Construction of highly stable two–step W–methods for ordinary differential equations

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Abstract. We describe the construction of linearly implicit two–step W–methods of high stage order and desirable stability properties for the numerical solution of stiff differential systems. The presented methods are demonstrated to be A–stable and L–stable when the stepsize is held constant. They also preserve good stability properties in a variable stepsize environment under quite demanding conditions imposed on the stepsize pattern.

Key Words. Two–step W–methods, stiff differential systems, A–stability, L–stability

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1 Introduction

In this paper we investigate the class of linearly implicit two–step W–methods with parallel stages for the numerical solution of ordinary differential equations (ODES)

$$\begin{cases} y' = f(t,y), \quad t \in [t_0, T], \\ y(t_0) = y_0, \end{cases} \tag{1.1}$$

$f : \mathbb{R} \times \mathbb{R}^m \to \mathbb{R}^m$. These methods were investigated in recent papers [16], [19], [15] and [17] and for a time step from t_n to $t_{n+1} = t_n + h_n$ have the following form

$$\begin{cases} Y_{ni} = y_n + h_n \sum_{j=1}^{s} a_{ij} k_{n-1,j}, \\ (I - h_n \gamma_i T_n) k_{n,i} = f(t_n + c_i h_n, Y_{ni}) + h_n T_n \sum_{j=1}^{s} \gamma_{ij} k_{n-1,j}, \\ y_{n+1} = y_n + h_n \sum_{i=1}^{s} \Big(b_i k_{ni} + v_i k_{n-1,i} \Big), \end{cases} \tag{1.2}$$

$i = 1, 2, \ldots, s$, $n = 1, 2, \ldots$. Here, T_n is some matrix of dimension $m \times m$. This matrix affects the efficiency, accuracy and stability properties of (1.2) and the choice $T_n = \frac{\partial f}{\partial y}(t_n, y_n)$ leads to the ROW–methods, see e.g., Kaps and Rentrop [12]. Schmitt and Weiner [18] discussed Krylov W–methods in which the matrices T_n are of low rank. These matrices are projections of the Jacobian matrix $\frac{\partial f}{\partial y}(t_n, y_n)$ into a nested sequence of some Krylov subspaces.

We will represent the method (1.2) by the table of its coefficients

$$\begin{array}{c|c|c} G & A & \Gamma \\ \hline c^T & b^T & v^T \end{array} = \begin{array}{ccc|ccc|ccc} \gamma_1 & & & a_{11} & \cdots & a_{1s} & \gamma_{11} & \cdots & \gamma_{1s} \\ & \ddots & & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ & & \gamma_s & a_{s1} & \cdots & a_{ss} & \gamma_{s1} & \cdots & \gamma_{ss} \\ \hline c_1 & \cdots & c_s & b_1 & \cdots & b_s & v_1 & \cdots & v_s \end{array}.$$

We will always assume that the abscissas $c_1, \ldots, c_s$ are constant. However, the coefficients G, Γ, A, b and v may depend on the ratio of consecutive stepsizes $\sigma_n = h_n / h_{n-1}$.

It was demonstrated in [16], [15], [17] that the method (1.2) is convergent with order $p^* = \min\{q+1, p\}$ for arbitrary matrices T_n if the starting errors satisfy the conditions $\|y(t_0) - y_0\| = O(h^p)$, $\|y'(t_0 + c_i h_0) - k_{0,i}\| = O(h^p)$, $i = 1, 2, \ldots, s$, $h = \max\{h_i\}$, and the coefficients of the method (1.2) satisfy the simplifying assumptions $C(q)$, $\Gamma(q)$ and $B(p)$ defined by

$$
\begin{array}{lll}
C(q): & \displaystyle\sum_{j=1}^{s} a_{ij}(c_j - 1)^{l-1} = \sigma_n^{l-1}\frac{c_i^l}{l}, & l = 1, 2, \ldots, q, \\
\Gamma(q): & \displaystyle\sum_{j=1}^{s} \gamma_{ij}(c_j - 1)^{l-1} = -\gamma_i \sigma_n^{l-1} c_i^{l-1}, & l = 1, 2, \ldots, q, \\
B(p): & \displaystyle\sum_{j=1}^{s} b_j \sigma_n^{l-1} c_j^{l-1} + \sum_{j=1}^{s} v_j (c_j - 1)^{l-1} = \frac{\sigma_n^{l-1}}{l}, & l = 1, 2, \ldots, p.
\end{array}
$$

In this paper we describe the construction of highly stable methods (1.2) with respect to the test equation

$$
y' = \lambda y, \quad t \geq 0, \tag{1.3}
$$

$\lambda \in \mathbb{C}$, where $T_n = \lambda$ for all n. We restrict our attention to methods (1.2) which satisfy $C(q)$, $\Gamma(q)$ and $B(p)$ with $p = q = s$. These conditions are stronger than required for convergence of order p. However, as demonstrated in [16] for Prothero–Robinson problem, the resulting methods do not suffer from order reduction phenomenon [8]. Moreover, these methods have a simple form of the local discretization error which is easier to estimate and control in a reliable way in a variable stepsize environment than for methods satisfying $C(p-1)$, $\Gamma(p-1)$ and $B(p)$, compare [9].

