Some secant approximations for Rosenbrock W-methods

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Abstract

Here we present a class of W-methods for stiff ODEs based on some special approximations of the Jacobian matrices that allow to reduce the number of order conditions. The approximations considered are modifications of some rank-1 updates, known from quasi-Newton methods. Two new embedded W-methods of order 3 and 4 are constructed and tested on some classical stiff equations arising from the semidiscretization of parabolic problems.

1 Introduction

In this paper we consider the autonomous initial value problem

$$\begin{cases} y' = f(y), \\ y(t_0) = y_0, \end{cases} \tag{1}$$

where $f : \mathbb{R}^N \to \mathbb{R}^N$, $y_0 \in \mathbb{R}^N$. In particular we are interested in the stiff case where an implicit solver is required.

An s-stage W-method for (1) is a special type of linearly implicit Runge-Kutta method defined by

$$\begin{array}{c} (I - h\gamma W)k_i = hf\left(y_m + \sum_{j=1}^{i-1} \alpha_{ij} k_j\right) + hW \sum_{j=1}^{i-1} \gamma_{ij} k_j, \quad i = 1, ..., s, \\ y_{m+1} = y_m + \sum_{i=1}^{s} b_i k_i, \end{array} \tag{2}$$

where $\gamma, \alpha_{ij}, \gamma_{ij}, b_i,\ i, j = 1, ..., s$, are the coefficients of the method and $W \in \mathbb{R}^{N \times N}$ is a certain approximation of the Jacobian $J = J(y_m)$. As well known, the special cases of $W = J$ and $W = 0$ lead to ROW-methods and explicit Runge-Kutta methods respectively. We refer to [5] and [21] for a comprehensive treatment of linearly implicit Runge-Kutta methods and the special classes of Rosenbrock, ROW- and W-methods.

Since the paper of Steihaug and Wolfbrandt [19], in order to face large dimensional problems many authors have proposed ideas for overcoming the most important drawback of ROW-methods (and of all implicit methods), that is, the explicit use of the Jacobian matrix at each step and the consequent solution of the s linear systems for the computation of k_i, $i = 1, ..., s$. In particular, among the others, we remember [8] and [24], where the authors examine the possibility of reusing the Jacobian of a previous step, and [16], [25], where a Krylov approach for the solution of the linear systems enables to avoid the explicit computation of the Jacobian, getting a so-called matrix-free W-method.

In this paper we present some new approaches for solving stiff ODEs by W-methods based on the use of the well known Broyden's updates [2] and the Schubert's update [17]. Actually the idea is not new since it was firstly proposed in [1] where the authors used the so-called good Broyden's update [3] for approximating the Jacobian at each step, starting with a certain approximation of $J(y_0)$. In this sense, we are particularly interested in stiff problems where a fixed approximation of the Jacobian (e.g. $W = J(y_0)$) does not represent a reliable approach. The first purpose of this paper is to extend this idea of [1] in order to make the update suitable for variable stepsize integration, that is necessary in order to create reliable codes based on the stepsize selection. The second one is to consider two other secant updates, the so-called bad Broyden's and Schubert's update.

All these updates are rank-1 updates that fulfil the secant equation

$$W_m(y_m - y_{m-1}) = f(y_m) - f(y_{m-1}), \tag{3}$$

and allow to have approximations of the type

$$W_m = J(y_m) + O(h), \tag{4}$$

where h is the discretization step. By (4), some of the order conditions of W-methods with arbitrary Jacobian approximations can be shifted to higher orders (see [21]). The use of the good and bad Broyden's updates allows to exploit the Sherman-Morrison formula for a fast computation of $(I - h\gamma W_m)^{-1}$ or to update the QR factorization, getting efficient tools for the linear algebra involved in (2) (see [4] for a wide background). On the other side, with the Schubert's update we are able to preserve the sparsity structure of the exact Jacobian and therefore to exploit the sparse factorization techniques for the computation of k_i, $i = 1, ..., s$.

In this paper we also construct two reliable W-methods based on the property (4). The first one, WB23, is an embedded 3(2)-order method with 4 internal stages and 3 function evaluations at each step. The basic method is L-stable and has B-order $q = 2$. The embedded method is strongly A-stable. The second one, WB34, is a 6 stages formula of order 4(3) where both methods are stiffly accurate. As for WB23, the basic method has B-order $q = 2$.

The paper is structured as follows. In Section 2 we describe the Broyden's and Schubert's approaches for the construction of reliable approximations of the Jacobian, showing also the so-called deterioration of the approximations. In Sections 3 and 4 we construct two embedded W-method of order 3 and 4 respectively. In Section 5 we provide some details about the numerical implementation. In Section 6 we present some numerical experiments, where our methods are compared with some other well-known ROW methods. In a final section we give some concluding remarks.

2 The rank-1 secant updates

For the construction of the Jacobian approximations W_m, $m \geq 0$, in this paper we consider three types of rank-1 secant updates. Before describing them we remember the following result [4].

Lemma 1 *(Sherman-Morrison) Let $u, v \in \mathbb{R}^n$ and assume that $A \in \mathbb{R}^{n\times n}$ is nonsingular. Then $A + uv^T$ is nonsingular if and only if $1 + v^T A^{-1} u \neq 0$. Furthermore*

$$\left(A + uv^T\right)^{-1} = A^{-1} - \frac{A^{-1}uv^T A^{-1}}{1 + v^T A^{-1} u}. \tag{5}$$

Now, starting with $W_0 = J(y_0)$ and setting $s_m = y_m - y_{m-1}$ and $q_m = f(y_m) - f(y_{m-1})$, $m \geq 1$, we consider the following methods for generating the secant sequence $\{W_m\}_{m\geq 0}$, $W_m \approx J(y_m)$.

1. The *good Broyden's update*, where, assuming $s_m \neq 0$,

$$W_m = W_{m-1} + \frac{(q_m - W_{m-1}s_m)s_m^T}{s_m^T s_m}, \qquad m \geq 1, \tag{6}$$

that implies

$$(I - h\gamma W_m) = (I - h\gamma W_{m-1}) - h\gamma \frac{(q_m - W_{m-1}s_m)s_m^T}{s_m^T s_m} \qquad m \geq 1.$$

The above formula remains a rank-1 update so that we can apply formula (5) to achieve $(I - h\gamma W_m)^{-1}$. This is substantially the same approach proposed in [1], but since we are interested in creating reliable codes we must take into account of the stepsize selection that leads to variable stepsize methods. Therefore the update relation (6) has to be slightly modified in order to address this requirement.

In this sense, for each $m \geq 1$, let h_m be the stepsize selected for the computation of y_m. We shall use the following formula

$$W_m = \frac{h_m}{h_{m+1}} \left(W_{m-1} + \frac{\left(q_m \frac{h_{m+1}}{h_m} - W_{m-1}s_m\right) s_m^T}{s_m^T s_m} \right), \qquad m \geq 1. \tag{7}$$

It is easy to show that the secant equation $W_m s_m = q_m$ remains true. The above formula allows to have the relation

$$(I - h_{m+1}\gamma W_m) = (I - h_m\gamma W_{m-1}) - h_m\gamma \frac{\left(q_m \frac{h_m}{h_{m+1}} - W_{m-1}s_m\right) s_m^T}{s_m^T s_m},$$

that is, a rank-1 update for the sequence $\{I - h_{m+1}\gamma W_m\}_{m\geq 1}$, not possible with (6), and necessary for applying formula (5) that leads to

$$(I - h_{m+1}\gamma W_m)^{-1} = (I - h_m\gamma W_{m-1})^{-1} + \frac{(I - h_m\gamma W_{m-1})^{-1}\gamma\,(h_{m+1}q_m - h_m W_{m-1}s_m)\, s_m^T\,(I - h_m\gamma W_{m-1})^{-1}}{s_m^T\left(s_m - (I - h_m\gamma W_{m-1})^{-1}\gamma\,(h_{m+1}q_m - h_m W_{m-1}s_m)\right)}, \quad (8)$$

if the hypotheses of Lemma 1 hold.

