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# MULTI-IMPLICIT PEER TWO-STEP W-METHODS FOR PARALLEL TIME INTEGRATION*

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**Abstract.**

Peer two-step W-methods are designed for integration of stiff initial value problems with parallelism across the method. The essential feature is that in each time step $s$ 'peer' approximations are employed having similar properties. In fact, no primary solution variable is distinguished. Parallel implementation of these stages is easy since information from one previous time step is used only and the different linear systems may be solved simultaneously. This paper introduces a subclass having order $s-1$ where optimal damping for stiff problems is obtained by using different system parameters in different stages. Favourable properties of this subclass are uniform stability for realistic stepsize sequences and a superconvergence property which is proved using a polynomial collocation formulation. Numerical tests on a shared memory computer of a matrix-free implementation with Krylov methods are included.

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*Key words:* parallel methods for stiff initial value problems, peer W-methods.

## 1 Introduction.

Recently the authors introduced a new class of time integration methods for the solution of large and stiff initial value problems

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

[10]. These methods have an inherent parallelism across the method since they employ $s$ stages which are totally independent within the actual time step. These stages depend on values from the previous step only leading to a two-step structure. An important difference to most standard schemes is that no extraordinary solution variable for $y$ with distinguished properties is computed.

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All $s$ stage solutions are peers sharing essentially the same accuracy and stability properties. As an example, singly-implicit methods being almost L-stable exist up to order 7 [10]. Also, the methods do not suffer from order reduction in stiff problems [11]. Method parallelism may be attractive in a computing environment with moderate parallelism using a black-box implementation of the right-hand side $f$. On large scale computers this parallelism still may simplify load balancing in adaptive space discretizations. Many approaches for parallel integration methods use parallel iteration schemes for non-parallel methods, e.g., [2, 6, 1]. A recent survey on classes of General Linear Methods with inherent parallelism can be found in [3].

The form of the 'Parallel Peer two-Step W-Methods' (PPSW-methods) is as follows. In each time step from $t_m$ to $t_{m+1} = t_m + h_m$ solutions $Y_{mi} \cong y(t_{mi})$, $i = 1, \ldots, s$, are computed as approximations at the points

$$t_{mi} := t_m + h_m c_i, \quad i = 1, \ldots, s, \tag{1.2}$$

which are not restricted to the time interval $[t_m, t_{m+1}]$. This means that the off-step nodes $c_i$ are not confined to $[0, 1]$. The time step consists of $s$ linearly implicit stages, $i = 1, \ldots, s$,

$$\begin{aligned}(I - \gamma_i h_m T_m) Y_{mi} \;=\; & \sum_{j=1}^{s} (b_{ij} I + h_m \gamma_{ij} T_m) Y_{m-1,j} \;+ \\ & + h_m \sum_{j=1}^{s} a_{ij} f(t_{m-1,j}, Y_{m-1,j}),\end{aligned} \tag{1.3}$$

where the reals $\gamma_i > 0$, $b_{ij}, \gamma_{ij}, a_{ij}$ are the parameters of the method. The matrix $T_m$ should be an approximation of the Jacobian $f_y(t_m, y(t_m))$ for stability reasons only. We point out that the right-hand side in (1.3) only uses information $Y_{m-1,j}$ from the previous time step and the left-hand side describes $s$ independent linear systems. The solution of these systems is expected to cause the main computational effort for realistic stiff problems of large dimension $n$. In [10] the first two authors analyzed the simpler, singly-implicit case for these schemes where the matrix in all $s$ stage equations is the same, $\gamma_i \equiv \gamma$, $i = 1, \ldots, s$. Such schemes may be used in sequential computations and it was found in [10], indeed, that they may already be competitive in this setting with existing standard codes. Still, the results were not fully satisfactory since singly-implicit methods lack optimal damping properties for very stiff problems. For parallel implementations the general multi-implicit case with different $\gamma_i$ is appropriate. With these methods optimal stiff damping is possible with the choice $A = (a_{ij})_{i,j=1}^{s} = -\Gamma$, $\Gamma = (\gamma_{ij})_{i,j=1}^{s}$ and we will consider only such methods in this paper. The diagonal matrix of the system parameters $\gamma_i$ is denoted by $G := \mathrm{diag}(\gamma_i)$.

While stability for very stiff problems is easily accomplished for the schemes (1.3), zero stability is not. This problem is aggravated through the fact that the coefficient matrices of nontrivial methods depend on the stepsize ratio

$$\sigma_m := h_m / h_{m-1} \leq \bar{\sigma}, \tag{1.4}$$

which we assume to be bounded from above (but not from below) by a positive constant. This makes it necessary to distinguish coefficients $A_m, \Gamma_m, G_m$ and $B_m = (b_{ij})_{i,j=1}^s$ from different time steps by the index $m$. Accuracy and stability questions are discussed in Section 2. There, we also employ a special choice of the diagonal parameter matrix $G_m$ introduced in [11] leading to a simple form of all coefficient matrices in a certain basis. This allows to prove uniform bounds for matrix products like $B_m B_{m-1} \cdots B_1$ and establishes the existence of stable peer methods of order $s-1$ for arbitrary $s$.

In Section 3 we discuss a polynomial collocation formulation of these special peer methods which may be of theoretical interest. However, we use this version also for proving superconvergence of order $s$ for constant stepsizes and special parameter choices. Accuracy and stability requirements still leave many degrees of freedom in the parameters of the methods. Here additional criteria may be discussed having a positive influence on method performance. For instance, large norms of the coefficients $B_m, A_m$ may lead to severe amplification of errors in nonlinear problems and numerical computations. Since all coefficient matrices are constructed in a monomial basis and transformed back by a Vandermonde similarity transformation we try to achieve moderate norms by analyzing the condition of this transformation in Section 5 for a special class of nodes $c_i$. A short discussion of variations in the form of the schemes (1.3) follows in Section 6. We conclude the paper with implementation details and numerical experiments on a parallel computer. Two example problems from parabolic systems are solved with an implementation using Krylov methods and compared with other existing software. One multi-implicit peer method constructed in [14] by brute-force search is included in the tests. Although it lacks the sound theoretical basis of the methods considered here it performs better in a few cases.

## 2 High order methods with structural stability.

Order conditions for the PPSW-methods have been derived in [10] by considering the local residuals

$$h_m \Delta_{mi} := (I - \gamma_i h_m T_m) y(t_{mi}) - \sum_{j=1}^{s} (b_{ij} I + h_m \gamma_{ij} T_m) y(t_{m-1,j}) - \\ - h_m \sum_{j=1}^{s} a_{ij} y'(t_{m-1,j}), \quad i = 1, \ldots, s. \tag{2.1}$$

Although the singly-implicit case $\gamma_i \equiv \gamma$ was considered only in [10] these conditions hold identically for arbitrary $\gamma_i$ and have the form

$$\Gamma(q):\ \gamma_i c_i^k + \sum_{j=1}^{s} \gamma_{ij} (c_j - 1)^k \sigma_m^{-k} = 0, \quad 0 \le k = 0 < q, \tag{2.2}$$

$$AB(q):\ c_i^k - \sum_{j=1}^{s} b_{ij} \left( \frac{c_j - 1}{\sigma_m} \right)^k - k \sum_{j=1}^{s} a_{ij} \left( \frac{c_j - 1}{\sigma_m} \right)^{k-1} = 0, \quad 0 \le k < q. \tag{2.3}$$

