \Pi_d\Delta_k + zG\Delta_k - \Delta_k \\ &= (\Pi_d + zG - I)\Delta_k, \end{aligned} \tag{4.2.40}$$

i.e., we have $\Delta_{k+1} = R(z_1, \ldots, z_d)\Delta_k$ with iteration matrix given by $R(z_1, \ldots, z_d) = I - \Pi_d^{-1}(I - zG)$. We observe that terms with U_{m-1} vanish in the error recursion (4.2.40). Hence, we have the same recursion as in [3, Eq. (4.11)]. Analogous to [3], we assume that all values z_j, $j = 1, \ldots, d$, are equal, i.e., $z_1 = \cdots = z_d \in \mathbb{C}^-$. Then, our statement follows immediately with the approach in [3]. We summarize this in the following theorem.

Theorem 4.2.10. *Let $z_j = \xi \in \mathbb{C}^-$ for all $j = 1, \ldots, d$ be given. If the iteration* (4.2.39) *is convergent for all $\xi \in \mathbb{C}^-$ with $|\arg(\xi) - \pi| \leq \alpha$ and for arbitrary predictors $U_{m,i}^0$, $i = 1, \ldots, s$, then it holds*

$$\alpha \leq \frac{\pi}{2(d-1)}. \tag{4.2.41}$$

In particular, an AMF peer method (4.2.11) *is at most A(α)-stable with angle α given by* (4.2.41). □

Again, we are also interested in characterizing stability of AMF peer methods for a fixed number of Newton steps $kmax \geq 1$. In this case, the predictor $U_{m,i}^0$ in the AMF peer scheme (4.2.11) influences stability. In [3], a very general predictor is considered to derive the stability matrix of the Newton iteration with AMF, namely

$$U_{m,i}^0 = \sum_{j=1}^{s} \widehat{b}_{ij} U_{m-1,j} + h_m \sum_{j=1}^{s} \widehat{a}_{ij} F_{m-1,j} + \sum_{j=1}^{i-1} \widehat{r}_{ij} U_{m,j} + h_m \sum_{j=1}^{i-1} \widehat{g}_{ij} F_{m,j}. \tag{4.2.42}$$

Predictors (4.2.42) with $\widehat{a}_{ij} = \widehat{r}_{ij} = 0$ for peer methods are introduced in [48]. Investigations and numerical tests in [3, 4] have shown that predictors of high order or predictors using stage values or function values of the current step have worse stability properties in the AMF case. Therefore, we shall deal with predictors for the Newton iteration in the form

$$U_{m,i}^0 = \sum_{j=1}^{s} \widehat{b}_{ij} U_{m-1,j}, \quad i = 1, \ldots, s \tag{4.2.43}$$

or in the compact representation $U_m^0 = \widehat{B} U_{m-1}$ with $\widehat{B} = \left(\widehat{b}_{ij}\right)_{i,j=1}^{s}$. We do not claim that this choice is optimal, but it is justified by former research and allows us a theoretical analysis. For completeness, we give the order conditions for predictors (4.2.43).

Definition 4.2.11. A predictor (4.2.42) is of order q if

$$\Delta_{m,i}^P = \mathcal{O}(h_m^{q+1}), \quad i = 1, \ldots, s,$$

where the residuals $\Delta_{m,i}^P$ are obtained when the exact solution $y(t_{m,i})$ is put into the predictor

$$\Delta_{m,i}^P := y(t_{m,i}) - \sum_{j=1}^{s} \widehat{b}_{ij} y(t_{m-1,j}) - h_m \sum_{j=1}^{s} \widehat{a}_{ij} y'(t_{m-1,j}) - \sum_{j=1}^{i-1} \widehat{r}_{ij} y(t_{m,j}) - h_m \sum_{j=1}^{i-1} \widehat{g}_{ij} y'(t_{m,j}).$$

□

Lemma 4.2.12. *A predictor* (4.2.43) *is of order q if and only if*

$$c_i^l - \sum_{j=1}^{s} \widehat{b}_{ij} \frac{(c_j - 1)^l}{\sigma^l} = 0, \quad i = 1, \ldots, s, \quad l = 0, 1, \ldots, q. \tag{4.2.44}$$

Proof. The statement follows by Taylor series expansion of the sufficiently smooth exact solution and putting these expansions into the residuals $\Delta_{m,i}^P$. ■

Remark 4.2.13. *The condition* $\Delta_{m,i}^P = \mathcal{O}(h_m^{q+1})$, $i = 1, \ldots, s$, *in Definition 4.2.11 is equivalent to*

$$U_{m,i}^0 - y(t_{m,i}) = \mathcal{O}(h_m^{q+1}), \quad i = 1, \ldots, s, \tag{4.2.45}$$

i.e., a predictor (4.2.42) *or* (4.2.43) *is of order q if the condition* (4.2.45) *is satisfied, see e.g. Theorem 4.2.2.* □

Remark 4.2.14. *Note that condition* (4.2.44) *for* $l = 0$ *leads to* $\widehat{B}\mathbb{1} = \mathbb{1}$ *and predictors of order* $q = s - 1$ *are given by* $\widehat{B} = V_0 V_1^{-1}$ *for constant step sizes.* □

The application of the AMF peer method (4.2.11) to the test equation (2.2.10) leads to a numerical recursion in the form

$$U_m = M_{kmax} U_{m-1}, \quad M_{kmax} := M_{kmax}(z_1, \ldots, z_d), \tag{4.2.46}$$

where the stability matrix M_{kmax} is implicitly defined from the relations

$$\Pi_d \left(U_m^{k+1} - U_m^k\right) = (B + zA)U_{m-1} + zG_0 U_m - (1 - \gamma z)U_m^k, \quad k = 0, \ldots, kmax - 1, \tag{4.2.47}$$

with $U_m := U_m^{kmax}$, predictor $U_m^0 = \widehat{B} U_{m-1}$, strictly lower triangular matrix $G_0 := G - \gamma I$ and AMF factor Π_d given by (3.2.22). For the simplest case $kmax = 1$, solving for M_1 in (4.2.46) and (4.2.47) gives

$$M_1 = \Big(\Pi_d I - zG_0\Big)^{-1} \Big(B + zA + (\Pi_d - 1 + \gamma z)\widehat{B}\Big). \tag{4.2.48}$$

Note that with $d = 1$, one obtains the usual stability matrix (4.1.5).

In the following, we prove a characterization of the stability of an AMF peer method at infinity. It turns out that the stability at infinity depends strongly on the predictor for the Newton iteration.

Theorem 4.2.15. *Let* $M_{kmax}(z_1, \ldots, z_d)$ *be the stability matrix defined by* (4.2.46) *and* (4.2.47) *for the AMF peer method* (4.2.11) *with* $kmax \geq 1$, *an AMF-splitting* $d \geq 2$ *and a predictor* $U_m^0 = \widehat{B} U_{m-1}$. *If* $z_i, z_j \to \infty$, *for at least two indices* $1 \leq i < j \leq d$, *then* M_{kmax} *tends to* $\widehat{B}$.

Proof. From (4.2.47), we have that

$$U_m^k = M^{(k)} U_{m-1}, \quad k = 0, \ldots, kmax,$$

for $M^{(k)} = M^{(k)}(z_1, \ldots, z_d)$, with $M^{(0)} = \widehat{B}$ and $M^{(kmax)} = M_{kmax}$. These matrices fulfil the recursion

$$\Pi_d \left(M^{(k+1)} - M^{(k)} \right) = B + zA + zG_0 M_{kmax} - (1 - \gamma z) M^{(k)}, \quad k = 0, \ldots, kmax - 1,$$

that is,

$$\Pi_d M^{(k+1)} = \mathcal{A} + \beta \left(\Pi_d M^{(k)} \right), \quad k = 0, \ldots, kmax - 1,$$

where $\mathcal{A} := B + zA + zG_0 M_{kmax}$ and $\beta := (\Pi_d - 1 + \gamma z)/\Pi_d$ is a scalar. Observe that $\lim\limits_{\substack{z_i, z_j \to \infty \\ i \neq j}} \dfrac{z}{\Pi_d} = 0$ and therefore $\beta \to 1$ if $z_i, z_j \to \infty$. From the latter recursion, we get explicitly

$$\Pi_d M_{kmax} = \left(\sum_{k=0}^{kmax-1} \beta^k \right) \mathcal{A} + \beta^{kmax} \Pi_d M^{(0)},$$

i.e.,

$$\left(I - \frac{z}{\Pi_d} \left(\sum_{k=0}^{kmax-1} \beta^k \right) G_0 \right) M_{kmax} = \frac{1}{\Pi_d} \left(\sum_{k=0}^{kmax-1} \beta^k \right) (B + zA) + \beta^{kmax} \widehat{B}.$$

Now, the result follows with $z/\Pi_d \to 0$ and $\beta \to 1$ taking $z_i, z_j \to \infty$. ■

4.2.4 Construction of an AMF peer method of order three

In this section, we describe the construction of a three-stage AMF peer method of order $p = 3$. As mentioned above, for stability reasons the predictor for the Newton iteration shall be considered in the optimization process. Furthermore, the choice of the predictor also influences accuracy. We consider the following predictors:

- `pr1`: Here is $U_m^0 = \widehat{B} U_{m-1}$ with $\widehat{B} = \mathbb{1} e_s^\top$. This predictor is only preconsistent, i.e., only $\widehat{B}\mathbb{1} = \mathbb{1}$ is satisfied. This predictor was proposed and used in [3,4]. However, due to the low order it requires at least $kmax = 2$, cf. Theorem 4.2.7. Therefore, we will use the following predictors requiring only $kmax = 1$. This allows a better comparison with linearly-implicit one-step and two-step W-methods.
- `pr2`: Here is $U_m^0 = \widehat{B} U_{m-1}$ with $\widehat{B} = V_0 V_1^{-1}$. This predictor is of order $q = s - 1$.
- `pr3`: Here is $\widehat{B} = (V_0 + y e_s^\top) V_1^{-1}$ and the predictor is of order $q = s - 2$ for any vector $y \neq 0$.

In the following, we give the construction principle of an AMF peer method with three stages and order $p = 3$. The construction is done for constant step sizes and we use `fmincon` from the optimization toolbox in MATLAB. We want to have good stability properties for $kmax = 1$ and we restrict to the case $d = 2$ in our numerical search. We choose the matrix B from the three-stage peer method in [58] giving optimal zero-stability. The nodes c_1 and c_2 with $c_3 = 1$ and the matrix G are constructed to give good stability by random walk. We choose randomly c and G and compute for these values A by Theorem 4.1.5 and predictor `pr2` guaranteeing order three with $kmax = 1$. Then, we consider the eigenvalues ξ of M_1 in (4.2.48) and compute for 40000 values of ξ running on the unit circle and for 100 equidistant points of z_1 in the real interval $[-1.e2, 0]$ the corresponding values z_2 and maximize with `fmincon` the angle α of the stability region with respect to z_2. Then, we slightly change the values of c and G randomly and accept the new values if the new angle α is larger. This was repeated 300 times. We finally found $\alpha \approx 36.8°$ for the method `Peer-3p` with predictor `pr2`.