2. The *bad Broyden's update*, that works directly on the inversions. This formula is easier and takes into account that in the practical implementation of a W-method (2), the matrix W_m is not explicitly used [5]. Setting $v_m = s_m - h_{m+1}\gamma q_m$, $m \geq 1$, and assuming $v_m \neq 0$, we use

$$(I - h_{m+1}\gamma W_m)^{-1} = (I - h_m\gamma W_{m-1})^{-1} + \left(\frac{s_m - (I - h_m\gamma W_{m-1})^{-1} v_m}{v_m^T v_m}\right) v_m^T. \quad (9)$$

Obviously we get then

$$(I - h_{m+1}\gamma W_m)^{-1} v_m = s_m,$$

so that secant equation $W_m s_m = v_m$ is fulfilled. Note that for h constant, using (5), if $v_m^T W_{m-1}s_m \neq 0$ the update (9) is equivalent to

$$W_m = W_{m-1} + \frac{(q_m - W_{m-1}s_m)v_m^T W_{m-1}}{v_m^T W_{m-1}s_m}. \quad (10)$$

On the contrary case, by Lemma 1, if $v_m^T W_{m-1}s_m = 0$ for a fixed $h > 0$ then $I - h\gamma W_m$ is singular.

3. The *Schubert's update*. When working with large systems with sparse Jacobian it could be important to maintain the sparsity pattern of the exact Jacobian during the integration. Indeed, one of the most important drawback arising when using the updates (7) and (9) is the fill-in phenomenon. Working with ODEs (1) arising for instance from the semidiscretization of PDEs we usually have to face large dimensional problems with sparse Jacobian, typically banded. Hence, in order to make our approach competitive with the standard ROW-methods, that are able to exploit such sparsity structure, we make use of the following update formula [3]. Setting

$$(P_Z(M))_{ij} := \begin{cases} 0 & if \quad Z_{ij} = 0 \\ M_{ij} & if \quad Z_{ij} = 1 \end{cases}, \qquad Z_{ij} := \begin{cases} 0 & if \quad (J(y_0))_{ij} = 0 \\ 1 & if \quad (J(y_0))_{ij} \neq 0 \end{cases},$$

and

$$(\mathbf{s}_i)_j := \begin{cases} 0 & if \quad Z_{ij} = 0 \\ s_j & if \quad Z_{ij} = 1 \end{cases}, \qquad \mathbf{s}_i \in \mathbb{R}^N, \tag{11}$$

we consider the update

$$W_m = W_{m-1} + P_Z(D^+(q_m - W_{m-1}s_m)s_m^T), \qquad m \geq 1, \tag{12}$$

where $D, D^+ \in \mathbb{R}^{N\times N}$ are diagonal matrices such that $D_{ii} = \mathbf{s}_i^T \mathbf{s}_i$, and

$$D_{ii}^+ = \begin{cases} 1/D_{ii} & if \ D_{ii} > 0, \\ 0 & if \ D_{ii} = 0. \end{cases}$$

Formula (12) fulfils the secant equation $W_m s_m = q_m$ unless $\mathbf{s}_i = 0$ with $(y_m)_i \neq 0$ for a certain i. Now, because of the sparsity assumptions, it would be a nonsense to consider the application of formula (5) for the computation of $(I - h_{m+1}\gamma W_m)^{-1}$, and it is more suitable to use a sparse LU factorization of $(I - h_{m+1}\gamma W_m)$.

Actually, there exists a formula for updating the LU factorization ([7]) but it is based on the updating of U and L^{-1}. Since L^{-1} generally looses the original bandwidth, this approach does not seem reliable.

Regarding the approximation properties of the above updates we have the following results, that give a measure of the so-called deterioration of the approximations.

Proposition 2 *Assume to work with the Euclidean norm $\|\cdot\|_2$. Let f be continuously differentiable and let J be Lipschitz continuous*

$$\|J(y_a) - J(y_b)\|_2 \leq \gamma \|y_a - y_b\|_2, \qquad y_a, y_b \in \mathbb{R}^N. \tag{13}$$

Then, assuming h constant, for $m \geq 1$ we have

1. *for the good Broyden's update (6)*

$$\|W_m - J(y_m)\|_2 \leq \|W_{m-1} - J(y_{m-1})\|_2 + \frac{3}{2}\gamma \|y_m - y_{m-1}\|_2; \tag{14}$$

2. *for the bad Broyden's update (10), if there exists $H > 0$ and $C > 0$ such that for $0 < h < H$*

$$\frac{|v_m^T W_{m-1} s_m|}{\|s_m\|_2 \|v_m^T W_{m-1}\|_2} \geq C, \quad m \geq 1, \tag{15}$$

then

$$\begin{aligned} \|W_m - J(y_m)\|_2 \leq & \left(1 + \frac{1}{C}\right) \|W_{m-1} - J(y_{m-1})\|_2 + \\ & \gamma\left(1 + \frac{1}{2C}\right) \|y_m - y_{m-1}\|_2. \end{aligned} \tag{16}$$

Proof. For the good Broyden's update (6) the result is well-known ([4] p.175). For the bad Broyden's update, by (10) we easily get

$$W_m - J(y_m) = (W_{m-1} - J(y_{m-1}))\left(I - \frac{s_m v_m^T W_{m-1}}{v_m^T W_{m-1} s_m}\right) + J(y_{m-1}) - J(y_m) + \frac{(q_m - J(y_{m-1})s_m)v_m^T W_{m-1}}{v_m^T W_{m-1} s_m}$$

By the assumptions on f we have the relation

$$\|q_m - J(y_m)s_m\|_2 \leq \frac{\gamma}{2}\|s_m\|_2^2, \tag{17}$$

and so, by (13) we get

$$\|W_m - J(y_m)\|_2 \leq \|W_{m-1} - J(y_{m-1})\|_2 \left\|I - \frac{s_m v_m^T W_{m-1}}{v_m^T W_{m-1} s_m}\right\|_2 + \gamma\left(1 + \frac{\|s_m\|_2 \left\|v_m^T W_{m-1}\right\|_2}{2\left|v_m^T W_{m-1} s_m\right|}\right)\|y_m - y_{m-1}\|_2 .$$

Finally, by (15) we get the thesis. ■

Proposition 3 *[14] Let f be continuously differentiable and assume that there exists $K = (K_1, ..., K_N) \in \mathbb{R}^N$, $K_i \geq 0$, such that*

$$\left\|e_i^T\left(J(y_a) - J(y_b)\right)\right\|_2 \leq K_i \|y_a - y_b\|_2, \qquad y_a, y_b \in \mathbb{R}^N.$$

Then for the Schubert's update we have

$$\|W_m - J(y_m)\|_F \leq \|W_{m-1} - J(y_{m-1})\|_F + \frac{3}{2}\|K\|_2 \|y_m - y_{m-1}\|_2, \tag{18}$$

where $\|\cdot\|_F$ denotes the Frobenius norm.

Under the hypothesis of the above propositions we can state that the deterioration of the approximations provided by the three updates is of the type

$$\|W_m - J(y_m)\| \leq c\,\|W_{m-1} - J(y_{m-1})\| + O(h), \quad m \geq 1,$$

where the constant c depends on the method and the norm chosen. Therefore, starting with the exact Jacobian $W_0 = J(y_0)$, the above property implies that for $m \leq N$ for some fixed N independent of h

$$W_m = J(y_m) + O(h), \quad 0 \leq m \leq N. \tag{19}$$

As mentioned in previous section, the above property allows to shift some of the order conditions of a W-method to higher orders. However, it is important to point out that using the above rank-1 updates we actually cannot control the deterioration of the approximations. The theoretical property given by (19) is fundamental to state the order conditions of the method, but the constant before the $O(h)$ term can become very large as m increases. Moreover, if we investigate the order of the method, when $h \to 0$ we have $m = c/h$ and hence $W_m = J(y_m) + O(1)$. For overcoming this problem, in practical implementation we adopt the restart of the methods. We refer to Section 5 for more details. Another reason that lead us to consider a periodic restart of the methods is that the results of Propositions 2-3 do not produces information about the preservation of the stability properties of the underlying method that follows from a particular choice of h.

