Two-step W-methods and their application to MOL-systems

R. Weiner [a], B.A. Schmitt [b], H. Podhaisky [a],

[a] *FB Mathematik und Informatik, Martin-Luther-Universität Halle-Wittenberg, Postfach, 06099 Halle, Germany*

[b] *Fachbereich Mathematik, Universität Marburg, Lahnberge, 35032 Marburg, Germany*

Abstract

Parallel two-step W-methods are linearly-implicit integration methods where the s stage values can be computed in parallel. We consider different types of such methods having order and stage order $s-1$ or s and favourable stability properties. A new class of two-step W-methods with peer variables is more robust with respect to stepsize changes since it possesses optimal damping at infinity. Numerical comparisons on a shared memory computer show the efficiency of the methods in combination with Krylov-techniques for MOL-systems.

Key words: Stiff ODEs, MOL, parallel two-step W-methods.

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1 Introduction

The method of lines (MOL) is a well-established approach for the solution of time-dependent partial differential equations. By a space discretization (Finite Differences, Finite Elements,...) the partial differential equations are transformed into a large system of ordinary differential equations

$$y' = f(t, y), \quad y(t_0) = y_0 \in \mathbb{R}^n. \tag{1.1}$$

This system is stiff, in general, and stiff integrators are required for the numerical solution. Among classical stiff integrators, linearly-implicit one-step

Email addresses: `weiner@mathematik.uni-halle.de` (R. Weiner),
`schmitt@mathematik.uni-marburg.de` (B.A. Schmitt),
`podhaisky@mathematik.uni-halle.de` (H. Podhaisky).

methods like ROW- and W-methods (e.g. RODAS [5]) are used frequently. However, due to the large dimension of (1.1) for higher dimensional partial differential equations special efforts have to be made for the efficient solution of the linear equations in linearly-implicit ROW- and W-methods. In the last years the combination of Krylov techniques with stiff integrators has become popular. Examples are ROWMAP [11], which combines the ROS4-methods [5] with a special Arnoldi process, and EXP4 [6] where a special W-method is combined with an efficient approximation of the product matrix-exponential $\times$ vector. An efficient multistep code is VODPK [2], which uses GMRES(l) within the BDF-code VODE.

In this paper we will consider possibilities to improve the performance of W-methods with respect to the following 2 directions:

1. Linearly-implicit one-step methods suffer from a low stage order, in general, which can lead to an order reduction for stiff problems.
2. One-step methods are not suited for parallel implementation with parallelism across the method.

These drawbacks can be overcome by using two-step W-methods.

In Section 2 we give an overview about two-step W-methods, both for sequential and parallel computers. We review stability and convergence results.

In Section 3 we consider the new class of parallel two-step W-methods with peer variables (PPSW-methods). In these methods s numerical solutions of equal importance are computed in parallel at each time step. We discuss the stability and convergence of the methods. With the help of simplifying assumptions methods of order $p = s - 1$ are constructed, which have stage order $s-1$ too. For the class of singly-implicit PPSW-methods, introduced in [10], order s can be obtained for constant stepsizes and appropriate parameter values.

In Section 4 we investigate the new class of multi-implicit PPSW-methods. We give special superconsistency conditions that allow to increase the order to $p = s$ for arbitrary stepsizes. In contrast to singly-implicit PPSW-methods the new methods can be stiffly accurate. Stiff accuracy leads to optimal damping properties for very stiff problems. These pay off in practical computations. We also discuss strong stability of the methods, which is important for convergence. By numerical search we construct special methods up to order 5 with good stability properties.

In Section 5 we apply parallel two-step W-methods to several MOL-systems. Our methods are implemented with the Krylov-method FOM [9] for the solution of the linear systems. The methods are tested on a shared memory computer and compared with the multistep Krylov-code VODPK. The results show the efficiency of the new multi-implicit PPSW-methods on parallel computers with few processors.

2 Two-step W-methods

In order to overcome the low stage order of classical one-step ROW- and W-methods the class of two-step W-methods was introduced by the authors in [7,8]. For problem (1.1) the most general form of these methods is

$$\begin{aligned} Y_{mi} &= u_m + h_m \sum_{j=1}^{i-1} \tilde{a}_{ij} k_{mj} + h_m \sum_{j=1}^{s} a_{ij} k_{m-1,j} \\ (I - h_m \gamma T_m) k_{mi} &= f(t_m + c_i h_m, Y_{mi}) + h_m T_m \sum_{j=1}^{i-1} \tilde{\gamma}_{ij} k_{m,j} + h_m T_m \sum_{j=1}^{s} \gamma_{ij} k_{m-1,j} \\ u_{m+1} &= u_m + h_m \sum_{i=1}^{s} (b_i k_{mi} + v_i k_{m-1,i}) \end{aligned} \tag{2.1}$$