`Peer-3p`:

$$
\begin{aligned}
c_1 &= -2.9533730202668934e{-}1, & c_2 &= 2.7898868351443451e{-}1, & c_3 &= 1.0000000000000000e{+}0,\\
b_{11} &= -8.1662611177702749e{-}1, & b_{12} &= 2.1923402764359148e{+}0, & b_{13} &= -3.7571416465888730e{-}1,\\
b_{21} &= -1.4739080635641988e{+}0, & b_{22} &= 3.4081212175550637e{+}0, & b_{23} &= -9.3421315399086491e{-}1,\\
b_{31} &= -2.2474449407963197e{+}0, & b_{32} &= 4.8389400465743577e{+}0, & b_{33} &= -1.5914951057780380e{+}0,\\
a_{11} &= -2.4958402814848576e{-}1, & a_{12} &= 1.4307145156245002e{-}1, & a_{13} &= 1.2660865099422125e{-}1,\\
a_{21} &= -4.1629649858929907e{-}1, & a_{22} &= -4.4656675421532926e{-}2, & a_{23} &= 2.6881930573707602e{-}1,\\
a_{31} &= -4.7607537878988360e{-}1, & a_{32} &= -5.1640334329837667e{-}1, & a_{33} &= 3.1945638945391092e{-}1,\\
g_{21} &= 8.1174591503861149e{-}1, & g_{31} &= 1.1122866874167001e{+}0, & g_{32} &= 9.3100440445960064e{-}1,\\
\gamma &= 2.0746250806871228e{-}1.
\end{aligned}
$$

For this method, we tried to find a vector y in predictor `pr3` giving better stability. We again consider the values for z_1 and ξ above. Changing y randomly we arrived at $\alpha \approx 58.9°$ for predictor `pr3` with

$$
y_1 = -5.5681213479506908e{-}1, \quad y_2 = -1.3706134560744183e{+}0, \quad y_3 = -3.0942441202856021e{+}0.
$$

Again, `Peer-3p` with predictor `pr3` and $kmax = 1$ is of order three. We also tried to take into account the error constant of predictor `pr3`. Unfortunately, with this approach one can find vectors y and predictors `pr3` with smaller error constants, but the angle α decreases. Therefore, we choose the vector y giving the largest angle α with respect to our procedure.

With Theorem 4.2.15, the stability at infinity of an AMF peer method is characterized by the eigenvalues of $\widehat{B}$. For predictor `pr1`, one has $\xi_1 = 1,\ \xi_2 = \cdots = \xi_s = 0$ whereas for predictor `pr2`, since $\widehat{B} = V_0 V_1^{-1} = V_0 P V_0^{-1}$, we have that $\xi_i = 1,\ i = 1, \ldots, s$. For `pr3` used in the tests with the three-stage method `Peer-3p`, we have $\xi_1 = \xi_2 = 1$, $\xi_3 \approx 0.248$.

In Figures 4.2.1 and 4.2.2, we show the stability regions for peer method `Peer-3p` with `pr2` and `pr3` when $d = 2$ and $kmax = 1$ for $z_1 = z_2 \in \mathbb{C}^-$. Note that for increasing $|z_1|$, the angle α decreases. However, for many practically relevant values of z_1 the stability region is sufficiently large and in both cases, stability is observed at least for all $z_1 = z_2 \in \mathbb{R}^-$.

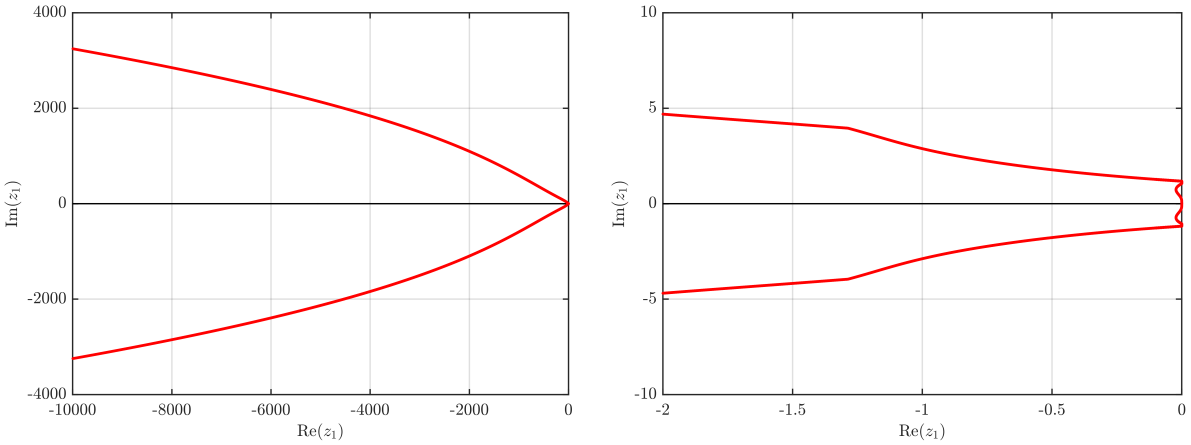

Figure 4.2.1: Stability region $\varrho(M_1(z_1, z_2)) < 1$ of peer method `Peer-3p` with `pr2` when $d = 2$ and $kmax = 1$ for $z_1 = z_2 \in \mathbb{C}^-$ (*left*) and zoomed at the origin (*right*).

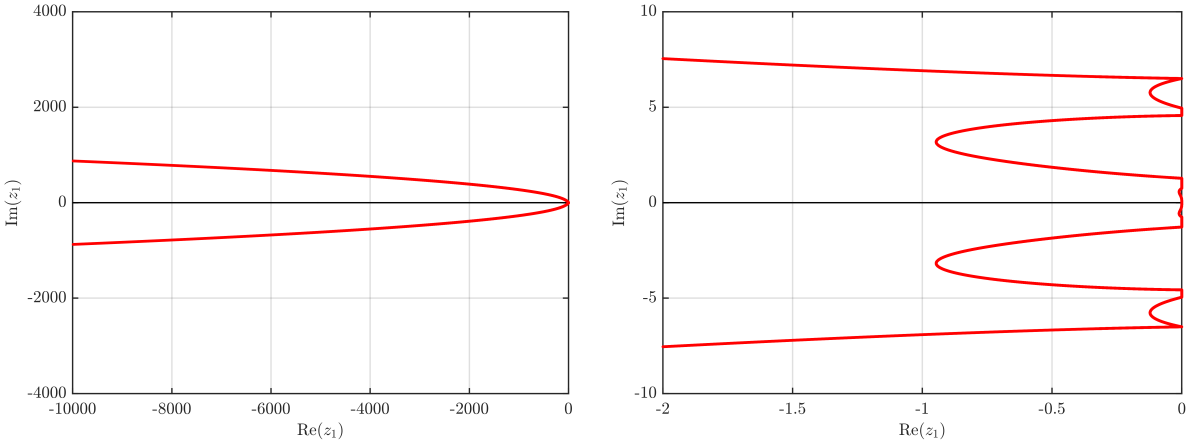

Figure 4.2.2: Stability region $\varrho(M_1(z_1, z_2)) < 1$ of peer method `Peer-3p` with `pr3` when $d = 2$ and $kmax = 1$ for $z_1 = z_2 \in \mathbb{C}^-$ (*left*) and zoomed at the origin (*right*).

4.3 IMEX peer methods with approximate matrix factorization

In this section, we focus on systems of ordinary differential equations with stiff and non-stiff parts in the form

$$y'(t) = f(t, y(t)) + g(t, y(t)), \quad y(t_0) = y_0 \in \mathbb{R}^n, \quad t \in [t_0, t_e]\,, \tag{4.3.49}$$

where $f\colon \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n$ represents the stiff part and $g\colon \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n$ the non-stiff part. The stiff part is treated with an implicit method and the non-stiff part with an explicit method. With this strategy, advantages of implicit and explicit methods are combined instead of using a single explicit or implicit method. Hence, the non-stiff part is solved with an explicit method due to their lower costs and the stiff part is treated with an implicit method due to their better stability properties. This means that in contrast to explicit methods, which require small step sizes for stiff problems, step sizes for implicit methods are not restricted by stability. With this approach, one obtains so-called implicit-explicit (IMEX) methods which are investigated frequently in the literature. IMEX Runge–Kutta methods [1, 6, 20] require additional coupling conditions between the explicit and implicit part. Due to this, the construction of methods of high order is difficult. In IMEX schemes based on general linear methods (GLMs), this drawback can be avoided because of the high stage order. Hence, peer methods are well suited and their construction is rather simple.

IMEX peer methods for systems (4.3.49) are recently introduced and investigated by Soleimani *et al.* [58, 60] via partitioned peer methods and by Lang *et al.* [42] via an extrapolation ansatz. An s-stage IMEX peer method for the solution of an initial value problem (4.3.49) is given by

$$\begin{aligned} U_{m,i} = &\sum_{j=1}^{s} b_{ij} U_{m-1,j} + h_m \sum_{j=1}^{s} a_{ij} f(t_{m-1,j}, U_{m-1,j}) + h_m \sum_{j=1}^{i} g_{ij} f(t_{m,j}, U_{m,j}) \\ &+ h_m \sum_{j=1}^{s} \widetilde{a}_{ij} g(t_{m-1,j}, U_{m-1,j}) + h_m \sum_{j=1}^{i-1} \widetilde{g}_{ij} g(t_{m,j}, U_{m,j}), \quad i = 1, \dots, s. \end{aligned} \tag{4.3.50}$$

Here B, A, $\widetilde{A}$, G and $\widetilde{G}$ are the parameters of the method where G is a lower triangular matrix with $g_{ii} = \gamma > 0$ and $\widetilde{G}$ is a strictly lower triangular matrix. The stage values $U_{m,i},\ i = 1, \dots, s$, are approximations to the exact solution $y(t_{m,i})$ where $t_{m,i} = t_m + c_i h_m$. Again, the nodes c are assumed to be pairwise distinct and constant with $c_s = 1$. In general, the coefficients of an IMEX peer method depend on the step size ratio σ. In the following, we summarize some results from [58, 60]. Again, order conditions can be derived by substituting the exact solution into the method and making a Taylor series

expansion of the residuals, cf. Section 4.1. With

$$\mathbb{AB}_i(l) := c_i^l - \sum_{j=1}^{s} b_{ij}\frac{(c_j-1)^l}{\sigma^l} - l\sum_{j=1}^{s} a_{ij}\frac{(c_j-1)^{l-1}}{\sigma^{l-1}} - l\sum_{j=1}^{i} g_{ij}c_j^{l-1},$$

$$\widetilde{\mathbb{AB}}_i(l) := c_i^l - \sum_{j=1}^{s} b_{ij}\frac{(c_j-1)^l}{\sigma^l} - l\sum_{j=1}^{s} \widetilde{a}_{ij}\frac{(c_j-1)^{l-1}}{\sigma^{l-1}} - l\sum_{j=1}^{i-1} \widetilde{g}_{ij}c_j^{l-1},$$

the following theorem can be stated.

Theorem 4.3.1 ([58]). *An IMEX peer method* (4.3.50) *is consistent of order p if and only if*

$$\mathbb{AB}_i(l) = \widetilde{\mathbb{AB}}_i(l) = 0, \quad \textit{for all } i = 1,\dots,s \textit{ and } l = 0,\dots,p. \qquad \square$$

With the notations (2.2.9), the following corollary can be shown.