Remark 4 *It is worthwhile nothing that the hypothesis (15) of Proposition 2 is actually rather common when solving ODEs where the function f arises from the discretization of sectorial operators. In such cases the field of values of the Jacobian $F(J(y_m))$ is typically strictly contained in the left-(right-)half complex plane. Hence, starting with $W_0 = J(y_0)$ and maintaining h sufficiently small, we can construct the sequence $\{W_m\}_{m>0}$ such that $F(W_m)$ remains strictly contained in the left-(right-)half complex plane. Moreover, observing that*

$$v_m^T W_{m-1} s_m \approx s_m^T W_{m-1} s_m, \quad as \quad h \to 0,$$

for such kind of problems we fall within the hypothesis (15).

Remark 5 *We must observe that property (19) is also attained with $W_m = J(y_0)$, but clearly this choice does not allow to fulfil the secant equation (3) that is the main reason that lead us to consider the above described rank-1 updates.*

3 An embedded WB-method of order 3

In this section we present an embedded W-method of order 3(2), based on the property $W_m = J(y_m) + O(h)$ attainable with formulas (7), (9) and (12). We call for convenience WB-method any W-method based on these updates. Since we want the basic method to be stiffly accurate and with B-order $q = 2$, it is not difficult to show that we need at least $s = 4$ internal stages. Starting from the general formula

$$(I - h\gamma W)k_i = hf\left(y_m + \textstyle\sum_{j=1}^{i-1} \alpha_{ij} k_j\right) + hW \textstyle\sum_{j=1}^{i-1} \gamma_{ij} k_j, \quad i = 1, ..., s,$$
$$y_{m+1} = y_m + \textstyle\sum_{i=1}^{s} b_i k_i,$$

the parameters $\gamma, \alpha_{ij}, \gamma_{ij}, b_i$, $i, j = 1, ..., s$, have to be chosen in order to fulfil certain conditions to obtain a fixed consistency order. We set as usual

$$\alpha_i = \sum_{j=1}^{i-1} \alpha_{ij}, \quad \beta_{ij} = \alpha_{ij} + \gamma_{ij}, \quad \beta_i = \sum_{j=1}^{i-1} \beta_{ij}, \qquad i, j = 1, ..., s.$$

Defining $b = (b_1, ..., b_s)^T$, $\beta = (\beta_{ij})$, $e = (1, ..., 1)^T$, $\alpha^k = \left(\alpha_1^k, ..., \alpha_s^k\right)^T$, in matrix form the conditions to be fulfilled up to order 3 are given by (see [21])

$$\begin{array}{lll} p=1 & \text{(R1)} & b^T e = 1 \\ p=2 & \text{(R2)} & b^T \beta e = 1/2 - \gamma \\ p=3 & \text{(R3a)} & b^T \alpha^2 = 1/3 \\ & \text{(R3b)} & b^T \beta^2 e = 1/6 - \gamma + \gamma^2 \\ & \text{(W3)} & b^T \alpha = 1/2 \end{array} \tag{20}$$

Actually, we have a simplified set of conditions because we are working with an autonomous systems and with $W_m = J(y_m)+O(h)$, $m \geq 0$, (see again [21] for details). Hence, with respect to a ROW-method the only additional condition is (W3), that, for nonautonomous system, is a condition of order 2.

When a ROW-method is applied for semidiscretized PDEs or PDAEs the following condition has to be fulfilled in order to avoid order reduction (see e.g. [6], [12] and [22])

$$b^T \overline{\beta}^j (2\overline{\beta}^2 e - \alpha^2) = 0, \quad p-2 \leq j \leq s-1, \quad \text{if } p \geq 3, \tag{21}$$

where $\overline{\beta} = \beta + \gamma I$. The condition (21) allows to have B-order $q \geq 2$. In our case, since we want $p = 3$ with $s = 4$, using (20) the conditions (21) become

$$\begin{array}{ll} \text{(B1)} & b_4 \beta_{43} \beta_{32} \alpha_2^2 = 2\gamma^4 - 2\gamma^3 + \gamma^2/3 \\ \text{(B2)} & b_3 \beta_{32} \alpha_2^2 + b_4 \left(\beta_{42} \alpha_2^2 + \beta_{43} \alpha_3^2\right) = 2\gamma^3 - 3\gamma^2 + 2\gamma/3 \\ \text{(B3)} & b_4 \beta_{43} \beta_{32} \beta_2 = 0 \end{array} \tag{22}$$

We remember the following.

Definition 6 *A ROW-method satisfying*

$$\beta_{si} = b_i, \quad i = 1, ..., s-1, \quad b_s = \gamma \quad \textit{and} \quad \alpha_s = 1, \tag{23}$$

is called stiffly accurate.

Methods which satisfies (23) yield asymptotically exact results for the Prothero - Robinson problem $y' = \lambda(y - \varphi(x)) + \varphi'(x)$ (see [5]). Since we want our method to be stiffly accurate, by inserting (23) into (20)-(22) we get the simplified set of conditions

$$\begin{array}{ll} \text{(R1')} & b_1 + b_2 + b_3 = 1 - \gamma \\ \text{(R2')} & b_2 \beta_2 + b_3 \beta_3 = 1/2 - 2\gamma + \gamma^2 \\ \text{(R3a')} & b_2 \alpha_2^2 + b_3 \alpha_3^2 = 1/3 - \gamma \\ \text{(R3b')} & b_3 \beta_{32} \beta_2 = 1/6 - 3\gamma/2 + 3\gamma^2 - \gamma^3 \\ \text{(W3')} & b_2 \alpha_2 + b_3 \alpha_3 = 1/2 - \gamma \\ \text{(B1')} & b_3 \beta_{32} \alpha_2^2 = 2\gamma^3 - 2\gamma^2 + \gamma/3 \\ \text{(B3')} & b_3 \beta_{32} \beta_2 = 0 \end{array} \tag{24}$$

Conditions (R3b') and (B3'), require

$$1/6 - 3\gamma/2 + 3\gamma^2 - \gamma^3 = 0.$$

Among the three real solutions of the above equation, $\gamma \approx 0.43586$ produces an L-stable method (see [15] for a proof) so that we make this choice. Looking at (B1'), (B3'), since 0.43586 is not a root of $2\gamma^3 - 2\gamma^2 + \gamma/3$ we find $\beta_2 = 0$. Therefore, the conditions (24) become

$$\begin{array}{ll} \text{(R1')} & b_1 + b_2 + b_3 = 1 - \gamma \\ \text{(R2")} & b_3\beta_3 = 1/2 - 2\gamma + \gamma^2 \\ \text{(R3a')} & b_2\alpha_2^2 + b_3\alpha_3^2 = 1/3 - \gamma \\ \text{(W3')} & b_2\alpha_2 + b_3\alpha_3 = 1/2 - \gamma \\ \text{(B1')} & b_3\beta_{32}\alpha_2^2 = 2\gamma^3 - 2\gamma^2 + \gamma/3 \end{array} \tag{25}$$

Now, if we set $\alpha_{43} = 0$, $\alpha_{42} = \alpha_{32}$, $\alpha_{41} = \alpha_{31}$, in order to have only three function evaluations, we get $\alpha_3 = 1$, and the only free parameters are α_2 and α_{31} (or α_{32}). Regarding the embedded method, it has to fulfil

$$\begin{array}{ll} \text{(E1)} & \bar{b}_1 + \bar{b}_2 + \bar{b}_3 + \bar{b}_4 = 1 \\ \text{(E2)} & \bar{b}_3\beta_3 + \bar{b}_4(1-\gamma) = 1/2 - \gamma \end{array} \tag{26}$$

Since the stability function $R(z)$ of a ROW-method is given by (see [5])

$$R(z) = 1 + zb^T(I - z\overline{\beta})^{-1}e,$$

the following result follows by direct computation.

Proposition 7 *Let a ROW-method which satisfies (24) be given. For the embedded method with stability function $\overline{R}(z)$ satisfying (26) we have*

$$\bar{b}_4 = \frac{-\gamma^3\overline{R}(-\infty) + \gamma^3 + \gamma/2 - 2\gamma^2}{1/2 - 2\gamma + \gamma^2}. \tag{27}$$

Relation (27) allows to define $\bar{b}_4$ in order to get a strongly A-stable method or even an L-stable method (cf. [13], [15]). If we chose to have $\overline{R}(-\infty) = 0$ we get $\bar{b}_4 = b_4$ but this choice would lead to a poorly accurate method, because it would tend to underestimate the local error. Hence we choose $\bar{b}_4 = \gamma/2$ obtaining a strongly A-stable method with $|\overline{R}(-\infty)| \approx 0.48$. We still have one free parameter, $\bar{b}_2$ (or $\bar{b}_1$). We set $\bar{b}_2$ in order to fulfil the higher order condition

$$\bar{b}_2\alpha_2 + \bar{b}_3\alpha_3 + \bar{b}_4\alpha_4 = 1/2. \tag{28}$$

The coefficients of the embedded method, that we call WB23 are collected in Table 1; α_2 and α_{31} have been chosen experimentally by testing the method on some Prothero-Robinson equations.

