Implicit Parallel Peer Methods for stiff initial value problems

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Dedicated to Professor Karl Strehmel on the occasion of his seventieth birthday

Abstract

A class of implicit two-step integration methods is introduced having s stages which may be computed in parallel. Since all stage solutions are approximations with equal accuracy and stability properties these methods were attributed as 'peer' methods. Using a special result on Vandermonde matrices we identify one subclass of order $s-1$ which is zero stable for general stepsize sequences. A further analysis for singularly perturbed problems shows that no order reduction occurs and the accuracy is essentially determined by the regularity of the smooth component. These results are backed by several numerical examples even including one differential algebraic problem.

Key words: Parallel methods for stiff ODEs, peer methods, singularly perturbed problems

1 Introduction

Recently the first two authors introduced a new class of linearly implicit integration methods for the solution of stiff initial value problems

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

with parallelism across the method [7]. It employs a set of s solution variables $Y_{m1}, \ldots, Y_{ms}$ per time step $t_m \to t_{m+1}$. Since these s variables share essentially the same properties and there is no principal solution variable as in many other methods these new schemes were denoted as peer methods. We now introduce an

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implicit version of these methods in two-step form. Generalization to more steps is obvious but will not be considered here. Within the time step $t_{m+1} = t_m + h_m$ the scheme uses off-step points $t_{mi} = t_m + h_m c_i$ with fixed nodes c_i, $i = 1, \ldots, s$. Stage approximations $Y_{mi} \cong y(t_{mi})$ at these points are computed for $i = 1, \ldots, s$ by

$$Y_{mi} - h_m \gamma_i f(t_{mi}, Y_{mi}) = \sum_{j=1}^{s} b_{ij} Y_{m-1,j} + h_m \sum_{j=1}^{s} a_{ij} f(t_{m-1,j}, Y_{m-1,j}). \tag{2}$$

The reals $\gamma_i > 0$ and a_{ij}, b_{ij} are the parameters of the scheme. Since the right-hand side in (2) uses only information from the previous step these s stages can be processed in parallel. It is convenient to introduce the coefficient matrices

$$G := \mathrm{diag}(\gamma_1, \ldots, \gamma_s), \quad A := (a_{ij})_{i,j=1}^{s}, \; B := (b_{ij})_{i,j=1}^{s} \tag{3}$$

and the step vectors $Y_m = (Y_{mi})_{i=1}^{s}$ and $f(Y_m) = (f(Y_{mi}))_{i=1}^{s}$. Due to the two-step nature the coefficients of higher order methods have to depend on the time grid and we will denote this dependence by an additional step index m. With these notations the scheme (2) takes on the more compact form

$$Y_m - h_m (G_m \otimes I) f(Y_m) = (B_m \otimes I) Y_{m-1} + h_m (A_m \otimes I) f(Y_{m-1}) \tag{4}$$

for autonomous systems which we discuss from now on, for simplicity. In deriving high order methods it is found that the coefficients have to depend on the stepsize ratios in the grid. It is assumed that these stepsizes ratios

$$\sigma_m := h_m / h_{m-1} \le \bar{\sigma}. \tag{5}$$

are bounded from above by some $\bar{\sigma} > 1$. However, no lower bound is imposed since this may be a severe restriction in practice. Further abbreviations are $\mathbb{1} = (1, \ldots, 1)^{\mathsf{T}}$, and e_i for the ith unit vector. The spectral radius of a matrix is denoted by ρ.

We start the discussion of the scheme (2) in Section 2 with an interpretation as General Linear Methods and by introducing basic stability notions. Section 3 is devoted to the derivation of order conditions. Considering high order methods with good stability it is found that the similarity transformation of the diagonal matrix G_m in (3) by Vandermonde matrices plays a crucial role. A simple representation of such matrices from Section 4 is used in Section 5 to construct a subclass being stable for general stepsize sequences. Since implicit methods might be especially suited for very stiff problems we analyze them for singularly perturbed problems in Section 6. Finally, numerical examples for such problems are presented in Section 7.

2 Structural properties of the scheme

The method (2) was motivated by certain reformulations of the Parallel Peer two-Step W-methods (PPSW methods) introduced recently by the first two authors [7]. However, the form of this scheme (2) also reminds on multistep methods, especially BDF-methods for $A = 0$. The main difference to BDF methods is that several approximations are computed here in each time step and the solution values used are not confined to the time grid $\{t_m\}$. The scheme (2) also has an interpretation as a General Linear Method (GLM), [1]. At the expense of increasing the number of variables the general version may be written as

$$\left(\begin{array}{c} Y_m \\ \hline K_m \\ Y_m \end{array}\right) = \left(\begin{array}{c|cc} G & A & B \\ \hline I & 0 & 0 \\ G & A & B \end{array}\right) \left(\begin{array}{c} hf(Y_m) \\ \hline K_{m-1} \\ Y_{m-1} \end{array}\right),$$

with Y_m and $K_m = hf(Y_m)$ as additional internal resp. external variables. The restricted version with $A = 0$ uses only Y_m as internal and external variables yielding the GLM form

$$\left(\begin{array}{c} Y_m \\ \hline Y_m \end{array}\right) = \left(\begin{array}{c|c} G & B \\ \hline G & B \end{array}\right) \left(\begin{array}{c} hf(Y_m) \\ \hline Y_{m-1} \end{array}\right).$$

Methods of this type have not yet been discussed in the literature.