For two-step W-methods the coefficients $A = (a_{ij})$, $\widetilde{A} = (\tilde{a}_{ij})$, $\Gamma = (\gamma_{ij})$, $\widetilde{\Gamma} = (\tilde{\gamma}_{ij})$, $b = (b_i)$ and $v = (v_i)$ depend on the stepsize ratio $\sigma_m = h_m/h_{m-1}$, γ is constant. For $A = \Gamma = 0$ and $v = 0$ we obtain a classical W-method or a ROW-method for autonomous systems and $T_m = f_y(u_m)$. Using the stage values of the previous time step allows to increase the stage order of these methods. Indeed, methods of order and stage order s have been constructed in [8] with the help of simplifying assumptions. The stability of the methods is also considered there in the following way. Application to the test-equation

$$y' = \lambda y, \quad \Re\lambda < 0, \tag{2.2}$$

with constant h leads to the recursion

$$\begin{pmatrix} hK_m \\ u_{m+1} \end{pmatrix} = M(z) \begin{pmatrix} hK_{m-1} \\ u_m \end{pmatrix}$$

with $K_m = (k_{mi})$ and with the stability matrix

$$M(z) = \begin{pmatrix} W\beta & W\,\mathbb{1} \\ b^T W \beta + v^T & 1 + b^T W\,\mathbb{1} \end{pmatrix}, \tag{2.3}$$

where the notations $z = h\lambda$, $\beta = A + \Gamma$, $\widetilde{\beta} = \widetilde{A} + \widetilde{\Gamma}$, $\mathbb{1} = (1, ..., 1)^T$ and $W = z[(1 - z\gamma)I - z\widetilde{\beta}]^{-1}$ are used.

We call the method A-stable if $\varrho(M(z)) < 1$ for $\Re z < 0$, and L-stable if in addition $\varrho(M(\infty)) = 0$. For very stiff problems the property

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

is desirable, which is equivalent to

$$\lim_{z\to\infty} e_{s+1}^T M(\infty) = 0. \tag{2.4}$$

Methods satisfying (2.4) are derived in [8]. These methods perform well on sequential computers. With the special choice $\widetilde{A} = \widetilde{\Gamma} = 0$ all s stage values Y_{mi}, k_{mi} can be computed in parallel. Such parallel methods have been constructed and analyzed in an earlier paper [7]. It was shown, that despite the smaller number of parameters methods of order and stage order s exist at least up to $s = 8$. These methods also satisfy (2.4).

Parallel methods with stage number $s = 2, 3, 4$ were tested on small problems using LU-decomposition and on MOL-systems using FOM. The numerical results demonstrate that the methods are efficient for $s = 2, 3$. Their weakness, however, is some critical dependence on the stepsize ratio in the stiff case since the stability matrix $M(\infty)$ depends on powers of σ up to σ^{s-1}. This makes the construction of robust methods and their implementation for higher s very difficult. In the next section we therefore propose a new class of parallel methods which do not suffer from this drawback, at least for $z \to \infty$.

Remark 2.1 *Cao et al. [3] also consider parallel two-step W-methods but only with strictly lower triangular coefficient matrices A and Γ. This restricts the number of parameters considerably.*

3 Parallel 'Peer' two-step W-methods

Dropping the distinguished solution variable u from (2.1) we consider Parallel 'Peer' two-step W-Methods (PPSW methods) of the form

$$(I - \gamma_i h_m T_m) Y_{mi} = \sum_{j=1}^{s} \Big(b_{ij} I + h_m \gamma_{ij} T_m\Big) Y_{m-1,j} + h_m \sum_{j=1}^{s} a_{ij} f\Big(t_{m-1,j}, Y_{m-1,j}\Big), \tag{3.1}$$

$i = 1, \ldots, s$. Here the numerical solutions Y_{mi} are approximations to the exact solution $y(t_{mi}) = y(t_m + h_m c_i)$. Obviously, with s processors all s values Y_{mi} can be computed in parallel. The matrix T_m should be an approximation to the Jacobian $f_y(t_m, y(t_m))$ for stability reasons only. In fact, the accuracy of these methods is derived for arbitrary T_m in the sense of W-methods. Introducing the stage vectors $Y_m = (Y_{mi})_{i=1}^s \in \mathbb{R}^{sn}$ and $G := \mathrm{diag}(\gamma_i)$ a compacter version of the PPSW-method is

$$(I - h_m G \otimes T_m) Y_m = (B \otimes I + h_m \Gamma \otimes T_m) Y_{m-1} + h_m (A \otimes I) F(t_{m-1}, Y_{m-1}), \quad (3.2)$$

where $F(t_{m-1}, Y_{m-1}) = (f(t_{m-1,1}, Y_{m-1,1})^T, ..., f(t_{m-1,s}, Y_{m-1,s})^T)^T$. Again, the coefficients of the method depend on $\sigma_m := h_m/h_{m-1}$. In contrast to PTSW-methods we have no special highlighted value u_{m+1} but s solution values of equal importance. One immediate consequence is the existence of a continuous extension of these methods. However, special stability requirements, similar to zero-stability for multistep methods, have to be met.

The coefficients will be determined in order to obtain a method that is of high order, has good stability properties and is robust with respect to stepsize changes. While the first goal can be easily achieved with the help of simplifying assumptions, the other two points are more difficult.

3.1 Convergence

The accuracy of the PPSW methods may be analyzed in a standard way by considering the residuals Δ_{mi}, which are obtained when the exact solution is put into the method:

$$h_m \Delta_{mi} := (I - \gamma_i h_m T_m) y(t_{mi}) - \sum_{j=1}^{s} \Big(b_{ij} + h_m \gamma_{ij} T_m\Big) y(t_{m-1,j}) - h_m \sum_{j=1}^{s} a_{ij} y'(t_{m-1,j}), \quad (3.3)$$

