Two-step W-methods with parallel stages

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Abstract

Two-step W-methods are linearly implicit time-stepping methods using s external stages that may be processed in parallel. Methods with order $s+1$ and stage order s exist. Appropriate generalizations for the concepts of A- and L-stability are derived as well as necessary conditions for A-stability and sufficient conditions for stiff accuracy. We construct methods of order four where no order reduction occurs in the Prothero-Robinson equation. Already in a sequential variable stepsize implementation some of these methods are competitive with standard ROW-codes on test problems from the literature. Tests using a very simple parallelization are promising.

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1 Introduction

The numerical solution of stiff initial value problems

$$y' = f(t,y), \quad y(t_0) = y_0, \tag{1.1}$$

with right hand side $f : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n$ is of great practical interest especially for large dimensions n. The linearly-implicit ROW- and W-methods like GRK4T ([5], [4]) and RODAS [4] are very efficient for such problems. However, these methods are not suited for a parallel implementation with parallelism across the method. Intensive work is being done on parallel methods for initial value problems, many results can be found in the textbook [1].

Recently, numerical tests on a parallel computer have shown the efficiency of special explicit two-step Runge-Kutta-methods (that allow an efficient parallel implementation) for nonstiff problems [2]. In this paper we combine the parallel potential of such methods with the good properties of ROW- and W-methods for stiff systems and consider linearly-implicit two-step methods having s external stages. For a time step from t_m to $t_{m+1} = t_m + h_m$ the methods have the following form,

$$\begin{aligned} Y_{mi} &= u_m + h_m \sum_{j=1}^{s} a_{ij} k_{m-1,j}, \\ (I - h_m \gamma_i T_m) k_{mi} &= f(t_m + c_i h_m, Y_{mi}) + h_m T_m \sum_{j=1}^{s} \gamma_{ij} k_{m-1,j}, \quad i = 1, \ldots, s, \\ u_{m+1} &= u_m + h_m \sum_{i=1}^{s} (b_i k_{mi} + v_i k_{m-1,i}). \end{aligned} \tag{1.2}$$

Important properties of the methods depend on the choice of the matrix T_m. The best (but most expensive) choice with respect to stability and accuracy is $T_m = f'(t_m, u_m)$ and leads to a

ROW-type method. With the other extreme, $T_m = 0$, the methods reduce to explicit two-step RK-methods which are not suited for stiff problems. We assume that the off-step points are simple, $c_i \neq c_j$, $i \neq j$, and that $\gamma_i > 0$, $i = 1, \ldots, s$. We note, that the s external stages can be processed in parallel with arbitrary γ_i. However, in a sequential implementation or a parallel implementation with some parallel preprocessing of the large matrix $I - h_m \gamma T_m$ it may be an advantage to have only one single parameter $\gamma_i \equiv \gamma$. Since the analysis of this confluent case is also simpler we will concentrate on it here.

In this paper we start the investigation of these methods with some theoretical properties that are independent of the computing environment. Numerical tests show that some methods are competitive with classical ROW-methods already in a sequential implementation and, hence, should be good candidates for parallel computations.

In Section 2 we give simplifying assumptions for the construction of methods having higher order and stage order and prove convergence results. A consequence of their two-step structure is that the coefficients of these methods depend on the stepsize ratio and have to be recomputed from a small linear system if that ratio changes. However, for large n this cost is negligible.

In Section 3 we consider linear stability properties and transfer some well-established concepts like A- and L-stability to these two-step methods. Especially stiffly accurate methods possess favourable stability properties that pay off in practical computations.

Classical ROW-methods encounter strong order reduction when applied to the Prothero-Robinson test equation. But this is not the case for two-step W-methods due to their high stage order. B-convergence results are given in Section 4.

Numerical results with a first sequential implementation using automatic stepsize control show the efficiency of our methods also in comparison with popular ROW-codes, see Section 5. A simple parallelization demonstrates their potential for parallel computations.

The following notations are used. The coefficients of the method are collected in the $s \times s$-matrices $A = (a_{ij})$, $\Gamma = (\gamma_{ij})$, $G = \mathrm{diag}(\gamma_i)$ and s-vectors $b = (b_i)^T$, $v = (v_i)^T$. The unit basis vectors are denoted by e_i, $i = 1, \ldots, s$ and $\mathbb{1} = (1, \ldots, 1)^T$ is the vector of ones. $\mathbb{C}_- := \{z \in C : \mathrm{Re} z \leq 0\}$ is the left complex halfplane.

2 Simplifying assumptions and convergence

This section begins the analysis of the two-step W-methods introduced in Section 1 with some convergence results. The main difficulty in the analysis of these methods is due to the fact that in addition to the approximations u_m for the solution values $y(t_m)$ the time step recursion is inflated by the vectors Y_{mi}, k_{mi}. Since the role of these vectors is not a priori clear it is also not evident what a sensible definition for consistency of these methods should be. Hence, in order to avoid ambiguities, we call our attention directly to convergence estimates. It turns out, that the stage increments k_{mi} will be rather good approximations for the derivative of y. So, we consider the residual errors η_m and δ_{mi} that appear when the exact values $y(t_m)$ and $y'(t_m + c_i h_m)$ are substituted for u_m and k_{mi} in (1.2):

$$\tilde{Y}_{mi} = y(t_m) + h_m \sum_{j=1}^{s} a_{ij} y'(t_{m-1} + c_j h_{m-1})$$

$$(I - h_m \gamma_i T_m) y'(t_m + c_i h_m) = f(\tilde{Y}_{mi}) + h_m T_m \sum_{j=1}^{s} \gamma_{ij} y'(t_{m-1} + c_j h_{m-1}) + \delta_{mi} \tag{2.1}$$

$$y(t_{m+1}) = y(t_m) + h_m \sum_{i=1}^{s} b_i y'(t_m + c_i h_m) + h_m \sum_{i=1}^{s} v_i y'(t_{m-1} + c_i h_{m-1}) + \eta_m$$

Since the potential for stepsize adaptation is very important for time stepping schemes we will try to avoid stepsize restrictions as far as possible and introduce the stepsize ratios $\sigma_m := h_m/h_{m-1}$. For simplicity we will only write σ if the index is clear from the context. The residual errors in (2.1) can be analysed with the help of the following simplifying assumptions:

$$
\begin{aligned}
C(q):&\quad \sum_{j=1}^{s} a_{ij}(c_j - 1)^{l-1} = \sigma^{l-1}\frac{c_i^l}{l}, \quad l = 1, ..., q\\
\Gamma(q):&\quad \sum_{j=1}^{s} \gamma_{ij}(c_j - 1)^{l-1} = -\gamma_i \sigma^{l-1} c_i^{l-1}, \quad l = 1, ..., q,\\
C\Gamma(r):&\quad \sum_{j=1}^{s}(a_{ij} + \gamma_{ij})(c_j - 1)^{l-1} = \sigma^{l-1}\left(\frac{c_i^l}{l} - \gamma_i c_i^{l-1}\right), \quad l = 1, ..., r,\\
B(p):&\quad \sum_{j=1}^{s} b_j \sigma^{l-1} c_j^{l-1} + \sum_{j=1}^{s} v_j (c_j - 1)^{l-1} = \frac{\sigma^{l-1}}{l}, \quad l = 1, ..., p.
\end{aligned}
\tag{2.2}
$$

Note, that $C(q)$ and $\Gamma(q)$ imply $C\Gamma(q)$. A method is said to have stage order q if the conditions $C(q)$ and $\Gamma(q)$ are satisfied.

It is readily seen in (2.2) that the coefficients of the methods will depend on the stepsize ratio σ and have to be recomputed in a practical implementation after changes in σ. But this will not affect the efficiency of the methods if the dimension n is large which is the situation of practical interest. We also will neglect this dependence on σ_m in our notation (but not in the analysis) by avoiding an additional index m on the coefficients of the method. Since the stepsizes used in a practical computation with stiff systems may have different magnitudes we will not restrict the relation between maximal and minimal stepsize. We only assume that the stepsize changes are bounded, i.e., that there exist constants $\hat{\sigma}$ and $\tilde{\sigma}$ such that

$$\tilde{\sigma} \le \sigma_m = h_m/h_{m-1} \le \hat{\sigma}. \tag{2.3}$$

And we assume that the coefficients of the method are bounded under this condition (2.3). This is no severe restriction for methods of primary interest.

