Two-step W-Methods for stiff ODE systems

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Abstract. We study a new class of time integration methods based on a s-stage linearly implicit two-step scheme. The convergence of the methods can be shown with the help of some simplifying assumptions. We derive some L- and L(α)-stable two-step W-methods (TSW-methods) with $s = 2$ and $s = 3$ of order $p = s$ and stage order $q = s$. Numerical comparisons show the efficiency of the methods, especially in combination with Krylov-techniques for large stiff systems.

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1 Introduction

For the numerical approximation of the solution $y(t)$ of a system of ordinary differential equations

$$y' = f(t, y), \quad y(t_0) = y_0 \in \mathbb{R}^n, \tag{1}$$

we propose a new class of two-step W-methods (TSW-methods). For a timestep from $t_m \to t_{m+1}$ with stepsize $h_m := t_{m+1} - t_m$ we compute the numerical solution $u_{m+1} \approx y(t_{m+1})$ by the s-stage scheme

$$Y_{mi} = u_m + h_m \sum_{j=1}^{s} a_{ij} k_{m-1,j} + h_m \sum_{j=1}^{i-1} \tilde{a}_{ij} k_{m,j}, \tag{2a}$$

$$(I - h_m \gamma T_m) k_{m,i} = f(t_m + c_i h_m, Y_{mi}) + h_m T_m \sum_{j=1}^{s} \gamma_{ij} k_{m-1,j} + h_m T_m \sum_{j=1}^{i-1} \tilde{\gamma}_{ij} k_{mj}, \tag{2b}$$

$$u_{m+1} = u_m + h_m \sum_{j=1}^{s} \left(b_j k_{m,j} + v_j k_{m-1,j} \right), \tag{2c}$$

with a problem dependent matrix $T_m \in \mathbb{R}^{n,n}$, usually an approximation to the Jacobian $f_y(t_m, u_m)$. If we choose $\tilde{a}_{ij} = \tilde{\gamma}_{ij} = 0$ we obtain the recently introduced class of parallel two-step W-methods, PTSW-methods [9, 10, 11]. In these methods all s stage values can be computed in parallel. On

the other side, if we have $a_{ij} = \gamma_{ij} = v_i = 0$ in the scheme we will get classical (one-step) ROW- and W-methods, e.g. [6]. The aim of this paper is to make use of the generalization to construct methods which a more efficient than PTSW-methods in a non-parallel computing environment.
TSW-methods fit into the framework of general linear methods. Recently, Butcher and Jackiewicz (e.g. [1, 2]) studied some related fully implicit methods suitable for stiff problems. Explicit two-step methods with $T_m = 0$ have been applied successfully to nonstiff problems, e.g. Cong et al. [4].
In Section 2 we give simplifying assumptions for the construction of methods with s stages having order s and stage order s.
In Section 3 we describe the construction of particular L- and L(α)-stable methods with $s = 2$ and $s = 3$.
Section 4 contains a description of the implementation of TSW-methods.
Numerical experiments in Section 5 show the potential of the new class of integration methods.

2 Order conditions and linear stability

2.1 Order conditions

We insert exact values and study the local residual errors.

Lemma 1 (simplifying assumptions). *Let $y(t)$ be sufficiently smooth. Denote $h = h_{m-1}$ and $\sigma h = h_m$ with a bounded stepsize ratio σ. If we insert exact values $y(t_m)$ for u_m, $y(t_m + c_i h_m)$ for Y_{mi}, and $y'(t_m + c_i h_m)$ for k_{mi} in the scheme* (2), *then we have*

$$-y(t_m + c_i\sigma h) + y(t_m) + \sigma h \sum_{j=1}^{s} a_{ij} y'(t_m + (c_j - 1)h) + \sigma h \sum_{j=1}^{i-1} \tilde{a}_{ij} y(t_m + c_j\sigma h) = \mathcal{O}(h^{q+1}) \quad \text{(3a)}$$

$$h_m \gamma T_m y'(t_m + c_i\sigma h) + \sigma h T_m \left[\sum_{j=1}^{s} \gamma_{ij} y'(t_m + (c_j - 1)h) + \sum_{j=1}^{i-1} \tilde{\gamma}_{ij} y'(t_m + c_j\sigma h) \right] = \mathcal{O}(h^{q+1}) \quad \text{(3b)}$$

$$-y(t_m + h) + y(t_m) + \sigma h \sum_{j=1}^{s} \big(b_j y'(t_m + c_j\sigma h) + v_j y'(t_m + (c_j - 1)h) \big) = \mathcal{O}(h^{p+1}) \quad \text{(3c)}$$

with an arbitrary matrix T_m if and only if the simplifying assumptions

$$C(q): \quad \sigma^l c_i^l / l! = \sigma \sum_{j=1}^{s} a_{ij} (c_j - 1)^{l-1}/(l-1)! + \sigma^l \sum_{j=1}^{i-1} \tilde{a}_{ij} c_j^{l-1}/(l-1)!, \quad l = 1, \ldots, q \quad \text{(4a)}$$

$$\Gamma(q): \quad -\gamma \sigma^l c_i^{l-1}/(l-1)! = \sigma \sum_{j=1}^{s} \gamma_{ij} (c_j - 1)^{l-1}/(l-1)! + \sigma^l \sum_{j=1}^{i-1} \tilde{\gamma}_{ij} c_j^{l-1}/(l-1)!, \quad l = 1, \ldots, q \quad \text{(4b)}$$

for $i = 1, \ldots, s$, and

$$B(p): \quad \sigma^l / l! = \sigma^l \sum_{i=1}^{s} b_i c_i^{l-1}/(l-1)! + \sigma \sum_{i=1}^{s} v_i (c_i - 1)^{l-1}/(l-1)!, \quad l = 1, \ldots, p, \quad \text{(4c)}$$

hold.