$i = 1, \ldots, s$. By Taylor expansion at t_m we observe that

$$h_m T_m (\gamma_i y(t_{mi}) + \sum_{j=1}^{s} \gamma_{ij} y(t_{m-1,j})) = O(h_{m-1}^{q+1})$$

holds if the condition

$$\Gamma(q): \quad \gamma_i c_i^k + \sum_{j=1}^{s} \gamma_{ij} (c_j - 1)^k \sigma^{-k} = 0, \quad k = 0, \ldots, q-1 \quad (3.4)$$

with $\sigma = \sigma_m$ is satisfied for a sufficiently smooth solution. Secondly, it holds that

$$y(t_{mi}) - \sum_{j=1}^{s} b_{ij} y(t_{m-1,j}) - h_m \sum_{j=1}^{s} a_{ij} y'(t_{m-1,j}) = O(h_{m-1}^{q})$$

if condition

$$AB(q): \quad c_i^k - \sum_{j=1}^{s} b_{ij} (c_j - 1)^k \sigma^{-k} - k \sum_{j=1}^{s} a_{ij} (c_j - 1)^{k-1} \sigma^{1-k} = 0, \quad k = 0, \ldots, q-1, \quad (3.5)$$

is true. We can summarize this in the following Lemma:

Lemma 3.1 *If the simplifying assumptions* $\Gamma(q)$ *and* $AB(q+1)$ *are satisfied with* $q \geq 1$ *and the solution* y *is sufficiently smooth then the residuals (3.3) for the scheme (3.1) are of order* q*, i.e.,* $\|\Delta_m\| = O(h_{m-1}^q)$.

Convergence results for PPSW-methods for variable stepsizes can be derived in the same manner as for multistep methods, see e.g. [4]. Here the exact solution is considered as a perturbed solution of (3.1) and the difference of numerical and exact solution is estimated with the help of Lemma 3.1 and the stability of the method.

Definition 3.1 *The PPSW-method* (3.1) *is called stable, if*

$$\|B_{m+l}B_{m+l-1}\cdots B_{m+1}B_m\| \leq M \tag{3.6}$$

for all m *and* $l \geq 0$*. Here the index reflects the dependence on the stepsize ratio* σ*.*

Theorem 3.1 *Let the simplifying assumptions* $AB(p+1)$ *and* $\Gamma(p)$ *be satisfied and* $\sigma_m \leq \sigma_{max}$*. Assume that the method is stable and has bounded coefficients. Let the starting values satisfy* $\|Y_{0i} - y(t_0 + c_i h_0)\| = \mathcal{O}(h_0^p)$.
Then the PPSW-method is convergent of order p*.*

Proof. Analogously to [4] using Lemma 3.1. ■

Using the simplifying conditions we will construct methods which satisfy the assumptions of Lemma 3.1 with $q = s - 1$ or s. The stability (3.6) requires more effort and additional restrictions on σ_m, in general.

3.2 Stability

We apply PPSW-methods to the test equation of A-stability $y' = \lambda y$ with constant stepsize h and $T_m = \lambda$. As usual we denote $z = h\lambda$. For the vectors $Y_m = \big(Y_{mi}\big)$ we obtain the recursion

$$Y_m = M(z)Y_{m-1}, \quad M(z) := (I - zG)^{-1}(B + z\beta), \quad \beta = A + \Gamma. \tag{3.7}$$

Definition 3.2 *The PPSW-method* (3.1) *is called* A*-stable resp.* $A(\alpha)$*-stable if* $\rho(M(z)) < 1$ *in the open left complex halfplane,* $z \in \mathbb{C}_- := \{z \in \mathbb{C} : \Re z < 0\}$ *resp. for* $|arg(z) - \pi| < \alpha$*. It is called* L*-stable (*$L(\alpha)$*-stable) if, additionally,* $\rho(M(\infty)) = 0$.

Due to

$$M(\infty) = -G^{-1}\beta$$

optimal damping properties for very stiff problems are obtained with $\beta = 0$.

Definition 3.3 *A PPSW-method with $\beta = 0$ is called* stiffly accurate.

For the convergence of the method (cf. Theorem 3.1), on the other hand, stability of $M(0) = B$ is required. The condition $AB(1)$ reads $B_m \mathbb{1} = \mathbb{1}$ and introduces one eigenvalue 1 for all values of σ_m.

Definition 3.4 *A PPSW-method is called strongly stable if for $\sigma = 1$ the eigenvalues λ_i of the matrix B satisfy*

$$\lambda_1 = 1, \quad |\lambda_i| < 1,\ i = 2, ..., s.$$

We now turn to the construction of special PPSW-methods of higher order with good stability properties.

3.3 PPSW1-methods

We introduce the following notations

$$V = (c_i^{j-1})_{i,j=1}^s, \quad P = \left(\binom{j-1}{i-1} \right)_{i,j=1}^s, \quad S_m = \mathrm{diag}(1, \sigma_m, \ldots, \sigma_m^{s-1}), \quad (3.8)$$
$$D = \mathrm{diag}(1, ..., s), \quad \widehat{D} = \mathrm{diag}(0, 1, ..., s-1), \quad F_0 = (\delta_{i-1,j}).$$

Requiring the condition $\Gamma(s)$ leads to the explicit relation

$$\Gamma = -G\Theta, \quad \Theta := V S_m P V^{-1}. \tag{3.9}$$

The matrix Θ describes the polynomial extrapolation from the subgrid $\{t_{m-1} + h_{m-1}c_i,\ i = 1, \ldots, s\}$ to $\{t_m + h_m c_i,\ i = 1, \ldots, s\}$. In a similar way, explicit solutions for the order conditions (3.5) may be obtained by requiring $AB(s)$. In this case, (3.5) has the form $0 = V - BVP^{-1}S_m^{-1} - AVP^{-1}S_m^{-1}F_0^T\widehat{D}$ with the matrices introduced above and may be solved for the matrix B yielding

$$B = \Theta - \sigma_m AVDF_0^T V^{-1} = \Theta - \sigma_m(\beta + G\Theta)VDF_0^T V^{-1}. \tag{3.10}$$

Here, the identity $PF_0^T\widehat{D} = DF_0^T P$ was used.

