J Appl Math Comput (2012) 38:389–406
DOI 10.1007/s12190-011-0485-0

JAMC

Implicit peer methods for large stiff ODE systems

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Received: 11 October 2010 / Published online: 15 May 2011

Abstract Implicit two-step peer methods are introduced for the solution of large stiff systems. Although these methods compute s-stage approximations in each time step one-by-one like diagonally-implicit Runge-Kutta methods the order of all stages is the same due to the two-step structure. The nonlinear stage equations are solved by an inexact Newton method using the Krylov solver FOM (Arnoldi's method). The methods are zero-stable for arbitrary step size sequences. We construct different methods having order $p = s$ in the multi-implicit case and order $p = s - 1$ in the singly-implicit case with arbitrary step sizes and $s \leq 5$. Numerical tests in MATLAB for several semi-discretized partial differential equations show the efficiency of the methods compared to other Krylov codes.

Keywords Implicit peer methods · Large stiff systems · Zero-stability · FOM

Mathematics Subject Classification 65L05 · 65L06

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1 Introduction

In [8] two of the authors introduced the class of linearly-implicit parallel peer methods for the solution of stiff initial value problems

$$y'(t) = f(t, y(t)), \quad t \in [t_0, t_e], \qquad y(t_0) = y_0, \tag{1}$$

$f : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n$. These methods are characterized by the fact that the stage values share same accuracy and stability properties. Later the methods were generalized in several directions, in [10] implicit parallel methods were considered, in [7] sequential linearly-implicit methods were introduced. In [9] linearly-implicit parallel peer methods were combined with the full orthogonalization method (FOM) and were used for the solution of large stiff systems of ordinary differential equations resulting from the semidiscretization of partial differential equations with the method of lines (MOL).

In this paper we will combine these approaches and consider s-stage sequential implicit peer methods for large stiff systems. This means that Newton's method will be used for the solution of the nonlinear stage equations. The solutions of the linearized systems, however, will be approximated by FOM in order to keep the computational effort low for large dimensions. The proposed class of peer methods has the form

$$Y_{m,i} = \sum_{j=1}^{s} b_{ij} Y_{m-1,j} + h_m \sum_{j=1}^{i} g_{ij} F_{m,j}, \quad i = 1, 2, \ldots, s. \tag{2}$$

In each time step from t_m to $t_{m+1} = t_m + h_m$ it computes stage solutions $Y_{m,i} \cong y(t_{m,i})$, $i = 1, 2, \ldots, s$, as approximations at the points

$$t_{m,i} := t_m + h_m c_i, \quad i = 1, 2, \ldots, s.$$

In this paper we consider methods with

$$0 \le c_1 < c_2 < \cdots < c_s = 1.$$

The stage derivatives are denoted by $F_{m,i} = f(t_m + h_m c_i, Y_{m,i})$, $i = 1, 2, \ldots, s$. Introducing stacked vectors

$$Y_m = \begin{pmatrix} Y_{m,1} \\ Y_{m,2} \\ \vdots \\ Y_{m,s} \end{pmatrix}, \qquad F(t_m, Y_m) = \begin{pmatrix} f(t_m + c_1 h_m, Y_{m,1}) \\ f(t_m + c_2 h_m, Y_{m,2}) \\ \vdots \\ f(t_m + c_s h_m, Y_{m,s}) \end{pmatrix}$$

a compact form of the scheme (2) is

$$Y_m = (B_m \otimes I) Y_{m-1} + h_m (G_m \otimes I) F(t_m, Y_m). \tag{3}$$

Here the coefficients are collected in the matrix $B_m = (b_{ij})_{i,j=1}^{s}$ and the lower triangular matrix $G_m = (g_{ij})_{i,j=1}^{s}$ which may depend on the step size ratio σ_m defined by $h_m = \sigma_m h_{m-1}$.

Remark 1 It is possible to include also $f(t_{m-1}, Y_{m-1})$ in (2). However, in this case L-stability ($M(\infty) = 0$, cf. (13)) is not possible. Furthermore the stability investigations become much more delicate. For explicit methods it is more suitable to consider this extension [13]. Calvo et al. [2] construct explicit peer methods of this type of order $2s - 1$.

When direct solvers are used for the solution of the linear equations, the singly-implicit choice

$$G_m = \gamma I + G_0 \tag{4}$$

with a strictly lower triangular matrix G_0 is advantageous, since only one LU decomposition per time step is needed. In combination with Krylov solvers, however, the multi-implicit choice with

$$G_m = \mathrm{diag}(\gamma_1, \gamma_2, \ldots, \gamma_s) + G_0,$$

can be used and the additional parameters may be used to improve the properties of the method.

The order and stage order of an s-stage peer method are limited to $p = s - 1$, in general. For special nodes and constant step size methods of order of convergence $p = s$ were constructed in [7]. In this paper we consider different choices for G_m. In the most general case, choosing G_m multi-implicit and σ-dependent, we construct methods of order of consistency and convergence $p = s$. If G_m does not depend on σ_m the order of consistency $p = s$ can be ensured for constant h only. Even when using Krylov solvers singly-implicit methods with (4) are of interest if preconditioning is considered. For this case we derive order conditions ensuring only order of consistency $p = s - 1$ but order of convergence $p = s$ for constant step sizes.