Proof. Follows by Taylor-series expansion. □

The local error bounds given by the simplifying assumptions in Lemma 1 imply convergence for the global errors

$$\varepsilon_m = \|y(t_m) - u_m\|, \quad \nu_{m+1} = \max_{i=1}^{s} \|y'(t_m + c_i h_m) - k_{mi}\| \tag{5}$$

as stated in the following theorem.

Theorem 1. *Assume that the initial errors satisfy $\varepsilon_0 = \mathcal{O}(h^p)$ and $\nu_0 = \mathcal{O}(h^q)$ with $p, q \in \mathbb{N}$. Let the coefficients of the method and the stepsize ratio be bounded, i.e. $\sigma_m = h_m/h_{m-1} < \sigma_{\max}$. If the method (2) satisfies the simplifying assumptions $C(q)$, $\Gamma(q)$ 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.*

Proof. Analogously to the proof of Theorem 2.1 in [10]. □

If a method satisfies $C(q)$ and $\Gamma(q)$ we say the method has stage order q. We collect the coefficients of the method (2) in the matrices and vectors

$$A := (a_{ij}),\ \Gamma := (\gamma_{ij}),\ b := (b_i),\ v := (v_i),\ \tilde{A} := (\tilde{a}_{ij}), \quad \text{and} \quad \tilde{\Gamma} = (\tilde{\gamma}_{ij}). \tag{6}$$

We consider methods with $C(s), \Gamma(s)$ (i.e. stage order s) and $B(s)$. Using the matrices

$$V_0 = (c_i^{j-1}), P = \left(\binom{j-1}{i-1}\right)_{i,j=1}^{s}, D = \operatorname{diag}(i), S = \operatorname{diag}(\sigma^{i-1}), C = \operatorname{diag}(c_i), V_1 = V_0 P^{-1} \tag{7}$$

we have a compact representation of the simplifying assumptions:

$$C(s): \qquad CV_0 = (AV_1 S^{-1} + \tilde{A} V_0) D \tag{8a}$$

$$\Gamma(s): \qquad -\gamma V_0 = (\Gamma V_1 S^{-1} + \tilde{\Gamma} V_0) \tag{8b}$$

$$B(s): \qquad \mathbb{1}^T = (b^T V_0 + v^T V_1 S^{-1}) D, \tag{8c}$$

where $\mathbb{1}^T = (1, \dots, 1)$ denotes a vector with s ones. We assume that the parameters $c_i, \gamma, \tilde{\gamma}_{ij}, b_i$ and $\tilde{a}_{ij}$ do not depend on the stepsize ratio σ. The remaining parameters a_{ij}, γ_{ij} and v_i may depend on σ and can be obviously calculated from (8) by solving small linear systems.

2.2 Linear stability

Applied to the linear scalar test equation $y' = \lambda y$ with $z = h_{m-1}\lambda$, $\sigma = h_m/h_{m-1}$ we get a matrix recursion for the numerical solution with $K_m := [k_{m1}, \dots, k_{ms}]^T$

$$\begin{pmatrix} h_m K_m \\ u_{m+1} \end{pmatrix} = M(z) \begin{pmatrix} h_{m-1} K_{m-1} \\ u_m \end{pmatrix} \tag{9}$$

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

$$M(z) = \begin{pmatrix} \sigma W(z)\beta & W(z)\mathbb{1} \\ \sigma(b^T W(z)\beta + v^T) & 1 + b^T W(z)\mathbb{1} \end{pmatrix} \tag{10}$$

with $\beta := A + \Gamma$, $\tilde{\beta} := \tilde{A} + \tilde{\Gamma}$ and $W(z) = [(1 - z\gamma)I - z\tilde{\beta}]^{-1} z$. It is clearly visible from (10) that the matrix $M(z)$ depends on σ. But, less obvious, β and v^T depend on σ too. From the simplifying assumptions C(s), Γ(s) and B(s) (i.e. Eq. (8)) we derive

$$\beta = [CV_0 D^{-1} - \gamma V_0 - \tilde{\beta} V_0] S V_1^{-1} = [CV_0 D^{-1} + W_\infty^{-1} V_0] S V_1^{-1}, \quad \text{with } W_\infty := W(\infty) = -(\gamma I + \tilde{\beta})^{-1}. \tag{11}$$

For constant step size (i.e. $\sigma = 1$) the stability of the numerical scheme is governed by the spectral radius of the amplification matrix. This leads to the following definition.