For fixed nodes these order conditions are linear restrictions on the remaining parameters of the method. So $s$ conditions can be applied without difficulty and by requiring $\Gamma(s)$ and $AB(s)$ the following matrix representations are obtained [10]

$$\Gamma_m := -G_m\Theta_m, \qquad \Theta_m := VS(\sigma_m)PV^{-1}, \tag{2.4}$$

$$B_m := \Theta_m - \sigma_m A_m V D F_0^{\mathsf{T}} V^{-1}. \tag{2.5}$$

These equations use the Vandermonde matrix $V := (c_i^{j-1})_{i,j=1}^s$, the Pascal matrix $P := \big(\binom{j-1}{i-1}\big)_{i,j=1}^s$, the shift $F_0 := (\delta_{i-1,j})_{i,j=1}^s$, where $\delta_{ij}$ means the Kronecker symbol, and the diagonal matrices $D := \mathrm{diag}(1,\ldots,s)$ and

$$S(\sigma) := \mathrm{diag}(1,\sigma,\ldots,\sigma^{s-1}). \tag{2.6}$$

Considering the linear test problem $y' = \lambda y$ with $\mathrm{Re}\,\lambda \le 0$ and using $T_m = \lambda$ the stability matrix of the scheme is obtained as

$$M(z) := (I - zG_m)^{-1}(B_m + z\beta_m), \quad z = h_m\lambda,$$

see [10]. The matrix $\beta_m := A_m + \Gamma_m$ governs the behaviour of the scheme for very stiff problems since $M(\infty) = -G_m^{-1}\beta_m$. In the paper [10], where singly-implicit methods with $G_m = \gamma I$ were discussed, it was not possible to choose optimal stiff damping $M(\infty) = 0$ due to loss of zero stability. In the present paper, however, we will demonstrate that this restriction does not hold for general multi-implicit methods (1.3) since we can choose $\beta_m = 0$ and still preserve zero stability. For such methods the stability matrix takes the simple form

$$M(z) = (I - zG_m)^{-1}B_m, \qquad A_m = -\Gamma_m. \tag{2.7}$$

With this choice stability and damping for $z \to \infty$ are very satisfactory. Therefore we discuss only this version in the rest of the paper and write these stiffly accurate methods down with the time stepping vectors $Y_m = (Y_{mi})_{i=1}^s$,

$$\begin{aligned}(I - h_m G_m \otimes T_m)Y_m \;=\; & (B_m \otimes I)Y_{m-1} + \\ & + h_m(A_m \otimes I)\big(f(Y_{m-1}) - (I \otimes T_m)Y_{m-1}\big).\end{aligned} \tag{2.8}$$

The stability of these schemes for $z \to 0$ is still an issue. In [10] it was shown that $M_m(0) = B_m$ has the form

$$B_m = (I - G_m E)\Theta_m, \qquad E = VDF_0^{\mathsf{T}}V^{-1}. \tag{2.9}$$

Equations (2.4) and (2.9) indicate that it is convenient to get rid of the common similarity transform with the Vandermonde matrix and to consider

$$\begin{aligned}\tilde{B}_m &:= V^{-1}B_m V = S(\sigma_m)P - \tilde{G}_m D F_0^{\mathsf{T}} S(\sigma_m)P, \\ \tilde{G}_m &:= V^{-1}G_m V.\end{aligned} \tag{2.10}$$

The matrix $S(\sigma_m)P$ is upper triangular with diagonal entries $\sigma_m^{i-1},\ i = 1,\ldots,s$ and $DF_0^{\mathsf{T}}S(\sigma_m)P$ is strictly upper triangular. Hence, we observe that the simple

choice $G_m = \gamma I$ is ruled out by the requirement of zero stability for $\sigma_m > 1$, see [10]. The structure of the matrix $\tilde{G}$ has to be rich enough to cancel large entries in the main diagonal of $S(\sigma_m)P$.

The multi-implicit methods in [14] were found by a brute force search with coefficients

$$\gamma_i^{(m)} = \frac{\bar{\gamma}_{0i}}{1 + \sigma_m \bar{\gamma}_{1i}}, \quad i = 1, \ldots, s-1. \tag{2.11}$$

With this $\sigma$-dependent ansatz larger stepsize ratios $\bar{\sigma}$ in (1.4) could be obtained. The last parameter $\gamma_s$ was determined by one condition $AB(s+1)$, i.e.,

$$\frac{1}{\gamma_s} = \sigma \sum_{j=1}^{s} \frac{1}{1 + \sigma - c_j}, \tag{2.12}$$

ensuring local order $s$ for the stage approximation $Y_{ms}$. This property may be used in stepsize control, see Section 7.

In this paper, however, we construct another class of stable methods explicitly. The construction is based on the fact that we associate the $s$ parameters $\gamma_i^{(m)}$ (their choice may also depend on $\sigma_m$) with the function values of a polynomial $g_m$ at the nodes $c_i$, i.e.

$$\gamma_i^{(m)} = g_m(c_i), \quad i = 1, \ldots, s, \; g_m(x) = \sum_{j=0}^{s-1} g_j^{(m)} x^j. \tag{2.13}$$

Introducing the diagonal matrix $C = \mathrm{diag}(c_i)$ this means that we have $G_m = g_m(C)$. However, it is our purpose to exploit the triangular structure of the different matrices in $\tilde{B}_m$, (2.10), where the transformed matrix $\tilde{G}_m$ appears.

LEMMA 2.1. *Let $\phi(x) = \prod_{i=1}^{s}(x - c_i) = \sum_{j=0}^{s} \phi_j x^j$ be the node polynomial and consider the corresponding Frobenius companion matrix*

$$F := \begin{pmatrix} 0 & 0 & \ldots & -\phi_0 \\ 1 & 0 & \ldots & -\phi_1 \\ & \ddots & \ddots & \vdots \\ & & 1 & -\phi_{s-1} \end{pmatrix}.$$

*Then, with parameters $\gamma_i^{(m)}$ as defined in* (2.13) *we have*

$$\tilde{G}_m = V^{-1} g_m(C) V = g_m(F) = \sum_{j=0}^{s-1} g_j^{(m)} F^j.$$

PROOF. From the property $c_i^s = -\sum_{j=1}^{s} \phi_{j-1} c_i^{j-1}$ follows $CV = VF$, or $V^{-1}CV = F$. □

It is easily seen that the matrix power $F^j$, $j < s$, has exactly $j$ nontrivial subdiagonals. For general polynomials $g_m$ the dependence on the coefficients $\phi_j$

may be quite complicated in this representation of $\tilde{G}_m$. However, we note that a representation which is linear in the coefficients $\phi_j$ and the elements of the last row of $\tilde{G}_m$ is possible and was given in [11].

In (2.10) the matrix $\tilde{G}_m$ is multiplied by the matrix $F_0^{\mathsf{T}}$ and its columns are shifted to the right. So, the subdiagonals of $\tilde{G}_m$ move to the diagonal of $\tilde{B}_m$ and the product $\tilde{G}_m D F_0^{\mathsf{T}}$ is still upper triangular if $g_m$ is a linear polynomial. Based on this observation we now introduce the family of multi-implicit peer two-step W-methods (1.3) based on the choice

$$\gamma_i^{(m)} = g_0^{(m)} + g_1^{(m)} c_i,\ i = 1, \dots, s \iff \tilde{G}_m = g_0^{(m)} I + g_1^{(m)} F, \tag{2.14}$$

which is a special case of formula (20) in [11]. With (2.14) $\tilde{G}_m$ has Hessenberg form. This choice leads to the following explicit form

$$\tilde{B}_m = \big(I - g_1^{(m)} \hat{D} - g_0^{(m)} F_0^{\mathsf{T}} \hat{D}\big) S(\sigma_m) P \tag{2.15}$$

of the matrix that governs zero stability. The matrix $\hat{D} = \operatorname{diag}(0, 1, 2, \dots, s-1)$ is a shifted version of $D$. For later reference we note that this formula for $\tilde{B}$ is independent of the nodes $c_i$ and extends to arbitrary $s \in \mathbb{N}$. Hence, each matrix $\tilde{B}_m$ may be regarded as a principal submatrix of an infinite triangular matrix. The eigenvalues of $\tilde{B}_m$ are given by the diagonal elements

$$\tilde{b}_{ii} = \sigma_m^{i-1}\big(1 - (i-1) g_1^{(m)}\big), \quad i = 1, \dots, s. \tag{2.16}$$

With this choice, zero-stability even for variable stepsizes is easily obtained.