As the methods have a two-step character, zero-stability is a crucial point for peer methods. In Sect. 2 we derive the order conditions and present a construction principle that ensures zero-stability for all step size sequences. In Sect. 3 we use some remaining degrees of freedom to increase the order of the methods. Different types of methods with constant and variable matrix G_m are discussed. In Sect. 4 we present special methods with good stability and accuracy properties for $s = 3, 4, 5$. Furthermore, we discuss implementation issues like the choice of starting approximations for the Newton process, error estimation and stopping criteria for the iterative methods. Finally, in Sect. 5 numerical results for several MOL problems are given. We compare the MATLAB implementation of our methods with the Krylov one-step codes ROWMAP [12] and EXP4 [3].

2 Order conditions and linear stability

The order conditions for peer methods can be derived by replacing $Y_{m,i}$ and $Y_{m-1,i}$ in (3) by values of the solution $y(t)$ and using $f(t_{m,i}, y(t_{m,i})) = y'(t_{m,i})$. Since this is done simultaneously for all stages, there is no difference between order and stage

order and hence no order reduction for stiff problems. Taylor series expansion gives

$$y(t_m + c_i\sigma h_{m-1}) = \sum_{l=0}^{p} \frac{(c_i\sigma_m h_{m-1})^l}{l!} y^{(l)}(t_m) + \mathcal{O}(h_{m-1}^{p+1}),$$

$$y(t_{m-1} + c_i h_{m-1}) = \sum_{l=0}^{p} \frac{((c_i-1)h_{m-1})^l}{l!} y^{(l)}(t_m) + \mathcal{O}(h_{m-1}^{p+1}),$$

$$\sigma_m h_{m-1} y'(t_m + c_i\sigma_m h_{m-1}) = \sum_{l=1}^{p} \sigma_m h_{m-1} \frac{(c_i\sigma_m h_{m-1})^{l-1}}{(l-1)!} y^{(l)}(t_m) + \mathcal{O}(h_{m-1}^{p+1}).$$

For a compact notation, we use the node vector $c = (c_1, c_2, \ldots, c_s)^\top$ and the operator $z := h_{m-1}\frac{d}{dt}$ in the following definition.

Definition 1 For $z \to 0$ and $\sigma_m > 0$ let the peer method (3) satisfy

$$\exp(\sigma_m c z) = B_m \exp((c-1)z) + G_m\sigma_m z \exp(\sigma_m c z) + \mathcal{O}(z^{p+1}), \tag{5}$$

with $p \in \mathbb{N}_0$ and the exponentials of the vectors are defined componentwise. Then, the method is *preconsistent* if $p \geq 0$ and *consistent of order* p if $p \geq 1$.

For constant step sizes, (5) simplifies to

$$\exp(cz) = B\exp((c-1)z) + Gz\exp(cz) + \mathcal{O}(z^{p+1}), \quad z \to 0. \tag{6}$$

Let the nodes c_i be pairwise distinct. Then, by the order conditions for $p = s-1$ in (5), one of the matrices B_m or G_m is uniquely determined by the other. Solving for B_m we re-write (5) in matrix form collecting the coefficients of $\frac{z^l}{l!}$ in columns. This gives

$$V_0 S = B_m V_1 + G_m V_0 D F_0^\top S \tag{7}$$

and hence

$$B_m = (V_0 - G_m V_0 D F_0^\top) S V_1^{-1}, \tag{8}$$

where the matrices are given by

$$\begin{aligned} &(V_0)_{i,j} = c_i^{j-1}, \qquad (V_1)_{i,j} = (c_i-1)^{j-1}, \\ &(F_0)_{i,j} = \delta_{i,j+1} = \begin{cases} 1 & i = j+1, \\ 0 & i \neq j+1, \end{cases} \\ &S = \operatorname{diag}(1, \sigma_m, \sigma_m^2, \ldots, \sigma_m^{s-1}) \quad \text{and} \quad D = \operatorname{diag}(1, 2, \ldots, s). \end{aligned} \tag{9}$$

Besides consistency, convergence of the methods requires zero-stability, at least. This problem will be discussed now.

Definition 2 A peer method (3) is *zero-stable*, if

$$\|B_{m+l}B_{m+l-1}\cdots B_{m+1}B_m\| \le K$$

holds for some constant $K < \infty$ and for all m and $l \ge 0$.

The uniform boundedness of arbitrary matrix products required in Definition 2 is a very difficult theoretical question. It is easily verified for special matrix families, only. Our construction of the methods in the next section uses such a family. Now, convergence for variable grids with $0 < \sigma_{\min} < \sigma_m < \sigma_{\max}$ follows analogously to [7].