Definition 1 (A-stability, L-stability). We call the set $\mathcal{S} = \{z \in \mathbb{C} : \varrho(M(z)) < 1\}$ with the matrix $M(z)$ defined in (10) for $\sigma = 1$ stability domain of the TSW-method. The method is called A(α)-stable if $\{z \in \mathbb{C} : |\arg(z) - \pi| \leq \alpha\} \subseteq \bar{\mathcal{S}}$. We call a method *stiffly accurate* if for all fixed $u_m, k_{m-1,i}, \quad i = 1, \ldots, s$ the condition

$$\lim_{|z| \to \infty} u_{m+1} = 0 \tag{12}$$

holds. A method is called L(α)-stable if it is A(α)-stable and (12) is fulfilled. It is said to be A-stable resp. L-stable if $\alpha = 90°$. $\square$

The stiff-accuracy-condition (12) is equivalent to a vanishing last row in the stability matrix $M(z)$ for $|z| \to \infty$, i.e. $e_{s+1}^T M(\infty) = 0$. This can be satisfied also for variable stepsize and gives raise to the following lemma.

Lemma 2 (stiff accuracy). *Let $C(s), \Gamma(s)$ and $B(s)$ be satisfied. Then we have $e_{s+1}^T M(\infty) = 0$ iff $c_k = 1$ for some k and*

$$b^T = -e_k^T W_\infty^{-1} = e_k^T [\gamma I + \tilde{\beta}], \quad v^T = e_k \beta. \tag{13}$$

Proof. The nontrivial part is from $e_{s+1}^T M(\infty) = 0$ to (13). Let $e_{s+1}^T M(\infty) = 0$, i.e.

$$b^T W_\infty \beta + v^T = 0, \quad \text{and} \quad 1 + b^T W_\infty \mathbb{1} = 0, \tag{14}$$

be satisfied. We can compute v^T from the first relation. Putting this into $B(s)$ and using (11) gives

$$\mathbb{1}^T = (b^T V_0 - b^T W_\infty [C V_0 D^{-1} + W_\infty^{-1} V_0]) D \tag{15}$$

$$\mathbb{1}^T = -b^T W_\infty C V_0. \tag{16}$$

Reordering of the right part from (14) and (16) gives

$$b^T W_\infty V_0 = -\mathbb{1}^T, \quad \text{and } 1 = -b^T W_\infty C V_0 e_s.$$

Hence, $b^T W_\infty = -\mathbb{1}^T V_0^{-1}$ and $1 = \mathbb{1}^T V_0^{-1} C V_0 e_s$ hold. The latter is equivalent to $c_k = 1$ and (13) follows immediately. $\square$

For $k = s$, Eq.(13) reduces to

$$b^T = -e_s^T W_\infty^{-1} = e_s^T [\gamma I + \tilde{\beta}], \quad v^T = e_s^T \beta, \quad c_s = 1. \tag{17}$$

3 Construction of particular methods

3.1 Preliminaries

In the following we restrict our discussion to the case:

$$C(s), \Gamma(s), B(s), \tilde{\Gamma} = 0, \quad \text{and Eq. (17)}. \tag{18}$$

The remaining free $(s^2 + 2)/2$ parameters $\gamma, c_1, \ldots, c_{s-1}, \tilde{a}_{21}, \ldots, \tilde{a}_{s,s-1}$ should not depend on the stepsize ratio σ. We do not claim that these assumptions are optimal. But they made it easier for us to find good parameter sets. For this search we tried a lot of different heuristics. Some of them involved rather technical computations made feasible by the power of computer algebra systems. We used different criterions: the magnitude of the leading error constant $|C_{p+1}|$, the angle α of the L(α)-stability, a critical stepsize ratio σ_{crit} (defined below) and the norm of the coefficient matrices A and Γ.

We define the leading error constant C_{s+1} by the residual error in $B(s+1)$, i.e.

$$(s+1)!C_{s+1} = 1 - \left[b^T C V_0 + v^T (C-I) V_1 \sigma^{-s}\right] e_s(s+1). \tag{19}$$

It is clear that from $C_{s+1}=0$ follows B$(s+1)$ and vice versa. Note, that for a TSW-method satisfying (17) the condition B$(s+1)$ is linear in the parameters $\tilde{a}_{s,i}$.

To measure the sensitiveness of the method with regard to consecutive step size enlargements we define a critical stepsize ratio by $\sigma_{\text{crit}} = \inf\limits_{\sigma>0}\{\varrho(G_\infty(\sigma)) > 1\}$ with $G_\infty(\sigma) := W_\infty \beta$.

To compute (numerically) the angle α of the L(α)-stability by $\alpha = \inf\limits_{z\in\partial\mathcal{S}}\{|\arg(z)-\pi|\}$ we need (an approximation to) the boundary $\partial\mathcal{S}$ of the stability domain of TSW-method under consideration. Instead of working with the stability matrix $M(z)$ directly, we define a polynomial $p(x,z)$ in x and z of degree s by

$$p(x,z) := x^{-1}(1-z\gamma)^s \det(xI - M(z)), \tag{20}$$

and compute the roots z for fixed x lying on the unit circle. Since we have

$$\partial\mathcal{S} \subseteq \{z : \exists x \text{ with } |x| = 1 \text{ and } p(x,z) = 0\} =: R$$

we obtain α from $\alpha = \inf\limits_{z\in R}\{|\arg(z)-\pi|\}$.

Remark 1. To see that $p(x,z)$ is a polynomial in z (i.e. we do not need the exponent $s+1$ instead of s in the definition (20)) one may consider $T^{-1}M(z)T$ with a transformation $T = \begin{pmatrix} I & \\ b^T & 1\end{pmatrix}$. To see that $p(x,z)$ is a polynomial in x we note, that due to the stiff accuracy (17) we have $\det(M(z)) = 0$.