Remark 2.1 *For methods with stage order $q = s$ and c_i given the coefficients a_{ij} and γ_{ij} are uniquely determined by (2.2) and bounded due to (2.3). So, for lower order methods it is always possible to find bounded coefficients for bounded stepsize ratios (2.3).*

As we mentioned above we will consider the stage increments k_{mi} as being approximations for derivatives of y. So we now discuss bounds for the global errors

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

The following stability lemma will be useful.

Lemma 2.1 *Let the elements of nonnegative sequences (ε_m), (ν_m) satisfy*

$$\begin{pmatrix}\varepsilon_{m+1}\\ \nu_{m+1}\end{pmatrix} \le \begin{pmatrix}1 + a h_m & b h_m\\ c & bc\, h_m\end{pmatrix}\begin{pmatrix}\varepsilon_m\\ \nu_m\end{pmatrix} + h_m \begin{pmatrix}f_m\\ g_m\end{pmatrix}, \quad m = 0, 1, ...$$

with nonnegative constants a, b, c and $f_m, g_m, h_m \geq 0$ and let $\sum_{j=0}^{m} h_j \leq (t_e - t_0)$, $L := a + bc$. Then, under condition (2.3) holds

$$\max\{\varepsilon_m, \nu_m\} \leq C e^{L(t_e - t_0)}(\varepsilon_0 + bh_0\nu_0 + (t_e - t_0)\max_j\{f_j + h_j g_j\}), \quad m = 0, 1, \dots .$$

Proof. With the relation

$$\begin{pmatrix} 1 + ah_m & bh_m \\ c & bch_m \end{pmatrix} \leq \begin{pmatrix} 1 + ah_m \\ c \end{pmatrix} \begin{pmatrix} 1 & bh_m \end{pmatrix} =: R_m$$

we obtain

$$\begin{pmatrix} \varepsilon_{m+1} \\ \nu_{m+1} \end{pmatrix} \leq \prod_{i=0}^{m} R_{m-i} \begin{pmatrix} \varepsilon_0 \\ \nu_0 \end{pmatrix} + \sum_{j=0}^{m} h_{m-j} \prod_{i=0}^{j-1} R_{m-i} \begin{pmatrix} f_{m-j} \\ g_{m-j} \end{pmatrix}$$

Now, using the rank-1 structure of $R_m = v_m w_m^T$, $v_m^T := (1 + ah_m, c)$, $w_m^T := (1, bh_m)$ we see, that $R_m \cdots R_{m-k} = v_m \big(\prod_{l=0}^{k-1} w_{m-l}^T v_{m-l-1} \big) w_{m-k}^T$ and obtain the bound

$$\prod_{l=0}^{k-1} w_{m-l}^T v_{m-l-1} = \prod_{l=0}^{k-1} (1 + ah_{m-l-1} + bch_{m-l}) \leq e^{(a+bc)(t_e - t_0)},$$

since $\sum_{j=0}^{m} h_{m-j} \leq t_e - t_0$. Now, with

$$v_m w_{m-j+1}^T \begin{pmatrix} f_{m-j} \\ g_{m-j} \end{pmatrix} = v_m (f_{m-j} + bh_{m-j+1} g_{m-j}) \leq C \max_{l=0}^{m}\{f_l + h_l g_l\} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

and a similar estimate for the product containing the initial values the statement follows. ∎

The lemma is used to prove our main convergence result. For simplicity we consider autonomous problems only. The choice of the system matrix T_m in the implicit step has some influence on convergence. It turns out, that one order condition (2.2) can be saved if $T_m \cong f'(u_m)$. The maximal stepsize will be denoted $h = \max_m h_m$.

Theorem 2.1 *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 be bounded under the restriction (2.3) on the stepsize ratios.*
a) If the method (1.2) satisfies the simplifying assumptions $C(q)$, $\Gamma(q)$ and $B(p)$, then for arbitrary matrices T_m it is convergent of order $p^* := \min\{q + 1, p\}$, i.e.,

$$\varepsilon_m = \mathcal{O}(h^{p^*}), \quad \nu_m = \mathcal{O}(h^{p^*}). \tag{2.4}$$

b) Let $C(q-1)$, $\Gamma(q-1)$, $C\Gamma(q)$ and $B(p)$ hold with $p, q \geq 1$. If T_m satisfies $T_m = f_y(u_m) + \mathcal{O}(h)$, then (2.4) is true again.

Proof. a) Using Taylor expansion in (2.1), the simplifying assumptions and the restriction (2.3) the following estimates are obtained,

$$\widetilde{Y}_{mi} = y(t_m + c_i h_m) + \mathcal{O}(h_m^{q+1}), \quad \delta_{mi} = \mathcal{O}(h_m^{q+1}), \quad \eta_m = \mathcal{O}(h_m^{p+1}).$$

Subtraction of (1.2) from (2.1) yields

$$\begin{aligned}
(I - h_m \gamma_i T_m)(y'(t_m + c_i h_m) - k_{mi}) &= f(y(t_m + c_i h_m) + \mathcal{O}(h_m^{q+1})) - f(Y_{mi}) \\
&\quad + h_m T_m \sum_{j=1}^{s} \gamma_{ij} (y'(t_{m-1} + c_j h_{m-1}) - k_{m-1,j}) + \mathcal{O}(h_m^{q+1}) \\
y(t_{m+1}) - u_{m+1} &= y(t_m) - u_m + h_m \sum_{i=1}^{s} b_i (y'(t_m + c_i h_m) - k_{mi}) \\
&\quad + h_m \sum_{i=1}^{s} v_i (y'(t_{m-1} + c_i h_{m-1}) - k_{m-1,i}) + \mathcal{O}(h_m^{p+1}).
\end{aligned}$$

With the Lipschitz-continuity of f we obtain from these equations the estimate

$$\begin{pmatrix}\varepsilon_{m+1}\\ \nu_{m+1}\end{pmatrix} \le \begin{pmatrix}1+\mathcal{O}(h_m) & \mathcal{O}(h_m)\\ \mathcal{O}(1) & \mathcal{O}(h_m)\end{pmatrix}\begin{pmatrix}\varepsilon_m\\ \nu_m\end{pmatrix} + h_m\begin{pmatrix}\mathcal{O}(h^{p^*})\\ \mathcal{O}(h^{p^*-1})\end{pmatrix} \tag{2.5}$$

with $p^* = \min\{q+1, p\}$. The statement follows now by direct application of Lemma 2.1.
b) The first part of the proof applies here with order $\min\{p,q\} \ge 1$ and shows that

$$T_m = f_y(y(t_m)) + \mathcal{O}(h), \tag{2.6}$$

since $T_m = f_y(u_m) + \mathcal{O}(h)$, by assumption. Taylor expansion now gives

$$\widetilde{Y}_{mi} = y(t_m + c_i h_m) - h_m^q A + \mathcal{O}(h_m^{q+1})$$

with

$$A = \frac{1}{(q-1)!}\Big(\frac{c_i^q}{q} - \sum_{j=1}^{s} a_{ij}(c_j-1)^{q-1}\frac{1}{\sigma_m^{q-1}}\Big)\, y^{(q)}(t_m)$$

Now, for the residual errors δ_{mi} we see that

$$\begin{aligned}\delta_{mi} &= (I - h_m\gamma_i T_m)y'(t_m + c_i h_m) - f\Big(y(t_m + c_i h_m) - h_m^q A + \mathcal{O}(h_m^{q+1})\Big)\\ &- h_m T_m \sum_{j=1}^{s}\gamma_{ij} y'(t_m + (c_j-1)h_m/\sigma_m)\\ &= (I - h_m\gamma_i T_m)y'(t_m + c_i h) - y'(t_m + c_i h) + h_m^q f_y(y(t_m))A\\ &- h_m T_m \sum_{j=1}^{s}\gamma_{ij}\sum_{l=1}^{q+1} y^{(l)}(t_m)\frac{(c_j-1)^{l-1}h_m^{l-1}}{(l-1)!\sigma_m^{l-1}} + \mathcal{O}(h_m^{q+1})\end{aligned}$$