Theorem 1 *Zero stability and order p of consistency guarantee convergence of order p.*

Since linearly-implicit peer methods with the stronger property of *optimal zero-stability* have been shown to be very efficient in [7] we require this property also for implicit methods. Optimal zero-stability means that for all step size ratios B_m has one eigenvalue equal to one (this follows from preconsistency) and all other eigenvalues are zero. For that we consider the transformed matrix $Q_m = V_1^{-1}B_m V_1$. By (8), we obtain

$$Q_m = P(I - V_0^{-1}G_m V_0 D F_0^\top)S, \tag{10}$$

where P is the Pascal matrix defined by $P = \left(\binom{j-1}{i-1}\right)_{i,j=1,2,\ldots,s} = V_1^{-1}V_0$. We require $Q_m - e_1 e_1^\top$ to be strictly upper triangular. Introducing $\mathrm{tril}(\cdot)$ as the lower triangular part of a matrix including the diagonal, i.e.

$$\mathrm{tril}(X) := \sum_{j=1}^{s}\sum_{i=j}^{s} e_i^\top X e_j e_i e_j^\top,$$

this condition can be written in the form

$$\mathrm{tril}(Q_m - e_1 e_1^\top) = 0. \tag{11}$$

Obviously, the condition (11) is not affected by the diagonal matrix S which can be omitted. Now, with (10) the condition (11) can be written as a linear system for the matrix G_m in the form

$$\mathrm{tril}(V_1^{-1}G_m V_0 D F_0^\top) = \mathrm{tril}(P) - e_1 e_1^\top = I - e_1 e_1^\top. \tag{12}$$

Since the first column on both sides of (12) is zero the condition represents effectively only $s(s-1)/2$ constraints. The remaining degrees of freedom are used in the following sections to construct methods of higher order of convergence $p = s$.

Applying the peer methods (2) with constant step size h to the test equation $y' = \lambda y$ leads to a recursion $Y_m = M(z)Y_{m-1}$ with the stability matrix

$$M(z) = (I - zG)^{-1}B, \tag{13}$$

where $z = h\lambda$. A-stability and A(α)-stability can now be defined using the set

$$\{z : \rho(M(z)) < 1 : z \in \mathbb{C}\}$$

as stability domain [7]. Note that $\mathrm{diag}(G) > 0$ implies $\lim_{z\to\infty} M(z) = 0$, i.e. A($\alpha$)-stable methods are also L(α)-stable.

3 Construction of optimally zero-stable methods of order $p = s$

3.1 Construction of multi-implicit methods

In order to obtain optimally zero-stable methods of the maximum order $p = s$ we use all degrees of freedom in the method by using a lower triangular matrix G_m with a general diagonal. This is appropriate from a computational point of view in the case when the stage equations are solved by iterative methods. We start with the representation (8), giving order of consistency $p = s - 1$. Since optimal zero-stability (12) implies only $s(s-1)/2$ conditions for the $s(s+1)/2$ coefficients g_{ij} of the matrix G_m we use the remaining s parameters to obtain order $p = s$ of consistency. The additional condition (5) for z^s reads

$$c^s = \sigma_m^{-s} B_m (c - \mathbf{1})^s + s G_m c^{s-1}, \tag{14}$$

where $\mathbf{1} = (1, \ldots, 1)^\top$. Together with (12) this gives a complete set of $s(s+1)/2$ linear equations for the elements of G_m. Theoretically, this system can be singular for special values of c_i. However, in our numerical search where we considered $0 \le c_i \le 1$ this did not occur.

The construction is summarized in the following theorem.

Theorem 2 *Let the matrix B_m be defined by (8), where the coefficients of the lower triangular matrix G_m are the solutions of (12) and (14). Then the peer method is optimally zero-stable and has order of consistency $p = s$ for variable step sizes. Hence, it is convergent of order $p = s$ for arbitrary step size sequences.*

Unfortunately, (12) and (14) imply that G_m depends on σ_m and has to be recomputed after step size changes during the integration process. In order to avoid this computation, especially for methods with many stages, we also consider methods with a frozen coefficient G, independent of m. Practical advantages of this choice will be seen in the numerical tests. Of course, in this case order of consistency $p = s$ is achieved for constant step sizes only.

Theorem 3 *Let the matrix B_m be defined by (8), where the coefficients of the constant lower triangular matrix G are the solutions of (12) and (14) for $\sigma_m = 1$. Then the peer method is optimally zero-stable and is convergent of order $p = s - 1$ for arbitrary step size sequences and of order $p = s$ for constant step sizes.*

If the step sizes are not varying too strongly, we can expect a better performance of these methods compared to methods of order $p = s - 1$.

3.2 Construction of superconvergent singly-implicit methods

In *singly-implicit methods* the elements in the diagonal of the matrix G are all equal to γ. We also use a constant matrix $G_m = G$. This choice has the advantage that the coefficient matrix $(I - h\gamma T)$ with $T \approx f_y$ is the same for all the implicit stages. Hence, some computational work can be saved if a direct solver is used for the linear systems or if preconditioning is used in iterative solvers.

The second advantage is that the derivation of the methods simplifies considerably as the matrices G and B depend only linearly on γ. This can be seen immediately by substituting $G = G_0 + \gamma I$ into (8). For constant step sizes this yields $B = B_0 + \gamma B_1$ with

$$B_0 = (V_0 - G_0 V_0 D F_0^\top) V_1^{-1} \quad \text{and} \quad B_1 = -V_0 D F_0^\top V_1^{-1}.$$

Also, the condition (12) for zero-stability simplifies since it is independent of γ due to

$$\begin{aligned} \operatorname{tril}(V_1^{-1} G V_0 D F_0^\top) &= \operatorname{tril}(V_1^{-1} G_0 V_0 D F_0^\top + \gamma P D F_0^\top) \\ &= \operatorname{tril}(V_1^{-1} G_0 V_0 D F_0^\top) = I - e_1 e_1^\top. \end{aligned}$$

Hence, the matrices B_0, B_1 and G_0 are uniquely determined by the nodes (c_i). In the second step γ has to be chosen in a certain way, which is discussed now.