3.2 Methods with $s=2$ stages

We have three parameters: c_1, γ and $\tilde{a}_{21}$. We follow two ideas: (a) methods with $\varrho(M(\infty)) = 0$ and (b) methods with $B(3)$ for $\sigma = 1$. As we see below, the intersection of (a) and (b) is not empty: four fixed methods satisfying B(3) and $\varrho(M(\infty)) = 0$ exist.

(a) Methods with $\varrho(M(\infty)) = 0$. At first glance this requirement seems to be rather strong. For L-stability we need $\varrho(G_\infty) < 1$ only. However, we have seen some advantages in numerical experiments with PTSW-methods (see [10]) from $\varrho(G_\infty) = 0$ when we used a Krylov-method for solution of the linear stage equations. For a stiffly accurate TSW-method $\varrho(M(\infty)) = 0$ is identical with $\varrho(G_\infty) = 0$. For $\sigma = 1$ we obtain

$$G_\infty = \frac{1}{2\gamma^2(c_1-1)}\begin{bmatrix} -\gamma\, c_1\,(c_1 - 2\,\gamma) & -\gamma\,\left({c_1}^2 - 2\,c_1 + 2\,\gamma\right) \\ \tilde{a}_{2,1}{c_1}^2 - \gamma + 2\,\gamma^2 & \tilde{a}_{2,1}{c_1}^2 - 2\,\tilde{a}_{2,1}c_1 - 2\,\gamma\,c_1 + 3\,\gamma + 2\,\gamma^2 c_1 - 4\,\gamma^2 \end{bmatrix}.$$

From $\det(G_\infty) = 0$ follows

$$\tilde{a}_{21} = ({c_1}^2\gamma - {c_1}^2 - 2\,\gamma^2 c_1 + c_1 + 2\,\gamma^2 - \gamma)/c_1^2. \tag{21}$$

And then $\mathrm{tr}(G_\infty) = 0$ leads to

$$c_1 = 1 + \gamma^2 - 2\,\gamma \pm \sqrt{1 + 10\,\gamma^2 - 6\,\gamma + \gamma^4 - 4\,\gamma^3} \tag{22}$$

Hence, for every positive γ with $\gamma \notin [0.300102, 0.448377]$ we have two methods with $\varrho(M(\infty)) = 0$ defined by (22),(21) and (18). The leading error constant C_3 is independent of the choice made on c_1, we have $C_3 = \frac{5}{12} + 3/2\,\gamma^2 - 2\gamma$, i.e. for $\gamma \approx 0.2584$ and $\gamma \approx 1.0749$ we satisfy B(3). With (22), we find two different knots c_1 for each γ. A disadvantage of the two methods with $\gamma \approx 1.0749$ is the relative large magnitude of $c_1 \approx 1.577$ resp. $c_1 \approx -1.566$ and hence none of them is included into the numerical experiments. We obtain

$$p(x,z) = (-1+z\gamma)^2 x^2 - 1/2\,\left(2+2\,z\gamma^2+3\,z-8\,z\gamma\right)x + 1/2\,z\left(1+2\,\gamma^2-4\,\gamma\right).$$

Using this polynomial we compute the angle α of L(α)-stability. We find a monotone relationship, see Fig. 1. For $\gamma > 0.29$ all methods are L-stable. If we choose $\gamma = 1-1/2\sqrt{2}$ then we have $\varrho(G_\infty) = 0$ also for $\sigma \neq 1$, i.e. $\sigma_{\text{crit}} = \infty$. This gives us a L-stable method defined by

$$\gamma = 1-1/2\sqrt{2}, c_1 = 2\gamma, \tilde{a}_{21} = (1/2-\gamma)/(2\gamma), \quad \textbf{(TSW2A)}.$$

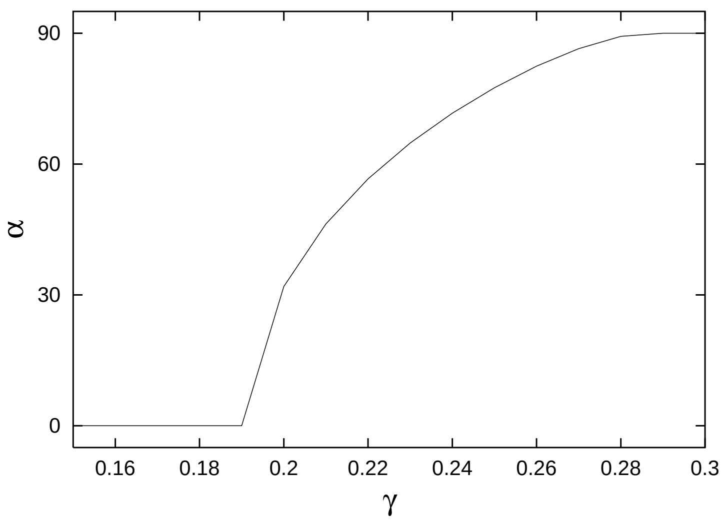

Figure 1: Angle α of L(α)-stability for methods with $s = 2$ and $\varrho(G_\infty) = 0$, i.e. methods which satisfy (21) and (22). For $\gamma > 0.29$ the methods remain L-stable.