THEOREM 2.2. *Let the coefficients of the method* (1.3) *be chosen with* $A_m = -\Gamma_m = G_m \Theta_m$ *and* $B_m$ *according to* (2.9). *Then with positive parameters* $\gamma_i^{(m)}$ *of the form* (2.14) *with* $g_1^{(m)} \in [g_*, g^*] \subseteq (0, \frac{2}{s-1})$ *and bounded* $g_0^{(m)}$, *there exists* $\bar{\sigma} > 1$ *such that* $\rho(B_m) = 1$ *holds for* $\sigma_m \le \bar{\sigma}$. *Moreover, for time grids obeying* $\sigma_m \le \bar{\sigma}$ *the following products are uniformly bounded,*

$$\|B_m B_{m-1} \cdots B_{m-k}\| \le K, \quad 0 \le k \le m,\ t_m \le t_e.$$

PROOF. Using parameters $g_1^{(m)}$ from the indicated interval it holds that $q := \max_{i=2}^{s} |1-(i-1)g_1^{(m)}| < 1$ in (2.16). So, with any $\bar{\sigma} \in (1, 1/q^{1/(s-1)})$ the diagonal elements of $\tilde{B}$ satisfy $\tilde{b}_{11} = 1$ and $|\tilde{b}_{ii}| \le \bar{\sigma}^{s-1} q < 1$, $i = 2, \dots, s$, for $\sigma_m \le \bar{\sigma}$. Optimal estimates for $\bar{\sigma}$ are presented after the proof. From the triangular form of $\tilde{B}_m$ follows that $\rho(B_m) = 1$ with only one simple eigenvalue of unit modulus. Since all matrices $\tilde{B}_m$ have triangular form the bound $\|B_m B_{m-1} \cdots B_{m-k}\| \le \kappa \|\tilde{B}_m \tilde{B}_{m-1} \cdots \tilde{B}_{m-k}\|$ holds with the condition number $\kappa = \|V\|\|V^{-1}\|$ of the Vandermonde matrix. With the assumed restrictions on the parameters $g_0, g_1$ and $\sigma_m$ there exists a nonnegative upper triangular matrix $\bar{B}$ such that $|\tilde{B}_m| \le \bar{B}$ entrywise. This matrix also has spectral radius $\rho(\bar{B}) = 1$ and only one single eigenvalue with modulus one. Hence, its powers are uniformly bounded. Since $|\tilde{B}_m \tilde{B}_{m-1} \cdots \tilde{B}_{m-k}| \le \bar{B}^{k+1}$ the statement follows. □

REMARK 2.1. It is easily seen that the supremum $\sigma_{\sup}$ of all stepsize ratios $\sigma_m > 1$, where a choice of $g_1$ with $\rho(B) < 1$ is possible, is the root of the polynomial equation (cf. [11])

$$(s-2)\sigma^{s-1} - (s-1)\sigma^{s-2} - 1 = 0,$$

in the interval $(0, 2/(s-1))$. The corresponding parameter $g_1$ is related to this one by $(1-g_1)\sigma_{\sup} = 1$. The following table contains numerical estimates for these values truncated to 4 digits.

(2.17)

| $s$ | 3 | 4 | 5 | 6 | 7 | 8 |
|---|---|---|---|---|---|---|
| $\sigma_{\sup}$ | 2.414 | 1.678 | 1.444 | 1.330 | 1.262 | 1.218 |
| $g_1$ | 0.5858 | 0.4039 | 0.3075 | 0.2481 | 0.2078 | 0.1788 |

The parameter $g_0^{(m)}$ is only slightly restricted by the positivity of the parameters $\gamma_i^{(m)}$ in (2.14),

$$g_0^{(m)} > -g_1^{(m)} \min_i c_i, \quad g_1^{(m)} > 0, \tag{2.18}$$

which we assume throughout the paper. Still, the choice of $g_0^{(m)}$ has some influence on the stability constant $K$ in Theorem 2.2.

## 3 Polynomial formulation of peer methods.

It is plain that the order conditions $\Gamma(q), AB(q)$ from the last section are rules for general polynomials of degree $q-1$. Considering only stiffly accurate methods with $A_m = -\Gamma_m$ we now write down these conditions for a polynomial $p$ of degree $q-1$ and obtain

$$\begin{aligned} &\Gamma(q)\colon \textstyle\sum_{j=1}^s \gamma_{ij} p(c_j) = \gamma_i p(1+\sigma_m c_i), \\ &AB(q)\colon \textstyle\sum_{j=1}^s b_{ij} p(c_j) = p(1+\sigma_m c_i) - \gamma_i \sigma_m p'(1+\sigma_m c_i), \end{aligned} \tag{3.1}$$

$i = 1, \ldots, s$. Here, it makes sense to consider the coefficients $\gamma_i$ as being function values of the polynomial $g_m$ introduced in (2.13). Interpolating the $s$ summation results in (3.1) by a polynomial $\psi$ of degree at most $s-1$, i.e., $\psi(c_i) = \sum_{j=1}^s b_{ij} p(c_j)$, $i = 1, \ldots, s$, yields the exact result

$$\psi(t) = p(1+\sigma_m t) - \sigma_m g_m(t) p'(1+\sigma_m t), \tag{3.2}$$

as long as $\max\{q, \deg(g_m)+q-1\} \le s-1$. This means that under the assumptions of Theorem 2.2 the identity (3.2) is true for polynomials $p$ of degree $s-1$ since $g_m$ has degree one. We now introduce the interpolation operator associated with the nodes $c_i$, i.e.,

$$Q : C^0 \to \Pi_{s-1}, \quad f \mapsto p,\ p(c_i) = f(c_i),\ i = 1, \ldots, s. \tag{3.3}$$

Here, $\Pi_k$ denotes the space of all polynomials with degree not greater than $k \in \mathbb{N}$. It is now possible to simplify the peer method (2.8) with these notations.

If $p \in \Pi_{s-1}$ is the polynomial which interpolates the approximations of the previous times step, $p(c_i) = Y_{m-1,i},\ i = 1, \ldots, s$, then the right-hand side of (2.8) is interpolated by the polynomial

$$p(1+\sigma_m t) - \sigma_m g_m(t) p'(1+\sigma_m t) - h_m g_m(t)\big((Qf(p)) - T_m p\big)(1+\sigma_m t).$$

Here, $(Qf(p))(1+\sigma_m t)$ means that the interpolation polynomial of the data $f(p(c_i))$, $i = 1, \ldots, s$, is evaluated at $1+\sigma_m t$. For general differential equations this polynomial has degree $s$. However, for the test equation $y' = \lambda y$ and the choice $T_m = \lambda$ the last term vanishes and the expression reduces to the polynomial $\psi$ from Equation (3.2). Considering now the interpolating polynomial $r \in \Pi_{s-1}$ of the most recent approximations, $r(c_i) = Y_{mi}$, $i = 1, \ldots, s$, the stage equations (2.8) correspond to the collocation conditions $(1 - z g_m(c_i)) r(c_i) = \psi(c_i)$, $i = 1, \ldots, s$, with $z = h_m \lambda$. They can be written in the form

$$Q\big((1 - z g_m) r\big) = \psi = p(1+\sigma_m \cdot) - \sigma_m g_m\, p'(1+\sigma_m \cdot). \tag{3.4}$$

For $z = 0$ we obtain the solution $r = \psi$. However, for $z \neq 0$ the expression $(1 - z g_m) r$ has degree $s$ and the interpolation error of $Q((1 - z g_m) r)$ is a constant multiple of the node polynomial $\phi$. In this case the collocation equation (3.4) may be solved easily, again.

LEMMA 3.1. *Let the peer method* (2.8) *with coefficient matrix* (2.9) *and a linear coefficient polynomial* $g_m(c) = g_0 + g_1 c$ *be applied to the test equation* $y' = \lambda y$, $\mathrm{Re}\lambda \leq 0$ *with initial values* $Y_{m-1,i} = p(c_i)$, $i = 1, \ldots, s$, *and* $p \in \Pi_{s-1}$. *Let* $z = h_m \lambda \neq 0$ *and* (2.18) *be satisfied and define* $w := (1/z - g_0)/g_1$. *Then, the collocation equation* (3.4) *is solved by the polynomial*

$$\begin{aligned} r(c) &= \frac{\psi(c)\phi(w) - \psi(w)\phi(c)}{\big(1 - z g_m(c)\big)\,\phi(w)}, \\ \psi(c) &= p(1+\sigma_m c) - \sigma_m g_m(c) p'(1+\sigma_m c). \end{aligned} \tag{3.5}$$

PROOF. Since $(1 - z g_m) r \in \Pi_s$ it holds that $Q((1 - z g_m) r) = (1 - z g_m) r - \mu\phi$ with an unknown constant $\mu$. Hence, the collocation equation (3.4) is equivalent with the polynomial identity

$$(1 - z g_m) r = \psi + \mu\phi.$$

Since the factor $1 - z g_m$ vanishes at the point $c = w$ the constant turns out to be $\mu = -\psi(w)/\phi(w)$. The point $w$ is not a zero of $\phi$ due to assumption (2.18). Hence, the assertion (3.5) follows. □

REMARK 3.1. (a) The function in (3.5) is indeed a polynomial of degree $s-1$ since the nominator vanishes at the point $c = w$ which is a simple zero of the denominator.