Unfortunately, singly-implicit methods with s stages do not have enough free parameters to satisfy the consistency conditions (6) up to order s even for constant step sizes. However, if the residual in the order condition (6) has a certain structure, we can still obtain methods which converge with order $p = s$. This concept is well-known and named *quasi-consistency* [6, 11], *superconvergence* [13] or *effective order* [1]. In [7], superconvergent linearly-implicit methods with Chebyshev nodes have been constructed. Here we generalize the construction to implicit methods and arbitrary nodes. The principal idea is to determine a constant vector $E \in \mathbb{R}^s$ with

$$Y_m = y(t_m + ch) - E h^s y^{(s)}(t_m) + \mathcal{O}(h^{s+1}). \tag{15}$$

Substituting (15) into (3) leads to the modified order condition

$$\exp(cz) - E z^s = B\left(\exp((c-1)z) - E z^s\right) + zG \exp(cz) + \mathcal{O}(z^{s+1}). \tag{16}$$

The modification with E has no influence on the lower order terms, but only on the z^s term which is now

$$\frac{1}{s!} c^s - E = B\left(\frac{1}{s!}(c-1)^s - E\right) + \frac{1}{(s-1)!} G c^{s-1}. \tag{17}$$

So, E must satisfy the rank-deficient linear system

$$(I - B_0 - \gamma B_1) E = r_0 + \gamma r_1, \tag{18}$$

with

$$r_0 = \frac{1}{s!} c^s - \frac{1}{(s-1)!} G_0 c^{s-1} - \frac{1}{s!} B_0 (c-1)^s, \tag{19}$$

$$r_1 = -\frac{1}{(s-1)!}c^{s-1} - \frac{1}{s!}B_1(c-1)^s. \tag{20}$$

Of course, (18) has a solution E if and only if the right hand side $r_0 + \gamma r_1$ lies in the image of $(I - B_0 - \gamma B_1)$. This finally leads to a polynomial condition for γ.

Theorem 4 *A singly-implicit peer method* (3), (4) *with* $c_i \neq c_j$ *for* $i \neq j$ *and* $c_s = 1$ *that is consistent of order* $s-1$ *and satisfies* (11) *is convergent of order* s *for constant step sizes if and only if* γ *is a root of the polynomial*

$$p(\gamma) = \det(I - B_0 - \gamma B_1 + (r_0 + \gamma r_1)e_s^\top). \tag{21}$$

Proof Multiplying (18) from the left by V_1^{-1} yields the system

$$V_1^{-1}(I - B)V_1 V_1^{-1} E = V_1^{-1}(r_0 + \gamma r_1). \tag{22}$$

Due to preconsistency the first column of $V_1^{-1}(I - B)V_1$ vanishes. Hence, we may move the last column $V_1^{-1}(r_0 + \gamma r_1)$ of the augmented system matrix to this place and consider the square matrix

$$M := V_1^{-1}(r_0 + \gamma r_1)e_1^\top + V_1^{-1}(I - B)V_1$$

instead. Now, (22) has a solution if and only if $V_1^{-1}(r_0 + \gamma r_1) \in \text{image}(V_1^{-1}(I - B)V_1)$. This is equivalent to M being singular since $\text{rank}(V_1^{-1}(I - B)V_1) = s - 1$ by (11), and we arrive at

$$0 = \det(M) = \det((r_0 + \gamma r_1)e_s^\top + I - B_0 - \gamma B_1) = p(\gamma).$$

Here, the identity $e_1^\top V_1^{-1} = e_s^\top$ due to $c_s = 1$ has been used. □

The condition $p(\gamma) = \det(M_0 + \gamma M_1) = 0$ with (21) corresponds to a generalized eigenvalue problem with the matrices

$$M_0 = r_0 e_s^\top + I - B_0,$$
$$M_1 = r_1 e_s^\top - B_1.$$

Since M_1 is always nonsingular we have

$$p(\gamma) = \det(M_0 + \gamma M_1) = \det(-M_0 M_1^{-1} - \gamma I)\det(-M_1) \tag{23}$$

and a method satisfying the assumptions of Theorem 4 is convergent of order s if and only if γ is an eigenvalue of the matrix $-M_0 M_1^{-1}$. Of course, only real positive eigenvalues are of practical interest.

Table 1 Multi-implicit methods of order $p = s - 1$ with constant G

	$s = 3$ s3	$s = 4$ s4	$s = 5$ s5
c_1	0.2965111264167650	0.1541463935325966	0.1899099193591592
c_2	0.6591161332612843	0.4910074678586249	0.3939885651937762
c_3	1.0000000000000000	0.7436397609359440	0.6590663408302807
c_4		1.0000000000000000	0.8872164547257527
c_5			1.0000000000000000
g_{11}	0.1683093491913489	0.0874788583307741	0.0786811387072333
g_{21}	0.3628778211882157	0.2831819427066078	0.1977990264420529
g_{31}	0.3787524476457439	0.3078491242818127	0.1911249255439913
g_{41}		0.3229398435452924	0.1795911264673902
g_{51}			0.1755057541315561
g_{22}	0.1680365348476524	0.1411579899501929	0.0849607580997951
g_{32}	0.3189836517418485	0.2371881675120290	0.2463905827322347
g_{42}		0.2358273071856336	0.2806687099884024
g_{52}			0.2847696294285085
g_{33}	0.1740621233869913	0.1319349339402774	0.1103220519021229
g_{43}		0.2402981159278471	0.2026225925156643
g_{53}			0.2330254931701668
g_{44}		0.1342671981394014	0.1131052451023614
g_{54}			0.1019794066232285
g_{55}			0.0934909359946043
α	86.3°	82.0°	73.7°
err	0.16	0.20	0.19