With (2.6) assumption $C\Gamma(q)$ yields

$$\delta_{mi} = \mathcal{O}(h\, h_m^q)$$

and (2.4) follows from (2.5) as before. ∎
For the discussion of methods with high stage order it is convenient to write the simplifying assumptions (2.2) in matrix form. We introduce the Vandermonde matrices

$$V_0 := \Big(c_i^{j-1}\Big)_{i,j} \in \mathbb{R}^{s\times q}, \quad V_1 := \Big((c_i-1)^{j-1}\Big)_{i,j} \in \mathbb{R}^{s\times q}, \tag{2.7}$$

and the diagonal matrices

$$D := \operatorname{diag}(1,2,\dots,q), \qquad S := \operatorname{diag}(1,\sigma,\dots,\sigma^{q-1}) \in \mathbb{R}^{q\times q}, \tag{2.8}$$

$$C := \operatorname{diag}(c_1,\dots,c_s), \qquad G := \operatorname{diag}(\gamma_1,\dots,\gamma_s) \in \mathbb{R}^{s\times s}. \tag{2.9}$$

By the binomial theorem the two Vandermonde matrices are related through the upper triangular Pascal matrix, $P_q = (p_{ij})_{i,j=1}^q$, $p_{ij} = \binom{j-1}{i-1}$ with the usual convention $p_{ij} = 0$ for $j < i$. The precise relation is

$$V_1 = V_0\begin{pmatrix}1 & -1 & 1 & \dots\\ & 1 & -2 & \\ & & 1 & \\ & & & \ddots\end{pmatrix} = V_0 P_q^{-1}, \quad V_0 = V_1 P_q.$$

Now, the simplifying assumptions (2.2) read

$$\begin{array}{lrcl} & C(q): & AV_0P_q^{-1} = & CV_0SD^{-1} \\ (2.10) & \Gamma(q): & \Gamma V_0 P_q^{-1} = & -GV_0S \\ & C\Gamma(r): & (A+\Gamma)V_0P_r^{-1} = & (CV_0D^{-1}-GV_0)S \\ & B(p): & b^TV_0S+v^TV_0P_p^{-1} = & \mathbb{1}^TSD^{-1}. \end{array}$$

3 Stability properties

We consider the properties of the scheme for the test-equation of A-stability $y' = \lambda y$ where the exact Jacobian $T_m = \lambda$ is used. Then, the recursion (1.2) depends on the sum $\beta := A + \Gamma$ of the coefficient matrices only and reduces to

$$\begin{pmatrix} h_mK_m \\ u_{m+1}\end{pmatrix} = M(z)\begin{pmatrix} h_{m-1}K_{m-1} \\ u_m\end{pmatrix}, \quad M(z) := \begin{pmatrix} \sigma W\beta & W\mathbb{1} \\ \sigma(b^TW\beta+v^T) & 1+b^TW\mathbb{1}\end{pmatrix}, \tag{3.1}$$

where $W := z(I - zG)^{-1}$ and $K_m := (k_{mi})_{i=1}^s$. For methods with high stage order the matrix β may be computed from the order conditions (2.2), respectively (2.10).

Lemma 3.1 *Let the method (1.2) satisfy $C\Gamma(s)$. Then, V_0 is regular and*

$$CV_0 = V_0F, \quad F := \begin{pmatrix} 0 & \cdots & & -\phi_0 \\ 1 & & & -\phi_1 \\ & \ddots & & \vdots \\ & & 1 & -\phi_{s-1}\end{pmatrix}$$

where F is the Frobenius companion matrix of the knot polynomial $\phi(t) = \sum_{j=0}^s \phi_j x^j := (x - c_1)\cdots(x - c_s)$ of the two-step W-method. Moreover,

$$\beta = A + \Gamma = (V_0FD^{-1} - GV_0)SP_sV_0^{-1}. \tag{3.2}$$

For equal parameters $\gamma_i \equiv \gamma$, i.e., $G = \gamma I$, an explicit representation is

$$SP_sV_0^{-1}\beta V_0(SP_s)^{-1} = SP_s(F - \gamma D)D^{-1} = SHD^{-1}, \tag{3.3}$$

with the Hessenberg matrix $H = \left(\binom{j}{i-1}(1-(j-i+1)\gamma)\right)_{i,j=1}^s - (\phi(1), \phi'(1), \ldots, \phi^{(s-1)}(1)/(s-1)!)^Te_s^T$ which has its last column modified by the vector of Taylor coefficients of ϕ at $t = 1$.

Proof. The multiplication CV_0 corresponds to a shift in columns $2\ldots s$ of V_0, and the entries $c_i^s = -\sum_{j=1}^s \phi_{j-1}c_i^{j-1}$ of the last column of CV_0 are combinations of the elements of V_0. In (3.2) the condition $C\Gamma(s)$ has been solved for β. The first $s-1$ columns of P_sF are shifted within P_s, the result for the last column follows by observing that $p_{ij}\phi_{j-1}$ is a Taylor coefficient of ϕ at $x = 0$ and that the terms containing $\phi_s = 1$ cancel out in the representation of H. ∎

Since the recursion of the scheme is inflated by s auxiliary values some care is necessary in transfering the usual stability notions, like A-stability. A straightforward generalization of stability concepts formulated in terms of some scalar stability function is their application to the spectral radius $\rho(M(z))$ which is a scalar function again. However, bounding the spectral radius by one is not sufficient to show that M^ℓ is uniformly bounded for $\ell \in \mathbb{N}$ which is the property needed for a convergence proof. Still other properties like L-stability which leads to a stronger error damping in the stiff case may be obtained by requiring less than the condition $\rho(M(\infty)) = 0$. So we adopt the following versions of the generalized notions of A- and L-stability.

Definition 3.1 *The scheme (1.2) is called A-stable, if there is a constant C such that the matrix from (3.1) (with $\sigma = 1$) satisfies*

$$\|M^\ell(z)\| \le C \textit{ for all } \ell \in \mathbb{N},\ z \in \mathbb{C},\ \operatorname{Re} z \le 0.$$

It is called $A(\alpha)$-stable, $\alpha \in (0, \frac{\pi}{2})$, if $M^\ell(z)$ is uniformly bounded for $\ell \in \mathbb{N}$ and z in the sector

$$W_\alpha := \{w \in \mathbb{C} : \ |\arg(w) - \pi| \le \alpha\}.$$

The scheme (1.2) is L-stable or $L(\alpha)$-stable, if it is A-stable or $A(\alpha)$-stable, respectively, and if

$$e_{s+1}^T M(z) \to 0 \quad \textit{for } z \to \infty. \tag{3.4}$$

A sufficient condition for A- resp. $A(\alpha)$-stability is that for all $z \in \mathbb{C}_-$ resp. $z \in W_\alpha$ holds $\rho(M(z)) \le 1$ and that eigenvalues of $M(z)$ lying on the unit circle have equal algebraic and geometric multiplicities. For L-stable schemes we do not require that the stage increments k_{mi} vanish for $z \to \infty$. But the error propagation $K_{m-1} \to u_{m+1}$ is cut off for infinite z.

Lemma 3.2 *The two-step method (1.2) satisfies (3.4) iff*

$$b^T G^{-1} \mathbb{1} = 1 \quad \textit{and} \quad v^T = b^T G^{-1} \beta. \tag{3.5}$$

Proof. With $\lim_{z\to\infty} W(z) = -G^{-1}$ (3.4) is equivalent to

$$-b^T G^{-1}\beta + v^T = 0, \quad 1 - b^T G^{-1} \mathbb{1} = 0. \quad \blacksquare$$

For high order methods the weight vectors b and v are fully determined by the condition (3.4).