(b) The two polynomials $r$ and $p$ representing the solution in two adjacent intervals do not fit continuously, in general. However, by considering

$$r(c) - p(1+\sigma_m c) = \frac{g(c)\big(z p(1+\sigma_m c) - \sigma_m p'(1+\sigma_m c)\big) - \phi(c)\psi(w)/\phi(w)}{1 - z g_m(c)}$$

it is seen that the jump at nodes $c = c_i,\ 1 \le i \le s$, is proportional to the residual of the extrapolated polynomial $p(1+\sigma_m\cdot)$ in the transformed differential equation $y' = zy$.

The simple case $z = 0$ is of special interest in Lemma 3.1. Since we will apply the following considerations in the next section with constant stepsize only, we will also restrict this discussion to the case $\sigma_m = 1$ where the coefficients of the method do not depend on $m$. Then the time stepping operator mapping the interpolating polynomial $p(c_i) = Y_{m-1,i},\ i = 1, \dots, s$, of $Y_{m-1}$ to the interpolator $r(c_i) = Y_{m,i},\ i = 1, \dots, s$, of $Y_m = BY_{m-1}$ is given by

$$\mathcal{B}\colon\ \Pi_k \to \Pi_k, \quad p \mapsto r,\ r(c) = p(1+c) - g(c)p'(1+c), \tag{3.6}$$

with $k = s - 1$, see (3.4). However, it is important to note that this mapping $\mathcal{B}$ is indeed an endomorphism of $\bigcup_{k\ge 0} \Pi_k$ since $g$ has degree one. This property corresponds to the upper triangular structure of $\tilde{B}_m$ in (2.15) since $\tilde{B}_m$ is the matrix representation of $\mathcal{B}$ in the monomial basis $\{c^{j-1} :\ 1 \le j \le k\}$. One advantage of this property is the ability to write the image of the difference of two arbitrary polynomials $p_1, p_2$ as the difference of the images

$$p_1 - p_2 \in \Pi_{s-1} \quad \Rightarrow \quad \mathcal{B}\big(Q(p_1 - p_2)\big) = \mathcal{B}(p_1 - p_2) = \mathcal{B}p_1 - \mathcal{B}p_2.$$

The eigenfunctions of the operator $\mathcal{B}$ may be ordered by increasing degree. The first ones are computed easily.

LEMMA 3.2. *Let $g(t) = g_0 + g_1 t$ be given. Then, $1 \in \Pi_0$ is the eigenfunction of $\mathcal{B}$ with eigenvalue $\lambda_1 = 1$, and $g - 1 \in \Pi_1$ is its eigenfunction belonging to $\lambda_2 = 1 - g_1$.*

PROOF. The identity $\mathcal{B}1 = 1$ is trivial. And the linear polynomial $g$ is mapped to $\mathcal{B}g = g_1 + (1 - g_1)g$, which yields $\mathcal{B}(g - 1) = \mathcal{B}g - 1 = (1 - g_1)(g - 1)$. □

This result shows that the coefficient function $g = 1 + (g - 1)$ is just the sum of the first two eigenfunctions of $\mathcal{B}$. It has an important consequence for the structure of the solution mapping $\mathcal{M}(z) : p \mapsto r$ in (3.5) which corresponds to the stability matrix $M(z)$ in (2.7). If we consider the image of the first eigenfunction $p = 1$ in (3.5) for $z \cong 0$ the quotient $\psi(w)/\phi(w) = \mathrm{O}(z^s)$ may be neglected. With $\psi = p = 1$ we obtain

$$\begin{aligned} r &= \mathcal{M}(z)1 = (1 + zg)1 + \mathrm{O}(z^2) = 1 + z1 + z(g - 1) + \mathrm{O}(z^2) \\ &= (1 + z)1 + z(g - 1) + \mathrm{O}(z^2). \end{aligned} \tag{3.7}$$

Since $\lambda_1 = 1$ is a simple eigenvalue of $\mathcal{M}(0) = \mathcal{B} : \Pi_{s-1} \to \Pi_{s-1}$ there exists a smooth curve $\lambda_1(z) = 1 + \mathrm{O}(z)$ near $z = 0$. And the decomposition (3.7) into eigenfunctions shows that $\lambda_1(z) = 1 + z + \mathrm{O}(z^2)$, cf. [16, §2.9]. Since all other eigenvalues are smaller than one in absolute value at $z = 0$, there is some hope for acceptable $A(\alpha)$-stability properties of these PPSW schemes. We remind that all eigenvalues vanish in the other limit $z \to \infty$.

## 4 Higher order and superconvergence.

For stiffly accurate methods (2.8) satisfying $\Gamma(s), AB(s)$ the leading error term in stage $i$ is given by,

$$
\begin{aligned}
& h_m\Delta_{mi} \\
(4.1) \qquad & = \frac{h_{m-1}^s}{s!}y^{(s)}(t_{m-1})\left((1+\sigma_m c_i)^s - \sum_{j=1}^s b_{ij}c_j^s - \sigma_m s\sum_{j=1}^s \gamma_{ij}c_j^{s-1}\right) + \\
& \quad + \mathrm{O}(h_{m-1}^{s+1}) \\
(4.2) \qquad & = \frac{h_{m-1}^s}{s!}y^{(s)}(t_{m-1})\big(\phi(1+\sigma_m c_i) - \gamma_i\sigma_m\phi'(1+\sigma_m c_i)\big) + \\
& \quad + \mathrm{O}(h_{m-1}^{s+1}),
\end{aligned}
$$

see (2.1) and [10, 14]. We recall that $\phi$ is the node polynomial of the method. Improving the order of the scheme by one requires that the $h_{m-1}^s$ term vanishes in (4.2) in all stages $i = 1, \ldots, s$. Such methods of order $s = 4$ have indeed been constructed in [14] by exploiting full freedom in the choice of the parameters $\gamma_i$. With the restrictions imposed by (2.18), however, no satisfactory methods could be found having global order $s$. Still, cancelling the $\mathrm{O}(h^s)$-error in the last stage only by (2.12) has its merits in error control, see Section 7.

In [10] superconvergence of order $s$ was observed with constant stepsizes even for singly-implicit PPSW methods. This superconvergence effect may also be beneficial with high accuracy computations when stepsize ratios cluster around one. The analysis given in [10] showed the cancellation of the leading error term for certain values of the single parameter $\gamma$. The essential property used there was the nilpotency of the lower block of the matrix $\tilde{B}$ beyond the first row using tedious algebraic computations. Here, we present a simpler proof using the collocation formulation of the peer method. Two properties are essential in proving superconvergence. The first one is due to the eigenvalue distribution of $B$ which leads to zero stability. Since one is the only eigenvalue not lying in the open unit disc, the powers $B^n$ converge to a rank-one matrix. Hence,

$$
\lim_{n\to\infty} B^n = B^\infty = \mathbb{1}v^{\mathsf{T}}, \quad v^{\mathsf{T}}\mathbb{1} = 1, \tag{4.3}
$$

where $v$ is the left eigenvector to the eigenvalue 1 of the matrix $B$. The corresponding right eigenvector is the vector $\mathbb{1}$ of ones, of course. The second essential property is the triangular form of $\tilde{B}$ in (2.15) which is equivalent with the operator $\mathcal{B}$ in (3.6) being an endomorphism of any space $\Pi_k$, $k \geq 0$.

As in [10, Theorem 9] we consider the errors $X_m = (Y_{mi} - y(t_{mi}))_{i=1}^s$ for constant stepsize $h_m \equiv h$. Then, all matrices $B_m$ are identical and we may drop the index $m$. And it is no restriction to consider the scalar case $n = 1$ for ease of writing. The error recursion reads

$$
\begin{aligned}
X_m &= BX_{m-1} - h\Delta_m + \mathrm{O}(h\|X_{m-1}\| + h^2\|\Delta_m\|) \\
&= -h\sum_{j=0}^{m-1} B^j\Delta_{m-j} + B^m X_0 + \sum_{j=1}^{m-1}\mathrm{O}(h\|X_{m-j}\| + h^2\|\Delta_{m-j+1}\|).
\end{aligned}
$$

Again, only the sum $\sum_{j=0}^{m-1} B^j \Delta_{m-j}$ needs consideration, all other terms are of order $h^s$ for sufficiently small initial errors $X_0$. If the eigenvalues of $B$ satisfy $\lambda_1 = 1$, $|\lambda_i| < 1$, $i \geq 2$, then we have $\rho(B - B^\infty) < 1$, see (4.3), and the series $\sum_{j=0}^{\infty} \|B^j - B^\infty\|$ converges since $B^j - B^\infty = (B - B^\infty)^j$. Hence, the $\mathrm{O}(h^{s-1})$ term in $X_m$ may be isolated in the form

$$X_m = -hB^\infty \sum_{j=0}^{m-1} \Delta_{m-j} + \mathrm{O}\Big(\max_{j=0}^{m-1} \|X_j\|\Big) + \mathrm{O}\Big(h \max_{j=1}^{m} \|\Delta_j\|\Big). \tag{4.4}$$