The application of (1.2) with $T_n = \lambda$ to (1.3) leads to the recurrence relation

$$
\begin{bmatrix} h_n K_n \\ y_{n+1} \end{bmatrix} = M(\sigma_n, z_n) \begin{bmatrix} h_{n-1} K_{n-1} \\ y_n \end{bmatrix},
$$

$n = 0, 1, \ldots$, where $z_n = h_n \lambda$,

$$
h_n K_n = \begin{bmatrix} h_n k_{n1} & \cdots & h_n k_{ns} \end{bmatrix}^T,
$$

and the amplification matrix $M(\sigma, z)$ is defined by

$$
M(\sigma, z) = \begin{bmatrix} \sigma\, W(z)(A + \Gamma) & W(z)\, e \\ \sigma \left(b^T W(z)(A + \Gamma) + v^T \right) & 1 + b^T W(z)\, e \end{bmatrix} \tag{1.4}
$$

with $W(z) = z(I - zG)^{-1}$ and $e = [1, \ldots, 1]^T \in \mathbb{R}^s$. The stability properties of (1.2) with respect to (1.3) depend on the product of matrices

$$M(\sigma_n, z_n)\, M(\sigma_{n-1}, z_{n-1}) \cdots M(\sigma_1, z_1), \tag{1.5}$$

$z_n = \sigma_n \sigma_{n-1} \cdots \sigma_1 z_0$, $z_0 = h_0 \lambda$. It is of interest to investigate if there exists a ratio $\sigma_{max} > 1$ such that (1.5) tends to zero as $n \to \infty$ for $\sigma_i \in [0, \sigma_{max}]$ and $\mathrm{Re}(z_0) < 0$. If this is the case we could consider this as a generalization of the concept of A–stability for variable stepsize methods (1.2). However, the asymptotic behaviour of (1.5) is very difficult to describe except for the special case where $\sigma_i = 1$ which corresponds to the fixed stepsize. Some progress in this direction was made recently by Guglielmi and Zennaro [6], [7] using the theory of joint spectral radius of a family of matrices and the concept of a polytope norm defined by its unit ball in $\mathbb{R}^s$. This approach will be illustrated in Section 6.

In this paper we will derive methods (1.2) which are A–stable and L–stable when the stepsize is held constant. In the case $p = q = s = 2$ we will also derive methods for which the stability matrix $M(\sigma, z)$ has a spectral radius less than one for $\mathrm{Re}(z) < 0$ and $\sigma \in [0, \sigma_{max}]$ for some $\sigma_{max} > 1$ which depends on the method. This is, of course, not sufficient to guarantee that (1.5) tends to zero as $n \to \infty$ and to obtain additional insight into stability properties of the resulting methods we study the asymptotic behaviour of these products numerically for various sequences $\{\sigma_i\}$ and $\{z_n\}$. These experiments demonstrate that for the methods derived in this paper the corresponding products (1.5) tend to zero as $n \to \infty$ for various stepsize patterns which are usually more demanding than one is likely to encounter in most practical applications.

2 Construction of highly stable W–methods

As already mentioned in Section 1 we will restrict our attention to the methods (1.2) with $p = q = s$. In this case the simplifying assumptions $C(p)$, $\Gamma(p)$ and $B(p)$ can be written in the matrix form

$$\begin{aligned}
&C(p): && A\, V_1 = C\, V_0\, S\, D^{-1},\\
&\Gamma(p): && \Gamma\, V_1 = -\, G\, V_0\, S,\\
&B(p): && b^T\, V_0\, S + v^T\, V_1 = e^T\, S\, D^{-1},
\end{aligned}$$

where

$$V_0 = \begin{bmatrix} e & c & \cdots & c^{p-1} \end{bmatrix}, \quad V_1 = \begin{bmatrix} e & c-e & \cdots & (c-e)^{p-1} \end{bmatrix},$$

$$C = \mathrm{diag}(c_1, c_2, \ldots, c_s), \quad D = \mathrm{diag}(1, 2, \ldots, s), \quad S = \mathrm{diag}(1, \sigma, \ldots, \sigma^{s-1}),$$

compare [16], [15], [17]. We will also assume that $\gamma_i = \gamma$, $i = 1, 2, \ldots, s$, which simplifies the implementation of (1.2) on sequential computers since only the LU–decomposition of the single matrix $I - h_n \gamma T_n$ is required at each step.

The conditions $C(p)$ and $\Gamma(p)$ uniquely determine the coefficient matrices A and Γ. We then enforce the order condition $B(p)$ and one of the following stability conditions.

1. The stability polynomial

$$p(\eta, z, \sigma) = \det(\eta I - M(z, \sigma))$$

of the method (1.2) has the form

$$p(\eta, z, \sigma) = \eta^s(\eta - R(z, \sigma)),$$

where the function $R(z, \sigma)$ is A–acceptable, i.e.,

$$|R(z, \sigma)| < 1 \quad \text{for} \quad \mathrm{Re}(z) < 0$$

and $\sigma \in [0, \sigma_{max}]$ for some $\sigma_{max} > 1$. This strategy (for $\sigma = 1$) was employed before in the construction of diagonally implicit multistage integration methods (DIMSIMs) in [3], [4], [5], [10], and general linear methods with inherent Runge–Kutta stability properties in [2].

This approach is technically very complicated and we were only able to carry it out for $p = q = s = 2$. For higher order methods this approach exhausts the capabilities of symbolic manipulation packages, even for $\sigma = 1$, i.e., for fixed stepsize methods.

The next two approaches describe the construction of highly stable methods for $\sigma = 1$. The verification of stability for variable stepsize methods is then carried out numerically in Section 6

2. The abscissas c_i are given in advance and the stability polynomial $p(\eta, z)$ of (1.2) is A–stable and L–stable, i.e., the roots $r_i(z)$, $i = 1, 2, \ldots, s+1$, of $p(\eta, z)$ satisfy the conditions

$$|r_i(z)| < 1 \quad \text{for} \quad \mathrm{Re}(z) < 0,$$

and

$$\lim_{z\to\infty} r_i(z) = 0.$$

Observe that this condition is stronger than that considered in [16], [17] where it was only required that $\lim_{z\to\infty} r_i(z) < 1$. This can be carried out using the Schur criterion, compare [14]. This strategy was employed before in the construction of highly stable two–step Runge–Kutta methods in [1] and [11].