Theorem 3.1 *Let $B(s)$ and $C\Gamma(s)$ be satisfied. Then (3.4) holds iff there is an index i, $1 \le i \le s$, with $c_i = 1$ and*

$$b^T = \gamma_i e_i^T, \quad v^T = e_i^T \beta.$$

Proof. Starting from $B(s)$ and using $C\Gamma(s)$ and (3.5) we get

$$\begin{aligned}
\mathbb{1}^T S D^{-1} &= b^T V_0 S + b^T G^{-1} \beta V_1 \\
&= b^T V_0 S + b^T G^{-1}(C V_0 D^{-1} - G V_0) S \\
&= b^T G^{-1} C V_0 S D^{-1} \qquad \Longleftrightarrow \\
\mathbb{1}^T &= b^T G^{-1} C V_0.
\end{aligned}$$

Hence, the vector $d^T = b^T G^{-1}$ has to satisfy the $s+1$ conditions $V_0^T C d = \mathbb{1}$ and $\mathbb{1}^T d = 1$, from (3.5). This is an overdetermined system

$$\sum_{i=1}^{s} c_i^l d_i = 1, \quad l = 0, \ldots, s. \tag{3.6}$$

Subtracting neighbouring equations yields

$$\sum_{i=1}^{s} c_i^l (c_i - 1) d_i = 0, \quad l = 0, \ldots, s-1.$$

This is a regular Vandermonde system for the unknowns $(c_i - 1)d_i$ and the existence of a nontrivial solution d requires $c_i = 1$ for some i. Then, the unique solution of (3.6) is $d = e_i$ leading to

$$b^T = d^T G = \gamma_i e_i^T, \quad v^T = b^T G^{-1} \beta = e_i^T \beta. \quad \blacksquare$$

In the following discussion we will concentrate on methods satisfying the condition of Lemma 3.2 with $i = s$,

$$c_s = 1, \quad b^T = \gamma_s e_s^T, \quad v^T = e_s^T \beta, \tag{3.7}$$

and call such methods *stiffly accurate* in accordance with the notion used for Runge-Kutta methods. For these methods the stability matrix M has rank s at most, since

$$M(z) = \begin{pmatrix} W \\ \frac{1}{1-\gamma_s z} e_s^T \end{pmatrix} \begin{pmatrix} \sigma\beta & \mathbb{1} \end{pmatrix}. \tag{3.8}$$

The following Lemma shows, that in the confluent case with only one γ the stability matrix $M(z)$ is only a slight modification of β with constant rank s for all z. This property gives some indication that it is hardly possible to strengthen the requirement (3.4). Even if we require $\rho(M(\infty)) = 0$ for some method with high stage order, see Table 4.1 below, the matrix $M(\infty)$ will be highly defective and very sensitive to perturbations.

Lemma 3.3 *Let $G = \gamma I$, $M(z)$ be given by (3.8) and β by (3.3). Then, rank$(M(z)) \equiv s$ and*

$$\rho(M(z)) = \rho\Big(SD^{-1}(\sigma w H + (1 + \gamma w)e_1 e_1^T)\Big), \quad w = \frac{z}{1 - \gamma z}.$$

At $z = \infty$ we have $\rho(M(\infty)) = (\sigma/\gamma)\rho(\beta) = (\sigma/\gamma)\rho(SD^{-1}H)$.

Proof. By the factorization (3.3) β and $F - \gamma D$ have rank $s - 1$, at least. For regular β the nullspace of M is one-dimensional and given by the span of $((\beta^{-1}\mathbb{1})^T, -\sigma)^T$. But for singular β the vector $\mathbb{1}$ is not in the range of β and the kernel of $M(z)$ is spanned by $(x^T, 0)^T$ where $\beta x = 0$. To see this, we use the property $\mathbb{1} = V_0 e_1$ and check whether $e_1 \in \text{range}(F - \gamma D)$. But this is not the case, since any nontrivial solution of $(F^T - \gamma D)y = 0$ has nonzero first component, and so, $e_1 \notin \ker(F^T - \gamma D)^\perp = \text{range}(F - \gamma D)$. The formula for $\rho(M)$ follows from the fact, that the spectral radius of the product (3.8) is not changed by interchanging the factors and from the properties $\mathbb{1} = V_0 e_1$, $P_s e_1 = e_1$, $\mathbb{1}^T P_s^{-1} = e_1^T$. $\blacksquare$

Necessary conditions for A-stability of some scheme can be obtained by looking at the behaviour of its stability function on the imaginary axis near the origin. In our notion of A-stability, see Definition 3.1, the spectral radius $\rho(M(z))$ takes the role of this function (with $\sigma = 1$). Since the eigenvalue one of $M(0)$ is simple and all the others are zero, for small z there exists a holomorphic curve of eigenvalues $\lambda(z)$ and eigenvectors $x(z)$ starting at $\lambda(0) = 1$, $x(0) = (0, 1)^T$, respectively, cf. [10]. Since eigenvalues depend continuously on the matrix, the other eigenvalue curves do not leave the unit disc for small z. A Taylor expansion of these curves can be obtained by expanding (3.8),

$$M(z) = \sum_{j=0}^{\infty} M_j z^j = \begin{pmatrix} 0 & 0 \\ v^T & 1 \end{pmatrix} + \sum_{j=1}^{\infty} \begin{pmatrix} I \\ \gamma_s e_s^T \end{pmatrix} G^{j-1}(\beta, \mathbb{1}) z^j,$$

and $x(z) = \sum_j x_j z^j$, $\lambda(z) = \sum_j \delta_j z^j$ and equating like powers of z in $M(z)x(z) - \lambda(z)x(z) = 0$. So we get the set of conditions

$$\sum_{j=0}^{\ell} (M_j - \delta_j I) x_{\ell - j} = 0, \quad \ell = 0, 1, \ldots. \tag{3.9}$$

These equations can be solved partially with the aid of the order conditions (2.2). In the following lemma we present only the first non-exact coefficient δ_{q+1} of $\lambda(z)$, despite the fact that also δ_{q+2} is required in the expansion of $|\lambda(iv)|-1$, $v\in\mathbb{R}$, for even orders q. But the formula for δ_{q+2} is rather lengthy and we were not able to construct A-stable methods of practical interest for this case so far (see the example at the end of this section).

Lemma 3.4 *Let $\sigma=1$. If the scheme satisfies the order conditions $C\Gamma(q)$ for some $q\le s$, then the matrix $M(z)$ from (3.8) possesses a holomorphic curve of eigenvalues $\lambda(z)$ and eigenvectors $x(z)$ near $z=0$ with $\lambda(0)=1$, $x(0)=(0,1)^T$. These curves have the form*

$$\begin{aligned}\lambda(z) &= \sum_{j=0}^{q}\frac{z^j}{j!}+\delta_{q+1}z^{q+1}+\delta_{q+2}z^{q+2}+O(z^{q+3}),\\ x(z) &= \begin{pmatrix}0\\1\end{pmatrix}+\sum_{j=1}^{q+1}\frac{z^j}{(j-1)!}\begin{pmatrix}(c-\mathbb{1})^{j-1}\\0\end{pmatrix}+O(z^{q+2}),\end{aligned}$$

where

$$\delta_{q+1}=\frac{1}{q!}\Big(e_s^T\beta(c-\mathbb{1})^q+\gamma_s\Big)=\frac{1}{q!}\Big(e_s^T\beta c^q-\frac{2^{q+1}-2}{q+1}+\gamma_s 2^q\Big)$$

Proof. The existence of the expansions for $\lambda(z)$ and $x(z)$ is a classical result [10]. Since the last component of x does not vanish in a neighbourhood of $z=0$ we may fix this component of $x(z)$ to the value one. This leads to $x_j^T=(\tilde{x}_j^T,0)$, $\tilde{x}_j\in\mathbb{C}^s$ for $j>0$ and we may write the condition (3.9) in the form

$$0=\begin{pmatrix}-\tilde{x}_\ell\\ v^T\tilde{x}_\ell\end{pmatrix}+\sum_{j=1}^{\ell-1}\begin{pmatrix}(G^{j-1}\beta-\delta_j I)\tilde{x}_{\ell-j}\\ \gamma_s^j v^T\tilde{x}_{\ell-j}\end{pmatrix}+\begin{pmatrix}G^{\ell-1}\mathbb{1}\\ \gamma_s^\ell-\delta_\ell\end{pmatrix}, \tag{3.10}$$

where we used the relation $v^T=e_s^T\beta$ as an abbreviation. For $\ell\le q+1$ the order conditions (2.10) can be used to replace the products $\beta\tilde{x}_{\ell-j}=\beta(c-\mathbb{1})^{\ell-j-1}/(\ell-j-1)!$ by $(c-\mathbb{1})^{\ell-j}/(\ell-j)!-G(c-\mathbb{1})^{\ell-j-1}/(\ell-j-1)!$. So, for $\ell\le q$ the sum of the terms $G^{j-1}\beta\tilde{x}_{\ell-j}$ becomes telescopic and the binomial formula can be applied to $\sum_j\delta_j\tilde{x}_{\ell-j}$. Note that this argument still applies for $\ell=q+1$ in the first s components of (3.10) since these conditions are independent of δ_{q+1}. This shows that the representation of $x(z)$ indeed holds up to order z^{q+1}.
The condition (3.10) can be solved for δ_ℓ by multiplication with the left eigenvector $(v^T,1)$ of M_0 eliminating $\tilde{x}_\ell$. This gives

$$\delta_\ell=\sum_{j=1}^{\ell-1}(v^TG^{j-1}\beta+(\gamma_s^j-\delta_j)v^T)\tilde{x}_{\ell-j}+v^TG^{\ell-1}\mathbb{1}+\gamma_s^\ell.$$