γ	=	$4.358665215084590e-01$			
α_{21}	=	$5.000000000000000e-01$	γ_{21}	=	$-5.000000000000000e-01$
α_{31}	=	$3.000000000000000e-01$	γ_{31}	=	$-6.509740048606094e-01$
α_{32}	=	$7.000000000000000e-01$	γ_{32}	=	$3.261356558646555e-01$
α_{41}	=	$3.000000000000000e-01$	γ_{41}	=	$-1.333333333333333e-01$
α_{42}	=	$7.000000000000000e-01$	γ_{42}	=	$-3.333333333333333e-02$
α_{43}	=	$0.000000000000000e-01$	γ_{43}	=	$-2.691998548417924e-01$
b_1	=	$1.666666666666667e-01$	$\bar{b}_1$	=	$5.666947609847634e-01$
b_2	=	$6.666666666666667e-01$	$\bar{b}_2$	=	$3.024769995389324e-01$
b_3	=	$-2.691998548417924e-01$	$\bar{b}_3$	=	$-8.710502127792520e-02$
b_4	=	$4.358665215084590e-01$	$\bar{b}_4$	=	$2.179332607542295e-01$

Table 1: set of coefficients for WB23.

4 An embedded WB-method of order 4

In general terms, the construction of an embedded W-method of order 4(3) is not very simple because there are 21 conditions for the basic method to get $p = 4$ and 8 conditions for the embedded method to achieve $p = 3$. However, with our assumptions of working with autonomous systems and approximations of the type $W = J + O(h)$ the situation is much simpler. We always refer to [21] for the complete set of order conditions.

We want both methods to be stiffly accurate and so the choice of $s = 6$ internal stages is necessary (see also the construction of RODAS in [5]). Hence, in our case the conditions for $p = 4$ are 11:

$$\begin{array}{lll}
p=1 & \text{(R1)} & b^T e = 1 \\
p=2 & \text{(R2)} & b^T \beta e = 1/2 - \gamma \\
p=3 & \text{(R3a)} & b^T \alpha^2 = 1/3 \\
 & \text{(R3b)} & b^T \beta^2 e = 1/6 - \gamma + \gamma^2 \\
 & \text{(W3)} & b^T \alpha = 1/2 \\
p=4 & \text{(R4a)} & b^T \alpha^3 = 1/4 \\
 & \text{(R4b)} & \varphi^T \overline{\alpha} \beta e = 1/8 - \gamma/3 \\
 & \text{(R4c)} & b^T \beta \alpha^2 = 1/12 - \gamma/3 \\
 & \text{(R4d)} & b^T \beta^3 e = 1/24 - \gamma/2 + 3\gamma^2/2 - \gamma^3 \\
 & \text{(W4a)} & b^T \overline{\alpha} \beta e = 1/6 - \gamma/2 \\
 & \text{(W4b)} & b^T \beta \alpha = 1/6 - \gamma/2
\end{array} \qquad (29)$$

where we define $\overline{\alpha} = (\alpha_{ij})$, and $\varphi = (b_1\alpha_1, ..., b_s\alpha_s)^T$

Moreover we want the relation (21) to be fulfilled, now with $p = 4$ and $s = 6$. Setting $c_1 = b^T\beta^4 e$, $c_2 = b^T\beta^2\alpha^2$, $c_3 = b^T\beta^5 e$, $c_4 = b^T\beta^3\alpha^2$, $c_5 = b^T\beta^4\alpha^2$, by

(21) we get the 4 additional conditions

$$
\begin{array}{ll}
\text{(B1)} & 2c_1 - c_2 = 2\gamma^4 - 4\gamma^3 + 5\gamma^2/3 - \gamma/6 \\
\text{(B2)} & 10\gamma c_1 - 3\gamma c_2 + 2c_3 - c_4 = 8\gamma^5 - 15\gamma^4 + 6\gamma^3 - 7\gamma^2/12 \\
\text{(B3)} & \begin{array}{l} 30\gamma^2 c_1 - 6\gamma^2 c_2 + 12\gamma c_3 - 4\gamma c_4 - c_5 = \\ \qquad 20\gamma^6 - 36\gamma^5 + 14\gamma^4 - 4\gamma^3/3 \end{array} \\
\text{(B4)} & \begin{array}{l} 42\gamma^3 c_1 - 10\gamma^3 c_2 + 14\gamma^2 c_3 - 10\gamma^2 c_4 - 5\gamma c_5 = \\ \qquad 40\gamma^7 - 70\gamma^6 + 80\gamma^3/3 - 5\gamma^4/2 \end{array}
\end{array}
\tag{30}
$$

After some computations we can simplify (30) into

$$
\begin{array}{l}
\gamma c_1 = -\frac{13}{14} c_3 \\
c_5 = \frac{15}{7}\gamma c_3 \\
c_4 = -2\gamma^5 + 3\gamma^4 - \gamma^3 + \frac{1}{12}\gamma^2 - \frac{12}{7} c_3 \\
\gamma c_2 = -2\gamma^5 + 4\gamma^4 - \frac{5}{3}\gamma^3 + \frac{1}{6}\gamma^2 - \frac{39}{21} c_3
\end{array}
\tag{31}
$$

Now our aim is to construct an embedded method such that both methods are stiffly accurate. We have to impose the condition (23) and also

$$
\overline{b}_i = \alpha_{si} = \beta_{s-1,i} \quad i = 1, ..., s-1, \quad \alpha_{s-1} = 1. \tag{32}
$$

Using firstly (23) and (R4c), (R4d), by the definitions of c_i, $i = 1, ..., 5$ we find

$$
\begin{array}{l}
c_1 = \gamma\left(1/24 - 2\gamma/3 + 3\gamma^2 - 4\gamma^3 + \gamma^4\right) + b_5\beta_{54}\beta_{43}\beta_{32}\beta_2 \\
c_2 = \gamma\left(1/12 - 2\gamma/3 + \gamma^2\right) + \\
\qquad \left(b_4\beta_{43}\beta_{32} + b_5\beta_{53}\beta_{32} + b_5\beta_{54}\beta_{42}\right)\alpha_2^2 + b_5\beta_{54}\beta_{43}\alpha_3^2 \\
c_3 = \gamma b_5\beta_{54}\beta_{43}\beta_{32}\beta_2 \\
c_4 = b_5\beta_{54}\beta_{43}\beta_{32}\alpha_2^2 + \\
\qquad \gamma\left(\left(b_4\beta_{43}\beta_{32} + b_5\beta_{53}\beta_{32} + b_5\beta_{54}\beta_{42}\right)\alpha_2^2 + b_5\beta_{54}\beta_{43}\alpha_3^2\right) \\
c_5 = \gamma b_5\beta_{54}\beta_{43}\beta_{32}\alpha_2^2
\end{array}
\tag{33}
$$

Now, by inserting (33) into (31) we find the necessary condition

$$
\frac{1}{24} - \frac{2}{3}\gamma + 3\gamma^2 - 4\gamma^3 + \gamma^4 = 0.
$$

Among the roots we chose $\gamma \approx 0.5279$ that leads to L-stability. With this choice and by (33) we find that (31) become simply

$$
\begin{array}{ll}
\text{(B1')} & b_5\beta_{54}\beta_{43}\beta_{32}\beta_2 = 0 \\
\text{(B2')} & b_5\beta_{54}\beta_{43}\beta_{32}\alpha_2^2 = 0 \\
\text{(B3')} & \begin{array}{l} \left(b_4\beta_{43}\beta_{32} + b_5\beta_{53}\beta_{32} + b_5\beta_{54}\beta_{42}\right)\alpha_2^2 + b_5\beta_{54}\beta_{43}\alpha_3^2 = \\ \qquad \gamma(2\gamma^4 - 10\gamma^3 + 9\gamma^2 - 7\gamma/3 + 1/6) \end{array}
\end{array}
\tag{34}
$$