3. The method (1.2) is stiffly accurate, i.e.,

$$c_s = 1, \quad b^T = \gamma\, e_s^T, \quad v^T = e_s^T\,(A+\Gamma),$$

$e_s = [0,\dots,1]^T \in \mathbb{R}^s$, compare [16], [15], [17], and the stability polynomial $p(\eta, z)$ of (1.2) is A–stable and L–stable. In this case the powers of the stability matrix $M(z,\sigma)$ depend on the powers of the $s\times s$ matrix $\widetilde{M}(z,\sigma)$ defined by

$$\widetilde{M}(z,\sigma) = \begin{bmatrix} \sigma\,(A+\Gamma) & e \end{bmatrix} \begin{bmatrix} w\, I \\ (1+\gamma\, w)\, e_s^T \end{bmatrix} = e\, e_s^T + w\Big(\sigma\,(A+\Gamma) + \gamma\, e\, e_s^T\Big),$$

where $w = z/(1-\gamma z)$.

These approaches will be illustrated in the next sections for the two–step W–methods with $p=q=s$ for $p=2$, 3 and 4.

3 W–methods with $p=q=s=2$

The stability polynomial of (1.2) with $\gamma_i = \gamma$ for $p=q=s=2$ has the form

$$p(\eta,z,\sigma) = (1-\gamma\, z)^2 \eta^3 - p_1(z,\sigma)\,\eta^2 + p_2(z,\sigma)\,\eta - p_3(z,\sigma),$$

where

$$p_1(z,\sigma) = 1 + p_{11}(\sigma)\, z + p_{12}(\sigma)\, z^2,$$
$$p_2(z,\sigma) = p_{21}(\sigma)\, z + p_{22}(\sigma)\, z^2,$$
$$p_3(z,\sigma) = p_{32}(\sigma)\, z^2.$$

We illustrate next the first strategy for construction of highly stable methods described in Section 2. Solving $B(2)$ for b_1 and b_2 and the system

$$p_{21}(\sigma) = 0, \quad p_{22}(\sigma) = 0, \quad p_{32}(\sigma) = 0$$

with respect to v_1, v_2, and γ leads to methods with

$$p(\eta, z, \sigma) = \eta^2\,(\eta - R(z,\sigma)),$$

where the function $R(z,\sigma)$ has the form

$$R(z,\sigma) = \frac{P(z,\sigma)}{Q(z,\sigma)} = \frac{1 + a(c_1,c_2,\sigma)\,z}{1 - b(c_1,c_2,\sigma)\,z}$$

which for $\sigma = 1$ reduces to the stability function $R(z,1) = (1+z/2)/(1-z/2)$ of the trapezoidal method for all choices of c_1 and c_2, $c_1 \neq c_2$. It can be verified that the Nørsett polynomial $E(y,\sigma) = |Q(i\,y,\sigma)|^2 - |P(i\,y,\sigma)|^2$ has, in general, a simple root at $\sigma = 1$. However, if $c_2 - c_1 = \sqrt{2}$ then $\sigma = 1$ is a double root of $E(y,\sigma)$ and this polynomial is nonnegative for $\sigma \in [0, \sigma_{max}]$ and all $y \in \mathbb{R}$, where $\sigma_{max} \approx 2.61217$. We can also verify that the poles of $R(z,\sigma)$ are in the positive half plane and we conclude that $R(z,\sigma)$ is A–acceptable for $\sigma \in [0,\sigma_{max}]$. The coefficients of the resulting method corresponding to $c_1 = 1 - \sqrt{2}$, $c_2 = 1$ and $\sigma = 1$ are listed below.

Method 1:

$$\begin{array}{c|c|c} G & A & \Gamma \\ \hline c^T & b^T & v^T \end{array} = \begin{array}{cc|cc|cc} \frac{1}{2} & & \frac{4-\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & \frac{\sqrt{2}-2}{4} & -\frac{\sqrt{2}}{4} \\ & \frac{1}{2} & -\frac{\sqrt{2}}{4} & \frac{4+\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & -\frac{\sqrt{2}+2}{4} \\ \hline 1-\sqrt{2} & 1 & \frac{\sqrt{2}}{8} & \frac{3\sqrt{2}}{8} & \frac{8-3\sqrt{2}}{8} & \frac{4-\sqrt{2}}{8} \end{array}.$$

To illustrate the second strategy described in Section 2 let us assume that $c = [0,1]^T$. Solving $B(2)$ with respect to v_1 and v_2 and then the system

$$p_{12}(1) = 0, \quad p_{22}(1) = 0, \quad p_{32}(1) = 0,$$

with respect to b_1, b_2 and γ we obtain the method whose coefficients, for $\sigma = 1$, are given below.

Method 2:

$$\begin{array}{c|c|c} G & A & \Gamma \\ \hline c^T & b^T & v^T \end{array} = \begin{array}{cc|cc|cc} \frac{3-\sqrt{3}}{2} & & 0 & 0 & 0 & \frac{\sqrt{3}-3}{2} \\ & \frac{3-\sqrt{3}}{2} & -\frac{1}{2} & \frac{3}{2} & \frac{3-\sqrt{3}}{2} & \sqrt{3}-3 \\ \hline 0 & 1 & \frac{18-11\sqrt{3}}{4} & \frac{5\sqrt{3}-6}{4} & \frac{5\sqrt{3}-8}{4} & \frac{\sqrt{3}}{4} \end{array}.$$

We can verify using the Schur criterion that the resulting methods is A–stable. Since

$$\lim_{z\to\infty} r_i(z,1) = 0,$$

where $r_i(z,1)$ are the roots of $p(\eta,z,1)$ the resulting method is also L–stable.