For $\ell=q+1$ the order conditions apply as before with the exception of the term $v^T\beta\tilde{x}_q=v^T\beta(c-\mathbb{1})^{q-1}/(q-1)!=v^Tc^q/q!-v^TGc^{q-1}/(q-1)!$. This computation leads to the second version of δ_{q+1} in the statement. A simplification is possible by observing that $v^Tc^q/q!$ may be replaced with $C\Gamma(q)$ and the binomial formula by

$$\frac{1}{q!}\beta c^q=\frac{1}{q!}\beta(c-\mathbb{1})^q+\frac{1}{(q+1)!}\big((c+\mathbb{1})^{q+1}-\mathbb{1}-c^{q+1}\big)-\frac{1}{q!}G\big((c+\mathbb{1})^q-\mathbb{1}\big).\quad\blacksquare$$

A necessary condition for A-stability is that the eigenvalue with $\lambda(0) = 1$ does not increase in modulus along the imaginary axis near the origin. By Lemma 3.4 we have

$$\lambda(iv) = e^{iv} + (\delta_{q+1} - \frac{1}{(q+1)!})(iv)^{q+1} + (\delta_{q+2} - \frac{1}{(q+2)!})(iv)^{q+2} + \mathcal{O}(|v|^{q+3}).$$

The requirement that the first nontrivial term in $|\lambda(iv)| - 1, v \in \mathbb{R}$, be negative leads to the conditions

$$\text{(3.11)} \qquad \begin{array}{rcll} \delta_{q+1} & < & \frac{1}{(q+1)!} & \text{for odd } q, \\ (-1)^{q/2}(\delta_{q+1} - \delta_{q+2}) & < & \frac{1}{q!(q+2)} & \text{for even } q. \end{array}$$

For high order methods with $q = s$ and $G = \gamma I$ Lemma 3.1 may be used in the representation of δ_{q+1} to show that it depends linearly on γ. In fact, using the relations $c^s = V_0 F e_s$, $e_s^T V_0 = \mathbb{1}^T$, $\mathbb{1}^T F = \mathbb{1}^T$ (by $\phi(1) = 0$) it is seen that

$$s!\,\delta_{s+1} - \frac{1}{s+1} = \gamma\phi(2) - \int_1^2 \phi(t)dt.$$

So, condition (3.11) may be easily fulfilled for methods with an odd number of stages by choosing γ appropriately.

Example: The following methods of order s given by the conditions $C(s)$, $\Gamma(s)$ and (3.7) with

$$\begin{array}{lll} s = 3: & c^T = (-1.5939207857, 2.5798409026, 1), & \gamma = 0.88591852578745, \\ s = 4: & c^T = (0.108081877988, 2.47847273755, 7.9263420118, 1), & \gamma = 1.4751505802, \end{array}$$

satisfy the necessary condition (3.11). We also have checked numerically that these methods are L-stable, in fact we found $\rho(M(z)) < 1$ for all $z \in \mathbb{C}_-$, $z \neq 0$. For instance, the three-stage method has a spectral radius $\rho(M(\infty)) \doteq 0.8454$. However, due to the strange placement of stage points c_i and large values in some error constants we did not find the 4-stage method of practical interest and did not use it in our numerical tests of the next sections.

4 Convergence for Prothero-Robinson equations

The error analysis in Section 2 applies to the nonstiff case only. It is well-known that one-step W- and ROW-methods may suffer from order reduction if applied to very stiff equations (e.g. [7]). This means, that the constants in the $\mathcal{O}(h^{p^*})$ estimate (2.4) may depend on the Lipschitz constant L of f making this estimate unrealistic in stiff situations where L is large. But those error terms that are independent of L, i.e., independent of the stiffness, may have an order well below the classical order p^*. This order reduction can already be observed for nonautonomous linear problems and one commonly accepted test equation for this case is the model problem of Prothero and Robinson [6]. B-convergence, i.e., convergence independent of the stiffness of the problem, has been discussed for Rosenbrock-type methods on some classes of stiff equations in [8]. However, those methods with a higher order of B-convergence do not have the optimal classical order. We will see now that the situation is better for two-step W-methods. Due to their high stage order almost no order reduction will occur.

We consider B-convergence of two-step W-methods for the Prothero-Robinson equation

$$\text{(4.1)} \qquad y' = \lambda(y - g(t)) + g'(t), \quad y(t_0) = g(t_0),$$

with $\lambda \in \mathbb{C}_-$ and exact solution $y(t) = g(t)$ and discuss error estimates with $\mathcal{O}$-constants not depending on λ. For simplicity we restrict our investigation to constant stepsizes and the case $G = \gamma I$ and we assume that the initial values are exact. Application of the two-step W-method (1.2) with $T_m = \lambda$ yields

$$(4.2)\qquad \begin{pmatrix} hK_m \\ y_{m+1} \end{pmatrix} = \underbrace{\begin{pmatrix} w\beta & w\mathbb{1} \\ wb^T\beta + v^T & 1 + wb^T\mathbb{1} \end{pmatrix}}_{M(z)} \begin{pmatrix} hK_{m-1} \\ y_m \end{pmatrix} + w \begin{pmatrix} G'(t_m)/\lambda - G(t_m) \\ b^T G'(t_m)/\lambda - b^T G(t_m) \end{pmatrix}$$

with $z = h\lambda$, $w = z/(1-\gamma z)$ and

$$G(t_m) = (g(t_m + c_1 h), ..., g(t_m + c_s h))^T, \quad G'(t_m) = (g'(t_m + c_1 h), ..., g'(t_m + c_s h))^T.$$

Residual errors $\triangle_K, \triangle_y$ are obtained after replacing K_m by $G'(t_m)$ and y_{m+1} by $g(t_{m+1})$:

$$(4.3)\qquad \begin{pmatrix} hG'(t_m) \\ g(t_{m+1}) \end{pmatrix} = M(z) \begin{pmatrix} hG'(t_{m-1}) \\ g(t_m) \end{pmatrix} + w \begin{pmatrix} G'(t_m)/\lambda - G(t_m) \\ b^T G'(t_m)/\lambda - b^T G(t_m) \end{pmatrix} + \begin{pmatrix} \triangle_K(t_m) \\ \triangle_y(t_m) \end{pmatrix}$$

We note, that these residual errors $\triangle_K, \triangle_y$ differ slightly from the ones defined in (2.1). The following theorems show that only a slight order reduction or no reduction at all occurs for $\lambda \to \infty$ in (4.1). Details depend on the stability properties of the two-step W-method.

Theorem 4.1 *Let the two-step W-method be A-stable and satisfy $C\Gamma(q)$ and $B(p)$. Then it is B-convergent of order $\tilde{p} = \min\{q, p\}$ for the Prothero-Robinson problem (4.1) with* $\operatorname{Re}\lambda < 0$.