(b) Methods with B(3). Condition $B(3)$ is linear in $\tilde{a}_{21}$. We can solve it for $\sigma = 1$, and with (18) we get

$$\tilde{a}_{21} = 1/6\,(5-12\,\gamma-3\,c_1+6\,\gamma\,c_1)/c_1, \tag{23}$$

with the free parameters c_1 and γ. Further, we satisfy B(3) also for $\sigma \neq 1$ iff

$$\gamma = \frac{3c_1-2}{6(c_1-1)} \tag{24}$$

holds. If we have (18) and (23), we can plot $\varrho(G_\infty)$ and α as functions of γ and c_1, see Fig. 2. L-stable methods exist for $\gamma > 0.7$ only.
For the computations, we choose the following method

$$c_1 = 1/3, \gamma = 1/4, \tilde{a}_{21} = 3/4, \qquad \textbf{(TSW2B)}. \tag{25}$$

TSW2B has $\varrho(G_\infty) = 1/3$ for $\sigma = 1$ and $\varrho(G_\infty) = 0$ for $\sigma = 3/2$. We see from (24) that condition $B(3)$ is satisfied. Since the method has $v^T = [0,0]$ B(3) holds for all σ. We compute $\alpha = 82.75°$ using the polynomial

$$p(x,z) = \left(\frac{1}{16}z^2 - 1/2\,z+1\right)x^2 + \left(-\frac{1}{48}z^2 - 1 - \frac{13}{24}\,z\right)x + \frac{1}{24}z. \tag{26}$$

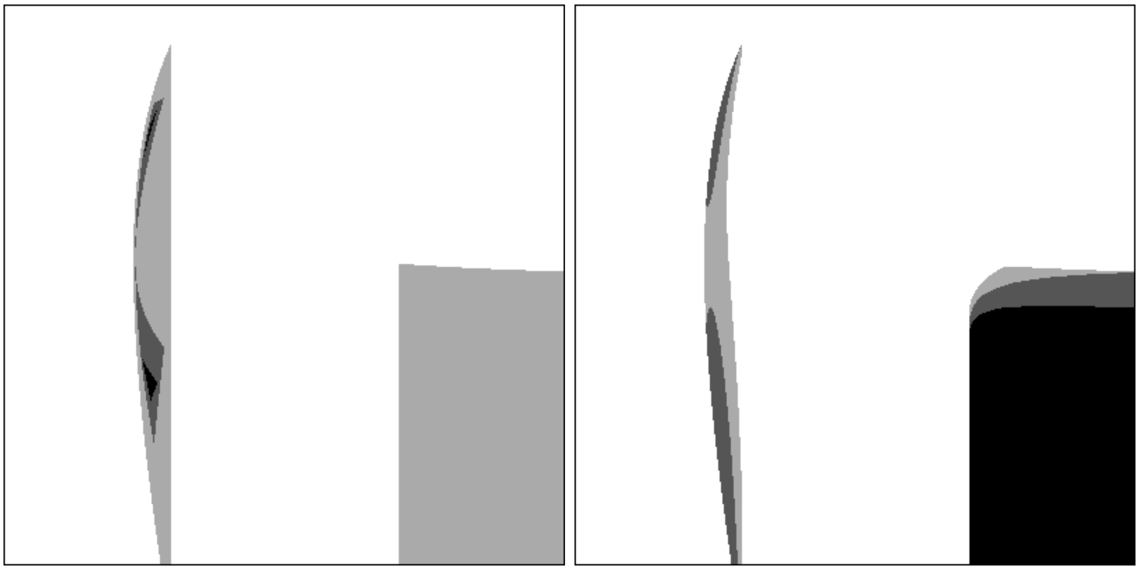

Figure 2: Spectral radius $\varrho(G_\infty)$ (left) and angle α of L(α)-stability (right) for TSW-methods with $s = 2$ stages satisfying B(3) depending on $\gamma \in [0,1]$ (x-axis) and $c_1 \in [0,1]$ (y-axis). The gray levels for the left picture are $\varrho \le 0.25$ (black), $\varrho \le 0.5$ (dark gray), $0.5 < \varrho \le 1$ (gray) and $\varrho > 1$ (white). In the right picture, we use black if $\alpha = 90°$ and gray levels for $\alpha > 80°$, $\alpha > 70°$ and white if $\alpha \le 70°$. We see L-stable methods for $\gamma > 0.7$ (right figure) but $\varrho < 0.25$ for $\gamma < 0.3$ (left) only.

3.3 Methods with $s = 3$ stages

Again, we assume the conditions summarized in (18). We have six parameters left: $c_1, c_2, \gamma, \tilde{a}_{21}, \tilde{a}_{31}$ and $\tilde{a}_{32}$. In the following, we analyze $\varrho(G_\infty) = 0$ for $\sigma = 1$. For parallel methods with $\tilde{a}_{21} = \tilde{a}_{31} = \tilde{a}_{32} = 0$ we would obtain the parallel methods derived in [10], e.g. PTSW3B. Here, we want to satisfy $\varrho(G_\infty) = 0$ by choosing appropriate $\tilde{a}_{21}, \tilde{a}_{31}, \tilde{a}_{32}$. We did the following computations with the help of Maple 7. They are not very difficult but some terms have large size. Let denote p_2, p_1 and p_0 the coefficients of the characteristic polynomial $\det(xI - G_\infty) = x^3 + p_2 x^2 + p_1 x + p_0$. From $p_0 = 0$ and $p_1 = 0$ we can derive $\tilde{a}_{31}$ and $\tilde{a}_{32}$ by solving a linear 2×2 system. Substituting this solution into p_2 gives a quadratic condition for $\tilde{a}_{21}$. If we fix c_1 we can plot the angle α of $L(\alpha)$-stability and the error constants as functions of γ and c_2 similar to Fig. 2. Using this approach we performed an exhaustive search. We present two methods:

- **(TSW3A)**

$$\gamma = 2/5, c_1 = 1/2, c_2 = 3/2,$$

$$\tilde{a}_{3,1} = \frac{1}{600}\,\frac{10130\,\tilde{a}_{2,1} + 6500\,\tilde{a}_{2,1}^2 - 19167}{75\,\tilde{a}_{2,1} - 83}, \tilde{a}_{3,2} = -\frac{1}{600}\,\frac{2650\,\tilde{a}_{2,1} - 2927}{75\,\tilde{a}_{2,1} - 83}$$

and $\tilde{a}_{21} = \frac{2711}{2200} - \frac{3}{2200}\sqrt{7561} \approx 1.113699076$. This method is L-stable. We have $|C_4| \approx 0.009$. $\sigma_{\text{crit}} = 1.528$.

- **(TSW3B)**

$$\gamma = 1/4, c_1 = 1/4, c_2 = 3/4, \tilde{a}_{21} = 1/2, \tilde{a}_{31} = 19/32, \tilde{a}_{32} = 5/32$$

This method is L(α)-stable with $\alpha \approx 83.49°$. We have $\varrho(G_\infty) = 0$ for all σ, i.e. $\sigma_{\text{crit}} = \infty$. We have $|C_4| = 23/1152 \approx 0.02$.

4 Implementation

One well-known advantage of W-methods is the straightforward implementation. For two-step W-methods some additional difficulties appear, namely the computation of starting values and the formulation for variable step size. We address these issues below. To avoid matrix-multiplications, it is common to work with transformated linear stage equations. We solve

$$(I - h_m \gamma T_m)(k_{m,i} + \xi_{mi}) = f(t_m + c_i h_m, Y_{mi}) + \xi_{mi} =: r_{mi}, \tag{27}$$

with $\xi_{mi} = \frac{1}{\gamma}\left[\sum_{j=1}^{s} \gamma_{ij} k_{m-1,j} + \sum_{j=1}^{i-1} \tilde{\gamma}_{ij} k_{m,j}\right]$ instead of (2b). Under assumption (18) the right hand sides r_{mi} satisfy $r_{mi} = \mathcal{O}(h_m^s)$ which is in interesting property especially if we use a Krylov method to solve (27).

To allow varying step size we need variable coefficients. In cases where the step size ratio σ changes we recompute a_{ij}, γ_{ij} and v_i using the simplifying assumptions (8). For larger ODE systems the small cost for these recomputations is negligible. The local error Err_{emb} is estimated by use of an embedded solution $\tilde{u}_{m+1}$, i.e.,

$$Err_{\text{emb}} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(\frac{u_{m+1,i} - \tilde{u}_{m+1,i}}{\texttt{ATOL} + \texttt{RTOL}|u_{m+1,i}|}\right)^2},$$

$$\tilde{u}_{m+1} = u_m + h_m \sum_{i=1}^{s}(b_{e,i} k_{m,i} + v_{e,i} k_{m-1,i}),$$

where **ATOL** and **RTOL** denote absolute and relative tolerances. We calculate the weights b_e, v_e of the embedded method by

$$b_e^T := 0.95 b^T, \qquad v_e^T := ((\mathbb{1}^T + \frac{1}{10} e_s^T) S D^{-1} - b_e^T V_0 S) V_1^{-1}.$$

Due to the '$\frac{1}{10}$'in the definition of v_e^T, condition B(s) is violated for the embedded method, i.e. we have $u_m - \tilde{u}_m = \mathcal{O}(h_m^s)$. For the computation of the starting values for the first step we use the RADAU code [7] for smaller problems and the one-step Krylov-W-code ROWMAP [12] for larger ones.

We consider two different implementations for TSW-methods:

1. For small systems LU decomposition for the solution of the linear systems is used. The Jacobian is approximated by finite differences. A heuristic is used to avoid frequent stepsize changes and expensive recomputations of the Jacobian, see [10].

2. For large systems we apply the full orthogonalization Arnoldi method for solving the s stage equations. For every stage, we start a new Krylov process. The dimension of the Krylov space is automatically adjusted such, that the residual error of the linear system in l_2-norm is less than $\texttt{KTOL} := \texttt{ATOL}/h$. The required Jacobian-vector products are approximated using finite differences. We compute a new stepsize h_{new} by

$$h_{\text{new}} = h_m \min(1.5, \max(0.75, Err_{\text{emb}}^{-1/s} \cdot 0.85)) \tag{28}$$

   If $Err_{\text{emb}} < 1$ we put $h_{m+1} = h_{\text{new}}$ otherwise we put $h_m := h_{\text{new}}$ and repeat the last time step.

We implemented the TSW-methods in FORTRAN. For the linear algebra we use BLAS and LAPACK. All computations were done in double precision. The codes can be obtained from the authors.

5 Numerical Results

We consider the following test problems:

- MEDAKZO from the CWI-IVP-testset [5]. The ODE system has 400 equations and a banded Jacobian.
- PLATE from [6]. The system is nonautonomous with 80 equations.
- BRUSS, the two-dimensional Brusselator equation, e.g. [8]. We choose the diffusion constant $D = 0.2$ and 100×100 grid points for the discretization.
- DIFFU2, a nonautonomous diffusion equation from [12]. We use 100×100 grid points.
- NILIDI from [12]. This problem originates from a scalar nonlinear diffusion equation semidiscretized using 100×100 grid points.