Consider next the third strategy described in Section 2. Assume that the method (1.2) is stiffly accurate, i.e., $c_2 = 1$, $b^T = \gamma\, e_2^T$ and $v^T = e_2^T\,(A+\Gamma)$. It can be verified that this implies that the condition $B(2)$ is automatically satisfied. The stability polynomial of the matrix $\widetilde{M}(\eta,z,\sigma)$ defined in Section 2 has the form

$$\widetilde{p}(\eta,z,\sigma) = (1-\gamma\, z)^2\eta^2 - \widetilde{p}_1(z,\sigma)\,\eta + \widetilde{p}_2(z,\sigma),$$

where

$$\begin{aligned} \widetilde{p}_1(z,\sigma) &= 1 + \widetilde{p}_{11}(\sigma)\, z + \widetilde{p}_{12}(\sigma)\, z^2, \\ \widetilde{p}_2(z,\sigma) &= \widetilde{p}_{21}(\sigma)\, z + \widetilde{p}_{22}(\sigma)\, z^2. \end{aligned}$$

We consider next the system

$$\widetilde{p}_{12}(1) = 0, \quad \widetilde{p}_{22}(1) = 0,$$

which has three solutions for c_1 and γ. Two solutions correspond to the methods whose coefficients for $\sigma = 1$ are listed below.

Method 3:

$$\begin{array}{c|c|c} G & A & \Gamma \\ \hline c^T & b^T & v^T \end{array} = \begin{array}{cc|cc|cc} \frac{3\pm\sqrt{3}}{2} & & \frac{3(5\pm3\sqrt{3})}{8} & \frac{9\pm7\sqrt{3}}{8} & \frac{-3(2\pm\sqrt{3})}{4} & \frac{\pm\sqrt{3}}{4} \\ & \frac{3\pm\sqrt{3}}{2} & \frac{-1\pm\sqrt{3}}{8} & \frac{9\mp\sqrt{3}}{8} & \frac{\mp\sqrt{3}}{4} & \frac{-6\mp\sqrt{3}}{4} \\ \hline 3\pm2\sqrt{3} & 1 & 0 & \frac{3\pm\sqrt{3}}{2} & \frac{-1\mp\sqrt{3}}{8} & \frac{-3(1\pm\sqrt{3})}{8} \end{array}.$$

It can be verified using the Schur criterion that these methods are A–stable as well as L–stable. These methods were also obtained in [15], [17].

4 W–methods with $p = q = s = 3$

We assume first that the abscissa vector c is given in advance and we choose $c = [0, \frac{1}{2}, 1]^T$. We then solve the system $B(3)$ for v_1, v_2, and v_3 and then try to choose the remaining parameters b_1, b_2, b_3, and γ in such a way that the resulting method has the desired stability properties for $\sigma = 1$, i.e., when the stepsize is kept constant. The stability polynomial of the method (1.2) with $p = q = s = 3$ (for $\sigma = 1$) has the form

$$p(\eta, z) = (1 - \gamma\, z)^3\, \eta^4 - p_1(z)\, \eta^3 + p_2(z)\, \eta^2 - p_3(z)\, \eta + p_4(z),$$

where

$$\begin{aligned} p_1(z) &= 1 + p_{11}\, z + p_{12}\, z^2 + p_{13}\, z^3, & p_2(z) &= p_{21}\, z + p_{22}\, z^2 + p_{23}\, z^3, \\ p_3(z) &= p_{32}\, z^2 + p_{33}\, z^3, & p_4(z) &= p_{43}\, z^3. \end{aligned}$$

Solving the system

$$p_{13} = 0, \quad p_{23} = 0, \quad p_{33} = 0, \quad p_{43} = 0,$$

with respect to b_1, b_2, b_3, and γ leads to four methods and it can be verified using the Schur criterion that one of them is A–stable and L–stable. The coefficients of this method for $\sigma = 1$ are listed below.

Method 4:

$$A = \begin{bmatrix} 0 & 0 & 0 \\ \frac{5}{24} & -\frac{2}{3} & \frac{23}{24} \\ \frac{7}{6} & -\frac{10}{3} & \frac{19}{6} \end{bmatrix}, \quad \Gamma = \begin{bmatrix} 0 & 0 & -1.21014 \\ -1.21014 & 3.63041 & -3.63041 \\ -3.63041 & 9.68111 & -7.26083 \end{bmatrix},$$

$$\gamma = 1.21014, \quad c = \begin{bmatrix} 0 & \frac{1}{2} & 1 \end{bmatrix}^T, \quad b = \begin{bmatrix} -6.45183 & 14.0277 & -5.23534 \end{bmatrix}^T,$$

$$v = \begin{bmatrix} 2.84496 & -3.13287 & -1.05264 \end{bmatrix}^T.$$

We consider next the case when the method (1.2) is stiffly accurate, i.e., $c_3 = 1$, $b^T = \gamma\, e_3^T$, and $v^T = e_3^T\,(A + \Gamma)$. Then the condition $B(3)$ is automatically satisfied. The stability polynomial $\widetilde{p}(\eta, z)$ of the matrix $\widetilde{M}(z, 1)$ defined in Section 2 has the form

$$\widetilde{p}(\eta, z) = (1 - \gamma\, z)^3\, \eta^3 - \widetilde{p}_1(z)\, \eta^2 + \widetilde{p}_2(z)\, \eta - \widetilde{p}_3(z),$$

where

$$\begin{aligned} \widetilde{p}_1(z) &= 1 + \widetilde{p}_{11}\, z + \widetilde{p}_{12}\, z^2 + \widetilde{p}_{13}\, z^3, \\ \widetilde{p}_2(z) &= \widetilde{p}_{21}\, z + \widetilde{p}_{22}\, z^2 + \widetilde{p}_{23}\, z^3, \\ \widetilde{p}_3(z) &= \widetilde{p}_{32}\, z^2 + \widetilde{p}_{33}\, z^3. \end{aligned}$$

Solving the system

$$\widetilde{p}_{13} = 0, \quad \widetilde{p}_{23} = 0, \quad \widetilde{p}_{33} = 0,$$

with respect to c_1, c_2, and γ we obtain eight methods and the method listed below is A–stable and L–stable.