Therefore, the system that we have to solve is given by (29) and (34). Looking at (B1') and (B2'), it is possible to show that the only possible choice is given by $b_5 = 0$ and $\beta_2 = 0$. Using (23) and (32) we then simplify the system

(29)-(34) into

(R1')	$b_1 + b_2 + b_3 + b_4 = 1 - \gamma$
(R2')	$b_3\beta_3 + b_4\beta_4 = 1/2 - 2\gamma + \gamma^2$
(R3a')	$b_2\alpha_2^2 + b_3\alpha_3^2 + b_4\alpha_4^2 = 1/3 - \gamma$
(R3b')	$b_4\beta_{43}\beta_3 = 1/6 - 3\gamma/2 + 3\gamma^2 - \gamma^3$
(W3')	$b_2\alpha_2 + b_3\alpha_3 + b_4\alpha_4 = 1/2 - \gamma$
(R4a')	$b_2\alpha_2^3 + b_3\alpha_3^3 + b_4\alpha_4^3 = 1/4 - \gamma$
(R4b')	$b_4\alpha_4\alpha_{43}\beta_3 = 1/8 - 5\gamma/6 + \gamma^2$
(R4c')	$b_3\beta_{32}\alpha_2^2 + b_4(\beta_{42}\alpha_2^2 + \beta_{43}\alpha_3^2) = 1/12 - 2\gamma/3 + \gamma^2$
(W4a')	$b_4\alpha_{43}\beta_3 = 1/6 - \gamma + \gamma^2$
(W4b')	$b_3\beta_{32}\alpha_2 + b_4(\beta_{42}\alpha_2 + \beta_{43}\alpha_3) = 1/6 - \gamma + \gamma^2$
(B3')	$b_4\beta_{43}\beta_{32}\alpha_2^2 = \gamma(2\gamma^4 - 10\gamma^3 + 9\gamma^2 - 7\gamma/3 + 1/6)$

Now from (R4b') and (W4a') we compute α_4. Setting α_2, α_3, we get then b_1, b_2, b_3, b_4 from (R1'),(R3a'),(W3'), (R4a'). From (R4c'), (W4b') and (B3') we get $\beta_{32}, \beta_{42}, \beta_{43}$. From (R3b') we obtain β_3 and from (R2') we find β_4. Then from (W4a') we compute α_{43}. For the remaining coefficients we proceed as follows. For α_{32} and α_{42} we use the additional conditions

$$\begin{aligned} b^T\overline{\alpha}\alpha &= 1/6 \\ \varphi^T\overline{\alpha}\alpha &= 1/8 \end{aligned} \tag{35}$$

that are conditions of order 3 and 4 respectively for a general W-method. Moreover, setting α_{52} arbitrarily we compute α_{53}, α_{53} using other two additional conditions

$$\begin{aligned} b^T\overline{\alpha}^2\alpha &= 1/24 \\ b^T\overline{\alpha}^2\beta e &= 1/24 - \gamma/6 \end{aligned}$$

that are both conditions of order 4. Table 2 collects the coefficients of the method here proposed that we call WB34. The remaining free parameters α_2, α_3 and α_{52} have been fixed experimentally.

γ	=	$5.728160624821350e-01$			
α_{21}	=	$5.200000000000000e-01$	γ_{21}	=	$-5.200000000000000e-01$
α_{31}	=	$2.851168665349716e-01$	γ_{31}	=	$-1.034772479328808e+00$
α_{32}	=	$6.248831334650284e-01$	γ_{32}	=	$6.501423878169246e-01$
α_{41}	=	$1.046681454850720e+00$	γ_{41}	=	$2.625385974420247e-01$
α_{42}	=	$-1.127221164631929e+00$	γ_{42}	=	$2.922670258511625e-01$
α_{43}	=	$3.910371962111624e-01$	γ_{43}	=	$-9.114397095544884e-01$
α_{51}	=	$8.451547656533995e-02$	γ_{51}	=	$1.574388804512719e-01$
α_{52}	=	$1.140000000000000e+00$	γ_{52}	=	$6.277349506307095e-02$
α_{53}	=	$-6.668002390497316e-02$	γ_{53}	=	$-5.710378229055593e-01$
α_{54}	=	$-1.578354526603668e-01$	γ_{54}	=	$-2.219906150909184e-01$
α_{61}	=	$2.419543570166118e-01$	γ_{61}	=	$0.000000000000000e-00$
α_{62}	=	$1.202773495063071e+00$	γ_{62}	=	$0.000000000000000e-00$
α_{63}	=	$-6.377178468105325e-01$	γ_{63}	=	$0.000000000000000e-00$
α_{64}	=	$-3.798260677512852e-01$	γ_{64}	=	$0.000000000000000e-00$
α_{65}	=	$5.728160624821350e-01$	γ_{65}	=	$-5.728160624821350e-01$
b_1	=	$2.419543570166118e-01$	$\bar{b}_1$	=	$2.419543570166118e-01$
b_2	=	$1.202773495063071e+00$	$\bar{b}_2$	=	$1.202773495063071e+00$
b_3	=	$-6.377178468105325e-01$	$\bar{b}_3$	=	$-6.377178468105325e-01$
b_4	=	$-3.798260677512852e-01$	$\bar{b}_4$	=	$-3.798260677512852e-01$
b_5	=	$0.000000000000000e-00$	$\bar{b}_5$	=	$5.728160624821350e-01$
b_6	=	$5.728160624821350e-01$	$\bar{b}_6$	=	$0.000000000000000e-00$

Table 2: set of coefficients for WB34.

Remark 8 *It's worthwhile nothing that conditions (35), that we chose for the basic method (and not satisfied by the embedded one), completes the set of conditions of order 3 for a general W-method. In this way, when the relation $W = J + O(h)$ deteriorates we lose only one order of consistency, getting an embedded W-method of order 3(2).*

Regarding WB23 of previous section, the situation is a bit more complicated, because the deterioration mentioned above influences only the order of the basic method, that drops to 2, whereas the condition (28) imposed for the embedded method guarantees the preservation of the order. Therefore, as local error estimator, WB23 can be negatively affected by the degree of the Jacobian approximations. Because of the small number of levels and the choice of having only 3 function evaluations per step, it is not possible to impose the necessary additional conditions for the basic method of WB23 for making it a method of order 3 for arbitrary approximation of the Jacobian.

5 Numerical implementation

In this section we want to provide some details concerning the practical implementation of the methods just proposed WB23 and WB34. Looking at (2) we observe that a direct implementation of such formula require, at each stage, the matrix vector multiplication $W \sum_{j=1}^{i-1} \gamma_{ij} k_j$ and the solution of a linear system with $(I - h\gamma W)$. As in [9], [5], the former operation can be avoided introducing the new stages

$$p_i = \gamma k_i + \sum_{j=1}^{i-1} \gamma_{ij} k_j, \quad i = 1, ..., s.$$

Defining the matrix $\Gamma = \gamma I + (\gamma_{ij})$, we can get the inverse relation

$$k_i = \frac{1}{\gamma} p_i - \sum_{j=1}^{i-1} \phi_{ij} p_j, \tag{36}$$

where $\Phi = (\phi_{ij}) = \frac{1}{\gamma} I - \Gamma^{-1}$ is a strictly lower triangular matrix. Inserting formula (36) into the general formulation (2) leads to

$$\begin{array}{c} (I - h\gamma W) p_i = h\gamma f \left(y_m + \sum_{j=1}^{i-1} a_{ij} p_j \right) + \gamma \sum_{j=1}^{i-1} \phi_{ij} p_j, \quad i = 1, ..., s, \\ y_{m+1} = y_m + \sum_{i=1}^{s} d_i k_i, \end{array} \tag{37}$$

where

$$(a_{ij}) = (\alpha_{ij})\, \Gamma^{-1} \text{ and } (d_1, ..., d_s) = (b_1, ..., b_s)\, \Gamma^{-1}.$$