For the first two problems we use LU-decomposition. BRUSS, DIFFU2 and NILIDI are solved using the TSW-methods combined with the Krylov method for the solution of the linear systems.

We measure the computing time in seconds on a SunFire computer and compare it with the accuracy at the endpoint of the time integration measured in a weighted l_2-norm. All computations were done on one CPU. The tolerances used are $\mathtt{ATOL} = \mathtt{RTOL} = 10^{-l}$, $l = 2, \ldots, 8$.

To evaluate the numerical efficiency of the TSW-methods we include computations with the following reference methods:

- the fourth order Rosenbrock method RODAS [6] (version of october 1996).
- the BDF-code VODPK (version of may 1997) [3] which uses GMRES for the solution of the linear equations.
- parallel two-step W-methods with two stages PTSW2A and PTSW2B
- parallel two-step W-methods with three stages PTSW3A and PTSW3B.

Discussion of the results. For PLATE and MEDAKZO (Fig. 3 and Fig. 4) the TSW-methods of order $p = 3$ TSW2B, TSW3A and TSW3B compete well with RODAS. The method TSW2A of order 2 is competitive for mild tolerances only.

Hardly any difference between TSW2A and TSW2B can be seen in the efficiency for the semidiscretized parabolic problems BRUSS, DIFFU2 and NILIDI (Fig. 5, 6 and 7). The best method in our tests using Krylov-techniques is TSW3B. It outperforms VODPK for BRUSS with tolerances less then 10^{-5} and for DIFFU2 and NILIDI for nearly all tolerances.

The numerical experiments give the clear answer "yes" to the introductory question of this paper whether PTSW-methods could be improved for non-parallel computing environment: in all examples we see sequential TSW-methods to be superior to the PTSW-methods for sequential computations.

These numerical results and other tests show the great potential of two-step W-methods. They can compete with well-known codes. Their main field of application seems to be the solution of large stiff systems in combination with Krylov techniques.

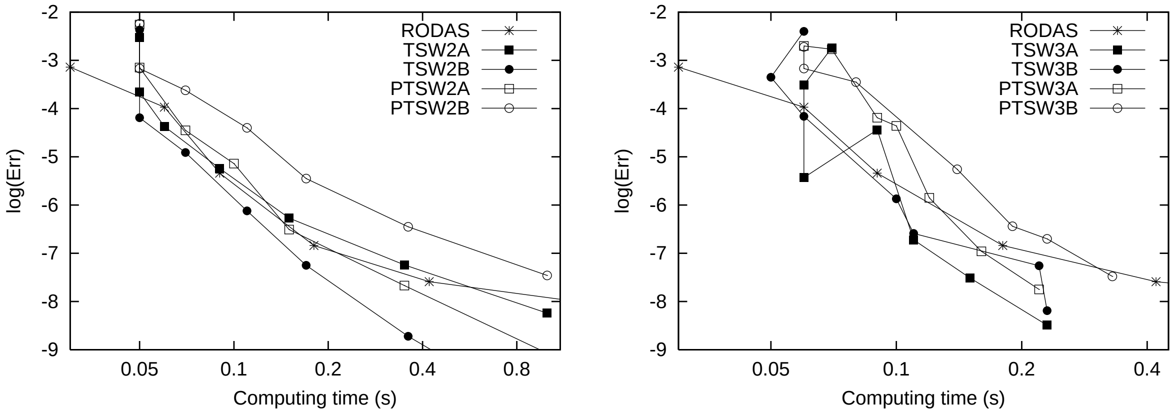

Figure 3: Results for PLATE.

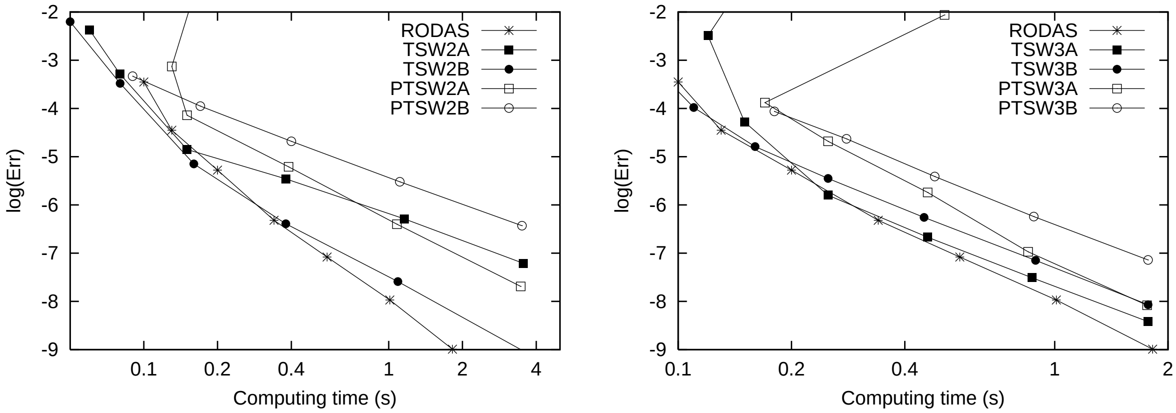

Figure 4: Results for MEDAKZO.