We observe, that for given coefficients G, β and nodes c_i all other coefficients are determined by $AB(s)$ and $\Gamma(s)$.

The structure of B in (3.10) is quite simple with the choice $G = \gamma I$. Such singly-implicit methods have been investigated in [10]. This class is also interesting for sequential implementations. The main results of [10] for these *PPSW1-methods* are:

- With one single γ stiff accuracy ($\beta = 0$) can not be obtained, since it implies that $M(0) = B$ has eigenvalues σ^{i-1}, $i = 1, ..., s$. So, the method cannot be stable in the sense of (3.6) for variable stepsizes.
- A fairly good choice of β that eliminates these unwanted eigenvalues is

$$\beta = V F_0 S_m D^{-1} V^{-1}. \tag{3.11}$$

- The choice (3.11) implies the following stability properties for arbitrary stepsize sequences

$$\begin{aligned} \beta_m \beta_{m-1} \cdots \beta_{m-s+2} &= 0 \\ B_m B_{m-1} \cdots B_{m-s+2} &= \mathbb{1} v^T \text{ with } v^T \mathbb{1} = 1. \end{aligned} \tag{3.12}$$

  Hence, the method is $L(\alpha)$-stable in a strong sense if it is $A(\alpha)$-stable. Furthermore (3.6) is satisfied for $\sigma_j \leq \sigma_{\max}$, i.e. the method converges of order $s - 1$.
- In the case of constant stepsizes superconvergence of order $p = s$ is possible for appropriate γ.

In [10] PPSW1-methods were tested on small stiff examples with LU-decomposition. For comparison purposes we include the following PPSW1-methods in our numerical tests on MOL-systems of high dimension:

PPSW1-4: $s = 4$, $\gamma = 0.468147$, $\alpha = 52°$

PPSW1-5: $s = 5$, $\gamma = 0.722499$, $\alpha = 79°$,

where α is the angle of $L(\alpha)$-stability and the knots are given by $c_{s-i+1} = \cos(\frac{(2i-1)\pi}{2s}) / \cos(\frac{\pi}{2s})$. The main drawback of PPSW1-methods is their lack of stiff accuracy. Although $\varrho(M(\infty))$ vanishes, the norm $\|M(\infty)\|$ can be quite large and may lead to serious error propagation for nonlinear problems. In the following section we will consider the new class of stiffly accurate PPSW2-methods.

4 Multi-implicit stiffly accurate PPSW-methods

We consider stiffly accurate methods ($\beta = 0$) in order to achieve optimal damping at infinity. It was mentioned in Section 3.3 that this property may not be obtained with one single γ and we have to consider multi-implicit methods with $G = \text{diag}(\gamma_i)$. They will be called *PPSW2-methods*. Now, the stability properties for very stiff systems are good by construction but (3.6) will be the weak point and requires special investigation.

For PPSW2 methods of order $s - 1$ free parameters are the knots c_i and

$G = \mathrm{diag}(\gamma_i)$. One option for the choice of G is improving the order to $p = s$ (*superconsistency*). By Theorem 3.1 this requires the simplifying conditions $\Gamma(s)$ and $AB(s+1)$. The matrix $\Gamma = -G\Theta$ from (3.9) already satsifies the first condition $\Gamma(s)$. But the second condition, $AB(s+1)$, for order s requires some computations. For $q = s+1$ the highest power c_i^s in (3.5) may be replaced by lower ones with the aid of the knot polynomial

$$\phi(t) := (t - c_1)\cdots(t - c_s). \tag{4.1}$$

since $\phi(c_i) = 0$. We now formulate the result on superconsistency.

Theorem 4.1 *Let the conditions $AB(s)$ and $\Gamma(s)$ be satisfied for the method (3.1), let ϕ be its knot polynomial (4.1) and $H = \max\{h_{m-1}, h_m\}$. If for some i, $1 \le i \le s$, the condition*

$$\phi(1 + \sigma_m c_i) = \gamma_i \sigma_m\, \phi'(1 + \sigma_m c_i) \tag{4.2}$$

holds, then the local residual in (3.3) satisfies $\Delta_{mi} = O(H^s)$. In fact, condition $AB(s+1)$ requires (4.2) for all $i = 1, \ldots, s$.

Proof. It is convenient to introduce the shifted variable $\tau = (c-1)/\sigma$ and the polynomial $\psi(\tau) = \sum_{k=0}^{s} \psi_k \tau^k := \phi(1 + \sigma\tau) = \phi(c)$ that satisfies $\psi((c_j - 1)/\sigma) = 0$, $j = 1, \ldots, s$. Using $A = -\Gamma$ and $\Gamma(s)$, the last equation in $AB(s+1)$ at the point c_i, $1 \le i \le s$, reads

$$\begin{aligned}
0 &= c_i^s - s\gamma_i c_i^{s-1} - \sum_{j=1}^{s} b_{ij}(c_j - 1)^s \sigma^{-s} \\
&= c_i^s - s\gamma_i c_i^{s-1} + \sigma^{-s} \sum_{k=0}^{s-1} \psi_k \sum_{j=1}^{s} b_{ij}(c_j - 1)^k \sigma^{-k} \\
&= c_i^s - s\gamma_i c_i^{s-1} + \sigma^{-s} \sum_{k=0}^{s-1} \psi_k (c_i^k - \gamma_i k c_i^{k-1}) \\
&= \sigma^{-s}(\psi(c_i) - \gamma_i \psi'(c_i)) = \sigma^{-s}(\phi(1 + \sigma c_i) - \gamma_i \sigma \phi'(1 + \sigma c_i)).
\end{aligned}$$

In the third line $\Gamma = -A$ and the order conditions $AB(s)$ and $\Gamma(s)$ have been used. ■

We note, that the superconsistency condition (4.2) may be written as the following rule for the choice of the parameter γ_i,

$$\frac{1}{\gamma_i} = \sigma \frac{\phi'(1 + \sigma c_i)}{\phi(1 + \sigma c_i)} = \sigma \sum_{j=1}^{s} \frac{1}{1 + \sigma c_i - c_j}. \tag{4.3}$$

Since the stability matrix (3.7) should have no poles on the negative real axis we have to satisfy (4.2) with $\gamma_i > 0$. Sufficient conditions on the knots c_i for that are easily obtained from (4.3).