4 Special methods and implementation issues

In the construction of the different types of methods described in Sect. 3 only the coefficients of the matrices B and G are fixed. The choice of the off-step nodes c_i is still free. To find good numerical schemes of the form (3), we perform a random walk search by varying the nodes c_i in the interval $[0, 1]$ in order to obtain large angles α of $L(\alpha)$-stability and a small norm of the $\mathcal{O}(h^{p+1})$ error term in (5) (for $\sigma_m = 1$) which we denote by err

$$\text{err} = \left\| \frac{1}{(p+1)!} c^{p+1} - \frac{1}{(p+1)!} B(c-1)^{p+1} - \frac{1}{p!} G c^p \right\|_2 .$$

We present three types of methods:

Table 2 Multi-implicit methods of order $p = s$

	$s = 3$ s3-sigma	$s = 4$ s4-sigma	$s = 5$ s5-sigma
c_1	0.3652686026916057	0.1184401720706515	0.1599044788394790
c_2	0.6887542583756895	0.3837335049954883	0.3886810267030429
c_3	1.0000000000000000	0.6844465289234397	0.5836944109189660
c_4		1.0000000000000000	0.8256259438802006
c_5			1.0000000000000000
α	85.4°	82.1°	67.9°
err	0.15	0.18	0.17

Matrix $G(\sigma)$ of s3-sigma:

$$g_{11} = \frac{0.1217562008972019\sigma^2 + 0.3153257129775683\sigma + 0.1802850861272289}{\sigma^2 + 1.726541567788656\sigma + 0.4935685268285777}$$

$$g_{21} = \frac{0.3000456289599450\sigma^3 + 0.7927752380513838\sigma^2 + 0.6240378735073610\sigma + 0.1556348476255093}{\sigma^3 + 2.324869601505632\sigma^2 + 1.526606748214190\sigma + 0.2953158861619276}$$

$$g_{31} = \frac{0.3179289434446160\sigma^3 + 0.8248259206820989\sigma^2 + 0.6348921595899917\sigma + 0.1562144929255245}{\sigma^3 + 2.324869601505632\sigma^2 + 1.526606748214190\sigma + 0.2953158861619276}$$

$$g_{22} = \frac{0.1451962276213406\sigma + 0.09677526815055233}{\sigma + 0.5983280337169764}$$

$$g_{32} = \frac{0.2808957982721961\sigma + 0.1874938170231784}{\sigma + 0.5983280337169764}$$

$$g_{33} = 0.1576628564887841$$

1. *Multi-implicit methods with the matrix G being independent of σ_m*
   The methods are of order $p = s - 1$ for general step sizes and of order $p = s$ for constant ones. The coefficient matrix $G_m = \mathrm{diag}(\gamma_1, \gamma_2, \ldots, \gamma_s) + G_0$ for $\sigma_m = 1$ is computed by (12) and (14) at the start. So $G_m = G$ is fixed during the integration process. The nodes, α and err of the methods used in our tests are given in Table 1.
2. *Multi-implicit methods with matrix G depending on σ_m*
   These methods have order of consistency $p = s$ also for variable step sizes. The coefficient matrix $G_m = \mathrm{diag}(\gamma_1, \gamma_2, \ldots, \gamma_s) + G_0$ for every σ_m is computed by (12) and (14). So G_m changes during the integration process and has to be recomputed with the actual step size ratio σ_m. The nodes, α and err of the methods used in our tests are given in Table 2. For $s = 3$ the table shows also $G(\sigma_m)$.
3. *Superconvergent singly-implicit methods*
   These methods are of order $p = s - 1$ for general step sizes and of order of convergence $p = s$ for constant ones. The coefficient matrix $G_m = \gamma I + G_0$ for $\sigma_m = 1$ is computed by (12) and (23). The nodes, α and err of the methods used in our tests are given in Table 3.

For all types of methods the matrix B_m is defined by (8).

Table 3 Superconvergent singly-implicit methods of order $p = s$

	$s = 3$ s3-single	$s = 4$ s4-single	$s = 5$ s5-single
c_1	0.4385371847140350	0.1661225026730741	0.2068377401453823
c_2	0.8743710492192502	0.4145497896735533	0.3951241118982431
c_3	1.0000000000000000	0.7042604619720084	0.6199266734460809
c_4		1.0000000000000000	0.8406000177315648
c_5			1.0000000000000000
g_{11}	0.1869928069686800	0.1205215848722439	0.0947726533677875
g_{21}	0.4358338645052150	0.2484272870004789	0.1882863717528655
g_{31}	0.4805420905198220	0.2243553795746857	0.1664873086357274
g_{41}		0.2112962998724116	0.1510411365150871
g_{51}			0.1531895778101022
g_{22}	0.1869928069686800	0.1205215848722439	0.0947726533677875
g_{32}	0.0809207247661426	0.3137825797242480	0.2466016246649778
g_{42}		0.3138914292536178	0.2590889022811201
g_{52}			0.2234013037887930
g_{33}	0.1869928069686800	0.1205215848722439	0.0947726533677875
g_{43}		0.3086897682008952	0.2236322387899814
g_{53}			0.2999378263874648
g_{44}		0.1205215848722439	0.0947726533677875
g_{54}			0.1166335518682632
g_{55}			0.0947726533677875
α	86.1°	83.2°	75.7°
err	0.06	0.05	0.05