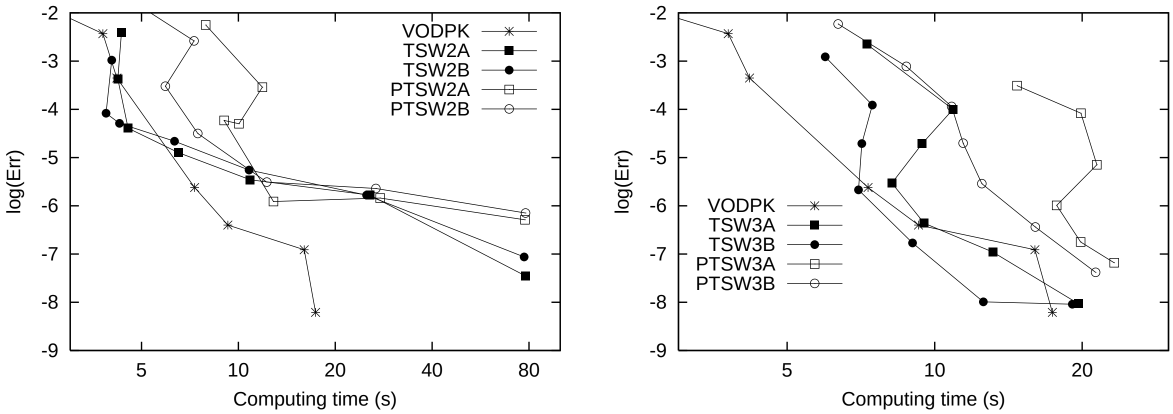

Figure 5: Results for BRUSS.

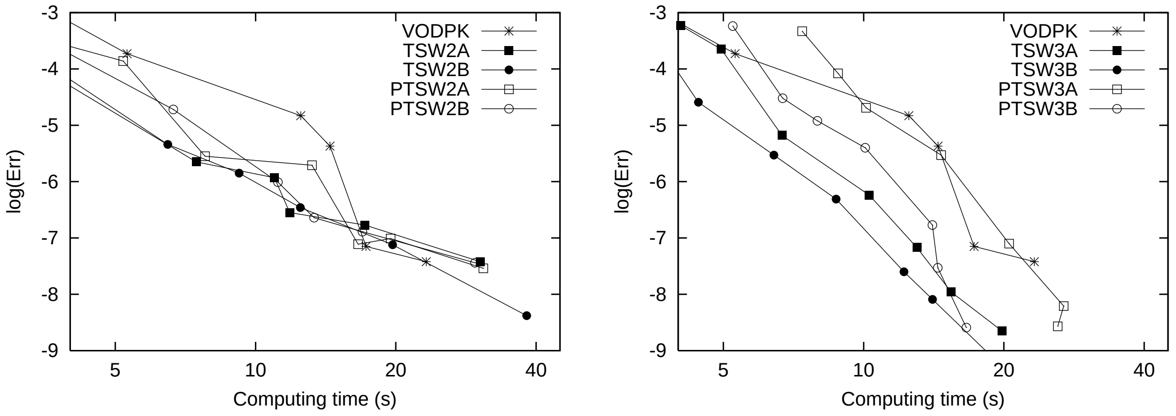

Figure 6: Results for DIFFU2.

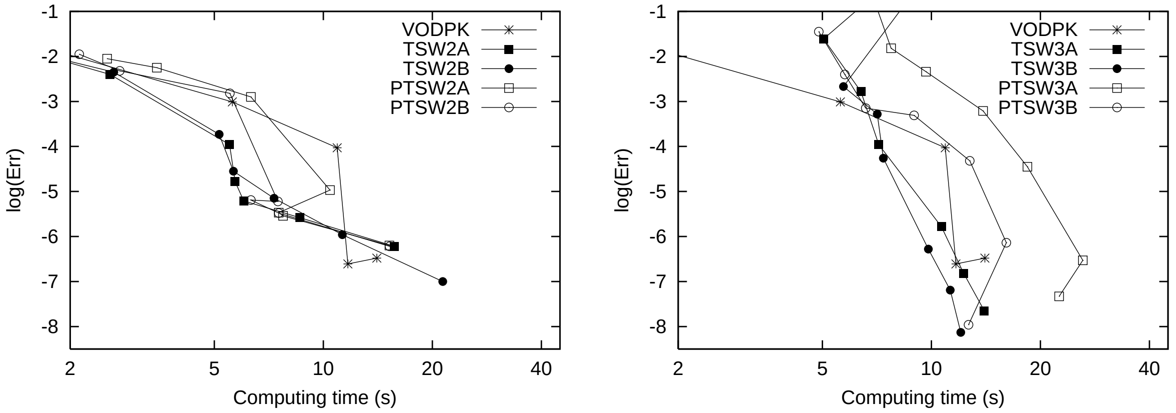

Figure 7: Results for NILIDI.

6 Conclusions

We are pleased to see that the new TSW-methods are competitive with production codes like RODAS for some small stiff test problems using LU decomposition. We see that this class of integration methods successfully incorporates some favorable properties, e.g. high stage order, robustness and cheap steps. Even more interesting is the performance for large stiff ODE systems were a Krylov method is used for the solution of the linear equations. This makes TSW-methods to be a notable option for the solution of more complex problems. Topics of further work include a detailed study of the Krylov process. We expect some advantages of using a multiple Arnoldi process with nested Krylov spaces as described in [12].

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