The left-hand side of (4) has the form of a backward Euler step and, hence, well-known results on solvability of the nonlinear systems in (4) apply. Sufficient conditions for solvability are $h_m\gamma_i\mu < 1$ [2, V.6] if μ is the one-sided Lipschitz constant of f.

With respect to stability properties we only consider the linear, autonomous test problem $y' = Jy$. Here, the scheme (4) reduces to the recursion

$$Y_m = (I - h_m G_m \otimes J)^{-1}(B_m \otimes I + h_m A_m \otimes J)Y_{m-1}. \tag{6}$$

Hence, Y_{m-1} is multiplied by a function $M_m(h_m J)$ of the matrix $h_m J$. This function M_m is the stability matrix of the scheme since inhomogeneous versions of (6) model the propagation of errors in the scheme (4). M_m is itself an $s \times s$-matrix and has the form

$$M_m(z) = (I - zG_m)^{-1}(B_m + zA_m), \quad z \in \mathbb{C}. \tag{7}$$

The index m reminds that all coefficients may depend on the stepsize ratio (5). For a constant stepsize h, however, M is independent of the step index m. Important special values of M_m yield the matrices

$$M_m(0) = B_m, \quad M_m(\infty) = -G_m^{-1}A_m. \tag{8}$$

They govern the propagation of very smooth or very stiff components, respectively.

Definition 1 *Let $M(.)$ be the stability matrix (7) of the method (2) for $\sigma = 1$. Then, the method is called* zero-stable, *if $\rho(M(0)) = 1$ and eigenvalues on the unit circle are simple. It is A-stable if $\rho(M(z)) < 1$ in the open left complex halfplane, $z \in \mathbb{C}_- := \{z \in \mathbb{C} : \ Rez < 0\}$ and L-stable if, additionally, $\rho(M(\infty)) = 0$.*

Due to (8) methods with optimal damping of stiff components are obtained by choosing $A_m = 0$ in (4), i.e., for BDF-like methods. Later on in this paper we will concentrate on this kind of methods.

3 Accuracy

The residual of the scheme (2) at the exact solution y may be computed by Taylor expansion around t_m. Use of the identity $f(y(t_{mi})) = y'(t_{mi})$ yields

$$\begin{aligned} h_m\Delta_{mi} &:= y(t_{mi}) - h_m\gamma_i y'(t_{mi}) - \sum_{j=1}^{s}\left(b_{ij}y(t_{m-1,j}) + h_m a_{ij}y'(t_{m-1,j})\right) \\ &= \sum_{k=0}^{q-1}\left(c_i^k - \gamma_i k c_i^{k-1} - \sum_{j=1}^{s} b_{ij}(\frac{c_j-1}{\sigma_m})^k - k\sum_{j=1}^{s} a_{ij}(\frac{c_j-1}{\sigma_m})^{k-1}\right)\cdot \\ &\quad \frac{h_m^k}{k!}y^{(k)}(t_m) + O(h_{m-1}^q). \end{aligned}$$

Here it is agreed upon that terms of the form kc_i^{k-1} evaluate to zero for $k = 0$. Then the condition $\Delta_{mi} = O(h_{m-1}^{q-1})$ is equivalent with

$$\begin{aligned} B(q): \quad & c_i^k - \sum_{j=1}^{s} b_{ij}(\frac{c_j-1}{\sigma_m})^k - k(\gamma_i c_i^{k-1} + \sum_{j=1}^{s} a_{ij}(\frac{c_j-1}{\sigma_m})^{k-1}) = 0, \\ & k = 0, \ldots, q-1. \end{aligned} \tag{9}$$

For $q = s$ this condition may be solved for the coefficient matrix B. Its representation is simplified by introducing the Vandermonde matrix $V = (c_i^{j-1})_{i,j=1}^s$, the Pascal matrix $P = \left(\binom{j-1}{i-1}\right)_{i,j=1}^s$, the diagonal matrices

$$S_m = \ \mathrm{diag}(1, \sigma_m, \ldots, \sigma_m^{s-1}), \tag{10}$$

and $D := \ \mathrm{diag}(1, \ldots, s)$. Then condition $B(s)$ reads $0 = V - GVDF_0^{\mathsf{T}} - B_m P^{-1}S_m^{-1} - A_m V P^{-1}S_m^{-1}DF_0^{\mathsf{T}}$. The matrix $F_0 = (\delta_{i-1,j})_{i,j=1}^s$ describes a shift. Using the identity $DF_0^{\mathsf{T}}S_m P = \sigma_m S_m P D F_0^{\mathsf{T}}$ [7] we obtain

$$B_m = (V - G_m V D F_0^{\mathsf{T}})S_m P V^{-1} - \sigma_m A_m V D F_0^{\mathsf{T}}.$$

This matrix is almost the same as for linearly-implicit PPSW methods, where A_m is replaced by $\beta_m = A_m + \Gamma_m$, [7], [10] and may be decomposed in the following way.