We now describe details of the implementation. The computation of each stage approximation $Y_{m,i}$ of the peer method requires the solution of the nonlinear system

$$Y_{m,i} - h_m g_{ii} F_{m,i} = \sum_{j=1}^{s} b_{ij} Y_{m-1,j} + h_m \sum_{j=1}^{i-1} g_{ij} F_{m,j}. \tag{24}$$

The terms on the right hand side are known and we denote them by w_i. So we have to solve the equation

$$0 = Y_{m,i} - h_m g_{ii} F_{m,i} - w_i =: g(Y_{m,i}). \tag{25}$$

Newton's method applied to (25) gives a sequence of linear systems of the form

$$\begin{aligned} (I - \delta_i T_i)\, \Delta Y_{m,i}^k &= w_i - Y_{m,i}^k + \delta_i f\big(Y_{m,i}^k\big) \\ Y_{m,i}^{k+1} &= Y_{m,i}^k + \Delta Y_{m,i}^k, \quad k = 0, 1, 2, \ldots, \end{aligned} \tag{26}$$

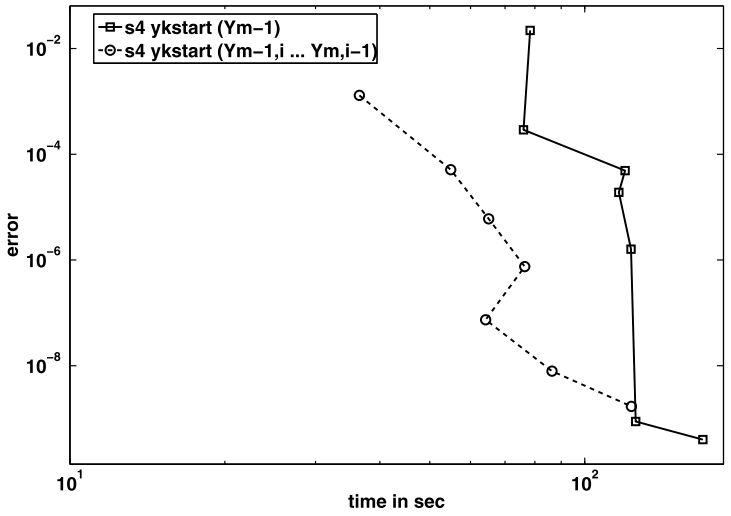

Fig. 1 Comparison of two initial guess strategies

where $T_i = \partial f(t_{m,i}, Y^k_{m,i})/\partial y$ and $\delta_i = h_m g_{ii}$. The value $Y^k_{m,i}$ is accepted as $Y_{m,i}$ when

$$\max_{j=1,2,\ldots,n} \frac{|(\Delta Y^k_{m,i})_j|}{\text{atol} + \text{rtol}|(Y_{m-1,i})_j|} \leq 0.1$$

holds. If this stopping criterion is not satisfied after 10 iterations we nevertheless set $Y_{m,i} = Y^{10}_{m,i}$ and leave it for the step size selection to decide whether this value is accurate enough.

The linear systems in (26) are solved iteratively by the Krylov method FOM with the maximal dimension of 20 for the Krylov space. The Krylov solution is accepted if the residual in (26) satisfies res $\leq$ ktol $\cdot$ atol. Here, atol is the absolute tolerance for the step size control of the integration method. We use ktol $= 0.1$ for peer-methods with 3 stages and ktol $= 0.01$ for peer-methods with 4 and 5 stages.

A crucial point is the computation of the initial guess $Y^0_{m,i}$ for Newton's method. We observe the best results in our tests when the initial guess is computed by an interpolation polynomial based on the s most recent stage values of the peer method. In stage i this means that $Y^0_{m,i}$ is computed by the $s-1$-degree polynomial fitted to the subgrid

$$\{t_{m-1} + h_{m-1}c_i, \ldots, t_{m-1} + h_{m-1}c_s, t_m + h_m c_1, \ldots, t_m + h_m c_{i-1}\}$$

and with the use of the stage vectors $Y_{m-1,i}, \ldots, Y_{m-1,s}, Y_{m,1}, \ldots, Y_{m,i-1}$. With this initial guess the methods perform far better than with the approximation $Y^0_{m,i}$ computed by the old stage values Y_{m-1} only. This can be seen in Fig. 1 where both strategies. are compared for method $s4$ and problem Nilidi (cf. Sect. 5) of dimension 40000.