Next we look at the leading $h^{s-1}$-terms of the local errors $\Delta_{m-j} \in \mathbb{R}^s$. By (4.2) they lie in a one-dimensional subspace of $\mathbb{R}^s$ spanned by the vector

$$\big(\phi(1+c_i) - \gamma_i \phi'(1+c_i)\big)_{i=1}^s = \big(\phi(1+c_i) - g(c_i)\phi'(1+c_i)\big)_{i=1}^s.$$

We note that its components have the form $(\mathcal{B}\phi)(c_i)$ with the mapping $\mathcal{B}$ from (3.6) in $\Pi_s$. Since the degree of $\mathcal{B}\phi$ exceeds $s-1$, the identity (3.2) for the interpolating polynomial $\psi \in \Pi_{s-1}$ of the data $(\mathcal{B}\phi)(c_i)$, $i = 1, \ldots, s$, has to be modified

$$\psi = Q\big(\phi(1+\cdot) - g\phi'(1+\cdot)\big) = \mathcal{B}\phi - \mu\phi, \tag{4.5}$$

see (3.3), with the constant $\mu = \frac{1}{s!}(\mathcal{B}\phi)^{(s)} = 1 - sg'$. Now it is clear that superconvergence occurs if the leading term $\mathcal{B}^\infty\psi$ in the global error vanishes.

THEOREM 4.1. *Let the method* (2.8) *satisfy* $AB(s)$ *and* $\Gamma(s)$. *Let the stepsize* $h$ *be constant and the parameters* (2.14) *be fixed with* $g_1 \in (0, 2/s)$. *Then, for a sufficiently smooth solution* $y$ *and initial errors* $X_0 = \mathrm{O}(h^s)$ *the error* $X_m$ *satisfies*

$$X_{mi} = -h^s(\mathcal{B}^\infty\phi)(c_i)\frac{g_1}{(s-1)!}\sum_{j=1}^{m} y^{(s)}(t_{m-j}) + \mathrm{O}(h^s), \quad i = 1, \ldots, s,\ m \geq 1.$$

*Moreover the properties* $\mathcal{B}^\infty\phi = 0$ *and* $X_{mi} = \mathrm{O}(h^s)$ *hold, if the system* $(I - \mathcal{B})u = \phi$ *has a solution* $u \in \Pi_s$, *i.e., if the problem*

$$g(t)u'(1+t) - u(1+t) + u(t) = \phi(t), \quad u(0) = 0, \tag{4.6}$$

*is solvable for* $u \in \Pi_s$.

PROOF. By (4.4) and (4.5) the $h^{s-1}$ term in the global error may be written in the form

$$X_{mi} = -\big(\mathcal{B}_{s-1}^\infty\psi\big)(c_i)\frac{h^s}{s!}\sum_{j=1}^{m} y^{(s)}(t_{m-j}) + \mathrm{O}(h^s).$$

Here, $\mathcal{B}$ is considered as a mapping $\Pi_{s-1} \to \Pi_{s-1}$ and we have added the index in the notation $\mathcal{B}_{s-1}$ in order to indicate the considered domain since the number of eigenvalues depends on it. The powers of $\mathcal{B}_{s-1}$ converge to $\mathcal{B}_{s-1}^\infty$ as long as the eigenvalues satisfy $1 - (i-1)g_1 \in (-1, 1]$, $i = 1, \ldots, s$, see (2.16). By (4.5)

the polynomial $\psi \in \Pi_{s-1}$ is the difference $\psi = \mathcal{B}_s\phi - \mu\phi$ of two polynomials of higher degree $s$. Since $\mathcal{B}_s$ is an extension of $\mathcal{B}_{s-1}$ we may easily write $\mathcal{B}_{s-1}\psi = \mathcal{B}_s\psi = \mathcal{B}_s^2\phi - \mu\mathcal{B}_s\phi$. But proceeding to higher powers we have to make sure that the sequence $\mathcal{B}_s^m$ converges, as well. Here, the condition $g_1 \in (0, \frac{2}{s})$ is required. Then we see that

$$\mathcal{B}_{s-1}^\infty\psi = \mathcal{B}_s^\infty(\mathcal{B}_s\phi - \mu\phi) = (1-\mu)\mathcal{B}_s^\infty\phi.$$

Since $1 - \mu = sg_1 \neq 0$ holds superconvergence occurs iff $\mathcal{B}_s^\infty\phi = 0$. This happens if $\phi$ has no component in the one-dimensional eigenspace of $\mathcal{B}_s$ belonging to the eigenvalue one. This is true, if $\phi$ lies in the range of $I - \mathcal{B}_s$, i.e., if there exists a polynomial $u \in \Pi_s$ with $(I - \mathcal{B}_s)u = \phi$. Then,

$$\mathcal{B}_s^\infty\phi = (\mathcal{B}_s^\infty - \mathcal{B}_s^\infty)u = 0.$$

Since the kernel of $I - \mathcal{B}_s$ consists of all constant functions, we may choose $u(0) = 0$ to make a possible solution unique. Then, the problem $(I - \mathcal{B}_s)u = \phi$ is equivalent with (4.6). □

REMARK 4.1. By the Fredholm alternative the equation $(I - \mathcal{B})p = \phi$ is solvable iff $\phi \perp \mathrm{Ker}(I - \mathcal{B})^*$. In order to avoid difficulties in defining the adjoint $\mathcal{B}^*$ we consider again the matrix representation $\tilde{B}$ of $\mathcal{B}$ in the monomial basis. Due to the triangular structure (2.15) of $\tilde{B}$ the components of the left eigenvector $\tilde{v}$ to the simple eigenvalue one are independent of the size of the matrix and the nodes $c_i$. The theorem shows that superconvergence with order $s$ occurs for an $s$-stage method if the inner product of $\tilde{v}$ and the coefficient vector $(\varphi^\mathsf{T}, 1) = (\phi_0, \ldots, \phi_{s-1}, 1)$ of the node polynomial $\phi$ vanishes, i.e. if

$$(\tilde{v}_1, \ldots, \tilde{v}_{s+1}) \begin{pmatrix} \varphi \\ 1 \end{pmatrix} = 0. \tag{4.7}$$

A conveniently scaled version of the vector $\tilde{v}$ is

$$\big(i!g_1^{i-1}\tilde{v}_i\big)_{i\geq 1} = \big(1, 1-g_0, 2(1-g_0)^2 - g_1, 6(1-g_0)^3 - 9g_1(1-g_0) + 2g_1^2, \ldots\big).$$

Looking for appropriate parameters $g_0, g_1$ one has to obey the restrictions imposed by zero-stability and positivity $\gamma_i > 0$ in (2.18).

## 5 Conditioning of the Vandermonde matrix.

Order $s-1$ and zero stability of the scheme may be obtained for arbitrary nodes $c_i$. In order to make a sensible choice for the remaining free parameters one should look for other criteria that may influence the properties of PPSW-methods. We recall that the stability analysis was performed for a linear autonomous model problem and after a change from a Langrangian to a monomial basis, see (2.10). This operation eliminated the nodes almost totally from the discussion. However, in practice, the scheme is applied to nonlinear problems and operates on function

values $Y_{mi}$. In a realistic analysis of nonlinear or numerical errors the norms of the coefficient matrices $A, B, \Gamma$ play a role, cf. [13]. It is to be expected that a large condition of the ubiquitous basis matrix $V$, see (2.4), (2.5), affects those norms adversely and may lead to serious error proliferation. This situation can be avoided to some extent if the condition

$$\mathrm{cond}_p(V) = \|V\|_p \|V^{-1}\|_p, \quad p \in \{2, F\}, \tag{5.1}$$

of the Vandermonde matrix is of moderate size. For the following analysis the isometric Euclidean ($p = 2$) and Frobenius norms ($p = F$) are of interest and appropriate nodes could be constructed by minimizing (5.1) for one of these norms. However, without restrictions on the nodes this is a very difficult task, cf. [7]. We therefore will make the analysis tractable by exploiting well-known properties of Chebyshev polynomials and consider only stretched Chebyshev nodes

$$c_i = \mu + \nu \cos\left(\frac{2s + 1 - 2i}{2s}\pi\right), \quad i = 1, \ldots, s. \tag{5.2}$$