Lemma 2 *If the method (2) satisfies $B(s)$, its coefficient matrix B_m is given by*

$$B_m = (I - G_m E)\Theta_m - \sigma_m A_m E, \quad \Theta_m = V S_m P V^{-1},\ E = V D F_0^{\mathsf{T}} V^{-1}. \tag{11}$$

The matrix Θ_m describes the polynomial extrapolation from the subgrid $\{t_{m-1} + h_{m-1}c_i,\ i = 1, \ldots, s\}$ to $\{t_m + h_m c_i,\ i = 1, \ldots, s\}$ and E is a difference operator with $E(\psi(c_i))_{i=1}^s = (\psi'(c_i))_{i=1}^s$ for polynomials ψ of degree $s-1$. The matrices Θ_m and E commute for $\sigma_m = 1$, since $E\Theta_m = \sigma_m \Theta_m E$, cf. [7]. Lemma 2 leads to the interpretation of the scheme (4) as a nonlinear corrector equation

$$\begin{aligned} \tilde{Y}_m &:= (\Theta_m \otimes I) Y_{m-1} \\ Y_m - h_m (G_m \otimes I) f(Y_m) &= ((I - G_m E) \otimes I)\tilde{Y}_m \\ &\quad + (A_m \otimes I)(h_m f(Y_{m-1}) - \sigma_m (E \otimes I) Y_{m-1}), \end{aligned}$$

to the extrapolated solution $\tilde{Y}_m$.

The decomposition (11) indicates that for eigenvalue discussions it is convenient to get rid of the common similarity transform with the Vandermonde matrix and to consider directly the matrices

$$\begin{aligned} \tilde{B}_m &:= V^{-1} B_m V = (I - \tilde{G}_m D F_0^{\mathsf{T}}) S_m P - \sigma_m \tilde{A}_m D F_0^{\mathsf{T}}, \\ &\quad \tilde{G}_m := V^{-1} G_m V, \quad \tilde{A}_m := V^{-1} A_m V. \end{aligned} \tag{12}$$

The matrix $S_m P$ is upper triangular with eigenvalues σ_m^k, $k = 0, \ldots, s-1$. Hence it describes an expanding map for $\sigma_m > 1$. The matrix $D F_0^{\mathsf{T}} S_m P$ is strictly upper triangular and essentially shifts the columns of its left operand $\tilde{G}_m$ to the right. So, in order to cancel the main diagonal of $S_m P$ one of the matrices $\tilde{G}_m$ or $\tilde{A}_m$ must have at least one nontrivial subdiagonal. Recalling the structure of the stability matrix (7) we essentially have two different attractive options:

1. *singly-implicit methods* with $G_m = \tilde{G}_m = \gamma^{(m)} I$: Since $\tilde{G}_m$ is diagonal, $A_m \neq 0$ is required for zero-stability. In [7] we found that the nilpotent matrix

   $$A_m = V F_0 S_m D^{-1} V^{-1} \tag{13}$$

   is a convenient choice. However, such methods do not possess optimal stiff damping since $M(\infty) = -\frac{1}{\gamma^{(m)}} A_m \neq 0$. Still, the spectral radius at infinity is zero, $(M(\infty))^s = 0$.

2. *multi-implicit stiffly accurate methods*: For stiffly accurate methods with $M(\infty) = 0$, i.e. $A_m = 0$, only the matrix $\tilde{G}$ may be used to cancel the diagonal of $S_m P$ in (12). This requires using different γ_i, i.e., a multi-implicit method.

Compared to linearly-implicit peer methods we expect the implicit methods (4) to be preferable in difficult situations like singularly perturbed problems. In these applications the behaviour in the stiff limit $z \to \infty$ is critical. Hence, we concentrate on the kind of methods from the second item and we will discuss in Section 5 a certain convenient choice which is based on the structural result of the following section.

4 Vandermonde similarity of diagonal matrices

By the definition $V\tilde{G} = GV$, the elements $\tilde{g}_{ij}$ of $\tilde{G}$ satisfy the conditions

$$\sum_{k=1}^{s} c_i^{k-1} \tilde{g}_{kj} = \gamma_i c_i^{j-1}, \quad i,j = 1,\ldots,n. \tag{14}$$

From every two adjacent columns the elements γ_i may be eliminated yielding

$$-\tilde{g}_{1,j+1} + \sum_{k=1}^{s-1} (\tilde{g}_{kj} - \tilde{g}_{k+1,j+1}) c_i^k + \tilde{g}_{sj} c_i^s = 0, \quad i = 1,\ldots,s, \tag{15}$$

and $j = 1,\ldots,s-1$. For each index j the equation (15) contains a polynomial of degree s which vanishes at all nodes c_i. So it must be a multiple of the node polynomial

$$\phi(c) = \prod_{i=1}^{s} (c - c_i) = \sum_{j=0}^{s} \phi_j c^j. \tag{16}$$

Hence the following linear relation holds among the elements of $\tilde{G}$

$$\tilde{g}_{kj} - \tilde{g}_{k+1,j+1} = \tilde{g}_{sj} \phi_k, \quad k,j = 1,\ldots,s-1. \tag{17}$$

This is a set of recursions which may be easily solved along diagonals beginning with the first or the last row of $\tilde{G}$.

Lemma 3 *Let mutually distinct nodes c_i, $i = 1,\ldots,s$ and an arbitrary diagonal matrix G be given. Then the elements of the transformed matrix $\tilde{G} = (\tilde{g}_{ij}) = V^{-1}GV$ have the representation*

$$\begin{aligned} \tilde{g}_{ij} &= \sum_{k=i}^{s} \phi_k \, \tilde{g}_{s,k+j-i}, \quad j \le i, \\ \tilde{g}_{i+1,j+1} &= -\sum_{k=0}^{i-1} \phi_k \, \tilde{g}_{s,k+j-i}, \quad j > i. \end{aligned} \tag{18}$$