Corollary 4.3.2 ([58]). *An IMEX peer method* (4.3.50) *is consistent of order $p = s$ if $B\mathbb{1} = \mathbb{1}$ and*

$$A = (CV_0 - GV_0D)D^{-1}SV_1^{-1} - \frac{1}{\sigma}B(C-I)V_1D^{-1}V_1^{-1}, \tag{4.3.51}$$

$$\widetilde{A} = (CV_0 - \widetilde{G}V_0D)D^{-1}SV_1^{-1} - \frac{1}{\sigma}B(C-I)V_1D^{-1}V_1^{-1} \tag{4.3.52}$$

hold. $\square$

Note that for pairwise distinct nodes c, the coefficient matrices A and $\widetilde{A}$ are uniquely defined by (4.3.51) and (4.3.52). The previous corollary means that the computation of A and $\widetilde{A}$ by (4.3.51) and (4.3.52) leads to IMEX peer methods of order of consistency $p = s$ for arbitrary coefficient matrices G, $\widetilde{G}$ and B satisfying the preconsistency $B\mathbb{1} = \mathbb{1}$. We will consider the constant matrix B, which has the property of zero-stability if the eigenvalues ξ_i of B have modulus less or equal to one and all other eigenvalues of modulus one are simple, cf. Definition 4.1.3. If $\xi_1 = 1$ and $\xi_i = 0$ for all $i = 2,\dots,s$, then the method is called optimally zero-stable. We give the following convergence result for IMEX peer methods.

Theorem 4.3.3 ([58]). *Let B, G and $\widetilde{G}$ in the IMEX peer method* (4.3.50) *be constant matrices. Let $B\mathbb{1} = \mathbb{1}$ and let A and $\widetilde{A}$ be given by* (4.3.51) *and* (4.3.52). *Let the IMEX peer method* (4.3.50) *be zero-stable. Let $h_{max} := \max\limits_m h_m$, $\max\limits_m \sigma_m \le \sigma_{max}$ and let $\varepsilon_0 = \mathcal{O}(h_0^s)$ hold for the starting values, then the IMEX peer method* (4.3.50) *is convergent of order $p = s$, i.e., $\varepsilon_m = \mathcal{O}(h_{max}^s)$, $h_{max} \to 0$.* $\square$

For stability, the scalar test equation with a stiff and non-stiff part

$$y'(t) = \lambda y(t) + \beta y(t) \tag{4.3.53}$$

is common for problems with stiff and non-stiff parts, cf. e.g. [58, 74, 76]. Here λ and β represent the eigenvalues of the Jacobian of the stiff and non-stiff part, respectively. The application of an IMEX peer method (4.3.50) with constant step size $h_m = h$ to the test equation (4.3.53) leads to a numerical recursion in the form

$$U_m = M(z,\widetilde{z})U_{m-1}, \quad M(z,\widetilde{z}) = (I - zG - \widetilde{z}\widetilde{G})^{-1}(B + zA + \widetilde{z}\widetilde{A}), \tag{4.3.54}$$

where $z := \lambda h$ and $\widetilde{z} := \beta h$ and $M(z,\widetilde{z})$ denotes the stability matrix. Note that $M(0,0) = B$. For $\widetilde{z} = 0$ and $z = 0$, we obtain the stability matrices of the implicit and explicit peer method, respectively. For an A-stable implicit peer method, we define the stability region of an IMEX peer method (4.3.50) by

$$\mathcal{S} := \left\{\widetilde{z} \in \mathbb{C}\colon \varrho(M(z,\widetilde{z})) \leq 1 \text{ for all } z \in \mathbb{C}^-\right\}. \tag{4.3.55}$$

If the implicit peer method of an IMEX peer method is only A(α)-stable, then the stability region $\mathcal{S}_\alpha$, cf. e.g. [13, 42]

$$\mathcal{S}_\alpha := \left\{\widetilde{z} \in \mathbb{C}\colon \varrho(M(z,\widetilde{z})) \leq 1 \text{ for all } z \in \mathbb{C}^- \text{ with } |\mathrm{Im}(z)| \leq \tan(\alpha)\,|\mathrm{Re}(z)|\right\} \tag{4.3.56}$$

is considered.

Remark 4.3.4. *In [58], stability investigations of IMEX peer methods with respect to a special test equation from weather prediction are discussed. This test equation is based on special properties of the acoustics equations, see e.g. [73]. IMEX peer methods of order three and order four are constructed which perform well for fast-wave–slow-wave problems [58].* □

Remark 4.3.5. *Superconvergence for IMEX peer methods has been investigated in several papers. In [55, 60], superconvergence for constant step sizes is discussed. Furthermore, superconvergent IMEX peer methods for variable step sizes are constructed recently in [56]. In this thesis, superconvergence of peer methods is not considered. This could be a topic of future work.* □

In the following, the stiff part is treated with an AMF peer method in the IMEX method. This adaptation allows the application of IMEX peer methods to problems of large dimension.

4.3.1 AMF IMEX peer methods

In this section, we consider non-autonomous systems of ordinary differential equations with a non-stiff part and a splitting of the stiff part into d terms in the form

$$\begin{aligned} y'(t) &= g(t,y(t)) + f(t,y(t)) = g(t,y(t)) + \sum_{j=1}^{d} f_j(t,y(t)), \quad t \in [t_0,t_e], \\ y(t_0) &= y_0 \in \mathbb{R}^n, \end{aligned} \tag{4.3.57}$$

where g represents the non-stiff part and f the stiff part. The idea is to combine the advantages of an AMF approach and an IMEX method. This allows for us to solve PDE problems which lead to high dimensional ODE systems with a non-stiff and stiff part. We again consider a corresponding splitting of the Jacobian for problems (4.3.57)

$$J_m = J_{m,0} + \sum_{j=1}^{d} J_{m,j}, \quad J_{m,j} = \partial_y f_j(t_{m-1,s}, U_{m-1,s}),$$

cf. Section 3.1. Here the matrix $J_{m,0}$ stands for the term of the Jacobian corresponding to the non-stiff part. In this section, an inexact AMF approach, i.e., $J_{m,0} \neq 0$, is considered. In this case, the AMF matrix

$$\Pi_d = \prod_{j=1}^{d} (I - h_m \gamma J_{m,j}) =: (I - h_m \gamma \widetilde{J}_m)$$

satisfies $\widetilde{J}_m = J_m - J_{m,0} + \mathcal{O}(h_m)$ and

$$(I - h_m \gamma \widetilde{J}_m) = (I - h_m \gamma J_m) + \mathcal{O}(h_m).$$

The computation of stage values $U_{m,i},\ i = 1, \ldots, s$, again requires the solution of systems of non-linear equations. The application of the simplified Newton's method leads to a recursion for AMF IMEX peer methods in the form

$$\begin{aligned} \Pi_d \Delta U_{m,i}^k &= \widetilde{w}_i - U_{m,i}^k + h_m \gamma f(t_{m,i}, U_{m,i}^k), \\ U_{m,i}^{k+1} &= U_{m,i}^k + \Delta U_{m,i}^k, \quad k = 0, 1, \ldots, kmax - 1, \\ U_{m,i} &= U_{m,i}^{kmax}, \quad i = 1, \ldots, s, \end{aligned} \tag{4.3.58}$$

with

$$\begin{aligned} \widetilde{w}_i := &\sum_{j=1}^{s} b_{ij} U_{m-1,j} + h_m \sum_{j=1}^{s} a_{ij} f(t_{m-1,j}, U_{m-1,j}) + h_m \sum_{j=1}^{i-1} g_{ij} f(t_{m,j}, U_{m,j}) \\ &+ h_m \sum_{j=1}^{s} \widetilde{a}_{ij} g(t_{m-1,j}, U_{m-1,j}) + h_m \sum_{j=1}^{i-1} \widetilde{g}_{ij} g(t_{m,j}, U_{m,j}), \\ i = 1, \ldots, s. & \end{aligned}$$

Again, $\widetilde{w}_i$ collects known stage and function values. The AMF matrix Π_d is given by (4.2.10) for a d-term-splitting $d \geq 2$ and $kmax$ denotes the maximal number of Newton steps.

For stability investigations of AMF IMEX peer methods, we combine the scalar test equation (4.3.53) with a stiff and non-stiff part with the linear test equation (4.2.35) for

splitting problems, i.e., we have

$$y'(t) = \sum_{j=1}^{d} \lambda_j y(t) + \beta y(t), \quad \mathrm{Re}(\lambda_j) \le 0, \quad j = 1, \ldots, s, \quad \mathrm{Re}(\beta) \le 0. \tag{4.3.59}$$

The application of an AMF IMEX peer method (4.3.58) with constant step sizes $h_m = h$ to the Equation (4.3.59) leads with the notations (3.2.20) to a numerical recursion in the form

$$U_m = \widetilde{M}_{kmax} U_{m-1}, \quad \widetilde{M}_{kmax} := \widetilde{M}_{kmax}\left(z_1, \ldots, z_d, \widetilde{z}\right), \tag{4.3.60}$$

where the stability matrix $\widetilde{M}_{kmax}$ is implicitly defined by

$$\begin{aligned} \Pi_d \left(U_m^{k+1} - U_m^k\right) = \left(B + zA + \widetilde{z}\widetilde{A}\right) U_{m-1} + \left(zG_0 + \widetilde{z}\widetilde{G}\right) U_m - (1 - \gamma z)\, U_m^k, \\ k = 0, \ldots, kmax, \end{aligned} \tag{4.3.61}$$

with $U_m := U_m^{kmax}$, predictor $U_m^0 = \widehat{B} U_{m-1}$, strictly lower triangular matrix $G_0 := G - \gamma I$ and AMF factor Π_d given by (3.2.22). For the simplest case $kmax = 1$, i.e., solving for $\widetilde{M}_1$ in (4.3.60) and (4.3.61) gives

$$\widetilde{M}_1 = \left(\Pi_d I - zG_0 - \widetilde{z}\widetilde{G}\right)^{-1} \left(B + zA + \widetilde{z}\widetilde{A} + (\Pi_d - 1 + \gamma z)\, \widehat{B}\right). \tag{4.3.62}$$

Note that for $\widetilde{A} = \widetilde{G} = 0$, we have the stability matrix (4.2.48) for AMF peer methods with $kmax = 1$. Analogously to Theorem 4.2.15, we show that stability at infinity of an AMF IMEX peer method is characterized by the eigenvalues of $\widehat{B}$.