Proof. Using Taylor expansion of (4.3) and the condition $C\Gamma(q)$ it follows that

$$\triangle_K(t_m) = \mathcal{O}(h^{q+1}).$$

Together with $B(p)$ this implies

$$\triangle_y(t_m) = \mathcal{O}(h^{\tilde{p}+1})$$

with $\tilde{p} = \min\{q, p\}$. Note, that the $\mathcal{O}$-terms depend on derivatives of the exact solution y but not on λ. Subtracting (4.2) from (4.3) yields for the global error

$$errk_{m+1} = G'(t_m) - K_m, \quad err_{m+1} = g(t_m + h) - u_{m+1}$$

the recursion

$$\begin{pmatrix} h\ errk_{m+1} \\ err_{m+1} \end{pmatrix} = M(z) \begin{pmatrix} h\ errk_m \\ err_m \end{pmatrix} + \begin{pmatrix} \triangle_K(t_m) \\ \triangle_y(t_m) \end{pmatrix}.$$

So, for exact initial values the error is given by

$$(4.4)\qquad u_{m+1} - g(t_{m+1}) = e_{s+1}^T \sum_{l=0}^{m} M^l(z) \begin{pmatrix} \triangle_K(t_{m-l}) \\ \triangle_y(t_{m-l}) \end{pmatrix}.$$

For A-stable methods, by definition, there exists a constant C_1 that is independent of λ such that

$$|u_{m+1} - g(t_{m+1})| \le (m+1) C_1 h^{\tilde{p}+1} = (t_{m+1} - t_0) C_1 h^{\tilde{p}}. \quad \blacksquare$$

Compared to the classical order $p^* = \min\{q+1, p\}$ obtained in Theorem 2.1 only one order is lost here in the usual case $p > q$. But for strongly A-stable methods no order reduction at all takes place since the following theorem establishes the order $\tilde{p}+1 \geq p^*$. There we also discuss the situation ([4])

$$h \to 0, \quad h\lambda \to \infty, \tag{4.5}$$

that is of special interest for smooth solutions but very stiff problems.

Theorem 4.2 *Let $\rho(M(\infty)) < 1$ and let $C\Gamma(q)$ and $B(p)$ be satisfied. Then, under assumption (4.5) holds*

$$|u_{m+1} - g(t_{m+1})| = \mathcal{O}(h^{\tilde{p}+1}), \quad \tilde{p} = \min\{q, p\}.$$

If the method is also stiffly accurate, (3.7), then we have the asymptotic behaviour

$$|u_{m+1} - g(t_{m+1})| \sim \frac{1}{z} h^{q+1} \text{ for } z \to \infty.$$

Proof. Under the first assumption $\sum_{l=0}^{m} \|M^l(z)\|$ is uniformly bounded for all m, $|z| \geq R$ in (4.4) and one order of h is gained.
In the second case, $B(q)$ is a consequence of (3.7) and $C\Gamma(q)$. Then, we have

$$u_{m+1} - g(t_{m+1}) = \triangle_y(t_m) + e_{s+1}^T M(z) \sum_{l=1}^{m} M^{l-1}(z) \begin{pmatrix} \triangle_K(t_{m-l}) \\ \triangle_y(t_{m-l}) \end{pmatrix}.$$

Since

$$\triangle_K(t_m) = -hw\gamma G'(t_m) + wG(t_m) - hw\beta G'(t_{m-1}) - w\mathbb{1}g(t_m)$$

it follows that

$$\begin{aligned}
\triangle_y(t_m) &= b^T \triangle_K(t_m) + g(t_m + h) - g(t_m) - hv^T G'(t_{m-1}) - hb^T G'(t_m) \\
&= \frac{1}{1-\gamma z}(- h\gamma g'(t_{m+1}) + g(t_{m+1}) - g(t_m) - he_s^T \beta G'(t_{m-1})) \\
&= \frac{1}{1-\gamma z}(\sum_{l=1}^{q} \frac{g^{(l)}(t_m) h^l}{(l-1)!} (\frac{1}{l} - \gamma - e_s^T \beta (c-1)^{l-1}) + \mathcal{O}(h^{q+1})) \\
&\sim \frac{1}{z} h^{q+1}
\end{aligned}$$

Finally, the observation

$$e_{s+1}^T M(z) = \frac{1}{1-\gamma z} (e_s^T \beta, 1)^T$$

finishes the proof. ■
We illustrate the theoretical results by making some experiments with three different two-step W-methods denoted by WMij, where i indicates the number of stages and j the classical order according to Theorem 2.1. All methods use $G = \gamma I$. Once the stage points c_i and the value of γ are fixed, all other coefficients of these methods are determined by the order and stability conditions given in Table 4.1.
With respect to our definitions the methods WM34 and WM44 are L(α)-stable while WM45 is A(α)-stable only. The methods do not satisfy the necessary conditions (3.11) for A-stability. The properties of the methods are summarized in Table 4.1, where the stability angles α were computed numerically.

Name	γ	$c_1, \ldots, c_s$	Conditions	$A(\alpha)$	$\rho(M(\infty))$
WM34	0.8494314722	-1.7119863088 2.3657253631 1	$C(3), \Gamma(3), B(4), (3.7)$	89.7°	0.8785299423
WM44	0.4564586673	-3.3252678057 -2.1053450642 -0.2660484528 1	$C(4), \Gamma(4), B(4), (3.7)$	68.4°	0
WM45	0.7535833817	-3.3397654896 -1.4870830356 0.5362026478 3.5569894699	$C(4), \Gamma(4), B(5),\ v = 0$	79.2°	0.9262701231

Table 4.1: Two-Step W-Methods

The figures 4.1 and 4.2 illustrate our theoretical results for the Prothero-Robinson equation (4.1) with solution

$$g(t) = \sin t, \quad t \in [0, 10].$$

Our two-step W-methods are compared with the Rosenbrock code GRK4T [5] of classical order 4. Since GRK4T cannot be applied directly to nonautonomous problems (but the two-step W-methods can), we use for all methods the autonomous form of (4.1) by adding an additional equation for t. The first Figure 4.1 shows the global error at the endpoint for a very stiff equation with $\lambda = -10^9$ and different stepsizes. In order to illustrate the advantage of stiffly accurate methods, satisfying (3.7), we also present the global error for fixed stepsize $h = 0.1$ but different λ in Figure 4.2.

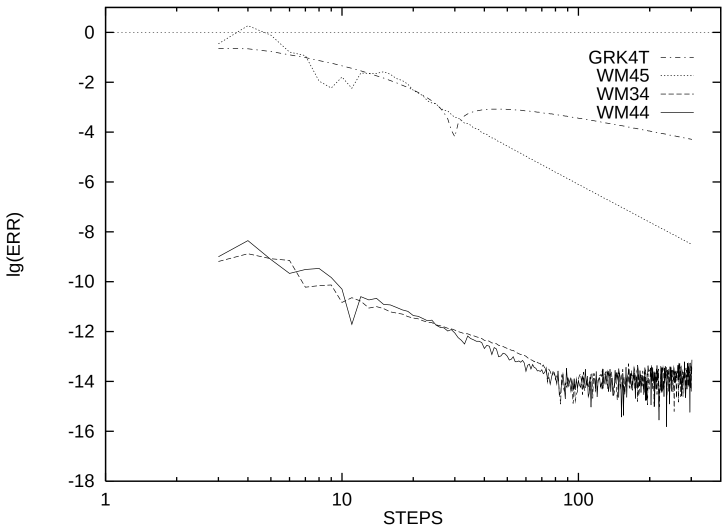

Figure 4.1: Error for fixed $\lambda = -10^9$.

The numerical results confirm those orders found in the theoretical analysis. For fixed large λ we observe the order reduction for GRK4T. The two-step W-methods, especially the stiffly accurate ones, are clearly superior here. And Figure 4.2 shows again the strong reduction of the global error by the factor z^{-1} for stiffly accurate methods.