Method 5:

$$A = \begin{bmatrix} -0.19063 & 0.0286272 & -0.828532 \\ -0.639433 & 2.7418 & 2.77941 \\ -0.137527 & 0.0582847 & 1.07924 \end{bmatrix},$$

$$\Gamma = \begin{bmatrix} -0.499644 & 0.0525853 & -0.763079 \\ -0.505399 & -1.78105 & 1.07631 \\ 0.298344 & -0.158761 & -1.34972 \end{bmatrix},$$

$$\gamma = 1.21014, \quad c = \begin{bmatrix} -0.990534 & 4.88178 & 1 \end{bmatrix}^T,$$

$$b = \begin{bmatrix} 0 & 0 & 1.21014 \end{bmatrix}^T, \quad v = \begin{bmatrix} 0.160817 & -0.100476 & -0.270479 \end{bmatrix}^T.$$

This method was also obtained in [15]. Interchanging c_1 and c_2 leads to an equivalent method which is also A–stable and L–stable. The coefficients of this method are not listed.

5 W–methods with $p = q = s = 4$

Proceeding similarly as in Section 3 we can also construct methods (1.2) with $p = q = s = 4$ which have good stability properties. Choosing the abscissas c_i to be uniformly distributed on the interval $[0, 1]$ leads to a method with coefficients given by

Method 6:

$$A = \begin{bmatrix} 0 & 0 & 0 & 0 \\ -\frac{1}{8} & \frac{37}{72} & -\frac{59}{72} & \frac{55}{72} \\ -\frac{8}{9} & \frac{31}{9} & -\frac{44}{9} & 3 \\ -\frac{25}{8} & \frac{93}{8} & -\frac{123}{8} & \frac{63}{8} \end{bmatrix},$$

$$\Gamma = \begin{bmatrix} 0 & 0 & 0 & -1.94429 \\ 1.94429 & -7.77715 & 11.6657 & -7.77715 \\ 7.77715 & -29.1643 & 38.8858 & -19.4429 \\ 19.4429 & -69.9944 & 87.493 & -38.8858 \end{bmatrix},$$

$$\gamma = 1.94429, \quad c = \begin{bmatrix} 0 & \frac{1}{3} & \frac{2}{3} & 1 \end{bmatrix}^T,$$

$$b = \begin{bmatrix} -324.747 & 967.148 & -925.943 & 289.764 \end{bmatrix}^T,$$

$$v = \begin{bmatrix} 157.894 & -399.336 & 308.045 & -71.8242 \end{bmatrix}^T.$$

Assuming next that (1.2) is stiffly accurate, i.e., $c_4 = 1$, $b^T = \gamma\, e_4^T$, and $v^T = e_4^T\,(A + \Gamma)$ we satisfy $B(4)$ and the resulting method is given below.

Method 7:

$$A = \begin{bmatrix} -0.321874 & 0.0950592 & -0.00454429 & -1.28538 \\ -0.446919 & 3.02612 & -0.0203008 & 2.66049 \\ 3.43758 & 13.7319 & 4.06365 & -6.82715 \\ -0.0839354 & 0.077553 & -0.00286957 & 1.00925 \end{bmatrix},$$

$$\Gamma = \begin{bmatrix} -0.93513 & 0.168541 & -0.00862624 & ,-1.16907 \\ -0.307764 & -2.46146 & -0.0400346 & 0.86497 \\ 1.05698 & 1.81535 & -2.46225 & -2.35436 \\ 0.287674 & -0.324876 & 0.0112255 & -1.91831 \end{bmatrix},$$

$$\gamma = 1.94429, \quad c = \begin{bmatrix} -1.51674 & 5.21939 & 14.406 & 1 \end{bmatrix}^T,$$

$$b = \begin{bmatrix} 0 & 0 & 0 & 1.94429 \end{bmatrix}^T,$$

$$v = \begin{bmatrix} 0.203738 & -0.247323 & 0.00835594 & -0.90906 \end{bmatrix}^T.$$

It can be verified using the Schur criterion that both methods listed above are A–stable and L–stable. We can also obtain A–stable and L–stable methods permuting the abscissas c_1, c_2, and c_3. The coefficients of these methods are not listed.

6 Numerical verification of stability

In this section we investigate numerically stability of the methods derived in Section 3, 4, and 5. Stability of the third method derived in Section 3 is governed by the 2×2 matrix $\widetilde{M}(z,\sigma)$ defined by

$$\widetilde{M}(z,\sigma) = \begin{bmatrix} \frac{3\sigma^2\left(1+\sqrt{3}(z-1)\right)z}{4(2-6z+3z^2)} & \frac{8+\left(3(\sqrt{3}-1)(\sigma^2-4\sigma)-4(\sqrt{3}+3)\right)z-3\sqrt{3}(\sigma-4)\sigma z^2}{4(2-6z+3z^2)} \\ \frac{\sigma^2\left(\sqrt{3}(1-z)-1\right)z}{4(2-6z+3z^2)} & \frac{8+\left((\sqrt{3}-1)(4\sigma-\sigma^2)-4(\sqrt{3}+3)\right)z+\sqrt{3}(\sigma-4)\sigma z^2}{4(2-6z+3z^2)} \end{bmatrix}.$$

We will follow the approach of Guglielmi and Zennaro [6], [7] to find conditions which imply that the product

$$\widetilde{M}(z,\sigma_n)\,\widetilde{M}(z,\sigma_{n-1})\cdots\widetilde{M}(z,\sigma_1) \tag{6.1}$$

is bounded or tends to zero as $n \to \infty$ for fixed value of $z = \bar{z}$. This seems to be justified if the spectrum of the problem (1.1) scaled by the average stepsize of the method (1.2) is concentrated near this value of $\bar{z}$. The boundedness of (6.1) would follow if we can find a polytope norm $\|\cdot\|_*$ in $\mathbb{R}^2$, compare [6], [7], such that for the induced matrix norm which will be denoted by the same symbol we have

$$\|\widetilde{M}(\bar{z},\sigma)\|_* \le 1 \tag{6.2}$$

for $\sigma \in [0,\sigma_{max}]$, $\sigma_{max} > 1$. These polytope norms are defined by their unit balls in $\mathbb{R}^2$. Define σ_{max} by

$$\sigma_{max} = \max\{\sigma :\ \rho(\widetilde{M}(\bar{z},\sigma)) = 1\},$$

where $\rho(M)$ is the spectral radius of M. These polytope norms $\|\cdot\|_*$ can be found by applying successively the matrix $\widetilde{M}(\bar{z},\sigma)$ to the set of initial points $\mathcal{S} = \{[1,0]^T,\ [0,1]^T,\ [-1,0]^T,\ [0,-1]^T\}$. If

$$\widetilde{M}^j(\bar{z},\sigma)\,P, \quad P \in \mathcal{S}, \quad j = 1,2,\ldots$$

are contained in a convex hull symmetric with respect to the origin of some points in $\mathbb{R}^2$ for $\sigma \in [0,\sigma_{max}]$, then this convex hull defines the unit ball of the