Theorem 4.3.6. *Let $\widetilde{M}_{kmax}\left(z_1, \ldots, z_d, \widetilde{z}\right)$ be the stability matrix defined by* (4.3.60) *and* (4.3.61) *for an AMF IMEX peer method* (4.3.58) *with $kmax \ge 1$, an AMF-splitting $d \ge 2$ and a predictor $U_m^0 = \widehat{B} U_{m-1}$. If $z_i, z_j \to \infty$, for at least two indices $1 \le i < j \le d$, then $\widetilde{M}_{kmax}$ tends to $\widehat{B}$.*

Proof. From (4.3.61), we have that

$$U_m^k = \widetilde{M}^{(k)} U_{m-1}, \quad k = 0, \ldots, kmax,$$

for $\widetilde{M}^{(k)} = \widetilde{M}^{(k)}\left(z_1, \ldots, z_d, \widetilde{z}\right)$, with $\widetilde{M}^{(0)} = \widehat{B}$ and $\widetilde{M}^{(kmax)} = \widetilde{M}_{kmax}$. These matrices fulfil the recursion

$$\begin{aligned} &\Pi_d \left(\widetilde{M}^{(k+1)} - \widetilde{M}^{(k)}\right) = B + zA + \widetilde{z}\widetilde{A} + \left(zG_0 + \widetilde{z}\widetilde{G}\right) \widetilde{M}_{kmax} - (1 - \gamma z)\, \widetilde{M}^{(k)}, \\ &k = 0, \ldots, kmax - 1, \end{aligned}$$

that is,

$$\Pi_d \widetilde{M}^{(k+1)} = \mathcal{A} + \beta \left(\Pi_d \widetilde{M}^{(k)}\right), \quad k = 0, \ldots, kmax - 1,$$

where $\mathcal{A} := B + zA + \widetilde{z}\widetilde{A} + \left(zG_0 + \widetilde{z}\widetilde{G}\right)\widetilde{M}_{kmax}$ and $\beta := (\Pi_d - 1 + \gamma z)/\Pi_d$ is a scalar. Observe that $\lim\limits_{\substack{z_i, z_j \to \infty \\ i \neq j}} \dfrac{z}{\Pi_d} = 0$ and therefore $\beta \to 1$ if $z_i, z_j \to \infty$. Furthermore, we have $\lim\limits_{\substack{z_i, z_j \to \infty \\ i \neq j}} \dfrac{\widetilde{z}}{\Pi_d} = 0$ for all $\widetilde{z} \in \mathbb{C}$. From the latter recursion, we explicitly get

$$\Pi_d \widetilde{M}_{kmax} = \left(\sum_{k=0}^{kmax-1} \beta^k \right) \mathcal{A} + \beta^{kmax} \Pi_d \widetilde{M}^{(0)},$$

i.e., we obtain with definition of $\mathcal{A}$, $\widetilde{M}^{(0)} = \widehat{B}$ and dividing by Π_d

$$\left(I - \left(\frac{z}{\Pi_d} G_0 + \frac{\widetilde{z}}{\Pi_d} \widetilde{G} \right) \sum_{k=0}^{kmax-1} \beta^k \right) \widetilde{M}_{kmax} = \left(\frac{1}{\Pi_d} B + \frac{z}{\Pi_d} A + \frac{\widetilde{z}}{\Pi_d} \widetilde{A} \right) \sum_{k=0}^{kmax-1} \beta^k + \beta^{kmax} \widehat{B}.$$

Now, the result follows with $z/\Pi_d \to 0$, $\widetilde{z}/\Pi_d \to 0$ for all $\widetilde{z} \in \mathbb{C}$ and $\beta \to 1$ taking $z_i, z_j \to \infty$. ■

In the following, we describe the construction of an AMF IMEX peer method of order three. We choose the implicit peer method `Peer-3p`, cf. Section 4.2.4, and try to find an associated explicit part. In detail, this means that the coefficients B, A, G, γ and the nodes c are given by method `Peer-3p` and $\widetilde{A}$ is computed by (4.3.52) for arbitrary coefficients $\widetilde{G}$, i.e., we have only the matrix $\widetilde{G}$ as free parameter. The construction is done for constant step sizes und we use `fminsearch` from the optimization toolbox in MATLAB. The matrix $\widetilde{G}$ is constructed to give good stability of the AMF IMEX peer method by random walk. Now, we describe the computation of the stability region $\mathcal{S}_\alpha$ of an AMF IMEX peer method. This approach was also applied for IMEX peer methods [42, 58] and IMEX general linear methods [13]. The stability region $\mathcal{S}_\alpha$ can be obtained for a given $\alpha \in \left[0, \frac{\pi}{2}\right)$ by intersection of all sets

$$\left\{ \widetilde{z} \in \mathbb{C} \colon \varrho(\widetilde{M}(z, \widetilde{z})) \leq 1 \text{ for fixed } z = -|y| / \tan(\alpha) + y\mathrm{i} \right\}, \quad \text{for all } y \in \mathbb{R},$$

which follows from the maximum principle. For $y = 0$, the set $\mathcal{S}_\alpha$ is independent of α and corresponds to the stability region of the explicit peer method. With $kmax = 1$, $d = 2$ and the choice $z_1 = z_2$, i.e., $z = 2z_1$, we obtain the stability matrix (4.3.62) of an AMF IMEX peer method in the form

$$\widetilde{M}_1(z_1, \widetilde{z}) = \left((1 - \gamma z_1)^2 - 2z_1 G_0 - \widetilde{z}\widetilde{G} \right)^{-1} \left(B + 2z_1 A + \widetilde{z}\widetilde{A} + \gamma^2 z_1^2 \widehat{B} \right).$$

We compute the boundary of the stability region $\mathcal{S}_\alpha$ by varying the eigenvalues $\xi = \mathrm{e}^{\mathrm{i}\varphi}$, $\varphi \in [0, 2\pi)$ on the unit circle for the eigenvalue problem $\widetilde{M}_1(z_1, \widetilde{z})\, x = \xi x$. This can be formulated as generalized eigenvalue problem for each $\widetilde{z}$ in the form

$$\left(B + 2z_1 A + \gamma^2 z_1^2 \widehat{B} + 2\xi z_1 G_0 - \xi (1 - \gamma z_1)^2 I \right) x = \widetilde{z} \left(-\widetilde{A} - \xi \widetilde{G} \right) x.$$

The set of eigenvalues $\widetilde{z}$ contains the boundary of the stability domain. We use different objective functions to obtain sufficiently large stability regions of the AMF IMEX peer methods, i.e., we take (i) the absolute value of the left boundary of the stability interval on the real axis, (ii) the absolute value of the stability interval on the imaginary axis, and (iii) the absolute value of the stability interval along the angle bisector in the complex plane. We choose the peer method `Peer-3p` with predictor `pr3`, i.e., we have A(α)-stability with $\alpha = 58.9°$, for $kmax = 1$ and $d = 2$, cf. Section 4.2.4. We used $\alpha = 55°$ and 500 discrete values $y \in [-5, 5]$ with $z_1 = -|y| / \tan(\alpha) + y\mathrm{i}$ and we take 2000 values for ξ on the unit circle. This was repeated for about 300 randomly chosen starting values for `fminsearch`. We have found the following explicit parts of the AMF IMEX peer methods in the cases (i), (ii) and (iii), denoted by `Peer-3p-real`, `Peer-3p-imag` and `Peer-3p-imre`, respectively. Note that AMF IMEX peer methods with larger stability regions may be found by a different strategy or by modifying the implicit part.

`Peer-3p-real`:

$$\begin{aligned}
\widetilde{a}_{11} &= -2.8464256019905126e{-}1, \widetilde{a}_{12} = 2.9103589994879552e{-}1, \widetilde{a}_{13} = 2.2116524272715354e{-}1,\\
\widetilde{a}_{21} &= -3.2906925168091749e{-}1, \widetilde{a}_{22} = -3.0448982937375967e{-}1, \widetilde{a}_{23} = 5.9310660005510829e{-}1,\\
\widetilde{a}_{31} &= -3.2394121976486833e{-}2, \widetilde{a}_{32} = -1.5957050812664859e{+}0, \widetilde{a}_{33} = 8.6933934580264116e{-}1,\\
\widetilde{g}_{21} &= 8.6752703583313661e{-}1, \widetilde{g}_{31} = 1.2477652655854138e{+}0, \widetilde{g}_{32} = 1.0887258591655815e{+}0.
\end{aligned}$$

`Peer-3p-imag`:

$$\begin{aligned}
\widetilde{a}_{11} &= -2.8464256019905126e{-}1, \widetilde{a}_{12} = 2.9103589994879552e{-}1, \widetilde{a}_{13} = 2.2116524272715354e{-}1,\\
\widetilde{a}_{21} &= -2.8462879857291067e{-}1, \widetilde{a}_{22} = -4.9205065253319446e{-}1, \widetilde{a}_{23} = 4.7324596884272573e{-}1,\\
\widetilde{a}_{31} &= -4.2776070728348103e{-}2, \widetilde{a}_{32} = -1.5719333546954230e{+}0, \widetilde{a}_{33} = 7.9378248418413022e{-}1,\\
\widetilde{g}_{21} &= 1.1305080370969471e{+}0, \widetilde{g}_{31} = 1.2715363552221052e{+}0, \widetilde{g}_{32} = 1.1271218533281994e{+}0.
\end{aligned}$$

`Peer-3p-imre`:

$$\begin{aligned}
\widetilde{a}_{11} &= -2.8464256019905126e{-}1, \widetilde{a}_{12} = 2.9103589994879552e{-}1, \widetilde{a}_{13} = 2.2116524272715354e{-}1,\\
\widetilde{a}_{21} &= -2.8077938579895633e{-}1, \widetilde{a}_{22} = -5.0829708968829245e{-}1, \widetilde{a}_{23} = 4.6286369295184270e{-}1,\\
\widetilde{a}_{31} &= -1.2274003705704250e{-}1, \widetilde{a}_{32} = -1.3198789110560626e{+}0, \widetilde{a}_{33} = 5.6808735054686043e{-}1,\\
\widetilde{g}_{21} &= 1.1532873373689738e{+}0, \widetilde{g}_{31} = 1.1614965748131793e{+}0, \widetilde{g}_{32} = 1.2907662900637291e{+}0.
\end{aligned}$$

In Figures 4.3.1–4.3.3, we give the stability regions of the constructed AMF IMEX peer methods (*black*) for $kmax = 1$, $d = 2$ and predictor `pr3` (*right*). For comparison, we also compute the stability regions with predictor `pr2` and $\alpha = 35°$ (*left*) and include the stability regions for the explicit peer methods (*blue circles*).

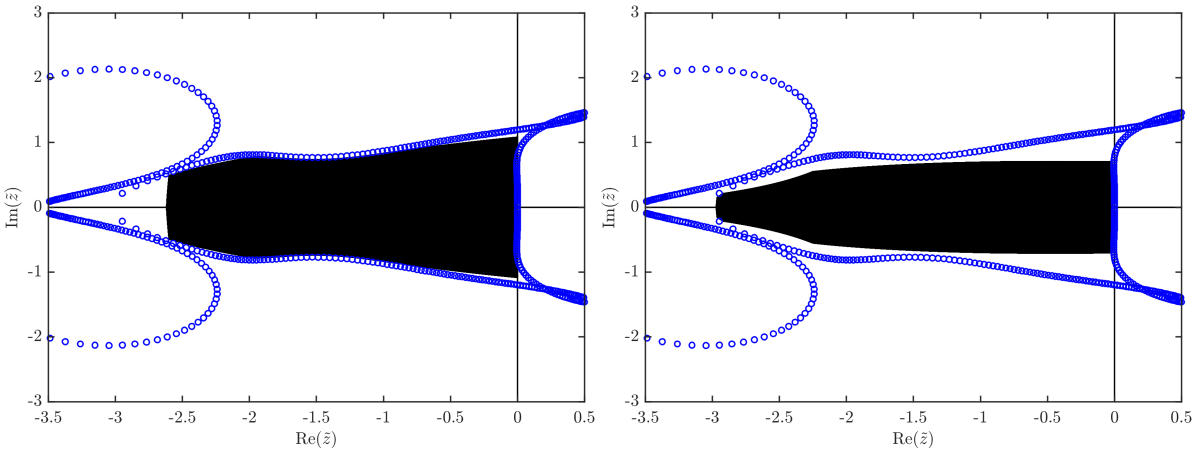

Figure 4.3.1: Stability region $\mathcal{S}_\alpha$ of AMF IMEX peer method `Peer-3p-real` for the test equation (4.3.59) with $kmax = 1$ and $d = 2$ (*black*) with `pr2` and $\alpha = 35°$ (*left*) and with `pr3` and $\alpha = 55°$ (*right*). Stability region of the explicit peer method (*blue circles*). The stability region of the IMEX method is optimized along the real axis.