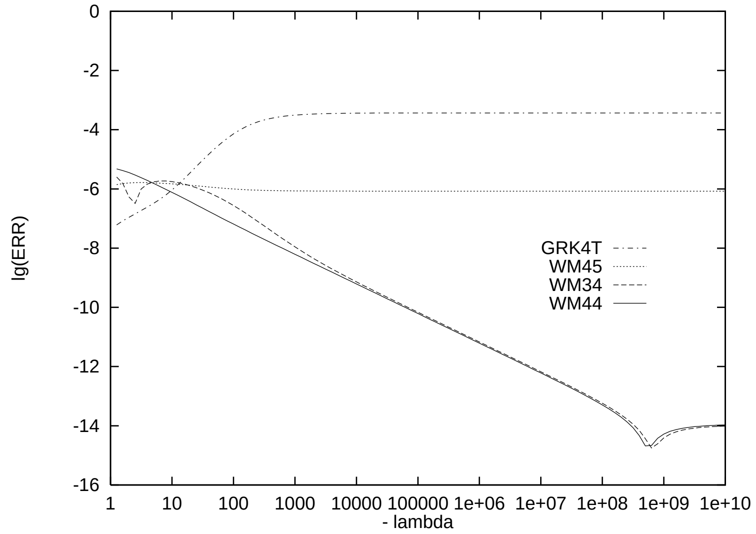

Figure 4.2: Error for fixed h.

5 Numerical results with stepsize control

Realistic experiments with the methods of Table 4.1 require a variable stepsize implementation which we present now. Since it is probably a good starting point for a parallel method if it is competitive with standard methods in sequential computations we first compare the sequential performance of our methods with the Rosenbrock codes ROS4 (11/1992, method GRK4T) and RODAS (10/1996), cf. [4], with default parameters. Both Rosenbrock methods have order 4.
First, we give some details of our implementation. The local error Err_{emb} is estimated by use of an embedded solution $\tilde{u}_{m+1}$, i.e.,

$$Err_{\mathrm{emb}} = \sqrt{\sum_{i=1}^{n} \left(\frac{u_{m+1,i} - \tilde{u}_{m+1,i}}{\mathtt{ATOL} + \mathtt{RTOL}|u_{m+1,i}|} \right)^2}, \quad \tilde{u}_{m+1} = u_m + h \sum_{s=1}^{s} (b_{e,i} k_{m,i} + v_{e,i} k_{m-1,i}),$$

where `ATOL` and `RTOL` denote absolute and relative tolerances. The weights for the embedded methods were chosen as $b_e^T := 0.95\ \gamma e_s^T$ and $v_e^T := ((\mathbb{1}^T + 0.1\ e_s^T)SD^{-1} - b^T V_0 S)V_1^{-1}$ for the L-stable methods WM34 and WM44. For WM45 $v_e := 0$ and $b_e := ((\mathbb{1}^T + 0.1 e_s^T)D^{-1}V_0^{-1}$ was used. Since the coefficients of the method depend on the stepsize ratio we avoid small changes in stepsize to save overhead for their recomputation (see the first case of (5.1)). So, the new stepsize h_{new} is computed by

$$h_{\mathrm{rel}} = \min\{2, \max\{1/2, Err_{\mathrm{emb}}^{-1/(q^*+1)} \cdot 0.85\}\}$$

$$h_{\mathrm{new}} = \begin{cases} h_{\mathrm{old}} & \text{if } h_{\mathrm{rel}} \in [0.95, 1.05] \\ h_{\mathrm{old}} \cdot h_{\mathrm{rel}} & \text{else,} \end{cases} \tag{5.1}$$

where q^* is the order of the embedded method. Since W-methods have full order with arbitrary matrices T_m we take advantage of unchanged stepsizes by re-using the old Jacobian matrix in this case to avoid matrix computations and factorizations. We do not claim this heuristic to be optimal. In fact, numerical experiments have shown that the performance of the two-step code depends critically on the chosen strategy for stepsizes and Jacobians. A detailed study of different heuristics is a topic of further work.

The starting values for the first time step are calculated by using the RADAU code from [3]. We take one step with RADAU and employ the continuous collocation RADAU solution to calculate $u(t_0 + c_i h_0)$. Since some of the knots c_i in Table 4.1 are negative, we avoid interpolation backwards in time by choosing a sufficient large stepsize $h_{\text{Radau}} = 5 \cdot h_0$.
The code is written in FORTRAN and is available from the authors. The Jacobian is approximated by finite differences. For matrix/vector operations we used the LAPACK/BLAS subroutines. The tests were performed on a HP/Convex X-Class with one processor except those marked "par" in Figure 5.5 below. For these parallel computations we used simple loop-base shared-memory parallelization. Our emphasis was not to achieve maximal speedup, we just wanted to indicate that the parallel implementation works well for large problems and gives encouraging performance improvements. Since one bottleneck for parallelism is the factorization of the Jacobian we expect a better parallel performance if we switch to approximate solution methods like Krylov methods. Krylov approximations are quite efficient within ordinary W-methods [9]. Their application to two-step methods will be a topic of further work.

Test Problems

The following test problems have been used for the numerical experiments:

- PLATE – A nonautonomous ODE of medium stiffness with $n = 80$ and dense Jacobian from [4].
- CUSP – An autonomous ODE system with $n = 96$ equations also from [4]. The Jacobian has a cyclic tridiagonal block structure and is treated as a full matrix in the ROW codes. For the W-methods we also tested a 7-band approximation as described in Hairer/Wanner [4].
- NILIDI – An autonomous nonlinear 2D diffusion problem, see [9]. The application of the method of lines gives an ODE system of dimension $n = 10^4 = 100 \times 100$. The upper and lower bandwidths of the Jacobian are $mu = 100$, $ml = 100$.

Discussion of the results

Each problem was solved for a series of torerances `ATOL`=`RTOL`=$10^{-2}, 10^{-3}, \ldots$. The figures below show plots of the integration time in seconds versus the error Err in the endpoint of the integration t_{end}, defined by

$$Err = \sqrt{\frac{1}{n} \sum_{i=1}^{n} \left(\frac{u_i - y_i(t_{\text{end}})}{1 + |y_i(t_{\text{end}})|} \right)^2} \ .$$

The best code for the problem PLATE for tolerances up to 10^{-8} is RODAS, see Fig. 5.3. For even stronger tolerances the Jacobian re-use heuristic pays off and the W-methods become superior. Only for crude tolerances is ROS4 competitive with the two-step W-methods.
For the problem CUSP the ROW-methods RODAS and ROS4 perform much better than the two-step methods if the Jacobian is treated as a full matrix, see Fig. 5.4. In contrast to the ROW-methods which need the exact Jacobian to achieve full order four the W-methods can use a cheap band approximation (see above) of the Jacobian. We demonstrate this with WM34band which is the best method for strong tolerances.
In order to test a loop-based parallelization of these W-methods we consider the larger example NILIDI which is more expensive in computing time. The results in Fig. 5.5 show, that ROS4

performs better than RODAS and is the best method for weak tolerances. For more stringent tolerances all three W-methods become more efficient than ROS4 even in the sequential version. The best W-method is WM34. For stringent tolerances the two-step W-methods benefit strongly from a larger number of Jacobian re-uses due to equal stepsizes in (5.1). This explains the steep slopes observed in Fig. 5.5. Parallel runs are indicated by the symbol "par$\{np\}$" where $\{np\}$ is the number of processors. The Jacobian is computed in parallel, but since its factorization is a sequential bottleneck for the parallel execution the speedup increases with the frequency of the Jacobian-reuse, i.e., for stronger tolerances. Hence, these experiments do not yet give a realistic picture of the parallel potential of the two-step W-methods since the cost is dominated here by the sequential factorization. But we expect a much better parallel performance if preconditioned iterative methods are used for the solution of the stage equations.