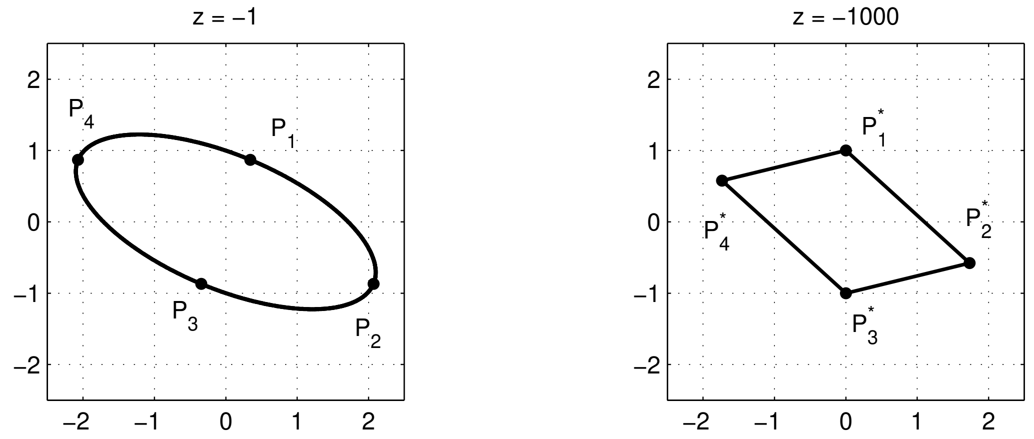

Figure 1: Unit balls for polytope norms $\|\cdot\|_*$ satisfying (6.2) for the matrix $\widetilde{M}(z,\sigma)$ for $z=-1$ (left graph) and $z=-1000$ (right graph).

polytope norm $\|\cdot\|_*$ satisfying (6.2). This process is illustrated for $z=-1$ for which $\sigma_{max}=2.70078$ and for $z=-1000$ for which $\sigma_{max}=1.90989$ and the corresponding unit balls are plotted in Fig. 1. On this figure $P_1=-P_3=[0.3446, 0.8692]^T$, $P_2=-P_4=[2.0712, 0.8680]^T$, $P_1^*=-P_3^*=[0,1]^T$, and $P_2^*=-P_4^*=[1.7331, -0.5789]^T$.

Stability properties of other methods constructed in Section 3, 4, and 5 are governed by stability matrices $M(z,\sigma)$ or $\widetilde{M}(z,\sigma)$ of dimensions 3×3, 4×4, or 5×5 and the approach of [6], [7] is more difficult to apply since we have to construct polytope norms in $\mathbb{R}^3$, $\mathbb{R}^4$, or $\mathbb{R}^5$. To investigate the stability of these methods we will instead monitor directly the behaviour of the products

$$M(z_n,\sigma_n)\,M(z_{n-1},\sigma_{n-2})\cdots M(z_1,\sigma_1) \tag{6.3}$$

or

$$\widetilde{M}(z_n,\sigma_n)\,\widetilde{M}(z_{n-1},\sigma_{n-2})\cdots \widetilde{M}(z_1,\sigma_1) \tag{6.4}$$

for some sequences of stepsize ratios $\{\sigma_n\}$ and complex numbers $\{z_n\}$. We have made the following choices:

1. Both sequences $\{\sigma_n\}$ and $\{z_n\}$ are generated randomly according to the formulas

$$\sigma_n=\left(\rho-\frac{1}{\rho}\right)\text{rand}+\frac{1}{\rho},$$

$$z_n = -1000\,\mathrm{rand} + (2\,\mathrm{rand} - 1)\,1000\,i,$$

$n = 1, 2, \ldots, N$, where rand is a random number with uniform distribution between 0 and 1 and ρ is a given ratio.

2. Sequences $\{\sigma_n\}$ and $\{z_n\}$ are given by

$$\sigma_n = \rho^{(-1)^n \sin\left(\frac{4\pi n}{N}\right)}, \quad z_n = \sigma_n\, z_{n-1},$$

$n = 1, 2, \ldots, N$, where z_0 is a given initial point.

3. Sequences $\{\sigma_n\}$ and $\{z_n\}$ are defined by

$$\sigma_n = \rho^{(-1)^n}, \quad z_n = \sigma_n\, z_{n-1},$$

$n = 1, 2, \ldots, N$, where z_0 is a given initial point. This choice corresponds to successively decreasing and increasing the stepsize by the ratio ρ.

Method	p	ρ_1	ρ_2	ρ_3
Method 1	2	3.86	2.84	1.83
Method 2	2	3.41	7.93	3.20
Method 3	2	4.23	14.1	4.48
Method 4	3	1.83	5.09	2.61
Method 5	3	2.26	4.62	2.29
Method 6	4	1.58	2.35	1.63
Method 7	4	1.70	4.60	2.34

Table 1: Ratios ρ_1, ρ_2, and ρ_3 corresponding to the sequences $\{\sigma_n\}$ and $\{z_n\}$ defined in 1. 2. and 3.