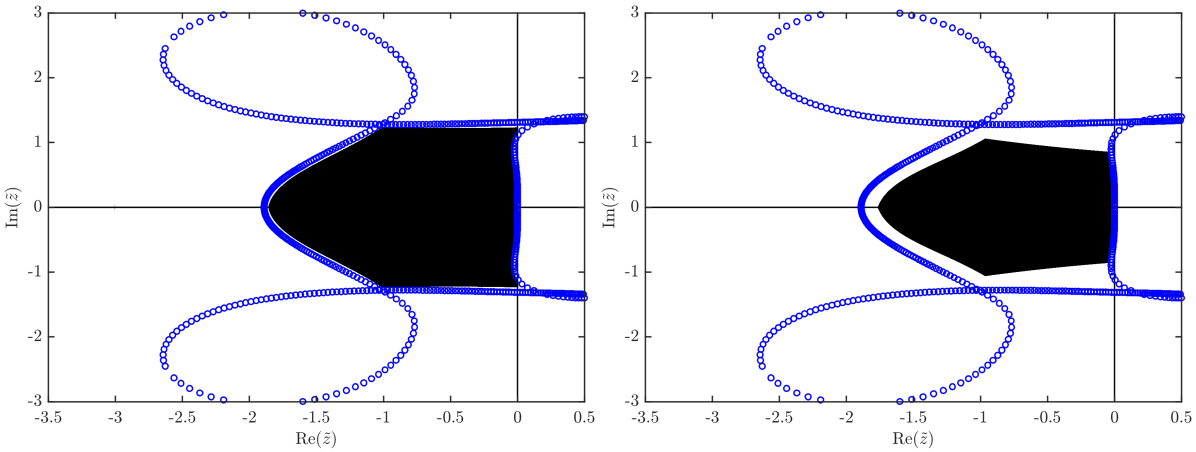

Figure 4.3.2: Stability region $\mathcal{S}_\alpha$ of AMF IMEX peer method `Peer-3p-imag` for the test equation (4.3.59) with $kmax = 1$ and $d = 2$ (*black*) with `pr2` and $\alpha = 35°$ (*left*) and with `pr3` and $\alpha = 55°$ (*right*). Stability region of the explicit peer method (*blue circles*). The stability region of the IMEX method is optimized along the imaginary axis.

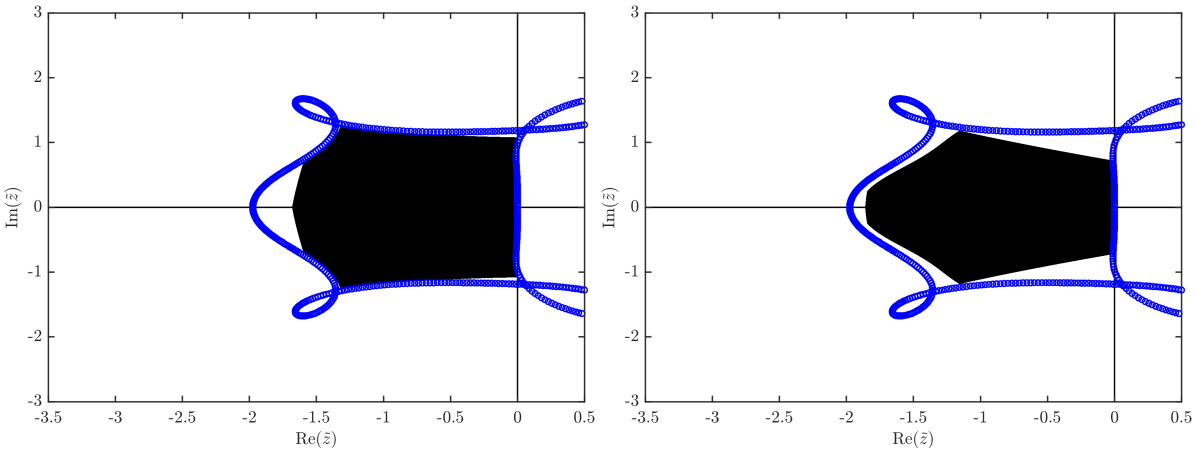

Figure 4.3.3: Stability region $\mathcal{S}_\alpha$ of AMF IMEX peer method `Peer-3p-imre` for the test equation (4.3.59) with $kmax = 1$ and $d = 2$ (*black*) with `pr2` and $\alpha = 35°$ (*left*) and with `pr3` and $\alpha = 55°$ (*right*). Stability region of the explicit peer method (*blue circles*). The stability region of the IMEX method is optimized along the angle bisector in the complex plane.

5 Numerical tests with approximate matrix factorization

In this chapter, we present our numerical experiments with one-step and two-step W-methods and peer methods with application of an approximate matrix factorization (AMF). The methods are tested on the autonomous 2D Brusselator problem, a linear model with homogeneous and time-dependent Dirichlet boundary conditions and a 2D diffusion–convection equation. In our tests with constant time step sizes, we compare the linearly-implicit W-methods with peer methods and illustrate the influence of different predictors in the AMF peer schemes. Furthermore, we consider the diffusion–convection problem with an inexact AMF approach and application of implicit-explicit (IMEX) peer methods.

5.1 Test examples

In this section, we present our test problems which are used in the numerical experiments. The test set consists of the autonomous 2D Brusselator problem, a linear diffusion model and a 2D diffusion–convection equation. For more details, we also refer to the references given below.

5.1.1 Brusselator problem

We consider the two-dimensional Brusselator problem with diffusion [27]

$$\begin{aligned} u_t &= 1 + u^2 v - (B+1)u + \alpha(u_{xx} + u_{yy}) + f(t,x,y), \\ v_t &= -u^2 v + Bu + \alpha(v_{xx} + v_{yy}), \\ \Omega &= [0,1]^2\,, \quad t \in [0,1]\,. \end{aligned} \tag{5.1.1}$$

We consider $\alpha = 0.1,\ B = 3$ and $f(t,x,y) = 0$. Initial conditions are given by

$$u(0,x,y) = 0.5 + y, \quad v(0,x,y) = 2 + 5x$$

and we consider homogeneous Neumann boundary conditions. We choose $m = 128$ and $m = 256$ uniform grid points in each dimension in space. The resulting autonomous

systems of ordinary differential equations (ODEs) are of dimension $n = 2m^2 = 32768$ and $n = 131072$, respectively. A reference solution is computed by `ode15s` from the MATLAB ODE-suite [57] with high accuracy. For an approximate matrix factorization (AMF) approach, the exact Jacobian for this problem is split into

$$J = J_x + J_y + J_r,$$

where J_x and J_y are the Jacobian matrices corresponding to the discretization of the diffusion term with central differences of second order in the x- and y-direction, respectively, and the Jacobian matrix J_r belongs to the reaction part. For a two-term-splitting, i.e., $d = 2$, we proportioned J_r to the Jacobians J_x and J_y of the diffusion part, respectively, i.e., we take $J_1 = J_x + \frac{1}{2}J_r$ and $J_2 = J_y + \frac{1}{2}J_r$. The Brusselator problem has already been considered for AMF peer methods in [3, 4].

5.1.2 Linear diffusion problem

We consider a linear diffusion equation with constant coefficients, e.g. [22, 52]

$$\begin{aligned} u_t &= u_{xx} + u_{yy} + g(t, x, y), \\ \Omega &= [0, 1]^2, \quad t \in [0, 1]. \end{aligned} \tag{5.1.2}$$

The inhomogeneity g is chosen appropriately to yield the exact solution

$$u(t, x, y) = \left(x(1 - x)y(1 - y) + \kappa \left((x + 1/3)^2 + (y + 1/4)^2\right)\right) \exp(t).$$

Initial and Dirichlet boundary conditions are taken from the exact solution. Again, we use central differences of second order for the discretization. Note that there is no space error, because the solution is a quadratic polynomial in x and y. For $\kappa = 0$, we have homogeneous Dirichlet boundary conditions, but for $\kappa = 1$, we obtain non-homogeneous time-dependent Dirichlet boundary conditions. We choose $m = 63$ and $m = 1023$ uniform grid points in each dimension in space, which lead to ODE systems of dimension $n = m^2 = 3969$ and $n = 1046529$, respectively. A reference solution and additional starting values are taken from the exact solution. We consider for AMF a two-term-splitting, where we split the Jacobian matrix in $J = J_x + J_y$. The Jacobian matrices J_x and J_y correspond to the discretization of the diffusion part in each spatial dimension.

5.1.3 Diffusion–convection problem

This problem is given by a diffusion–convection equation in the form, e.g. [70]

$$\begin{aligned} u_t &= \varepsilon(u_{xx} + u_{yy}) - yu_x + xu_y + g(t, x, y), \\ \varepsilon &= 0.1, \quad \Omega = [0, 1]^2, \quad t \in [0, 1]. \end{aligned} \tag{5.1.3}$$

The inhomogeneity g is chosen appropriately according to the exact solution

$$u(t,x,y) = \sin(\pi x)\sin(\pi y)(1 + 4xy\exp(-2\varepsilon\pi^2 t)).$$

Initial and boundary conditions are taken from the exact solution. We choose $m = 69$ and $m = 128$ uniform grid points in each dimension in space, which lead to ODE systems of dimension $n = m^2 = 4761$ and $n = 16384$, respectively. A reference solution is computed by `ode15s` with high accuracy. Again, we consider for this problem a two-term-splitting for AMF and proceed analogously to the Brusselator problem (5.1.1). For exact AMF, the Jacobian matrix of the convection part is added to the Jacobian matrices of the diffusion part, respectively, in such a way that a two-term-splitting $J = J_1 + J_2$ is obtained, with J_1 associated to $\varepsilon u_{xx} - yu_x$ and J_2 corresponding to $\varepsilon u_{yy} + xu_y$. For inexact AMF, the Jacobian matrix of the convection part is disregarded, i.e., we consider a splitting $J = J_1 + J_2$, where J_1 and J_2 correspond to the discretization of the diffusion part in each dimension in space.