Clearly, using the good and bad Broyden's updates, the use of the inversion formulas (8), (9), allows to compute the inverse of $(I - h\gamma W)$ by means of a rank-1 update at each step. However, when working with large problems with sparse Jacobian the use of the inversion formulas for these updates is quite inefficient because the inverses are full and hence all the necessary matrix operations to perfom the update are unable to exploit the sparsity structure of the problem. By (8), (9), since we can write

$$(I - h_{m+1}\gamma W_m)^{-1} = (I - h_1 \gamma W_0)^{-1} + u_0 v_0^T + ... + u_m v_m^T, \tag{38}$$

(h_1 being the first step) it is much more convenient to compute p_i, $i = 1, ..., s$, computing the LU factorization of $(I - h_1 \gamma W_0)$ and then storing the update vectors u_k, v_k, $k \geq 0$. In this way we also avoid the initial inversion, i.e., the explicit computation of $(I - h_1 \gamma W_0)^{-1}$. Since we are mainly interested in these kind of problems the methods have been implemented in this manner. For the good Broyden's update, since we also need the matrix W_m to perform the update of $(I - h_{m+1}\gamma W_m)^{-1}$ we use the recursion (similar to (38)) arising from (7). In this way, with respect to a standard ROW-method these two update approaches are able to work with only one factorization (unless we need to recompute the Jacobian) and the cost of the computation of the Jacobian is substituted by the cost for the computation of the update vectors. For the Schubert's update, the linear algebra cost is essentially the same of a ROW-method, but the cost for the computation of the Jacobian is substituted by the cost of the sparse operation (12).

In our numerical experiments, the stepsize selection that we adopt is given by the classical formula

$$h_{new} = h \min \left\{ fac_M, \max \left\{ fac_m, fac_s \left(\frac{tol}{err} \right)^{1/p} \right\} \right\}, \tag{39}$$

where we chose $fac_M = 5, fac_m = 0.2$ and $fac_s = 0.75$ when using the exact Jacobian, and the more conservative set $fac_M = 2, fac_m = 0.2$ and $fac_s = 0.75$, for the rank-1 updates. Because of the progressive deterioration of $W = J+O(h)$ we use $p-1$ instead of p in (39) for the W-methods.

Regarding the norm of the local error estimate LE we consider the formula

$$err_m = \sqrt{N^{-1}\sum_{i=1}^{N}\left(\frac{LE_i}{rtol\cdot(y_m)_i + atol_i}\right)^2},$$

where $atol \in \mathbb{R}^N$ and $rtol \in \mathbb{R}$ are the absolute and relative tolerances respectively, so that the stepsize is accepted if $err_m \leq rtol$.

As anticipated at the end of Section 2, an important remark regard the implementation of the WB-methods based on the updates considered. Formulas (14), (16) and (18) actually do not produce information about the degree of the deterioration of the approximations as m increases. Hence, besides the theoretical properties of these updates, we could have a fast deterioration of the spectral properties that affects the stability of the methods. However, the numerical experiments reveal that this drawback can be overcome quite simply by recovering the Jacobian at certain points during the integration. In this sense, our idea is to recompute the Jacobian (i.e., to restart the method) when a failed attempt occurs. Just to give an explanation of this idea let us consider the Prothero-Robinson equation

$$y' = \lambda(y - \varphi(t)) + \varphi'(t), \qquad \lambda = -500, \qquad \varphi(t) = 1/4\sin(t/4), \tag{40}$$

for $0 \leq t \leq 10$ and $y(0) = 1$. We integrate this equation (in the corresponding autonomous form) using the just explained implementation with the following methods: WB34, the ROW-method corresponding to the set of coefficients given in Table 2; WB34g and WB34b, the W-methods of Table 2 implemented with the updates (7) and (9) respectively with restart; WB34g-wr and WB34b-wr that are the same methods but without restart. The results, given in Fig.1, are exhaustive and confirm that the restart approach is necessary.

Regarding the sparse update, although it is always difficult to control the progressive deterioration of the approximations, the experiments on large and sparse problems reveal that this approach can often be implemented without restart. Evidently, the preservation of the sparsity structure of the Jacobian together with the theoretical properties of the update, lead to a negligible alteration of the stability properties of the underlying method. In any case, in all the experiments of the next section the WB-methods are always implemented with restart.

We have created a Matlab code `ROSWB` available at `http://univaq.it/~novati`. The code is written following the format used in THE MATLAB ODE SUITE [18] and allows to chose between WB23 and WB34 and also among some other well known ROW-methods. The code permits to switch between the three rank-1 updates presented, or to use the exact Jacobian (even numerically generated

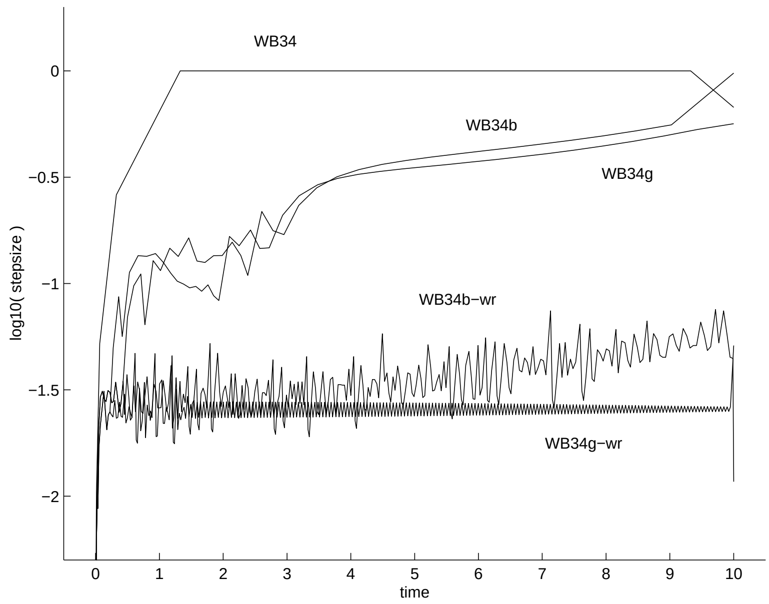

Figure 1: Stepsize curve of the WB34 method for the Prothero-Robinson problem (40) with and without restart.

by the Matlab function `numjac`), or also to keep it constant. We do not claim that the implementation here presented is the best possible, but since in our experiments we shall use it for each method, the comparisons that we are going to present are surely significative.

6 Numerical experiments

In this section we present some numerical experiments in which we compare the WB-methods with some classical ROW-methods implemented in `ROSWB`. In particular we consider RODASP by Steinebach [20], a 6-stage method of order 4, ROS3P [11], a 3-stage method of order 3, and ROS3PW [15], a 4-stage method of order 3.

In the first two experiments we want to test the ROW-methods WB23 and WB34. The aim is to test if the set of coefficients is actually well designed. We compare these methods with the above ROW-methods on the following well known test problems.

1. HIRES, the chemical reaction model proposed by Schäfer (see [5]). We integrate this problem from 0 to 50.
2. ROBER, the reaction of Robertson (see [5]). We integrate this problem from 0 to 10^{11}.

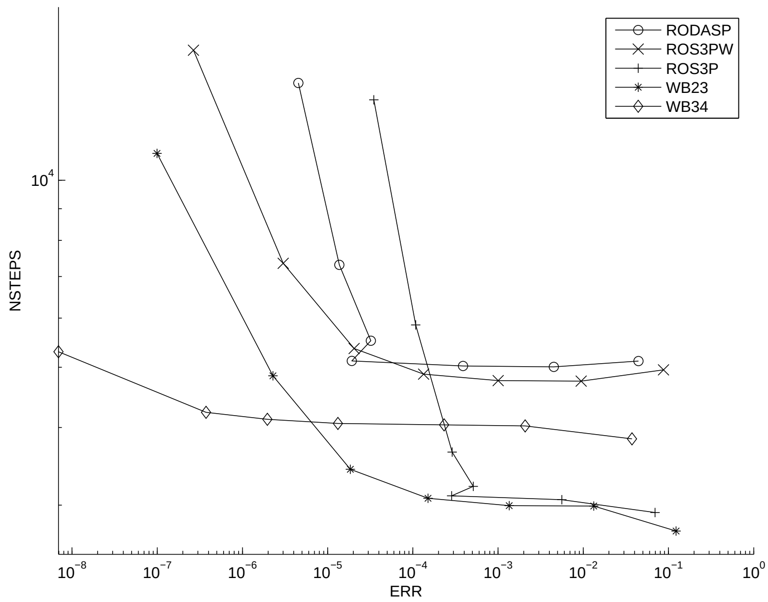

Figure 2: Number of steps - error diagram for HIRES.