Lemma 4.1 *a) For knots $c_i \in [0,1]$, $i = 1,\dots,s$ and any $\sigma > 0$ all γ_i, $i = 1,\dots,s$, are positive.*
b) For knots $c_s = 1$ and $c_i < 1$, $i = 1,\dots,s-1$ and any $\sigma > 0$ the last parameter in (4.3) is positive, $\gamma_s > 0$.

Since any stage error $Y_{mi} - y(t_{mi})$ depends on all previous errors $Y_{m-1,j} - y(t_{m-1,j})$ a global error $O(h^s)$ requires that *all* s conditions (4.2) are satisfied. In this case Lemma 4.1 leads to severe restrictions on the choice of the method parameters since all γ_i are fixed and the knots c_i are restricted to the unit interval. Here, it is difficult to find strongly stable PPSW2-methods. Those methods found by numerical search have all knots quite near 1 and their stability depends very critically on σ_m, see Figure 4.2. The following Table gives the knot-vector c and the angle of $L(\alpha)$-stability of special superconsistent methods:

Super2:	$s = 2,\ c = (0.85, 1),$	$\alpha = 90°$
Super3:	$s = 3,\ c = (0.85, 0.95, 1),$	$\alpha = 89°$
Super4:	$s = 4,\ c = (0.79, 0.915, 0.99, 1),$	$\alpha = 88°$

Requiring only one condition (4.2), for $i = s$, say, does not improve the global order $s-1$. But the higher local order of Y_{ms} can be used for error estimation. Considering the last component of the extrapolated values $(\Theta \otimes I)Y_{m-1}$ we have already an $\mathcal{O}(h^{s-1})$ approximation for Y_{ms}. Hence, the correction

$$Y_{ms} - \sum_j \theta_{sj} Y_{m-1,j} \tag{4.4}$$

is indeed a higher order estimate for the local error. Fixing γ_s by (4.3) the remaining γ_i, $i = 1,...,s-1$ (and the knots c_i) were optimized by a numerical search. Since γ_s now depends on σ we found it convenient to have such a dependence on all γ by using the ansatz

$$\gamma_i = \frac{\gamma_{0i}}{1 + \sigma\gamma_{1i}},\ \gamma_{0i} > 0, \gamma_{1i} \ge 0,\ i = 1,...,s-1. \tag{4.5}$$

Some fairly "good" strongly stable methods have been found but we think that they are not yet optimal. We present some of these methods by giving the vectors c, γ_0 and γ_1 and the angle of $L(\alpha)$-stability:

PPSW2-3: $s = 3, c = (-0.1, 0.7, 1), \gamma_0 = (2.55, 0.4005), \gamma_1 = (0.5, 0.5), \alpha = 90°$
PPSW2-4: $s = 4, c = (-0.38333, -0.25, 0.825, 1),$
$\gamma_0 = (0.584888524, 0.536977593, 0.467201038)$
$\gamma_1 = (0.472969203, 0.506264075, 0.496391355), \alpha = 83°$
PPSW2-5: $s = 5, c = (-1.09, -0.2290, 0.51, 0.63, 1),$
$\gamma_0 = (0.214789562, 0.249182503, 0.237832565, 0.245204742),$
$\gamma_1 = (0.566334104, 0.496228487, 0.518584061, 0.498857638), \alpha = 86°$

PPSW2-6: $s = 6, c = (-1.702, -0.51, -0.195797762, 0.155193392, 0.755672784, 1)$,
$\gamma_0 = (0.214789562, 0.249182503, 0.237832565, 0.245204742, 0.353848357)$,
$\gamma_1 = (0.566334104, 0.496228487, 0.518584061, 0.498857638, 0.502412430)$,
$\alpha = 81°$

Unfortunately, for PPSW2-methods we have no theoretical stability result like (3.12). However, for strongly stable methods (cf. Definition 3.4) we can prove the existence of an interval $[\sigma_a, \sigma_b]$ where the method is stable in the sense of (3.6).

Theorem 4.2 *Let the method be strongly stable. Then there exists an interval $[\sigma_a, \sigma_b]$ with $\sigma_a < 1 < \sigma_b$ such that the method is stable for stepsize sequences satisfying*

$$\sigma_a \leq \frac{h_m}{h_{m-1}} \leq \sigma_b \text{ for all } m \geq 1. \tag{4.6}$$