Considering methods with $A_m = 0$ the matrix $\tilde{G}$ contains the only free parameters of the method that influence its stability properties. The main advantage of Lemma 3 is the bilinear representation in terms of the coefficients ϕ_i of the node polynomial and the elements $\tilde{g}_{sj}$ of its last row. Hence, we use these elements $\tilde{g}_{sj}, j = 1,\ldots$ and

not the method parameters $\gamma_i, i = 1, \ldots, s$ in the following discussion. Of course, these original parameters may be recovered by the formula

$$\gamma_i = \sum_{j=1}^{s} \tilde{g}_{sj} \sum_{k=j}^{s} \phi_k c_i^{k-j}, \quad i = 1, \ldots, s, \tag{19}$$

which is easily obtained from (14) with $j = 1$ and (18). Since it may help in understanding the structure we display the matrix from Lemma 3 for $s = 3$,

$$\tilde{G} = \begin{pmatrix} \phi_1\tilde{g}_{31} + \phi_2\tilde{g}_{32} + \tilde{g}_{33} & -\phi_0\tilde{g}_{31} & -\phi_0\tilde{g}_{32} \\ \phi_2\tilde{g}_{31} + \tilde{g}_{32} & \phi_2\tilde{g}_{32} + \tilde{g}_{33} & -\phi_0\tilde{g}_{31} - \phi_1\tilde{g}_{32} \\ \tilde{g}_{31} & \tilde{g}_{32} & \tilde{g}_{33} \end{pmatrix}$$

The Lemma will be a main tool in the construction of a certain class of stable multi-implicit methods.

5 Stable high order multi-implicit methods

In designing singly-implicit PPSW methods in [7] it was found that choosing an upper triangular structure of $\tilde{B}$ led to robust stability properties for general stepsize sequences. The price to be paid there was some loss of damping in the stiff limit. Now, by a judicious choice of the parameters in the representation of $\tilde{G}$ from Lemma 3 we may obtain similar properties without loosing the optimal damping property $M(\infty) = 0$. We recall the observation that, due to the structure (11) of B_m, it was not possible to use $G = \gamma I$ with one single γ since the columns of the matrix $\tilde{G}$ are shifted to the right by the multiplication with F_0^{T}. But by this shift the subdiagonal of a general matrix $\tilde{G}$ is moved to the main diagonal and may be used to cancel the large entries of $S_m P$ in the main diagonal of $\tilde{B}_m$. So, by Lemma 3 it is convenient to choose $\tilde{g}_{s,s-1}, \tilde{g}_{ss} \neq 0$ only.

Theorem 4 *Let the coefficient matrices B_m of the scheme (2) be given by (11) with $A_m = 0$. Let the matrix $\tilde{G}$ be chosen by Lemma 3 with $\tilde{g}_{sj} = 0, j \leq s-2$, and $\tilde{g}_{s,s-1} \in (0, \frac{2}{s-1})$. Then, the parameters γ_i have the form*

$$\gamma_i = \tilde{g}_{ss} + \tilde{g}_{s,s-1}(\phi_{s-1} + c_i), \quad i = 1, \ldots, s, \tag{20}$$

and the method is zero stable. Moreover, there exists $\bar{\sigma} > 1$ such that with any monotonic matrix norm the uniform estimate

$$\|B_{m+k} \cdots B_{m+1} B_m\| \leq K, \quad k, m \geq 0, \tag{21}$$

holds for $t_m \leq t_e$ and stepsize sequences obeying (5). The constant K depends on $\bar{\sigma}$ only.

Proof Since only the last two elements $\tilde{g}_{sj}$ are nontrivial, the matrix $\tilde{G}$ has Hessenberg structure with constant subdiagonal elements $\tilde{g}_{i,i-1} = \tilde{g}_{s,s-1}$. Equation (20) is the version of (19) for this choice. Considering zero stability we look at the representation (12) of $\tilde{B}$. Here, the columns of $\tilde{G}$ are shifted to the right by the multiplication with $DF_0^{\mathsf{T}} S_m P$ and the resulting matrix $\tilde{B}$ is upper triangular. Its diagonal elements are given by $\tilde{b}_{11} = 1$ and

$$\tilde{b}_{ii} = \sigma_m^{i-1}(1 - (i-1)\tilde{g}_{s,s-1}), \quad i = 2, \ldots, s. \tag{22}$$

So, for any choice $\tilde{g}_{s,s-1} \in (0, \frac{2}{s-1})$ there exists $\bar{\sigma}$ and $q < 1$ such that $|\tilde{b}_{ii}| \le q$, $i = 2, \ldots, s$ for $\sigma_m \le \bar{\sigma}$. Optimal values for $\tilde{g}_{s,s-1}$ and $\bar{\sigma}$ are discussed after the proof.

Since the matrix V is the same in all steps the bound $\|B_{m+k} \cdots B_{m+1} B_m\| \le \kappa \|\tilde{B}_{m+k} \cdots \tilde{B}_{m+1} \tilde{B}_m\|$ may be used with the constant $\kappa = \|V^{-1}\|\|V\|$ as a first step in proving (21). Now, looking at the upper triangular matrices $|\tilde{B}_j|$ where the absolute value is taken elementwise, we observe the bound

$$|\tilde{B}_j| \le \begin{pmatrix} 1 & v^{\mathsf{T}} \\ 0 & C \end{pmatrix}, \quad \tilde{B}_j = \begin{pmatrix} 1 & v_j^{\mathsf{T}} \\ 0 & \tilde{B}_{22}^{(j)} \end{pmatrix},$$

with $C = qI + R$ and a strictly upper triangular matrix R, $R^{s-1} = 0$. By the binomial theorem the powers $\|C^k\| \le q^{k-s+1}\binom{k}{s-1}(q + \|R\|)^{s-1}$, $k \ge 2s-2$, are uniformly bounded and the series