In Figs. 2 and 3 we observe the results for the above problems in a number of steps-precision diagram. The number of steps ($NSTEPS$) is displayed as a function of the Euclidean norm of the error (ERR). The diagrams are obtained changing the value of $atol = rtol = TOL$.

Both results show that the coefficients of WB34 are actually well designed. The behavior of WB23 is also very interesting for HIRES (if compared with RODASP), especially for low tolerances.

Now we want show the performances of our methods on three equations arising from the semi-discretization of well-known parabolic problems. For each example, we compare the obtained numerical results for each methods with a reference solution for the given ODE. The computing time ($NSEC$) is displayed as a function of the Euclidean norm of the error (ERR). For each problem we set $atol = rtol = TOL$ and the methods have been applied with

$$TOL = 10^{-2}, 10^{-3}, ...$$

We consider the following problems.

1. The FitzHugh and Nagumo model

$$\begin{cases} \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - g(u) - v \\ \frac{\partial v}{\partial t} = \eta(u - \beta v) \end{cases}$$

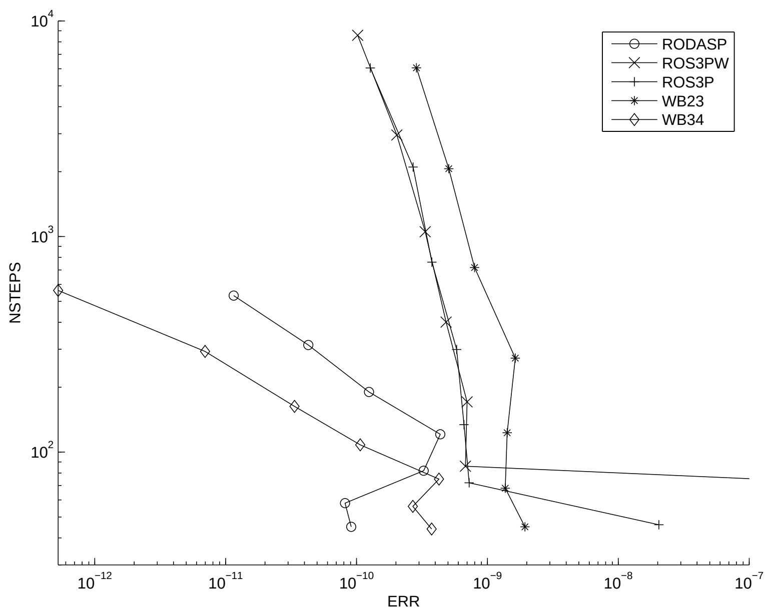

Figure 3: Number of steps - error diagram for ROBER.

where

$$f(u) = u(u - \alpha)(u - 1),$$

for $0 \le x \le 100$ and $0 \le t \le 400$, with boundary conditions

$$\frac{\partial u}{\partial x}(0,t) = -0.3, \qquad \frac{\partial u}{\partial x}(100,t) = 0,$$

and initial conditions

$$u(x,0) = v(x,0) = 0.$$

We discretize with the method of lines and central differences with mesh-size $\delta = 100/151$, getting a system of 300 equations. As in [5], we chose $\alpha = 0.139$, $\eta = 0.008$, and $\beta = 2.54$

2. The NILIDI problem [25], i.e., the two-dimensional nonlinear diffusion equation

$$\frac{\partial u}{\partial t} = e^u \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) + u\left(18e^u - 1\right),$$

on $[0,\pi/3] \times [0,\pi/3]$ and $0 \le t \le 1$. We consider Dirichelet boundary conditions and initial condition $u(x,y,0) = \sin(3x)\sin(3y)$. We discretize with central differences and the method of lines with $\delta = \pi/93$, getting a system of 900 equations.

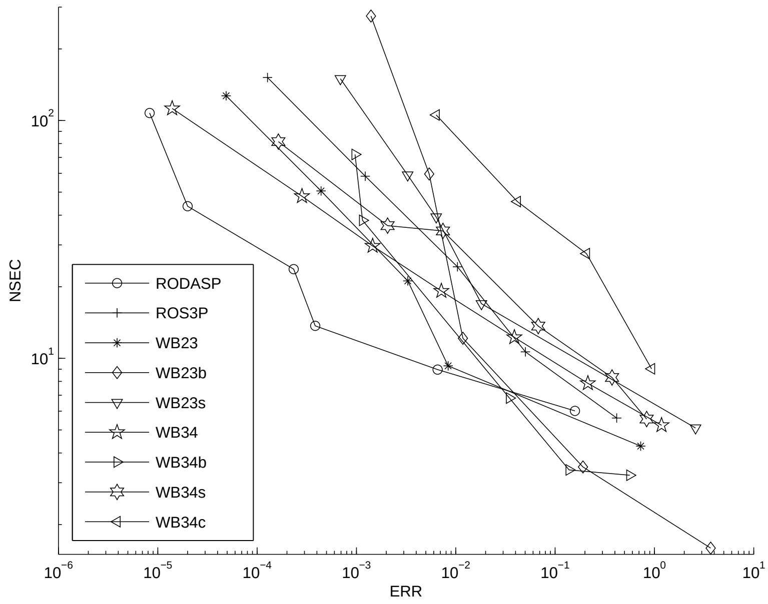

Figure 4: Work-precision diagram for the FitzHugh & Nagumo problem.

3. The equation

$$\frac{\partial u}{\partial t} = \nu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) - u\frac{\partial u}{\partial x} - u\frac{\partial u}{\partial y}, \tag{41}$$

on $[0, 1/2] \times [0, 1/2]$ and $0 \le t \le 0.1$, with $\nu = 0.1$. Initial and time-dependent boundary conditions are taken from the exact solution

$$u(x, y, t) = \frac{1}{1 + \exp\left(\frac{x+y-t}{2\nu}\right)}.$$

We discretize as before with $\delta = 1/42$ getting a system of 400 equations.

In Figs. 4, 5, 6, we can observe the results obtained. WBxxg, WBxxb and WBxxs, denote the WBxx method applied with the good Broyden's, bad Broyden's and Schubert's update respectively. Moreover WBxxc denotes the WBxx applied with $W_m = J(y_0)$. All methods are implemented with the stepsize selection (39) and with restart when a failed attempt occurs.

The results for the FitzHugh and Nagumo problem (Fig. 4) show that the best method is RODASP and also that the update approaches cannot outperform the use of the exact Jacobian. In particular for this example the methods based on the good Broyden's update are not suited. However it is interesting to observe the comparison between WB34s, WB34b and WB34c that show the improvement attainable using the updates with respect to the use of a constant

Jacobian. The behavior of ROS3PW is similar to that of ROS3P, and hence it is not represented. For the methods considered, in the following table (Table 3) we also report the statistics corresponding to the choice of $TOL = 10^{-6}$.

	SS	FA	FE	PD	DEC	LS	NSC	ERR
RODASP	894	10	5424	894	904	5424	43.6	2.00e-5
ROS3P	2864	6	5747	2864	2870	8610	151.6	1.27e-4
WB23	2426	4	7296	2426	2430	9720	127.0	4.87e-5
WB23b	3091	29	9334	29	30	15570	275.1	1.40e-3
WB23s	2837	0	8511	1	2837	11348	149.8	6.89e-4
WB34	629	1	3787	629	630	3780	29.6	1.45e-3
WB34b	1395	1	8375	2	2	9770	71.9	9.70e-4
WB34s	768	1	4613	2	769	4614	36.1	2.06e-3
WB34c	2127	1	12768	2	2128	12768	105.5	6.35e-3

Table 3. Statistics for the FitzHugh and Nagumo problem with $TOL = 10^{-6}$.
SS:succesful steps; FA: failed attempts; FE: function evaluations;
PD: partial derivatives; DEC: LU decompositions; LS: linear systems;
NSC: seconds; ERR: final error (Euclidean norm).

In Fig. 5 the results for the NILIDI equation are shown.. Here the best methods seem to be WB34, WB34b and WB34s. The behavior of WB23b and WB23s (not plotted) is very similar to that of WB23 and it is interesting the comparison of these methods with ROS3P and RODASP.