Proof. The proof is similar to the one for multistep methods, e.g. [4]. For better readability we underline the dependence on σ by writing $B(\sigma)$ in this proof. With (4.3), (4.5) and

$$B(\sigma) = \Theta(\sigma) - \sigma G(\sigma)\Theta(\sigma) V D F_0^T V^{-1},$$

the matrix $B(\sigma)$ depends continously on σ in a neighbourhood of $\sigma = 1$. By strong stability a matrix T exists with

$$T^{-1}B(1)T = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \varepsilon_2 & & 0 \\ & & \ddots & \ddots & \\ 0 & & \cdots & & \lambda_s \end{pmatrix}$$

and $\|T^{-1}B(1)T\|_1 = 1$. Since the eigenvalue 1 does not depend on σ due to $B(\sigma)\ \mathbb{1} = \ \mathbb{1}$ there exist $\sigma_a < 1 < \sigma_b$, such that

$$\|T^{-1}B(\sigma)T\|_1 = 1 \tag{4.7}$$

for all $\sigma \in [\sigma_a, \sigma_b]$. Hence,

$$\|\prod_{k=m}^{m+l} B_k\|_1 \leq \|T^{-1}\|_1 \|T\|_1 \text{ for all } m, l. \quad \blacksquare$$

As a consequence, the superconsistent methods are convergent of order $p = s$ and the methods with ansatz (4.5) are convergent of order $p = s - 1$ for variable stepsizes with

$$\sigma \in [\sigma_a, \sigma_b],$$

if the remaining assumptions of Theorem 3.1 are satisfied.

For larger s the bounds σ_a, σ_b calculated by Theorem 4.2 can be rather close to one. Computing the Jordan canonical form with MAPLE we have plotted the norm (4.7) of some PPSW2-methods over σ in Figure 4.1.

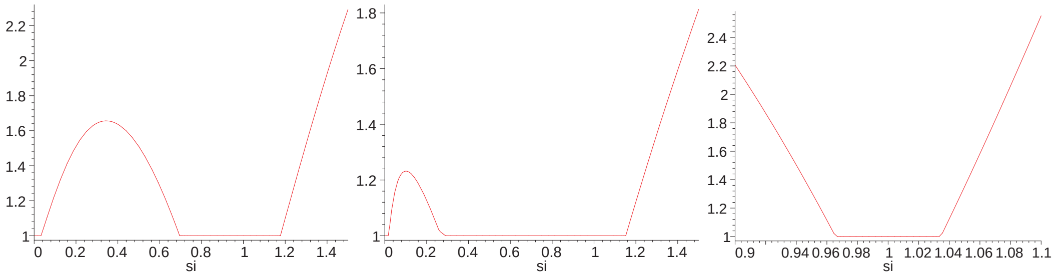

Fig. 4.1. Norm (4.7) for PPSW2-3, PPSW2-4 and PPSW2-5 over σ

The norm condition (4.7) is sufficient for stability. In order to get a feeling of the real size of $\prod_{k=0}^{m} B_k =: L^{(m)}$ we made a computation with varying σ_k. In this product each σ_k is constructed with a random value $r \in [0,1]$ and $\sigma := 0.1 + 2r$ and the restriction

$$\sigma_k = \max(2 - \sigma_{max}, \min(\sigma, \sigma_{max})).$$

As characteristic for the size of $L^{(m)}$ Figure 4.2 shows the maximal value of the elements of $L^{(m)}$ for $m = 1, ..., 10000$ as a function of σ_{max},

$$bnorm := \max_{m,i,j} |l_{ij}^{(m)}|.$$

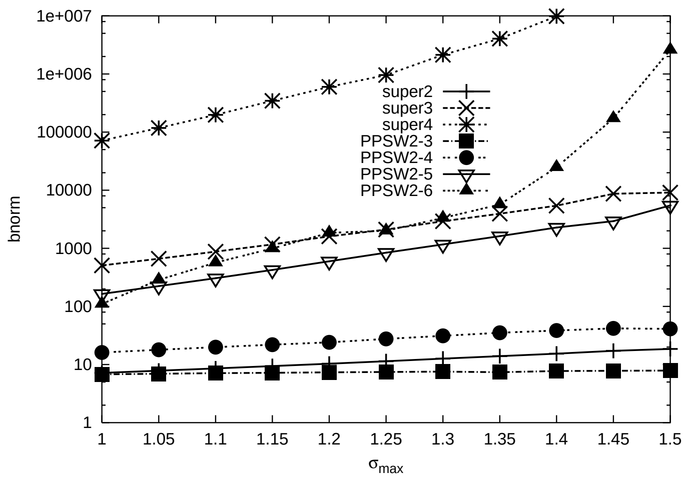

Fig. 4.2. bnorm for special PPSW-methods

Figure 4.2 impressively shows the superiority of methods having only one superconsistent stage and using (4.5). It also gives hints for the choice of σ_{max} in the implementation of PPSW2-methods.

5 Numerical Tests

In this section we apply PPSW1- and PPSW2-methods to MOL-systems. The tests are performed on a SunFire computer with shared memory and 8 Ultrasparc3 processors. For an s-stage PPSW-method s processors are used. The implementation is straight-forward using OpenMP. As usual, only the right-hand side has to be provided by the user. The error estimation is done for Y_{ms} by (4.4) for PPSW2-methods, and using an embedded solution of order $\mathcal{O}(h^{s-2})$ for PPSW1-methods. The new step-size is computed by standard rules, see e.g. [7]. In correspondence with Fig. 4.2 we limit the stepsize increase to $\sigma_{max} = 1.5$ for Super2, PPSW2-3,4 and to $\sigma_{max} = 1.2$ for the other methods. The linear systems are solved with the Krylov-method FOM. By synchronizing the processors for all s linear systems the same Krylov-dimension is used, i.e. the Krylov process is stopped if all s systems are solved with accuracy $rktol \cdot atol$. Here, $atol$ is the absolute tolerance for the step-size control of the integration method. The choice of the factor $rktol$ is very critical for the efficiency of the method. We used $rktol = 0.1$ for the methods of order 2 and 3, and $rktol = 0.001$ for the methods of order 4 and 5. No preconditioning was used since we wanted to concentrate on the comparison of the integrators. The starting values are computed with ROWMAP [11].