$$\sum_{k=2s-2}^{\infty} \|C^k\| \le (q + \|R\|)^{s-1} \sum_{k=2s-2}^{\infty} \binom{k}{s-1} q^{k-s+1}$$

converges. Hence, the products

$$|\tilde{B}_{m+k} \cdots \tilde{B}_{m+1} \tilde{B}_m| \le \begin{pmatrix} 1 & v^{\mathsf{T}} \\ 0 & C \end{pmatrix}^k = \begin{pmatrix} 1 & v^{\mathsf{T}} \sum_{j=0}^{k-1} C^j \\ 0 & C^k \end{pmatrix}$$

are uniformly bounded. □

By (22), the parameter $\tilde{g}_{s,s-1}$ is the critical one with respect to zero stability and its choice determines the maximal stepsize ratio $\bar{\sigma}$ for (21). The value of $\tilde{g}_{s,s-1}$ leading to a least upper bound $\sigma_{\sup}$ for $\bar{\sigma} < \sigma_{\sup}$ is given by the positive solution of the equation

$$(1 - \tilde{g})^{s-1} - (s-1)\tilde{g} + 1 = 0.$$

The following table contains numerical estimates for $\sigma_{\sup}$, truncated to 4 digits, and the corresponding value of $\tilde{g}_{s,s-1}$.

s	3	4	5	6	7	8
σ_{sup}	2.414	1.677	1.444	1.329	1.262	1.217
$\tilde{g}_{s,s-1}$	0.5858	0.4039	0.3075	0.2481	0.2078	0.1788

A hard restriction on the choice of the second parameter $\tilde{g}_{ss}$ comes from the positivity of the coefficients γ_i. By (20) it is required that

$$\tilde{g}_{ss} > -\tilde{g}_{s,s-1}(\phi_{s-1} + \min_i c_i).$$

Further insight in the stability properties may be obtained from the observation that with the choice (20) the matrix $\tilde{B}_m$ does not dependent on the nodes c_i but only on the two parameters $\tilde{g}_{s,s-1}$ and $\gamma_0 := \tilde{g}_{ss} + \tilde{g}_{s,s-1}\phi_{s-1}$. Since $\tilde{G}F_0^{\mathsf{T}} = \gamma_0 \operatorname{diag}(0,1,\ldots,1) + \tilde{g}_{ss}F_0^{\mathsf{T}}$, the matrix $\tilde{B}_m$ in (12) may be computed explicitly. With the diagonal matrix $\hat{D} = \operatorname{diag}(0,1,2,\ldots,s-1)$ we get

$$\tilde{B} = S_m\Big(I - \tilde{g}_{s,s-1}\hat{D} - \gamma_0 F_0^{\mathsf{T}}\hat{D}\Big)P. \tag{23}$$

The diagonal of this upper triangular matrix is $S_m(I - \tilde{g}_{s,s-1}\hat{D})$, cf. (22), and its spectral radius is one for $\sigma_m \le \bar{\sigma} < \sigma_{\sup}$, by construction.

We note that with the uniform stability estimate (21) standard convergence results from multistep methods [2] apply here. So, Theorem 7 from [7] may be easily adapted to the present situation establishing global order $s-1$ for methods satisfying condition $B(s)$ and the assumptions of Theorem 4. Instead of replicating this formulation we rather like to discuss more difficult situations in the following section.

6 Singularly perturbed problems

Fully implicit methods (2) with coefficient $A_m = 0$ have favourable properties in very stiff problems. We start by considering the scalar Prothero-Robinson-equation

$$y' = \lambda(y - u(t)) + u'(t),\ t \ge 0, \tag{24}$$

where $u(t)$ is some smooth function and $\operatorname{Re}\lambda < 0$. We note that u is a solution of the differential equation (24) which attracts all other solutions. This equation has been used for studying order reduction of Runge-Kutta and other methods in the limit $\operatorname{Re}\lambda \to -\infty$. In this limiting case the new methods (2) have a nice property known as strong S-stability [5].

Lemma 5 *With $t_{m-1} \in [t_0, t_e)$ consider one fixed step of the method (2) with $A_m = (a_{ij}) = 0$ applied to the equation (24). Then for Y_m holds that*

$$Y_{mi} - u(t_{mi}) \to 0 \quad \textit{for} \quad \textit{Re}\,\lambda \to -\infty.$$

Proof With $z = h\lambda$ the equation for stage i reads

$$(1 - \gamma_i z)(Y_{mi} - u(t_{mi})) = h\gamma_i u'(t_{mi}) - u(t_{mi}) + \sum_{j=1}^{s} b_{ij} Y_{m-1,j}.$$

Here it is evident that the difference $Y_{mi} - u(t_{mi})$ vanishes in the limit $\mathrm{Re}\,(1-\gamma_i z) \to \infty$. $\square$

This property partially carries over to singular perturbation problems of the form

$$\begin{aligned} x' &= p(x,z), \\ \epsilon z' &= q(x,z), \end{aligned} \tag{25}$$