5.2 Numerical results

In this section, we summarize the results of the numerical integration of the problems presented in Section 5.1 with the one-step AMF W-methods, two-step AMF W-methods and AMF peer methods described in Chapter 3 and Chapter 4. All numerical experiments are implemented in MATLAB. For the problems (5.1.1) and (5.1.3), the starting values for the two-step W-methods and peer methods are computed by `ode15s` with high accuracy. For the problem (5.1.2), these additional values are taken from the exact solution. For methods with $c_i < 0$, we use an adapted starting process to avoid moving outside the range of the time integration, cf. e.g. [64, p. 176]. We consider fixed step size integrations with $h = 2^{-l}$, $l = 3, \ldots, 12$, for the problem (5.1.1) and $h = 2^{-l}$, $l = 2, \ldots, 10$, for the problems (5.1.2) and (5.1.3), and calculate the global errors in the maximum norm at the endpoint of the time interval. In the pictures below, we show the logarithm of the obtained errors and the considered step sizes h (*left*) and we show the errors versus the number of calls to the linear system solver to respect different stage numbers (*right*).

Figures 5.2.1 and 5.2.2 show the results for the Brusselator problem (5.1.1).

The expected orders can be observed for all problems. For the peer method `Peer-3p`, one Newton step with predictors `pr2` and `pr3` is sufficient, cf. Theorem 4.2.2. The two-step W-method `TSW-3a` gives the most accurate results. Due to its higher order, the results with predictor `pr2` are more accurate than with `pr3`. Among the one-step W-methods, `W3` has problems for larger step sizes, but this method is more accurate than the other W-methods for smaller step sizes.

Results for the linear diffusion problem (5.1.2) are given in Figures 5.2.3–5.2.6.

For homogeneous boundary conditions, all methods perform well with their expected

orders. The accuracy of the two-step W-methods and peer methods is much better than for the one-step W-methods. Again, the results with predictor `pr2` are more accurate than with `pr3`. For time-dependent boundary conditions, all methods have problems for larger step sizes. For smaller step sizes, the two-step W-methods and peer methods are superior. For the one-step W-methods `W2` and `W3`, the order reduction for $m = 1023$ is clearly visible. With respect to the number of linear systems, method `W1` gives very good results for $m = 1023$.

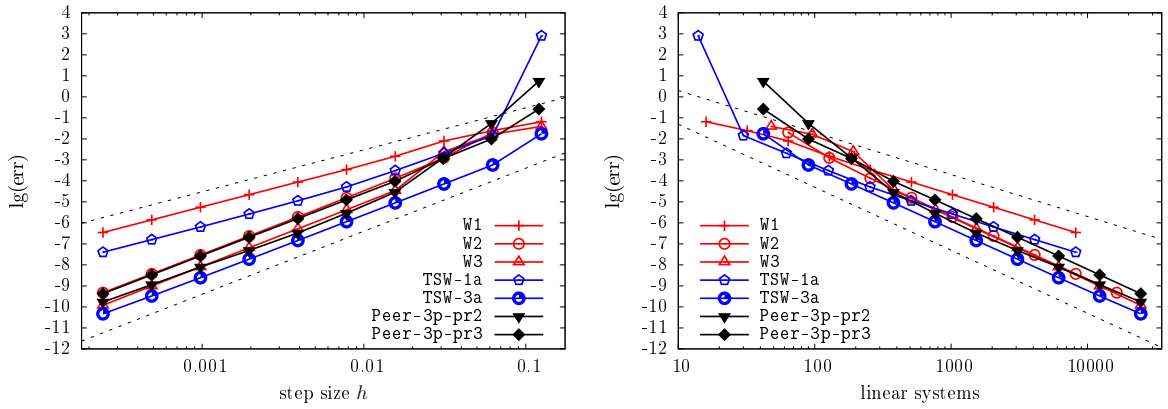

Figure 5.2.1: Results for Brusselator problem (5.1.1) with $m = 128$. For the peer method `Peer-3p`, predictors `pr2` and `pr3` with $kmax = 1$ are used. Lg(err) vs. step size h (*left*) and lg(err) vs. linear systems (*right*). Dashed straight lines with slopes corresponding to orders two and three are added for reference.

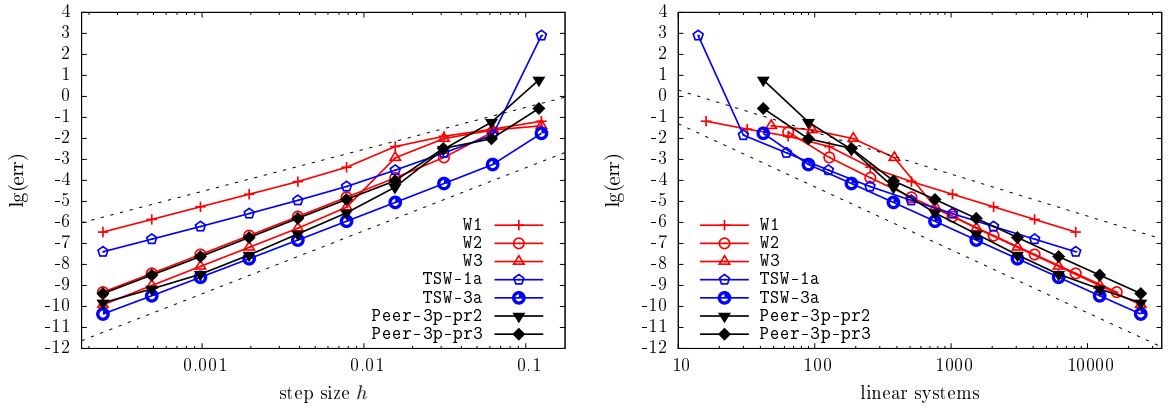

Figure 5.2.2: Results for Brusselator problem (5.1.1) with $m = 256$. For the peer method `Peer-3p`, predictors `pr2` and `pr3` with $kmax = 1$ are used. Lg(err) vs. step size h (*left*) and lg(err) vs. linear systems (*right*). Dashed straight lines with slopes corresponding to orders two and three are added for reference.

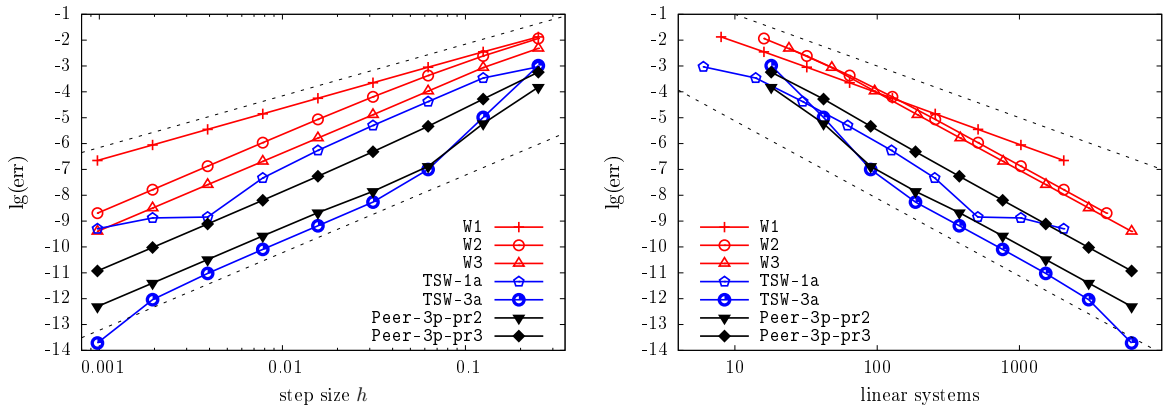

Figure 5.2.3: Results for linear diffusion problem (5.1.2) with homogeneous Dirichlet boundary conditions ($\kappa = 0$) and $m = 63$. For the peer method `Peer-3p`, predictors `pr2` and `pr3` with $kmax = 1$ are used. Lg(err) vs. step size h (*left*) and lg(err) vs. linear systems (*right*). Dashed straight lines with slopes corresponding to orders two and three are added for reference.

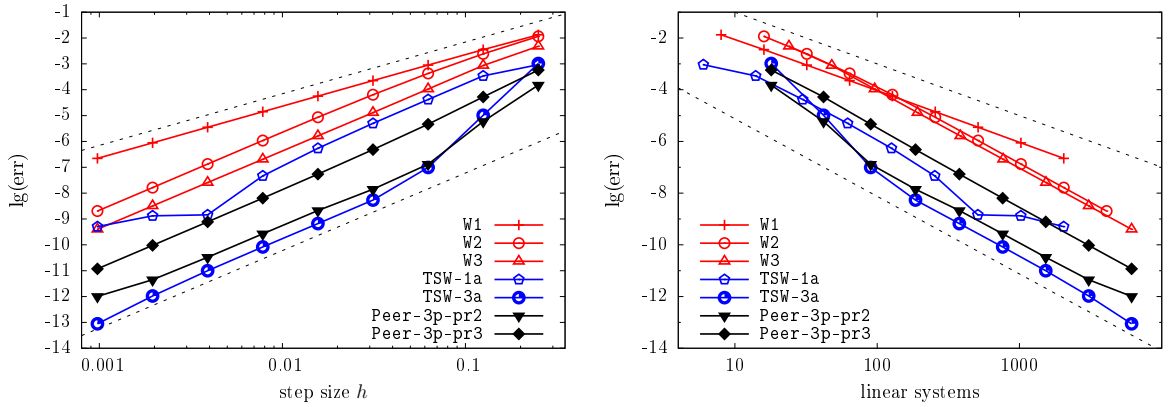

Figure 5.2.4: Results for linear diffusion problem (5.1.2) with homogeneous Dirichlet boundary conditions ($\kappa = 0$) and $m = 1023$. For the peer method `Peer-3p`, predictors `pr2` and `pr3` with $kmax = 1$ are used. Lg(err) vs. step size h (*left*) and lg(err) vs. linear systems (*right*). Dashed straight lines with slopes corresponding to orders two and three are added for reference.

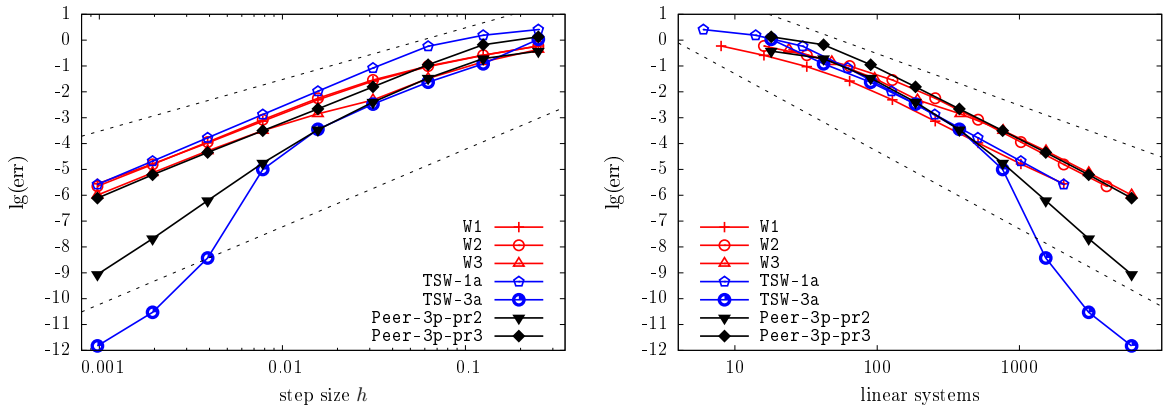

Figure 5.2.5: Results for linear diffusion problem (5.1.2) with time-dependent Dirichlet boundary conditions ($\kappa = 1$) and $m = 63$. For the peer method `Peer-3p`, predictors `pr2` and `pr3` with $kmax = 1$ are used. Lg(err) vs. step size h (*left*) and lg(err) vs. linear systems (*right*). Dashed straight lines with slopes corresponding to orders two and three are added for reference.