The parallel methods were compared with the sequential two-step W-method (2.1) TSW3B [8] and with VODPK [2]. In VODPK, which is a combination of the BDF code VODE with restarted GMRES(l), we used the default value $l = 5$.

The following problems were solved:

DIFFU: A nonautonomous 2D diffusion equation

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

The function f and the initial and Dirichlet boundary conditions are given by the exact solution $u(t, x, y) = \sin(\pi x)\sin(\pi y)(1 + 4xy \sin t)$. MOL with second order central differences on a 100×100 grid gives a stiff ODE-system of dimension $n = 10000$.

NILIDI: The nonlinear diffusion equation [11]

$$u_t = e^u(u_{xx} + u_{yy}) + u(18e^u - 1),$$

on $[0, \pi/3] \times [0, \pi/3]$, $\quad t \in [0, 1]$. Initial and boundary values are taken from the exact solution $u = e^{-t}\sin(3x)\sin(3y)$. By MOL on a 100×100 grid we get a stiff system of 10000 equations again.

FOOD: The 2-dimensional predator-prey model [1]

$$
\begin{aligned}
u_t^i &= d_i \triangle u^i + f^i(u^1, u^2), \quad i = 1, 2 \\
f^1(u^1, u^2) &= u^1(b_1 - a_1 u^2), \quad f^2(u^1, u^2) = u^2(b_2 - a_2 u^1) \\
d_1 &= 0.05,\ d_2 = 1,\ b_1 = 1,\ b_2 = -1000, \\
a_1 &= 0.1,\ a_2 = -100 \\
\frac{\partial u^i}{\partial n} &= 0 \text{ on } \partial\Omega,\ \Omega = [0,1]^2, \quad t \in [0,3], \\
u^1(0,x,y) &= 10 - 5\cos(\pi x)\cos(10\pi y) \\
u^2(0,x,y) &= 17 + 5\cos(10\pi x)\cos(\pi y).
\end{aligned}
$$

The dimension of the ODE system obtained by MOL is $n = 20000$.

BRUSSELATOR: The 2-dimensional stiff Brusselator

$$
\begin{aligned}
u_t &= \alpha(u_{xx} + u_{yy}) + 1 + u^2 v - 4u \\
v_t &= \alpha(v_{xx} + v_{yy}) + 3u - u^2 v \\
t &\in [0, 10], \quad (x, y) \in [0,1] \times [0,1], \quad \alpha = 0.2
\end{aligned}
$$

Standard Finite Differences on a 100×100 grid give 20000 equations.

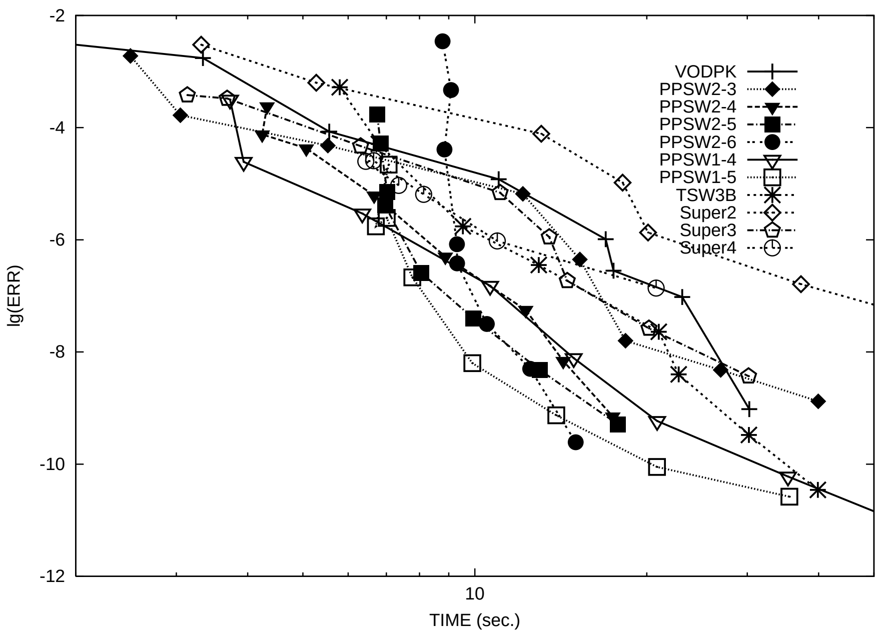

Fig. 5.3. Results for DIFFU

In Figures 5.3 – 5.6 we give precision-time diagrams for the test problems. The computing times are for s processors for the parallel methods and for computation with 1 processor for the sequential methods.