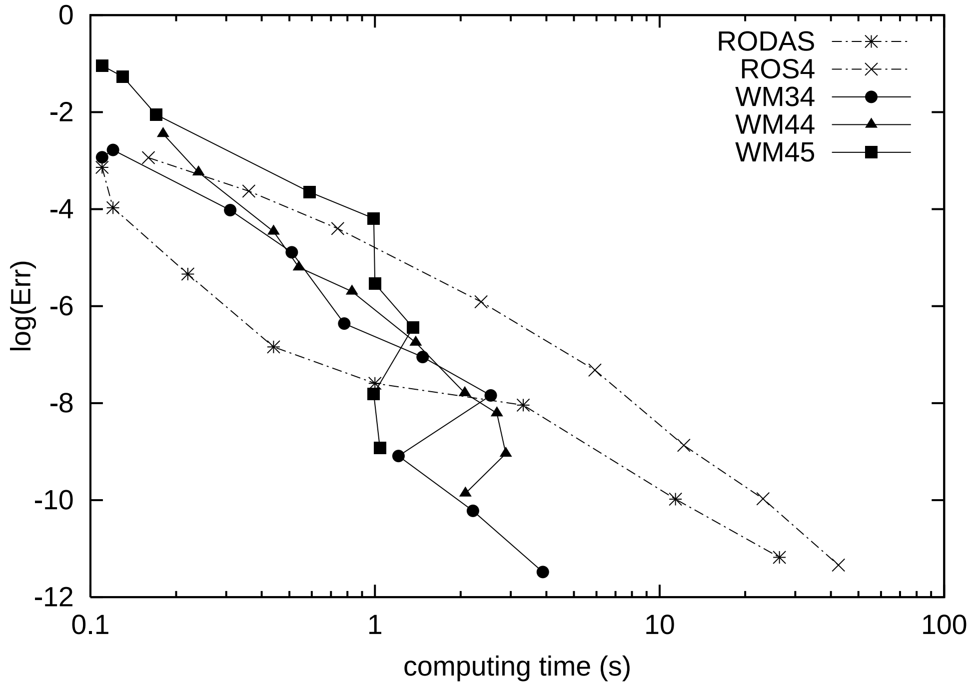

Figure 5.3: Results for problem PLATE

6 Conclusion

In this paper we have introduced a class of two-step W-methods which uses s external stages that can be processed in parallel. Methods having high stage order for variable stepsizes can be constructed easily with the help of simplifying assumptions. According to our analysis for constant stepsizes these methods possess good stability properties. Enhancement of these features for stiff systems is possible by a proper definition and the construction of stiffly accurate methods. Numerical results show that these methods can be competitive with other stiff codes even in a sequential implementation. Open problems so far are a sensitive dependence of some stability and error constants on stepsize changes.

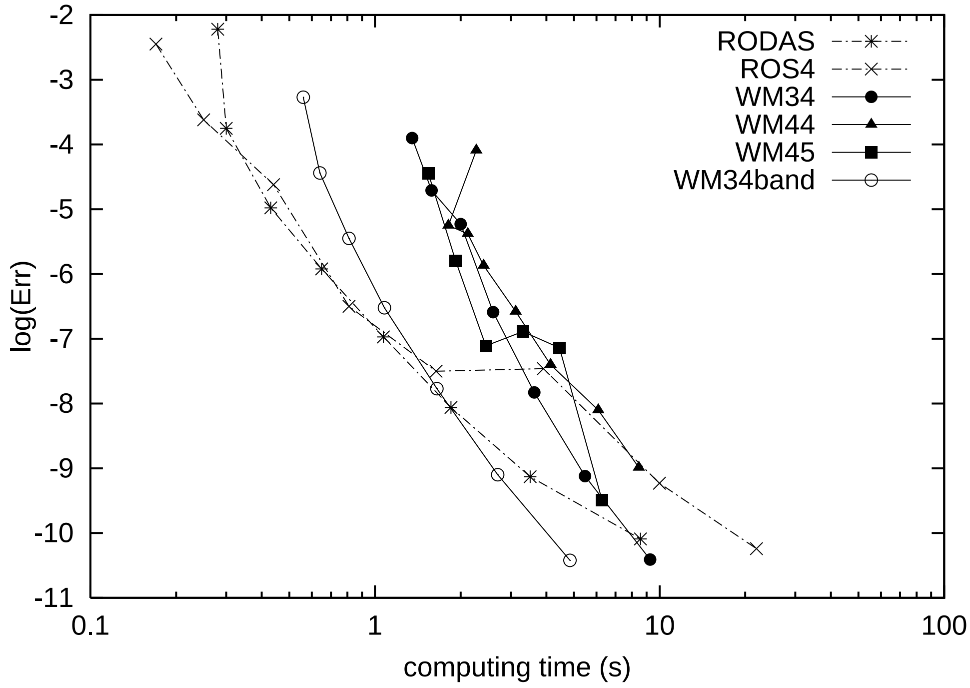

Figure 5.4: Results for problem CUSP

The methods are well suited for parallel implementation, especially if fast methods for the solution of the stage equations will be used. Such methods might include parallel factorizations of the Jacobian or iterative methods like Krylov methods. The robust and efficient parallel implementation will be a goal of future work.

References

[1] K. Burrage, *Parallel and sequential methods for ordinary differential equations*, Clarendon Press Oxford, 1995.

[2] N.H. Cong, H. Podhaisky, and R. Weiner, *Numerical experiments with some explicit pseudo two-step RK methods on a shared memory computer*, Computers Math. Applic. **36** (1998), no. 2, 107 – 116.

[3] E. Hairer and G. Wanner, *Stiff differential equations solved by Radau methods*, J. Comput. Appl. Math., to appear.

[4] ———, *Solving Ordinary Differential Equations II*, 2. ed., Springer-Verlag, 1996.

[5] P. Kaps and P. Rentrop, *Generalized Runge-Kutta methods of order four with stepsize control for stiff ordinary differential equations*, Numer. Math. **38** (1979), 55–68.

[6] A. Prothero and A. Robinson, *On the stability and accuracy of one step methods for solving stiff systems of ordinary differential equations*, Math. Comp. **28** (1974), 145–162.

[7] K. Strehmel and R. Weiner, *Linear-implizite Runge-Kutta Methoden und ihre Anwendung*, Teubner-Verlag Stuttgart-Leipzig, 1992.

[8] K. Strehmel, R. Weiner, and M. Büttner, *Order results for Rosenbrock type methods on classes of stiff equations*, Numer. Math. **59** (1991), 723–737.

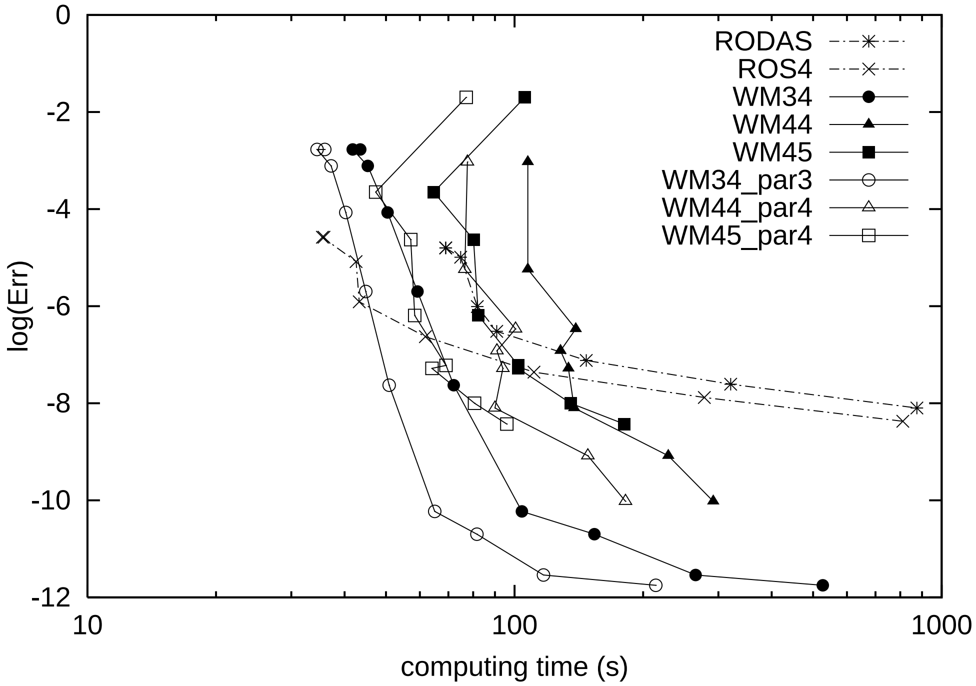

Figure 5.5: Results for problem NILIDI

[9] R. Weiner, B.A. Schmitt, and H. Podhaisky, *ROWMAP – a ROW-code with Krylov techniques for large stiff ODEs*, APNUM **25** (1997), 303–319.

[10] J.H. Wilkinson, *The Algebraic Eigenvalue Problem*, Clarendon Press, Oxford, 1965.

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