The starting values $Y_{0,i}$ for the first integration step are computed with ROWMAP. The step size control is performed in the standard way, i.e. the new step size is computed by

$$h_{\text{new}} = h_m \min\big(2, \max(0.2, 0.8 \cdot \text{est}^{\frac{-1}{q}})\big), \tag{27}$$

where

$$\text{est} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(\frac{p_i(t_{m+1,s}) - (Y_{m+1,s})_i}{\text{atol} + \text{rtol}|(Y_{m,s})_i|}\right)^2}. \tag{28}$$

The order is $q = s - 1$ for the methods of types 1 and 3 and $q = s$ for the methods of type 2. The error estimate (28) uses the vector interpolation polynomial $p(t) = [p_1(t), p_2(t), \ldots, p_n(t)]^\top$ based on the points $(t_{m+1,1}, Y_{m+1,1}), \ldots, (t_{m+1,s-1}, Y_{m+1,s-1})$ for methods of types 1 and 3 and the points $(t_{m+1}, Y_{m,s}), (t_{m+1,1}, Y_{m+1,1}), \ldots, (t_{m+1,s-1}, Y_{m+1,s-1})$ for type 2 methods.

We have implemented the peer methods in MATLAB.

5 Numerical tests

The implicit peer methods are compared with the MATLAB-codes ROWMAP (version of May 2009, http://numerik.mathematik.uni-halle.de/forschung/software/) and EXP4 (version of August 1998). ROWMAP [12] contains various ROW-methods and uses a special multiple Arnoldi process for the solution of the linear systems. We used the method GRK4T [5] (RM-GRK4T in the figures). EXP4 of Hochbruck, Lubich and Selhofer [3] is an exponential W-method with Krylov approximation for

$$\varphi_1(h\gamma A)v, \qquad \varphi_1(z) = (e^z - 1)/z, \qquad A = f_y(t_m, u_m).$$

In our tests we use difference approximations for products Av. This may be a disadvantage for EXP4, where an exact Jacobian is recommended.

We present results for the following test problems:

Bruss2D: The 2-dimensional Brusselator [3] given by

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

with Neumann boundary conditions. The diffusion constant is $\alpha = 0.02$ and the initial values are determined by

$$u(0, x, y) = 0.5 + y, \qquad v(0, x, y) = 1 + 5x.$$

Diffu2: The 2-dimensional diffusion equation [12]

$$u_t = \Delta u + f(t, x, y), \quad \Omega = [0, 1]^2, \quad t \in [0, 1].$$

Here the initial and the Dirichlet boundary values are taken from the exact solution

$$u(t, x, y) = \sin(\pi x)\sin(\pi y)(1 + 4xy\sin t)$$

and f is determined appropriately.

Nilidi: The nonlinear diffusion equation [12]

$$u_t = \mathrm{e}^u(u_{xx} + u_{yy}) + u(18\mathrm{e}^u - 1), \quad (x, y) \in \Omega = [0, \pi/3]^2, \quad t \in [0, 1]. \tag{29}$$

The initial and the Dirichlet boundary values are taken from the exact solution:

$$u(t, x, y) = \mathrm{e}^{-t}\sin(3x)\sin(3y).$$

Radiation: This problem is a system of two strongly nonlinear diffusion equations with a highly stiff reaction term. The dependent variables $E(t, x, y)$ (radiation energy) and $T(t, x, y)$ (material temperature) are defined on the unit square for $t > 0$, by means of

$$\begin{aligned} E_t &= \nabla \cdot (D_1 \nabla E) + \sigma(T^4 - E) \\ T_t &= \nabla \cdot (D_2 \nabla T) - \sigma(T^4 - E) \end{aligned} \tag{30}$$

with

$$\sigma = \frac{Z^3}{T^3}, \qquad D_1 = \frac{1}{3\sigma + \frac{\|\nabla E\|_2}{E}}, \qquad D_2 = kT^{\frac{5}{2}}$$

where

$$Z(x, y) = \begin{cases} Z_0 & \text{if } |x - \frac{1}{2}| \le \frac{1}{6} \text{ and } |y - \frac{1}{2}| \le \frac{1}{6} \\ 1 & \text{otherwise} \end{cases}$$

with $k = 5 \cdot 10^{-5}$ and $Z_0 = 1$ or $Z_0 = 5$. For $Z_0 = 5$ the nonlinear source term in (30) has a jump which makes the problem computationally more difficult. The initial values and details of the discretization can be found in [4].

For all problems we use central differences for semi-discretization and a grid resolution of $m = 100$ points in each space dimension ($m = 200$ for Nilidi), the overall dimension is denoted by n. All problems are solved for seven tolerances $tol = 10^{-2}, 10^{-3}, \ldots, 10^{-8}$ with rtol = atol = tol. The marks in Figs. 2–6 show the computing time (in seconds, logarithmic scale) plotted against the logarithm of the error at the endpoint in the norm

$$\text{error} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(\frac{u_i - \text{uex}_i}{1 + |\text{uex}_i|}\right)^2}. \tag{31}$$

The reference solutions uex are computed with high accuracy by standard integrators. The new methods solve all problems reliably. For crude tolerances the 3-stage methods are the best, for more strict tolerances the higher order methods are more