To obtain some insight into stability properties of the methods constructed in this paper we computed the products (6.3) or (6.4) for $N = 1000$ for $\{\sigma_n\}$ and $\{z_n\}$ defined above, where we have chosen $z_0 = -100$ for the sequences defined in 2. and 3. We have listed in Table 1 the maximum values of ρ, denoted by ρ_1, ρ_2, and ρ_3 (for the corresponding sequences $\{\sigma_n\}$ and

$\{z_n\}$ defined in 1., 2. or 3.) for which the norm of (6.3) or (6.4) is less than the machine epsilon $eps \approx 10^{-16}$.

The results presented in Table 1 indicate that the methods constructed in this paper are quite stable when the stepsize is changing rapidly as defined by 1. 2. or 3. In most applications the stepsize variations are rather mild and we can conclude that these methods are sufficiently stable for all practical purposes. We can also observe that the methods which are stiffly accurate have, in most cases, better stability properties than other methods which is reflected in larger values of ρ_1, ρ_2 and ρ_3 for the methods 3 and 7 and for the method 5 for the sequences $\{\sigma_n\}$ and $\{z_n\}$ defined in 1. than for the methods 2, 6 and 4.

7 Numerical experiments

To verify stability properties in a variable step size environment we have tested the methods constructed in Section 3, 4 and 5 on various well known stiff problems. The error estimation was performed by embedding technique analogously to the one adopted in [17] with $atol = rtol$ except for ROBER, where we have used $atol = 10^{-6}\,rtol$ as proposed in [8]. The Jacobian was evaluated at each time step.

For the two and three-stage Methods 1–5 the maximal stepsize increase was limited to $\sigma_{max} = 1.5$. Method 6 showed a nonsmooth behaviour for $\sigma_{max} = 1.5$ and failed for some problems, therefore we limited the stepsize increase for the four-stage methods to $\sigma_{max} = 1.1$. The numerical experiments also indicate that the stiffly accurate method 7 was not influenced by the larger value of σ_{max}.

We present the results for the following problems:

- The Prothero-Robinson equation

$$y' = \lambda(y - g(t)) + g'(t), \quad y(0) = g(0),$$

  with $\lambda = -10^6$, $g(t) = \sin(t)$, $t_e = 10$, and exact solution $y(t) = \sin(t)$.

- ROBER (see [8]) with $t_e = 10^8$.

- The Kreiss problem [13]

$$y' = R(t)\Lambda(\varepsilon)R^{-1}(t), \quad y(0) = \begin{pmatrix} 1 \\ 2.6 \end{pmatrix}, \quad 0 \le t \le 1,$$

with

$$R(t) = \begin{pmatrix} \cos(-\theta t) & \sin(-\theta t) \\ -\sin(-\theta t) & \cos(-\theta t) \end{pmatrix}, \quad \Lambda(\varepsilon) = \begin{pmatrix} -\frac{1}{\varepsilon} & 0 \\ 0 & -1 \end{pmatrix}.$$

We have used $\varepsilon = 10^{-4}$ and $\theta = 1$. The problem is therefore characterized by a strongly varying Jacobian.

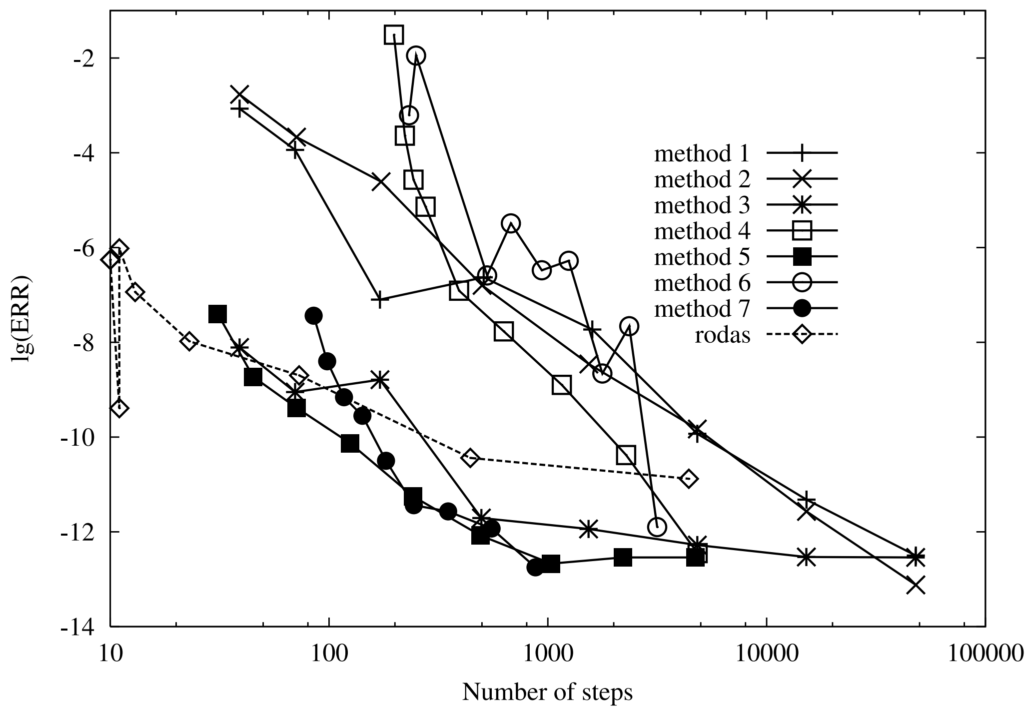

Figure 2: Results for Prothero-Robinson

Our aim was not to optimize the code with respect to the computing time but rather to consider the performance of the methods with respect to stability. As characterization of performance we therefore display the obtained accuracy versus the number of steps. To get some feeling how our methods compare with other codes we also display the results for the state of the art code RODAS [8]. Numerical comparisons of stiffly accurate two-step