We introduce the Chebyshev polynomials

$$\chi_k(\xi) := \cos(k \arccos(\xi)), \qquad k \geq 0, \tag{5.3}$$

and their transformed counterparts

$$q_1(c) := \frac{1}{\sqrt{2}}, \qquad q_k(c) = \chi_{k-1}\left(\frac{c - \mu}{\nu}\right), \ k \geq 2. \tag{5.4}$$

So, for $s \geq 1$ the polynomial $\phi(c) = 2(\nu/2)^s q_{s+1}(c)$ has the zeros (5.2). It is well known that Chebyshev polynomials satisfy certain orthogonality relations. Hence, the polynomials $q_1, \ldots, q_s$ form an orthonormal basis in the discrete inner product with the nodes (5.2), [5],

$$\frac{2}{s} \sum_{i=1}^{s} q_k(c_i) q_j(c_i) = \delta_{jk}, \quad 1 \leq k, j \leq s. \tag{5.5}$$

Introducing the upper triangular matrix $\Psi = (q_{jk})_{j,k=1}^{s}$ of the coefficients of $q_k(c) = \sum_{j=1}^{k} c^{j-1} \nu^{1-j} q_{jk}$ we see that the matrix

$$\big(q_k(c_i)\big)_{i,k=1}^{s} = V S(\nu)^{-1} \Psi \tag{5.6}$$

has orthogonal columns due to (5.5). By Taylor expansion, the elements of $\Psi$ are obtained as $q_{11} = 1/\sqrt{2}$ and

$$q_{jk} = \frac{1}{(j-1)!} \chi_{k-1}^{(j-1)}(\xi_0), \quad k \geq 2, \ \xi_0 := -\frac{\mu}{\nu}. \tag{5.7}$$

Its entries may be easily computed recursively by differentiation of the Chebyshev recursion $\chi_k(\xi) = 2\xi\chi_{k-1}(\xi) - \chi_{k-2}(\xi)$, $k \geq 2$. For example, the leading

$4 \times 4$-blocks of any matrix $\Psi$, $s \geq 4$, and its inverse are

$$\Psi = \begin{pmatrix} \frac{1}{\sqrt{2}} & \xi_0 & 2\xi_0^2 - 1 & \xi_0(4\xi_0^2 - 3) \\ & 1 & 4\xi_0 & 3(4\xi_0^2 - 1) \\ & & 2 & 12\xi_0 \\ & & & 4 \end{pmatrix},$$

$$\Psi^{-1} = \begin{pmatrix} \sqrt{2} & -\sqrt{2}\xi_0 & \sqrt{2}(2\xi_0^2 + 1) & -\sqrt{2}\xi_0(2\xi_0^2 + 3) \\ & 1 & -2\xi_0 & 3\xi_0^2 + \frac{3}{4} \\ & & \frac{1}{2} & -\frac{3}{2}\xi_0 \\ & & & \frac{1}{4} \end{pmatrix}.$$

Due to the orthogonality relation (5.5) the condition of $V$ may be expressed in terms of the parameters $\mu, \nu$ alone.

LEMMA 5.1. *Consider the Vandermonde matrix $V$ built with the nodes* (5.2). *Let $\Psi = (q_{jk})_{j,k=1}^{s}$ be the matrix of the Taylor coefficients* (5.7). *Then,*

$$\operatorname{cond}(V) = \operatorname{cond}(S(\nu)^{-1}\Psi),$$

*where the condition number may be computed in the spectral or the Frobenius matrix norm.*

PROOF. By (5.5) the matrix $Q = (q_k(c_i))_{i,k=1}^{s}$ satisfies $Q^{\mathsf{T}}Q = \frac{s}{2}I$. Now, with (5.6) follows $V = Q\Psi^{-1}S(\nu)$ and $V^{\mathsf{T}}V = \frac{s}{2}S(\nu)(\Psi^{-1})^{\mathsf{T}}\Psi^{-1}S(\nu)$. So, indeed we have $\|V\| = \frac{s}{2}\|\Psi^{-1}S(\nu)\|$ in any unitarily invariant norm. An analogous computation for $V^{-1}$ proves the lemma since the scaling factor $s/2$ drops out. □

The computation of the spectral condition $\operatorname{cond}_2$ is very difficult. So, for convenience, we discuss the Frobenius condition $\operatorname{cond}_F$. And for implementation purposes of the PPSW methods the last node will be fixed at $c_s = 1$. This couples the parameters $\mu, \nu$ and the condition $\operatorname{cond}(V)$ is a rational function of the stretching factor $\nu$ alone,

$$K(\nu) := \operatorname{cond}_F(S(\nu)^{-1}\Psi), \quad \text{where } \mu = 1 - \nu\cos\left(\frac{\pi}{2s}\right).$$

In fact, $\nu^{s-1}K(\nu)$ is a polynomial. Table 5.1 shows the values for the condition $K(\frac{1}{2})$, which corresponds to nodes $c_i \in (0, 1]$, and numerically computed minimal values for the function $K(\nu)$. Apparently, the parameters at the minimum behave like $\nu_{\min} \cong 1 + \frac{1}{2s-3/2}$ leading to nodes (5.2) with $c_1 < -1$. Since the minimum of $K$ is rather flat and it is a slight practical advantage to have nodes in $[-1, 1]$ we decided to use stretched Chebyshev points

$$c_i^C := \frac{\cos\left(\frac{2s+1-2i}{2s}\pi\right)}{\cos\left(\frac{\pi}{2s}\right)}, \quad i = 1, \ldots, s, \tag{5.8}$$

contained in the interval $[-1, 1]$. The row labelled $K_C$ in the table contains the values corresponding to (5.8) and shows that this choice is nearly optimal.

Table 5.1: Vandermonde condition numbers and minima

| $s =$ | 3 | 4 | 5 | 6 | 7 | 8 |
|---|---|---|---|---|---|---|
| $K(1/2)$ | 23.682 | 132.27 | 747.56 | 4257.2 | 24369 | 140001 |
| $K(\nu_{\min})$ | 4.5497 | 10.678 | 25.403 | 60.861 | 146.31 | 352.31 |
| $\nu_{\min}$ | 1.2098 | 1.1502 | 1.1172 | 1.0951 | 1.0795 | 1.0682 |
| $K_C$ | 4.5826 | 10.919 | 26.328 | 63.641 | 154.01 | 372.73 |

Compared to nodes $c_i \in [0,1]$ we see a dramatic decrease of the condition of the Vandermonde matrix. For example, with $s = 6$ stages the ratio $K(\frac{1}{2})/K_C$ is about 66 and this decrease is even more pronounced when the exact spectral condition is computed. In fact, for $s = 6$ the condition $\mathrm{cond}_2(V)$ drops from 3896.1 for $\nu = 1/2$ to 41.44 for the points (5.8) by a factor of 94. This improvement is visible in the numerical performance of higher-order methods (1.3). So, in Section 7 all methods with $s \geq 4$ stages are based on the stretched nodes (5.8). Unfortunately, the great width of the interval $[-1,1]$ leads to relatively large differences between the smallest and largest parameters $\gamma_1$ and $\gamma_s$. This is an issue when iterative methods are used for the stage equations since the condition of the matrix $I - h\gamma_i T$ is roughly $h\gamma_i\|T\|$ if the logarithmic norm of $h\gamma_i T$ is small. Due to this fact, for methods with $s \leq 3$ stages there is still an advantage of using nodes in a smaller interval.