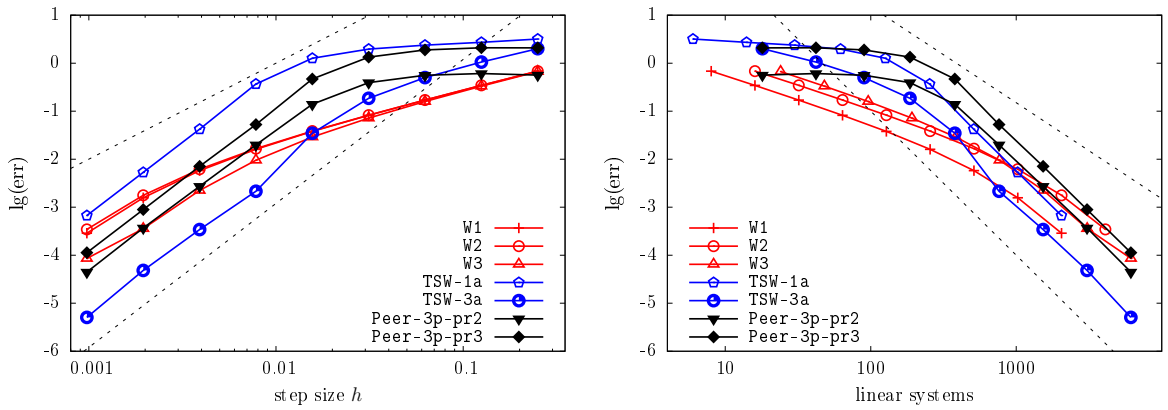

Figure 5.2.6: Results for linear diffusion problem (5.1.2) with time-dependent Dirichlet boundary conditions ($\kappa = 1$) and $m = 1023$. For the peer method `Peer-3p`, predictors `pr2` and `pr3` with $kmax = 1$ are used. Lg(err) vs. step size h (*left*) and lg(err) vs. linear systems (*right*). Dashed straight lines with slopes corresponding to orders two and three are added for reference.

Results for the diffusion–convection problem (5.1.3) are given in Figures 5.2.7–5.2.9.

For the peer methods, the influence of the predictor on the stability can be clearly seen in Figures 5.2.7 and 5.2.8. Whereas for the Brusselator and for the diffusion problem for `Peer-3p` with `pr2` one Newton step is sufficient, for the diffusion–convection problem, predictor `pr2` requires four steps for $m = 69$ and $m = 128$ to have stability. This can be explained by Figure 4.2.1. The advantage of predictor `pr3` with respect to stability is obvious. One Newton step, which is sufficient for order three, is also sufficient for stability. The two-step W-methods perform well. The one-step AMF W-methods have no stability problems. In Figure 5.2.9, the influence of the incorporation of the time derivative $\partial_t f$ in one-step AMF W-methods is demonstrated. As expected, the order drops down if the time derivative $\partial_t f$ is not computed.

Of all the problems, the two-step W-method `TSW-3a` performs best. The accuracy is clearly superior and there are, in general, no stability problems. The one-step W-methods have advantages only for large step sizes for the linear diffusion problem with $\kappa = 1$. In our tests among, the one-step W-methods `W3` is the best. The peer method `Peer-3p` with predictor `pr3` has no stability problems with $kmax = 1$. However, if stability with predictor `pr2` is sufficient, then `pr2` with $kmax = 1$ gives more accurate results.

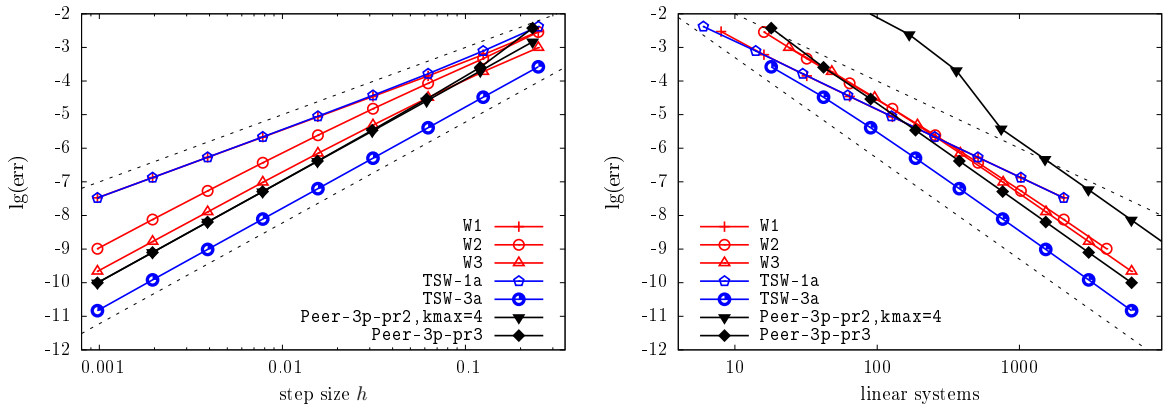

Figure 5.2.7: Results for diffusion–convection problem (5.1.3) with $m = 69$. For the peer method `Peer-3p`, predictor `pr2` with $kmax = 4$ and predictor `pr3` with $kmax = 1$ are used. Lg(err) vs. step size h (*left*) and lg(err) vs. linear systems (*right*). Dashed straight lines with slopes corresponding to orders two and three are added for reference.

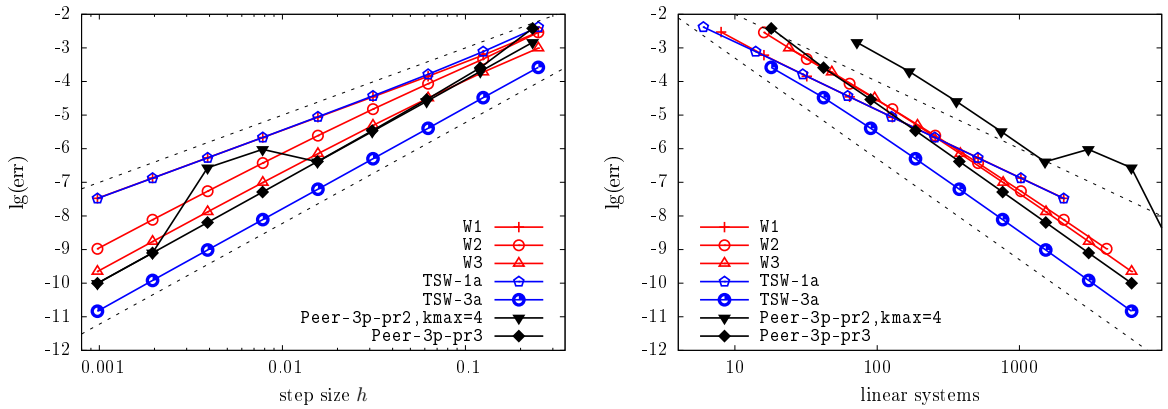

Figure 5.2.8: Results for diffusion–convection problem (5.1.3) with $m = 128$. For the peer method `Peer-3p`, predictor `pr2` with $kmax = 4$ and predictor `pr3` with $kmax = 1$ are used. Lg(err) vs. step size h (*left*) and lg(err) vs. linear systems (*right*). Dashed straight lines with slopes corresponding to orders two and three are added for reference.

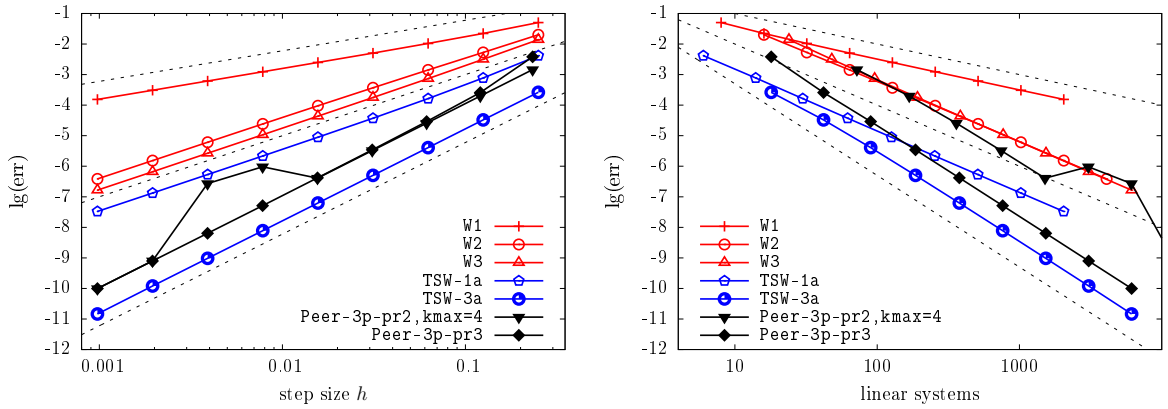

Figure 5.2.9: Results for diffusion–convection problem (5.1.3) with $m = 128$. For the peer method `Peer-3p`, predictor `pr2` with $kmax = 4$ and predictor `pr3` with $kmax = 1$ are used. The time derivative $\partial_t f$ is not used in the one-step AMF W-methods. Lg(err) vs. step size h (*left*) and lg(err) vs. linear systems (*right*). Dashed straight lines with slopes corresponding to orders one, two and three are added for reference.

5.3 Numerical tests with inexact AMF and IMEX peer methods

In this section, we present the numerical experiments with an inexact AMF approach, i.e., some parts of the Jacobian are not considered in the AMF approach with fully implicit peer methods. For comparison, we include the numerical results of the one-step W-methods `W1`, `W2` and `W3` and two-step W-methods `TSW1a` and `TSW3a` as presented above. We consider the diffusion–convection problem (5.1.3) and fixed time step sizes $h = 2^{-l}$, $l = 2\ldots,10$. For inexact AMF, the Jacobian of the convection part is disregarded, cf. Section 5.1.3.

Again, we compute the global errors in the maximum norm at the endpoint of the time interval. In Figure 5.3.1, we show the obtained errors versus the considered step sizes h (*left*) and the error versus the number of calls of the linear system solver (*right*). The influence of an inexact AMF approach can be clearly seen. For the peer method `Peer-3p` and predictor `pr2`, it again requires at least four Newton steps to have stability. In contrast to the exact AMF approach, we observe after one Newton step with predictor `pr3` only order two. With predictor `pr3`, at least two Newton steps are necessary for order three, cf. Theorem 4.2.4. Note that the achieved accuracy is not satisfactory in comparison with the one-step and two-step W-methods.