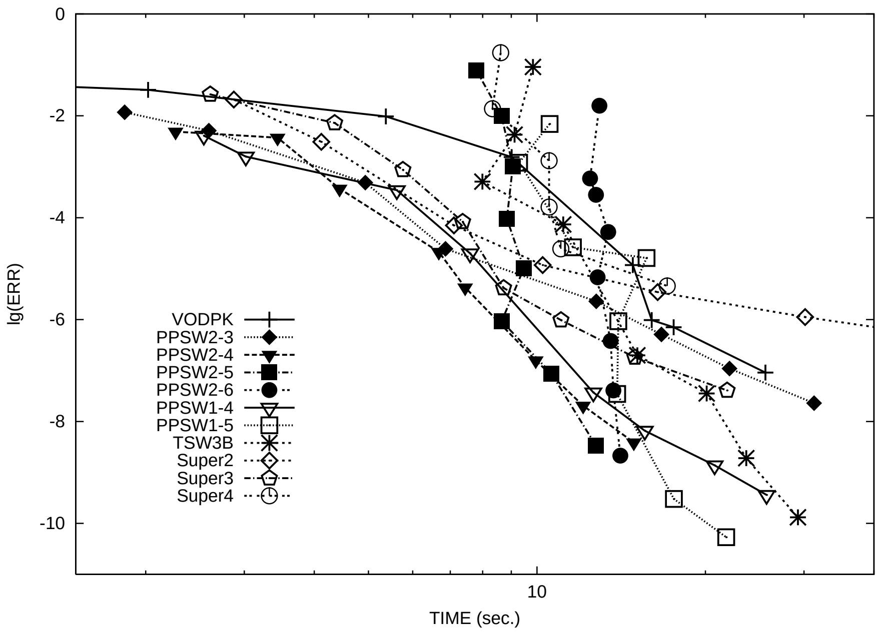

Fig. 5.4. Results for NILIDI

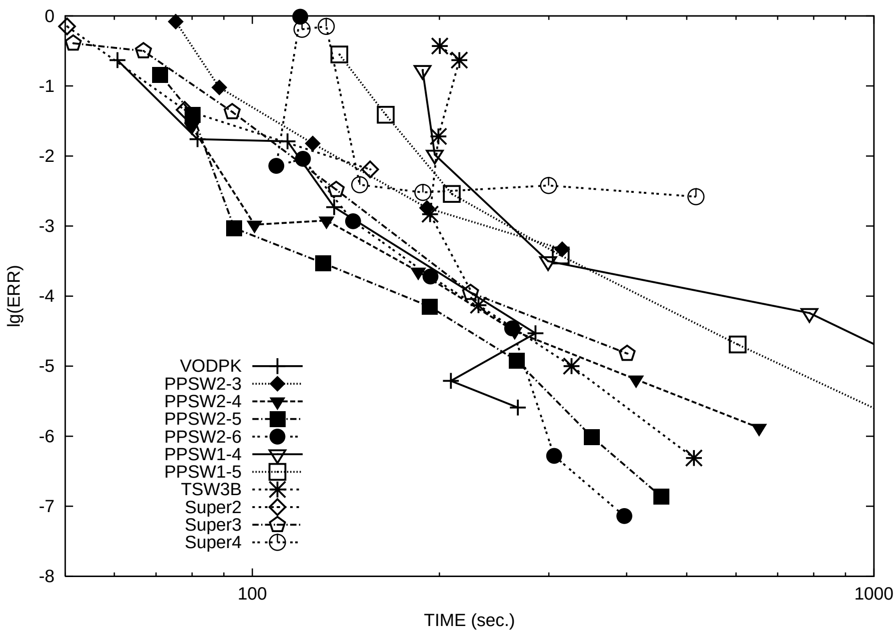

Fig. 5.5. Results for FOOD2

6 Conclusions

We discussed several variants of two-step W-methods and their stability and convergence properties. We also introduced the class of multi-implicit two-step Peer W-methods (PPSW2) which combine several attractive features for the parallel solution of large stiff problems. They are tailored to using indepen-

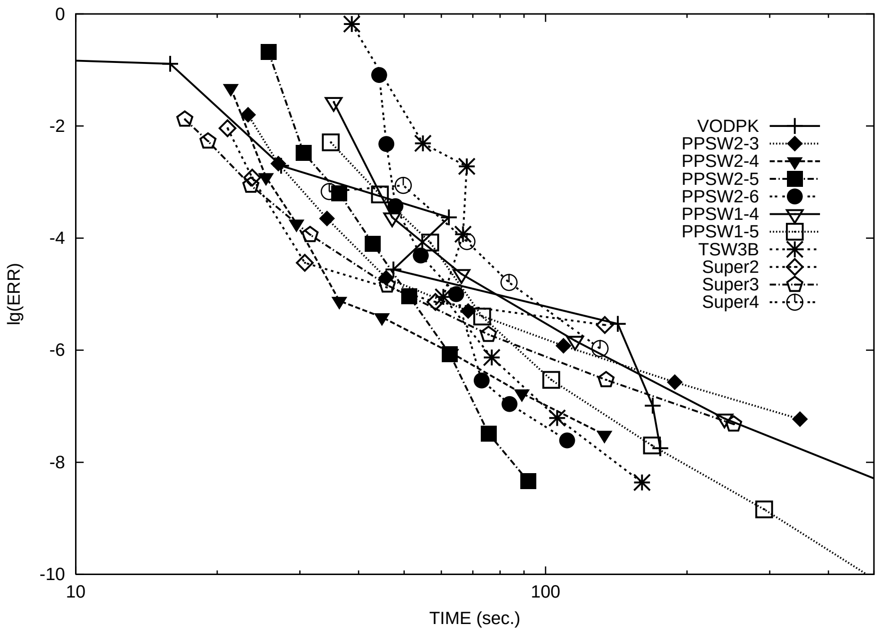

Fig. 5.6. Results for BRUSS

dent solution methods for the different stage equations like Krylov methods and provide optimal stiff damping due to their stiff accuracy. The numerical tests illustrate the theoretical results. The two sequential methods VODPK and TSW3B perform similarly. The new PPSW2-methods are more efficient than comparable PPSW1-methods. As suggested by the norm estimates in Figure 4.2 PPSW2-methods using error control with one single superconsistent stage are superior to fully superconsistent methods. Overall, PPSW2-methods are well designed for parallel computers with a few processors and are superior here to classical sequential codes like VODPK. A main topic of future work will be identification of other theoretical criteria that are critical for the performance of these methods. This should be the basis for the search for better methods with higher stage numbers s.

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