## 6 Variants of peer methods.

Considering the explicit form of the coefficient matrices $B_m = \Theta_m - G_m E\Theta_m$ (2.9), and $A_m = -\Gamma_m = G_m\Theta_m$ (2.4) of a PPSW-method (2.8) of order at least $s-1$ one sees that the system matrix $I - h_m G_m \otimes T_m$ appears on its right-hand side, too. Hence, this scheme may be written in the form

$$\begin{aligned}(I - h_m G_m \otimes T_m)\big(Y_m - (\Theta_m \otimes I)Y_{m-1}\big) \\ = \big((G_m\Theta_m) \otimes I\big)\big(h_m f(Y_{m-1}) - \sigma_m(E \otimes I)Y_{m-1}\big).\end{aligned} \tag{6.1}$$

Here, the relation $E\Theta_m = \sigma_m\Theta_m E$ [10] was used. This version has the form of a corrector equation with the extrapolated values $\tilde{Y}_m := (\Theta_m \otimes I)Y_{m-1}$ as a predictor and is well suited for implementing these methods. In fact, it is the only possible implementation if $T_m$ is only defined implicitly by using an iterative method for the corresponding system with the matrix $I - h_m G_m \otimes f'(\cdot)$ which we will do in the next section. In this context (6.1) has the additional advantage that the right-hand side is of order $h_m^s$ for smooth solutions and only a small correction term needs to be computed. In fact, according to the interpretation (3.1) the expression $f(Y_{m-1}) - \sigma_m(E \otimes I)Y_{m-1}$ is the difference between the computed derivative $f(Y_{m-1})$ and a difference approximation $\sigma_m(E \otimes I)Y_{m-1}$ of it. This error indicator is then extrapolated by the multiplication with $\Theta_m$.

Writing the right-hand side of (6.1) in its original form, $(\Theta_m \otimes I)f(Y_{m-1}) - (E\Theta_m \otimes I)Y_{m-1}$, a different interpretation is, that the difference approximation

$(E \otimes I)\tilde{Y}_m$ of the extrapolated solution is compared with the extrapolated function values $(\Theta_m \otimes I)f(Y_{m-1})$. Here, one might expect improvements by replacing this extrapolated information by more actual evaluations of $f$. This leads to the following 'one-leg' version

$$\begin{aligned} &\tilde{Y}_m := (\Theta_m \otimes I)Y_{m-1}, \\ &(I - h_m G_m \otimes T_m)(Y_m - \tilde{Y}_m) = (G_m \otimes I)\big(h_m f(\tilde{Y}_m) - (E \otimes I)\tilde{Y}_m\big) \end{aligned} \tag{6.2}$$

of the peer method. It is easily seen, that this version has the same order as (6.1) with identical coefficients. Also, the stability matrix (2.7) is the same. For more general problems, however, the schemes may behave differently. In fact, (6.2) may be interpreted as one simplified Newton step with initial guess $\tilde{Y}_m$ for the following implicit peer methods introduced in [11],

$$Y_m - h_m(G_m \otimes I)f(Y_m) = \big((I - G_m E) \otimes I\big)\tilde{Y}_m. \tag{6.3}$$

This is the stiffly accurate version of (4) in [11] with $A_m = 0$. Numerical experiments in [11] showed an improved performance of (6.3) compared to (6.1) for some very stiff, singularly perturbed problems. However, there is no order reduction for both schemes (6.3) and (6.1), and for less stiff problems there was no significant difference with sequential computations. From the practical point of view, however, there are some notable differences between the two peer-W versions. In an implementation of (6.1) on a distributed system each processor computes its own solution $Y_{mi}$ and the function evaluation $f(Y_{mi})$ and communicates both to all other processors. For (6.2) however, processor number $i$ may receive all old approximations $Y_{m-1,j}, j = 1, \ldots, s$, compute its own predictor $\tilde{Y}_{mi}$, the corresponding evaluation $f(\tilde{Y}_{mi})$, and solve its linear $n \times n$-system. Then, it sends only its new approximation $Y_{mi}$ to all others using half the communication of (6.1) for large problems. On a system with common memory however, (6.1) has the advantage that computed function evaluations $f(Y_{m-1})$ can be re-used after a step rejection. In the numerical tests of the next section the version (6.1) is used.

## 7 Numerical experiments.

Automatic stepsize control requires some means for estimating the local error. In the class of peer methods we consider again the two possibilities for such an estimate mentioned in [10]. For higher-order methods (e.g., $s \geq 4$) the solution $Y_{ms}$ may be compared with a predictor of order $s - 2$. For low order methods especially, a sound higher-order estimate $\mathrm{O}(h^s)$ of the local error may be obtained by using one 'superconsistent' stage $Y_{ms}$ with $\Delta_{ms} = \mathrm{O}(h^s)$ in (4.1). This additional order condition (2.12) may be satisfied by a proper choice of the parameter $g_0^{(m)}$ in (2.14). Based on these additional approximations the stepsize control is performed in a standard way with absolute and relative tolerances *atol* and *rtol*.

Since the class of multi-implicit PPSW methods is designed for parallel computing we performed tests on a SunFire computer with shared memory and 24

processors (Ultra III, 900 MHz, 8 MB Cache). Only the simple parallelism across the method is exploited by computing the $s$ stages on $s$ processors in parallel. Of course, additional processors could be used to parallelize the evaluation of the right-hand side $f$ (parallelism across the system) to further reduce computing time. However, such measures are problem-dependent and were not used in our tests. Direct methods for the solution of the stage systems are not attractive for solving the stage equations, since the high cost of a LU- or QR-decomposition limits the possible speed-up in parallel back substitutions. Also for reasons of efficiency iterative methods are an obvious alternative and we decided to use Krylov methods having favourable properties in the stiff ODE background. For each stage system the Arnoldi FOM method [9] is applied independently until a stopping criterion of the form

$$\textit{residual} \le \textit{rktol} \cdot \textit{atol} \tag{7.1}$$

is satisfied where *atol* is the absolute tolerance for the global integration error. Unfortunately, two reasons may lead to large differences in the iteration numbers for the different stages. The first one comes from the predictor-corrector interpretation of (6.1), where the right-hand sides and the corrections $Y_{mi} - \tilde{Y}_{mi}$ are much smaller for the first stages. This happens especially for $c_1 < 0$, where the computation of $\tilde{Y}_{m1}$ is no extrapolation at all. The second reason lies in the speed of convergence of FOM which is related to the condition number of the matrix $I - h\gamma_i J$, $J = f'(Y_{m-1,s})$. For a dissipative matrix $J$, satisfying $y^{\mathsf{T}} J y \le 0$, $y \in \mathbb{R}^n$, this condition number is proportional to $\gamma_i h \|J\|$. Here, the choice (2.14) leads to slower convergence for stages with $c_i \cong 1$ where the iteration already started with an inferior initial guess. In order to simplify the synchronization of the processors, the iteration in all stages is performed until the system for $Y_{ms}$ satisfies (7.1) with *rktol* given in Table 7.1.

The following multi-implicit peer methods have been selected for the presentation. The methods *mipeer's*' use all the features developed in this paper. They have order $s - 1$ and use $\gamma_i$ from (2.14). The parameter $g_1$ is taken from (2.17) and $g_0$ is determined to satisfy (4.7) yielding superconvergence for $\sigma = 1$.

The better conditioning with Chebyshev nodes is not yet decisive for three stages. So, for $s = 3$ we include the method *misup3*. Here $g_0$ is determined to satisfy (2.12) leading to order $s = 3$ in the last stage. This higher stage is used for error estimation and stepsize control. A detailed description of the methods is given in Table 7.1, where the last two columns contain the angle of $L(\alpha)$ stability and the iteration tolerance $rktol$ in (7.1). The values for $g_0, g_1$ are rounded to 4 digits. With the parameters specified in Table 7.1 the coefficients $A_m = -\Gamma_m$ and $B_m$ of the peer method are uniquely determined by (2.4), (2.14) and (2.9). Since the method *mipeer*6 from this class has shown no further improvement in performance we omit its results from the presentation. However, from [14] we include the special multi-implicit peer method *PPSW2-5* with nodes $c = (-1.09, -0.229, 0.51, 0.63, 1)$ and $\gamma_s$ from (2.12). The other parameters $\gamma_i$, $i = 1, \ldots, s-1$ have the form (2.11) with

Table 7.1: Peer methods used in the numerical experiments

| Method | $c_i$ | $\bar{\sigma}$ | $g_1$ | $g_0$ | $\alpha$ | *rktol* |
|---|---|---|---|---|---|---|
| *misup*3 | –0.094,0.242,1 | 2 | 0.386 | (2.12) | 88.8 | 0.1 |
| *mipeer*3 | $c_i^C$, (5.8) | 2 | 0.5858 | 0.9057 | 90 | 0.1 |
| *mipeer*4 | $c_i^C$, (5.8) | 1.4 | 0.4039 | 0.5443 | 90 | 0.1 |
| *mipeer*5 | $c_i^C$, (5.8) | 1.3 | 0.3075 | 0.3756 | 89.8 | 0.01 |

$$(\bar{\gamma}_{0i})_{i=1}^{s-1} = (0.2066, 0.1544, 0.32, 0.3304),$$
$$(\bar{\gamma}_{1i})_{i=1}^{s-1} = (0.5811, 0.4917, 0.5887, 0.4688).$$

These peer methods are compared with the Krylov codes VODPK [4] and ROWMAP [15] and the Runge–Kutta–Chebyshev code RKC [12, 8]. We note that the Krylov codes may profit from a good preconditioning while RKC does not. However, in our tests no preconditioning was applied. Unfortunately, we are not aware of any freely available code using parallel integration methods with iterative solution of stage equations which could have been used instead.