$x \in \mathbb{R}^{n_1}, z \in \mathbb{R}^{n_2}$, $n_1 + n_2 = n$, with $0 < \epsilon \ll 1$ if the derivative q_z is a dissipative matrix. Compared with (1) we have the identities $y^{\mathsf{T}} = (x^{\mathsf{T}}, z^{\mathsf{T}})$ and $f^{\mathsf{T}} = (p^{\mathsf{T}}, \frac{1}{\epsilon} q^{\mathsf{T}})$. Application of the scheme (2) is obvious and for the errors

$$(Y_{mi} - y(t_{mi}))_{i=1}^{s} = \begin{pmatrix} X_m \\ Z_m \end{pmatrix}$$

we obtain a recursion of the form

$$\begin{pmatrix} X_m \\ Z_m \end{pmatrix} = (\, I - h_m G_m \otimes \hat{f}_y \,)^{-1} \begin{pmatrix} (B_m \otimes I) X_{m-1} + h_m \xi_m \\ (B_m \otimes I) Z_{m-1} + h_m \zeta_m \end{pmatrix}. \tag{26}$$

Here, $\hat{f}_y$ is an appropriate integral mean value of the derivative and $(\xi_m^{\mathsf{T}}, \zeta_m^{\mathsf{T}}) = \Delta_m^{\mathsf{T}}$ are the residuals of the exact solution. For the methods from Section 5 they satisfy $\|\xi_m\|, \|\zeta_m\| = O(h_{m-1}^{s-1})$. The inverse in (26) has the following well-known representation [8],

$$\begin{aligned} (\, I - hG \otimes \hat{f}_y \,)^{-1} &= \begin{pmatrix} I - hG \otimes \hat{p}_x & -hG \otimes \hat{p}_z \\ -\frac{h}{\epsilon} G \otimes \hat{q}_x & I - \frac{h}{\epsilon} G \otimes \hat{q}_z \end{pmatrix}^{-1} \\ &= \begin{pmatrix} I + O(h) & O(\epsilon) \\ O(1) & (I - \frac{h}{\epsilon} G \otimes \hat{q}_z)^{-1} + O(\epsilon) \end{pmatrix}. \end{aligned} \tag{27}$$

There are two critical points in the analysis of the error recursion (26). The first one concerns the northwest block of the transfer matrix in (26) where we need a bound of the form $1 + O(h)$ for the product $(I - hG \otimes \hat{p}_x)(B_m \otimes I)$. Here, our analysis is restricted to a constant stepsize h where the coefficient matrices do not depend on the time t_m and we may drop the index m for them. For such grids and $\tilde{g}_{s,s-1} \in (0, \frac{2}{s-1})$ the method is zero stable and there exists a norm $\|\cdot\|_*$ in $\mathbb{R}^s$ equivalent with $\|\cdot\|_2$ such that $\|B\|_* = 1$. Since B is diagonalizable this norm can be chosen in the form $\|v\|_* = \|U^{-1} v\|_2$, $v \in \mathbb{R}^s$, where U is the eigenvector matrix of B. By using tensor products this norm may be extended to the spaces $\mathbb{R}^{sn_1}$ such that $\|B \otimes I\|_* = 1$. The second critical point is the second diagonal block of the matrix in (26). Here, we need the dissipativity of the matrix $G \otimes q_z$ which follows directly from that of q_z only in the Euclidean norm, since G is diagonal. Hence, we still use the spectral norm for the southeast block of the matrix in (26). In fact, under the assumption

$$\epsilon \le dh, \tag{28}$$

for some appropriate $d > 0$ and $h \le h_0$, there exists $\alpha < 1$ such that

$$\|(I - \frac{h}{\epsilon} G \otimes \hat{q}_z)^{-1}(B \otimes I) + O(\epsilon)\|_2 \le \alpha < 1.$$

Summarizing, we use separate norms for the X and Z components in (26) and obtain the following recursive bound for the errors

$$\begin{pmatrix} \|X_m\|_* \\ \|Z_m\|_2 \end{pmatrix} \le \begin{pmatrix} 1 + O(h) & O(\epsilon) \\ O(1) & \alpha \end{pmatrix} \begin{pmatrix} \|X_{m-1}\|_* + O(h\|\xi_m\|_*) \\ \|Z_{m-1}\|_2 + O(h\|\zeta_m\|_2) \end{pmatrix}. \tag{29}$$

A slight modification of the proof of Lemma 3.9 of [2] yields the following result.

Theorem 6 *Let the derivative q_z of the singularly perturbed problem (25) be dissipative, i.e. $u^\mathsf{T} q_z(x,z)u < 0$ for all $u \in \mathbb{R}^{n_2}$, $\|u\|_2 = 1$. Consider the scheme (2) with the coefficient set of Theorem 4 on a grid with constant stepsize h satisfying (28). Then, the residuals $(\xi_m^\mathsf{T}, \zeta_m^\mathsf{T}) = \Delta_m^\mathsf{T}$ of the scheme,*

$$\xi := \max\{\|\xi_j\|_* : jh \le t_e\}, \quad \zeta := \max\{\|\zeta_j\|_2 : jh \le t_e\},$$

satisfy $\xi = O(h^{s-1})$, $\zeta = O(h^{s-1})$. And, with an appropriate constant K, the errors X_m, Z_m can be estimated by

$$\begin{aligned} \|X_m\|_* &\le K(\|X_0\|_* + \epsilon\|Z_0\|_2 + \xi + \epsilon\zeta), \\ \|Z_m\|_2 &\le K(\|X_0\|_* + (\alpha^m + \epsilon)\|Z_0\|_2 + \xi + h\zeta). \end{aligned}$$