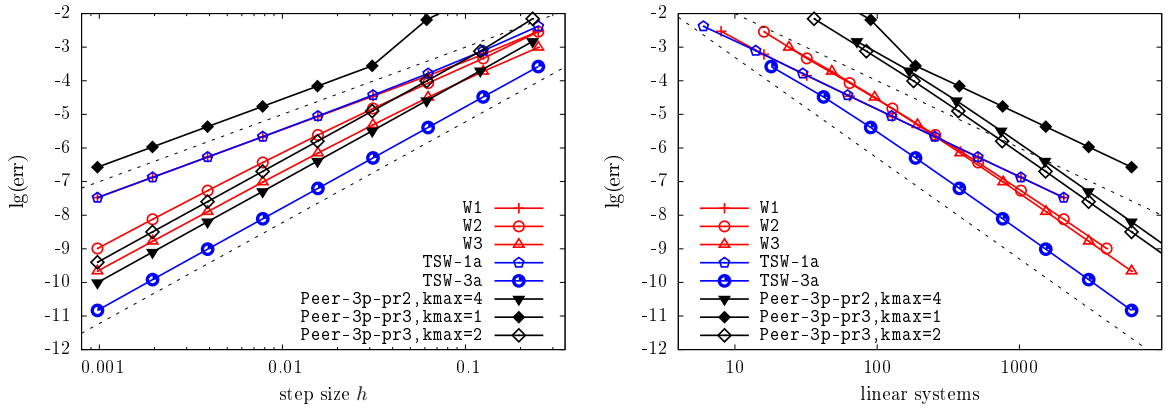

Figure 5.3.1: Results for diffusion–convection problem (5.1.3) with $m = 69$. For the peer method `Peer-3p`, an inexact AMF approach with predictor `pr2` with $kmax = 4$ and predictor `pr3` with $kmax = 1$ and $kmax = 2$ is used. Lg(err) vs. step size h (*left*) and lg(err) vs. linear systems (*right*). Dashed straight lines with slopes corresponding to orders two and three are added for reference.

Therefore, we consider in the following an inexact AMF approach where non-stiff convection parts are treated explicitly. We test our IMEX peer method `Peer-3p-imre`, cf.

Section 4.3, and consider the diffusion–convection problem (5.1.3) again. The results are given in Figure 5.3.2. For the peer method `Peer-3p-imre` with predictor `pr3`, only one Newton step is required for order three. The obtained accuracy is comparable to the case of an exact AMF approach with a fully implicit peer method, see Figure 5.2.7. Unfortunately, we even observe stability problems for the peer method `Peer-3p-imre` with predictor `pr2` for $kmax = 4$. This could be explained by the optimization process, where the peer method `Peer-3p-imre` is optimized only with respect to predictor `pr3`.

In general, inexact AMF combined with IMEX peer methods is a good choice for problems, where parts of the Jacobian are difficult to compute or some parts should be treated explicitly. Again, the proposed predictor `pr3` ensures the full order of the numerical scheme after one Newton steps and allows a reasonable comparison with linearly-implicit one-step and two-step W-methods.

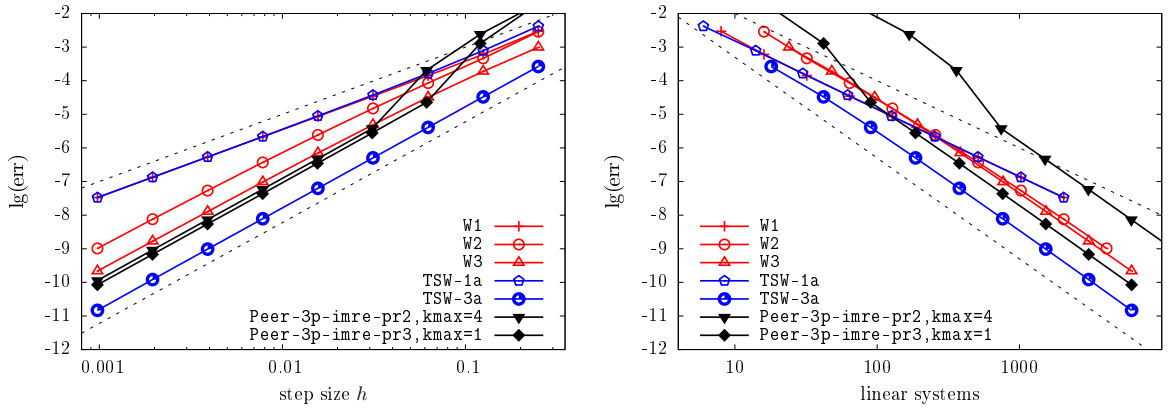

Figure 5.3.2: Results for diffusion–convection problem (5.1.3) with $m = 69$. For the AMF IMEX peer method `Peer-3p-imre`, predictor `pr2` with $kmax = 4$ and predictor `pr3` with $kmax = 1$ are used. Lg(err) vs. step size h (*left*) and lg(err) vs. linear systems (*right*). Dashed straight lines with slopes corresponding to orders two and three are added for reference.

6 Conclusions

In this thesis, we have investigated two-step W-methods and peer methods with application of an approximate matrix factorization (AMF). Two-step AMF W-methods are introduced and stability is studied. Appropriate two-step AMF W-methods up to order three are constructed for the solution of high dimensional initial value problems. Moreover, a stability result at infinity for two-step AMF W-methods is shown. Furthermore, a special class of stiffly accurate two-step W-methods of order $p^* = s + 1$ is elaborated. Methods up to five stages were found in a numerical optimization process and successfully tested on standard stiff test problems of small dimensions. Their performance is competitive compared to standard integration solvers like `RODAS` and `ode23s` in a variable step size implementation. One main contribution of this PhD thesis is the comparison of one-step W-methods with two-step W-methods and two-step peer methods in the context of AMF. In contrast to one-step AMF W-methods, the time derivatives are not incorporated in numerical two-step AMF schemes.

AMF peer methods using additional function values from the previous step are considered and developed. In our research, we have focussed on investigations for a fixed number of Newton steps in the AMF peer scheme. This allows a more convenient comparison of AMF peer methods with linearly-implicit one-step and two-step AMF W-methods. We have proved a stability result for AMF peer methods at infinity and have shown consistency and convergence of AMF peer methods in the setting of a fixed number of Newton steps. As it turned out, accuracy and stability are heavily based on the choice of the predictor in the Newton iteration. We have constructed a new three-stage AMF peer method of order three and propose a corresponding predictor. In comparison to the proposal by Beck *et al.* [3,4], this predictor guarantees order three for a three-stage AMF peer method after one step in the Newton iteration. Furthermore, its stability properties are promising.

We have tested our constructed two-step AMF W-methods and AMF peer methods on an autonomous 2D Brusselator problem, a linear model with homogeneous and time-dependent Dirichlet boundary conditions and a 2D diffusion–convection equation. Our results with constant time step sizes are compared to one-step AMF W-methods. For the problems with homogeneous boundary conditions, all methods perform well in our numerical experiments. The accuracy of two-step AMF W-methods and AMF peer methods is clearly superior compared to one-step methods. For time-dependent boundary conditions, all methods have problems for large time step sizes. In this case, one-step AMF W-methods are more robust in comparison to two-step AMF schemes, but for

smaller step sizes, an order reduction for one-step methods and high dimensional problems is clearly visible. With respect to stability, accuracy and robustness, our proposed predictor performs well in AMF peer methods for all considered problems. In general, the two-step W-method `TSW-3a` has been done best in our numerical tests. Due to the high accuracy, robustness and stability properties, this method can be recommended for practical use.

Many initial value problems arising from partial differential equations (PDEs) by discretization in space are composed of a stiff and a non-stiff part. For this reason, we have considered implicit-explicit (IMEX) peer methods with an AMF approach. We have recalled the recently introduced class of IMEX peer methods and have extended our AMF peer methods by considering a corresponding explicit part in the numerical scheme. An associated AMF IMEX peer method of order three with our proposed predictor is constructed. Our numerical tests on the 2D diffusion–convection equation with an inexact AMF approach confirm the theoretical results and show again that peer methods are also a good choice for problems where some non-stiff parts should be treated explicitly.

In our numerical experiments, we have observed that stability problems occur for AMF peer methods with a predictor of higher order. It requires a more proper stability analysis to understand this behaviour. Despite the fact that predictors using function values from the previous step are not stable in the AMF case, it could be considered a more general predictor in AMF peer schemes, for example, predictors using stage values from the current step. This could be a topic of future work.

Furthermore, we have considered fixed time step size integrations in our numerical tests with AMF. Two-step W-methods and peer methods are successfully applied in variable step size implementations. In [3, 4], AMF peer methods are also investigated for problems of convection–diffusion–reaction type with step size control. In further work, our proposed peer methods and predictors can also be treated in numerical tests with variable step size sequences.

IMEX methods have been intensively studied in the literature. In this thesis, we have restricted the study to the field of IMEX peer methods. Further investigations could be concerned with two-step W-methods and a splitting strategy. Like IMEX two-step Runge–Kutta methods [76] and two-step IMEX peer methods, a class of two-step IMEX W-methods could be promising due to their high stage order and favorable stability properties. In contrast to IMEX Runge–Kutta methods, see e.g. [1,6,20], no additional coupling conditions between an explicit and an implicit part and no order reduction for stiff problems should be expected.

In this PhD thesis, we have mainly focussed on two-dimensional PDEs in our stability investigations and numerical tests. In further work, it is interesting to study the behaviour for higher dimensions in space. Then convergence rates in the PDE-sense, i.e., when the step sizes in time and space are changed simultaneously, can also be investigated. Recently, González-Pinto *et al.* [23] have proved PDE-convergence of one-stage

AMF W-methods in the Euclidean norm and in the maximum norm for the linear diffusion problem. Optimal convergence rates are also obtained. For the one-step AMF W-method with $\gamma = \frac{1}{2}$ and time-dependent Dirichlet boundary conditions, nearly order two is proved in the Euclidean norm, whereas an order reduction to order one occurs in the maximum norm. These principles and convergence analysis could be extended to one-stage two-step AMF W-methods.

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Publikationsliste

[1] M. Klinge, D. Hernández-Abreu und R. Weiner. *A comparison of one-step and two-step methods with approximate matrix factorization.* Erscheint im J. Comput. Appl. Math. (2020). `https://doi.org/10.1016/j.cam.2019.112519`

[2] M. Klinge, H. Podhaisky und R. Weiner. *Two-step W-methods.* Zur Veröffentlichung eingereicht.

[3] M. Klinge und R. Weiner. *Strong stability preserving explicit peer methods for discontinuous Galerkin discretizations.* J. Sci. Comput. **75**, 1057–1078 (2018).

[4] M. Klinge, R. Weiner und H. Podhaisky. *Optimally zero stable explicit peer methods with variable nodes.* BIT Numer. Math. **58**, 331–345 (2018).

Eidesstattliche Erklärung

Hiermit erkläre ich an Eides statt, dass ich die vorliegende Dissertation selbständig, ohne fremde Hilfe Dritter und ohne Benutzung anderer als der angegebenen Quellen und Hilfsmittel angefertigt habe. Die aus anderen Werken wörtlich oder inhaltlich entnommenen Daten, Fakten und Konzepte sind unter Angabe der entsprechenden Quelle als solche gekennzeichnet.

Diese Arbeit wurde bisher weder im In- noch im Ausland in gleicher oder ähnlicher Form in einem anderen Prüfungsverfahren vorgelegt.

Halle (Saale), 12. Oktober 2021

Marcel Klinge