In Fig. 6 the results for the ODE arising from (41) are shown. The results of WB34g and WB34b are remarkable. Here the behavior of WB34 (not plotted) is similar to that of ROS3PW. The worst methods were WB23s and WB34c (not represented). For this experiment we also consider the numerical observed temporal order (p_{num}). We compute the Euclidean norm of the error at $t = 0.1$ with respect to the reference solution of the ODE (ERR in the tables below) applying the methods with constant stepsize h. All WB-methods are implemented without restart. Tables 4a, 4b, 4c, 4d, contain the results.

	ROS3PW		ROS3P		WB23	
h	ERR	p_{num}	ERR	p_{num}	ERR	p_{num}
2e-3	7.63e-8		9.19e-8		1.95e-8	
1e-3	9.90e-9	2.95	1.46e-8	2.66	2.54e-9	2.94
5e-4	1.27e-9	2.97	2.64e-9	2.46	3.25e-10	2.96
2.5e-4	1.60e-10	2.98	5.59e-10	2.24	4.15e-11	2.97

Table 4a - Problem (41). Observed temporal order
for the ROW-methods of order 3.

	RODASP		WB34	
h	ERR	p_{num}	ERR	p_{num}
2e-3	4.00e-9		3.04e-9	
1e-3	1.00e-9	2.00	2.54e-10	3.58
5e-4	2.50e-10	2.00	1.94e-11	3.71
2.5e-4	6.24e-11	2.00	1.51e-12	3.69

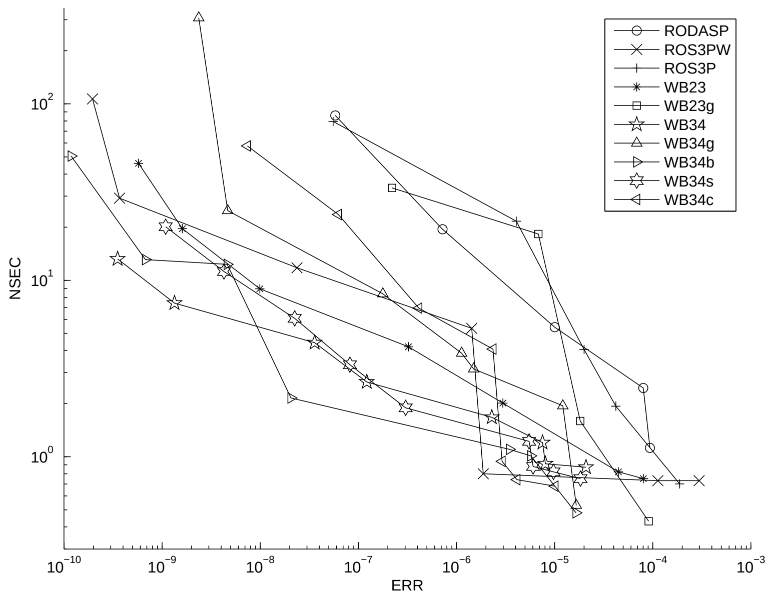

Figure 5: Work-precision diagram for the NILIDI problem.

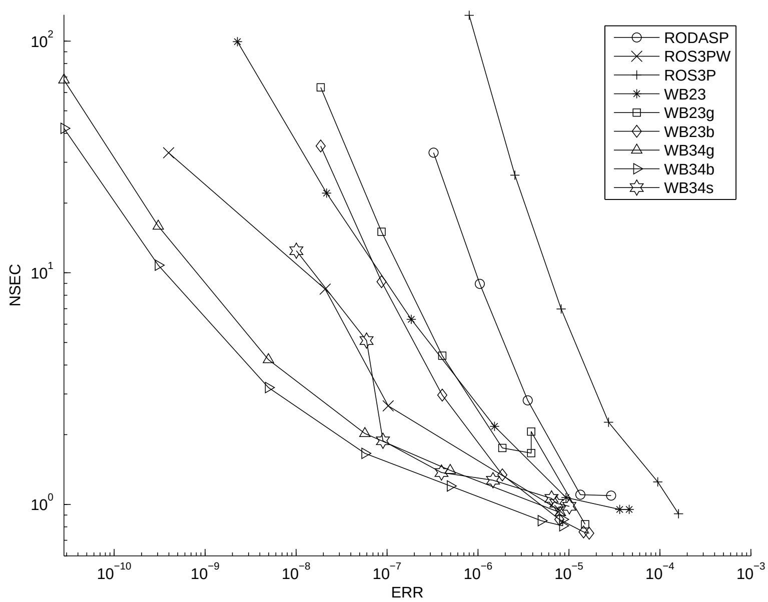

Figure 6: Work-precision diagram for the problem (41).

Table 4b - Problem (41). Observed temporal order
for the ROW-methods of order 4.

	WB23g		WB23b		WB23s		WB23c	
h	ERR	p_{num}	ERR	p_{num}	ERR	p_{num}	ERR	p_{num}
2e-3	5.27e-7		5.34e-7		3.22e-7		3.39e-5	
1e-3	1.57e-7	1.75	1.59e-7	1.75	9.23e-8	1.80	1.04e-5	1.71
5e-4	4.36e-8	1.85	4.38e-8	1.86	2.89e-8	1.67	2.92e-6	1.83
2.5e-4	1.15e-8	1.92	1.15e-8	1.92	8.21e-9	1.82	7.82e-7	1.90

Table 4c - Problem (41). Observed temporal order
for the W-methods based on the WB23 set of coefficients.

	WB34g		WB34b		WB34s		WB34c	
h	ERR	p_{num}	ERR	p_{num}	ERR	p_{num}	ERR	p_{num}
2e-3	9.11e-8		9.72e-8		1.39e-7		1.53e-5	
1e-3	1.62e-8	2.49	1.67e-8	2.54	2.05e-8	2.76	3.26e-6	2.24
5e-4	2.71e-9	2.58	2.74e-9	2.61	3.04e-9	2.75	5.71e-7	2.51
2.5e-4	4.08e-10	2.73	4.10e-10	2.74	4.37e-10	2.80	8.70e-8	2.72

Table 4d - Problem (41). Observed temporal order
for the W-methods based on the WB34 set of coefficients.

Looking at Tables 4a-4b, if we compare WB23 with ROS3P and ROS3PW, and WB34 with RODASP, either in terms of numerical order and accuracy, we can state that the WB-methods presented are well designed. Regarding the order reduction of the W-methods considered (Tables 4c and 4d), the results were expected (see the remark at the end of Section 4). However it is worth nothing that the WB34x methods have an observed order around the value $p_{num} = 2.75$, where the typical situation working with semidiscretized parabolic PDEs and inexact Jacobian is $p_{num} = 2$. This is due to the additional conditions (35). A final remark regards the comparison between the rank-1 updates and the use of time-lagged Jacobians. Here all W-methods are implemented without recovering the Jacobian, and hence, looking at the errors we can observe the improvements attainable with the rank-1 updates.

7 Concluding remarks

In previous section we saw that the WB-methods represent an efficient class of W-methods. The comparisons with the well known ROW-methods considered show that especially the W-methods based on the bad Broyden's update and on the Schubert's update are accurate and inexpensive for large problems with sparse Jacobian. The accuracy is substantially due to the secant equation (3) that allows to have a Jacobian approximations of the type

$$W_m = J(y_m) + O(h). \tag{42}$$

As to the computational cost, the use of the Broyden's updates allows to reduce drastically the number of LU decompositions (see Table 3). Moreover the computation of the rank-1 updates is quite inexpensive (especially for the bad Broyden's update). For the Schubert's update approach the computational cost of the sparse update is nearly negligible. On the other hand the progressive deterioration of (42) (that holds in particular for variable stepsize) forces the restart of the methods in order to assure the stability.

The results of the numerical experiments presented are encouraging because a deeper analysis on the stability properties attainable with the rank-1 updates (together with an accurate error analysis) should allow the realization of even more efficient algorithms, especially in what concerns the stepsize selection and restart strategies. Another possible improvement could regard the use of a symmetric sparse update, that consists in a rank-2 update, for problems where this property holds for the Jacobian. From literature (see for instance [4]), we know that this kind of update allows also the sequencing of the Cholesky factorizations that could lead to very efficient W-methods.

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