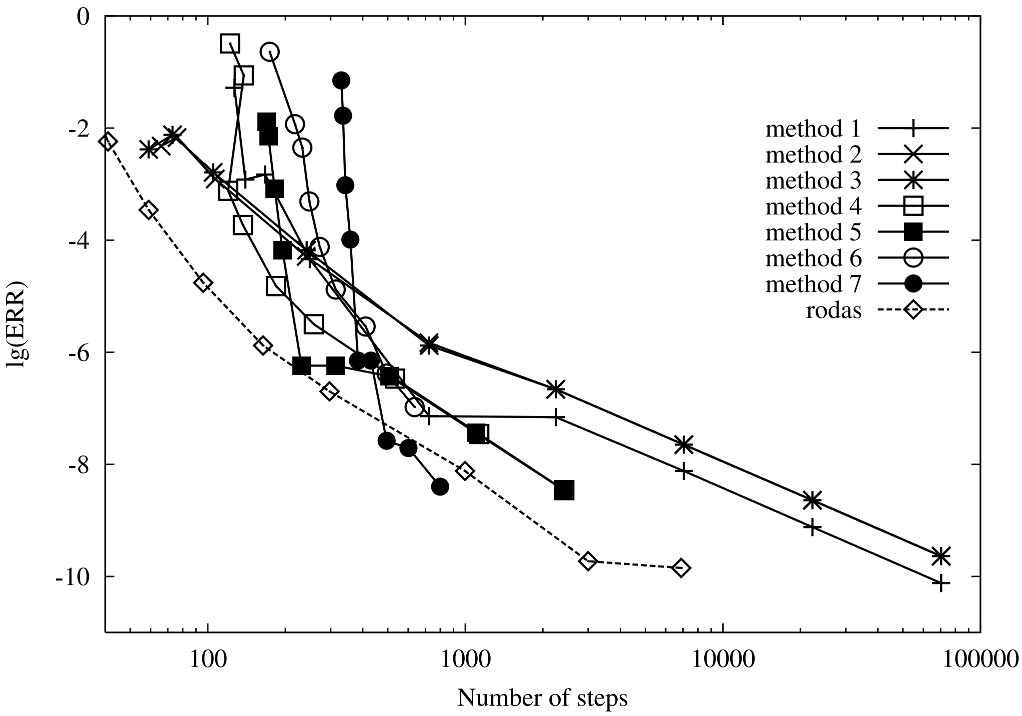

Figure 3: Results for the Kreiss problem

W-methods with other codes for larger problems with respect to computing time can be found in [17].

For the Prothero-Robinson equation the stiffly accurate methods are clearly superior, what can be explained by the convergence results for singularly perturbed problems for these methods ([19]).

For the other two problems the performance of the Methods 2 and 3 is nearly identical. The three and four-stage methods are also comparable. For larger tolerances Method 4 is superior for the nonautonomous Kreiss problem which may be due to the location of the abscissas c_i in $[0, 1]$. For the ROBER problem the Method 5 which is stiffly accurate seems to be advantegeous.

Observe that the Method 1 experiences difficulties for ROBER, which may be caused by the lack of L-stability.

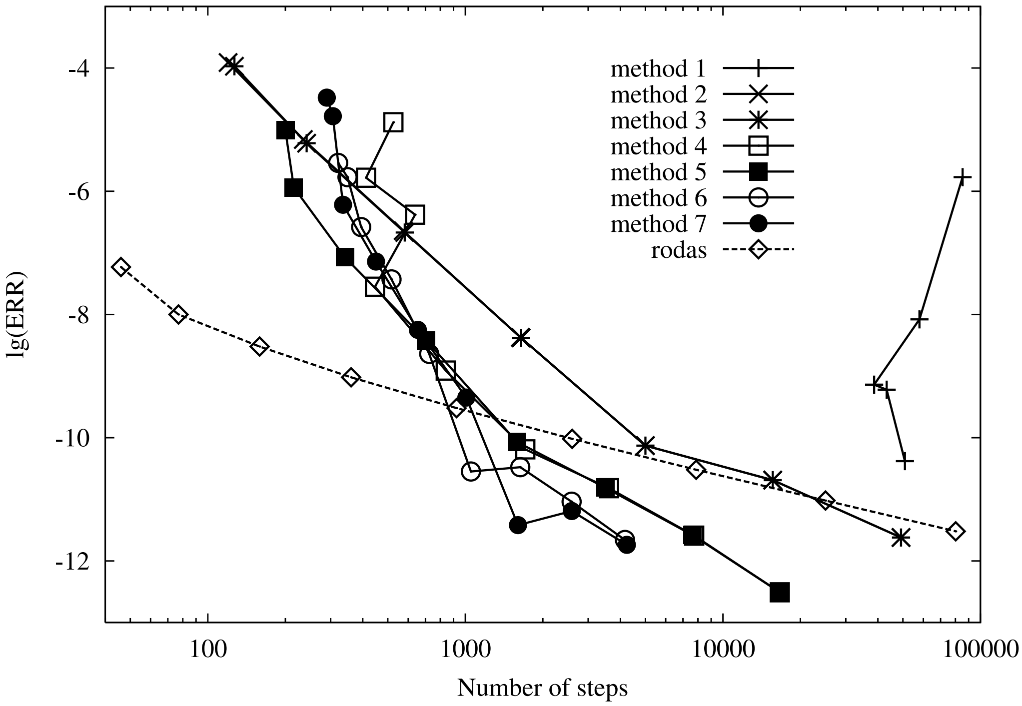

Figure 4: Results for ROBER

8 Concluding remarks

In this paper we described the construction of linearly implicit two–step W–methods with parallel stages of order p and stage order $q = p$ for $p = 2$, 3, and 4 which are appropriate for the numerical solution of stiff diffential systems. The derived methods are A–stable (Method 1) and A–stable as well as L–stable (Methods 2–7) if the stepsize of integration is held constant. It was also demonstrated numerically that these methods preserve good stability properties in a variable stepsize environment under very demanding conditions imposed on the stepsize pattern. The initial tests of these methods on various well known stiff systems are promising and indicate that these methods are competetive with state–of–the–art codes for stiff differential equations.

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