Proof The proof relies on the following estimates [2] for the eigenvalues and eigenvector matrix U for the matrix in (29), $\lambda_1 = 1 + O(h)$, $\lambda_2 = \alpha + O(\epsilon)$,

$$U, U^{-1} = \begin{pmatrix} 1 & O(\epsilon) \\ O(1) & 1 \end{pmatrix}.$$

In the direction of the first eigenvector of U there is no damping and the recursion (29) yields the contribution

$$O(\|X_0\|_* + \epsilon\|Z_0\|_2) + O(\xi + \epsilon\zeta).$$

In the second direction the damping factor is $\lambda_2 = \alpha + O(\epsilon) < 1$. Recursive application leads to uniformly bounded sums $\sum_{j\ge1} \lambda_2^j$ and the contribution at t_m is

$$\lambda_2^m O(\|X_0\|_* + \|Z_0\|_2) + hO(\xi + \zeta) \sum_{j=1}^{m} \lambda_2^j.$$

The back transformation with U^{-1} yields the estimate from the statement. □

Remark The error estimates for the x and z components are quite similar. The main difference between both components is the influence of their regularity on the error. The local error ζ is multiplied by small terms everywhere in the global estimate. Hence, in both components the error is essentially determined by the regularity of the smooth component x in the first place, similar to the situation in multistep methods [4].

7 Numerical examples

Many aspects of the implementation of the implicit scheme (2) are similar to the linearly-implicit PPSW-methods described on [7]. One crucial difference comes from the need to solve s nonlinear systems in (2). The absolute and relative tolerances for the Newton iteration were set to one tenth of the error tolerances for stepsize control. As initial guess for Newton's method the extrapolated values $\Theta_m Y_{m-1}$ are used, cf. (11), and a maximum of 10 simplified Newton iterations is performed. As error estimate for stepsize control we compare Y_{ms} with a predictor of order $s-2$ which does not use the value $Y_{m-1,1}$.

The implementation of the implicit methods is more complicated and more expensive than that of their linearly-implicit counterparts using the same coefficients (plus additional ones). Linearly-implicit two-step methods may also perform well for singularly perturbed problems, cf. [11]. So, the most intriguing question here is whether the increased effort for the scheme (2) pays back by improved stability properties. Hence, we restrict our testing to some small singularly perturbed problems with sequential computatuions. Since the implementation of the scheme may be easily adapted to differential equations of the form $Ly' = f(t,y)$ with constant matrix L, we also include one differential-algebraic problem with singular L, just for curiosity. We present results for the following three test problems.

- SINGP, cf. [6]: It is very stiff with $\epsilon = 10^{-12}$ on the time interval $t \in [0,1]$ with four equations,

$$\begin{aligned} \epsilon y_1' &= -y_1^2 - y_3^2 + y_4^4/y_2 - \epsilon y_3, \\ \epsilon y_2' &= -y_2 + y_4^4 - 2\epsilon y_2, \\ y_3' &= y_1, \\ y_4' &= -\tfrac{1}{2}|y_2|^{1/4}, \end{aligned} \qquad y(t) = \begin{pmatrix} \cos t \\ e^{-2t} \\ \sin t \\ e^{-t/2} \end{pmatrix}$$

- OREGO: The Oregonator reaction [2, IV.10] of dimension $n = 3$ on $t \in [0, 360]$.

- TAMP: The transistor amplifier form the CWI test set with $n = 8$ equations on the interval $t \in [0, 0.2]$. It is a stiff DAE of index 1 where the matrix L has rank 5.

From the class of methods derived in Section 5 we took only one 4-stage method (named **i4**) and one with 6 stages (**i6**). The nodes and the parameters $\tilde{g}_{s,s-1}$, $\gamma_0 := \tilde{g}_{ss} + \tilde{g}_{s,s-1}\phi_{s-1}$ of these methods are given by

meth.	$\tilde{g}_{s,s-1}$	γ_0	c_1	c_2	c_3
$i4$	0.4039283620	0.5511656641	−0.8583336	−0.1977341	0.1115533
$i6$	0.2480736013	0.2980736013	−1	−0.7320508	...

The last node is always $c_s = 1$ and the nodes of **i6** are stretched Chebychev nodes $c_i = -\cos((2i-1)\omega)/\cos(\omega)$, $i = 1, \ldots, s$, $\omega = \pi/(2s)$. Each of these methods is compared with the corresponding PPSW method [7] named **w4** and **w6**. As benchmark we used the code RODAS which has a computational effort comparable to method **w6**. The results are presented in the following Figures 1–3 where the implicit methods are distinguished by filled marks. The diagrams show logarithms of the final error at t_e over the total number of function calls (not including those for the Jacobian) on the horizontal axis.