The test problems are two parabolic equations discretized in space.

DIFFU: A nonautonomous 2D diffusion equation

$$u_t = u_{xx} + u_{yy} + f(t, x, y), \quad t \in [0, 10], \quad (x, y) \in [0, 1]^2.$$

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

RADIATION: This is the radiation-diffusion problem described in [8]. It consists of two coupled parabolic equations with nonlinear diffusion and a very stiff reaction term which produces a steep front for the chosen mass number $Z_0 = 5$. Discretization on two uniform cell centered meshes with $50 \times 50$ and $100 \times 100$ cells is considered.

The results are given for $atol = rtol$ from $10^{-1} - 10^{-6}$. For the hard RADIATION problem some methods, especially VODPK, fail for crude tolerances.

In the linear problem all *mipeer* methods behave smoothly with a clear lead for the higher order methods. The superiority of those methods compared to, e.g., RKC is mainly due to the parallelization. The picture changes at the nonlinear RADIATION problem. Here, the higher-order *mipeer* methods need sharp tolerances to show their potential. As a rule of thumb one might say, that *misup3* leads for crude tolerances, *mipeer5* for strong ones and that *mipeer4* shows the best overall performance. And the difference to the non-parallel methods RKC, ROWMAP and VODPK is even larger for the RADIATION problem. We want to note, that the speed-up for an $s$-stage peer method is near to the optimal value $s$ compared to the computing time of the same method on one processor.

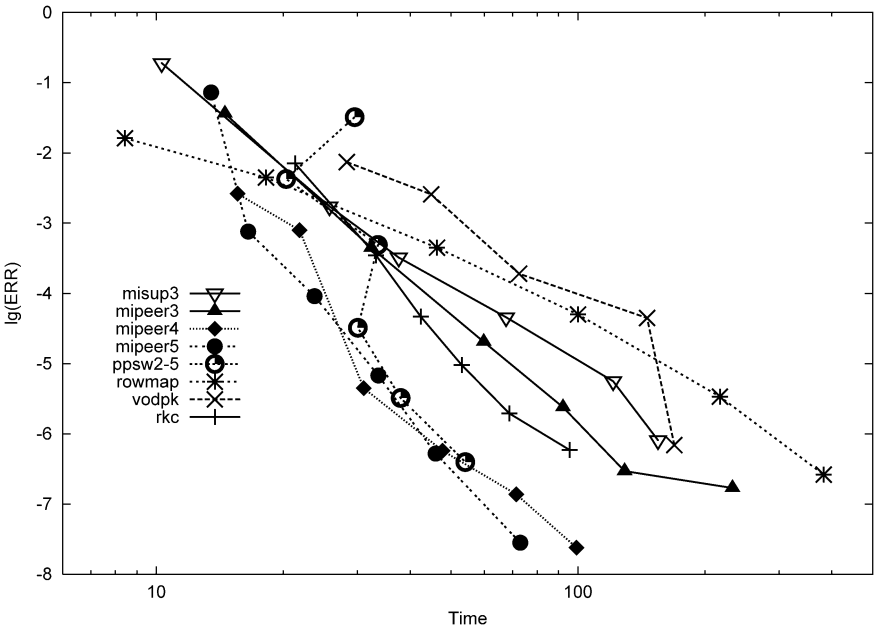


Figure 7.1: Results for DIFFU.

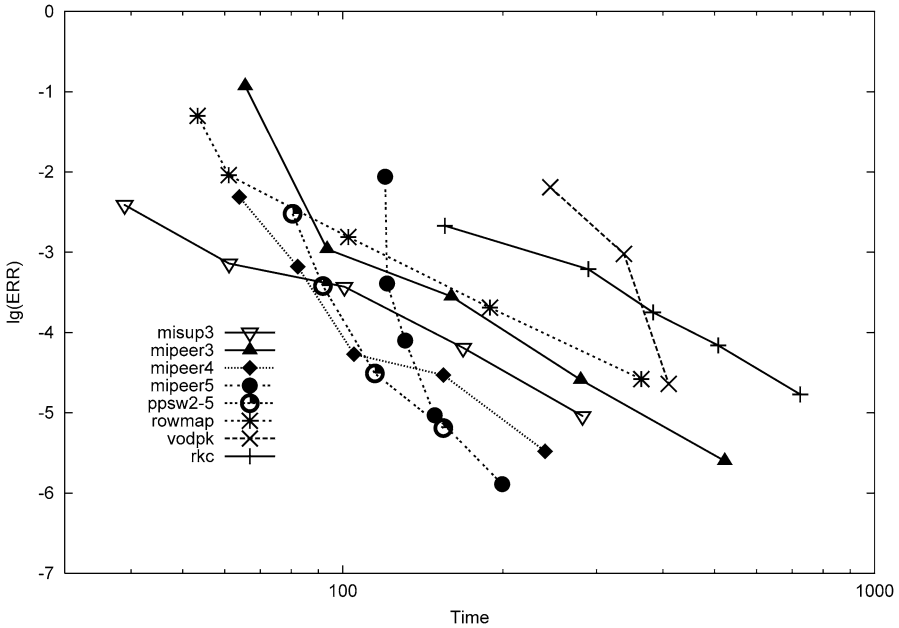


Figure 7.2: Results for RADIATION, $50 \times 50$-mesh.

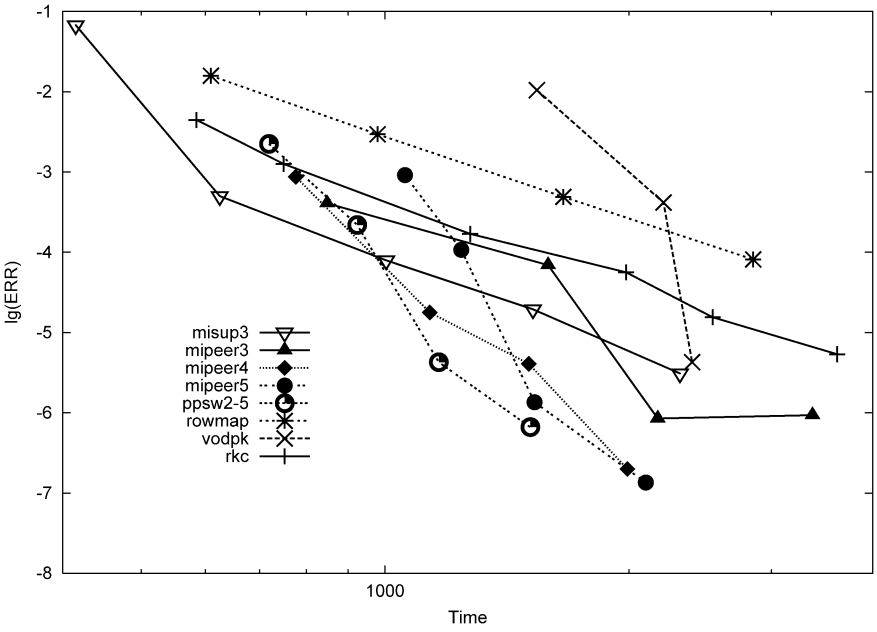


Figure 7.3: Results for RADIATION, $100 \times 100$-mesh.

It is interesting to look at the hand-made method *PPSW2-5* which is not backed by a strong stability result as in Theorem 2.2. Although it has problems for crude tolerances it sometimes outperforms all other methods. This is a clear motivation for future research on wider classes of peer methods.

**Conclusions.**

A special subclass of multi-implicit peer W-methods with high order has been investigated in this paper having a fairly strong theoretical background. Uniform stability estimates for realistic time grids can be proved and a polynomial collocation formulation widens the range of the applicable analysis. Additional results are concerned with superconvergence for constant stepsize and the condition of Vandermonde matrices. These results are used as additional criteria for choosing remaining free parameters in the subclass and lead to a quite deterministic construction principle. Numerical experiments show that an efficient implementation of these methods is possible and competitive with existing software. However, comparison with a hand-optimized method not belonging to this class indicates that superior peer methods may still be found in extensions of it.

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