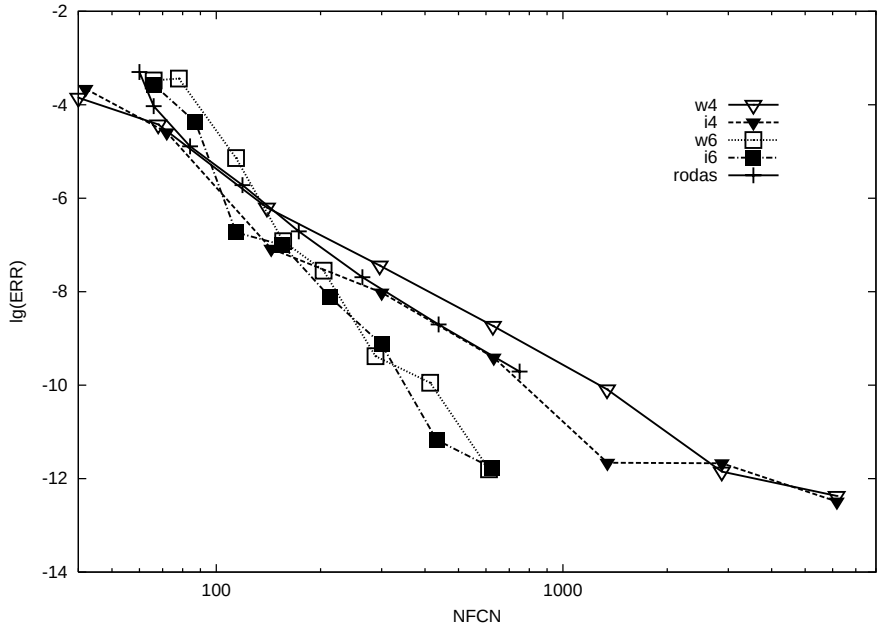

Figure 1: Results for SINGP

In these diagrams we make the following observations. Only for the four-stage methods there is a noticeable difference between implicit and linearly-implicit methods. However, we point out that in the TAMP example some marks are missing for the PPSW methods where they failed. This indicates that for mild tolerances, at least, the implicit methods (2) are more reliable than the linearly-implicit ones for extremely stiff problems. The benchmark code RODAS is outperformed for sharp tolerances. For the examples OREGO and TAMP, however, it is faster for less stringent tolerances probably due to a better estimate for the initial stepsize. We used a rather small and cautious guess for h_0.

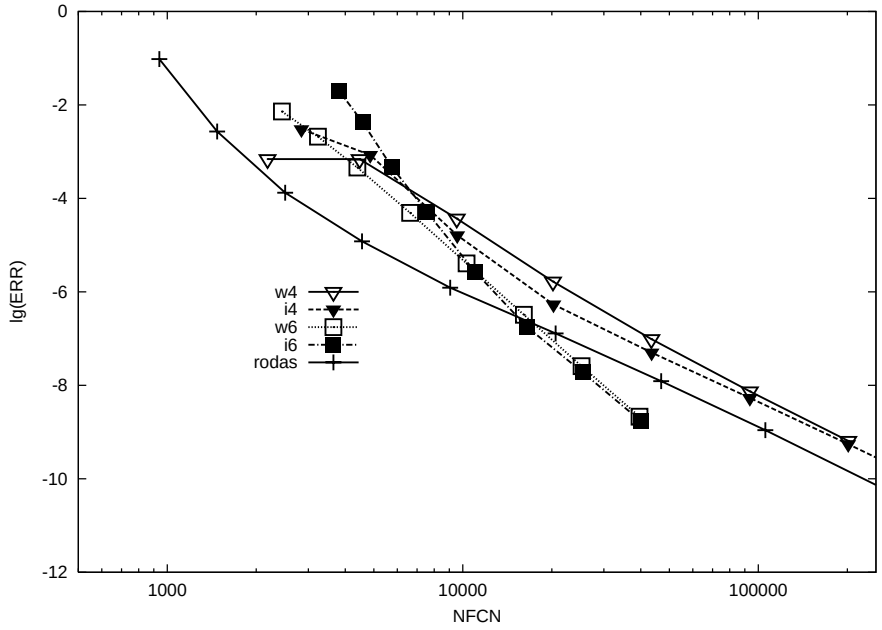

Figure 2: Results for OREGO

Conclusion

A fully implicit class of two-step methods was introduced having a set of solution variables with equal properties in s stages. The nonlinear systems in these stages are independent and may be solved in parallel on s processors. A subclass of methods is identified which have stage order $s-1$ and are stable for general stepsize sequences. In singularly perturbed problems no order reduction occurs and the error is essentially determined by the regularity of the smooth component. Numerical tests show that the methods perform well compared with existing software. However, they have an edge over related linearly-implicit peer methods only for very stiff problems and mild tolerances.

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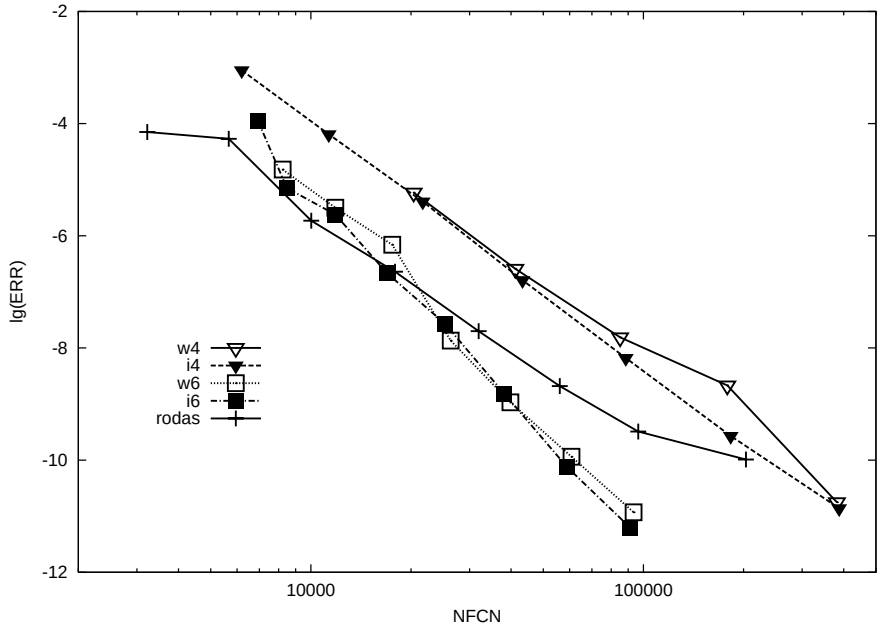

Figure 3: Results for TAMP

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