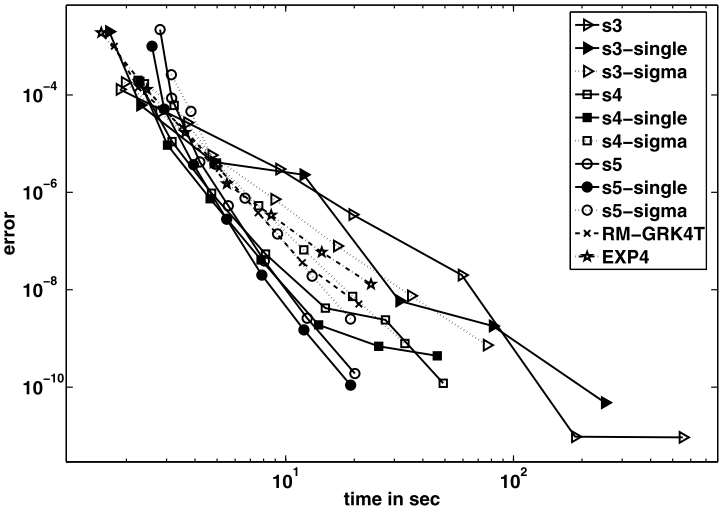

Fig. 2 Results for Bruss2D, $n = 20000$

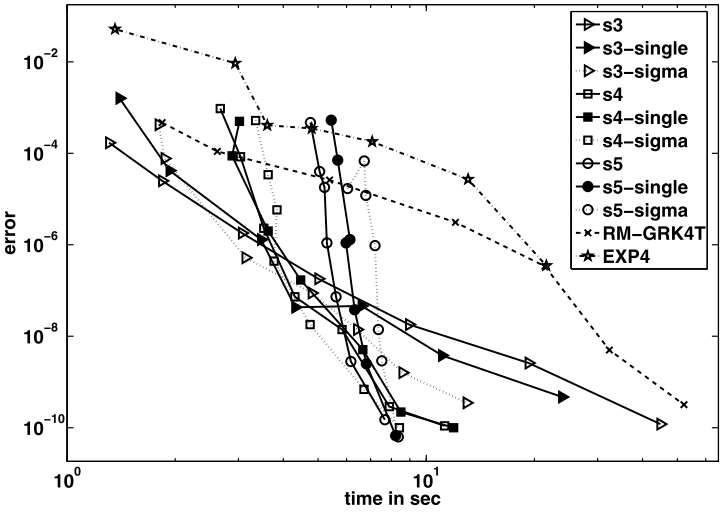

Fig. 3 Results for Diffu2, $n = 10000$

efficient. Among the 3-stage peer methods s3-sigma of order of consistency 3 is the best, for 4 and 5 stages the methods are comparable with advantages for the singly-implicit methods. This means, for lower accuracy we would use the method s3-sigma, for medium accuracy s4-single and for higher accuracy s5-single.

For the simple test problem Bruss2D and for Nilidi the performance of ROWMAP and EXP4 is similar to that of the peer methods, but for the other problems the implicit peer methods are clearly superior. Especially for the stiff Radiation problem with $Z_0 = 5$ and for the sharper tolerances the errors of all peer methods are at least

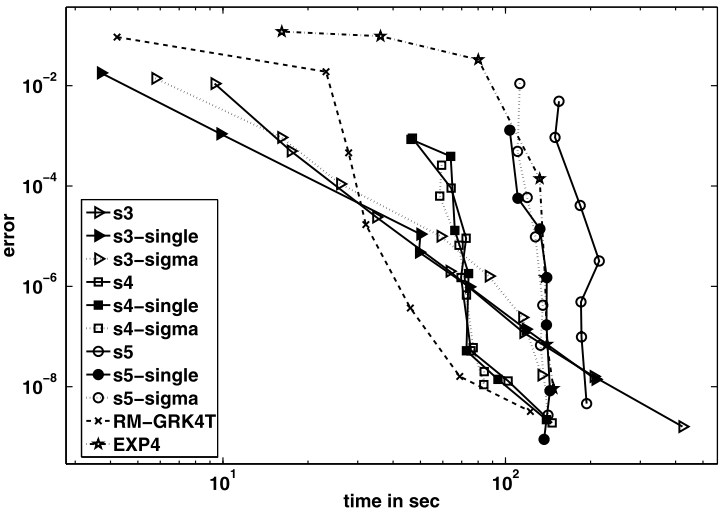

Fig. 4 Results for Nilidi, $n = 40000$

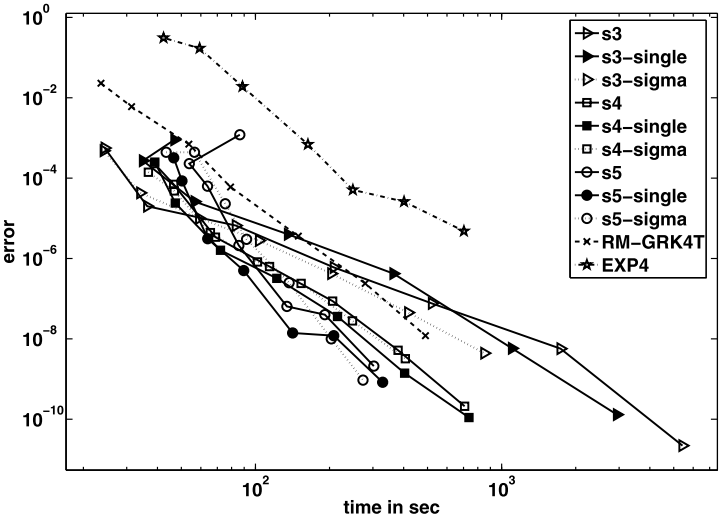

Fig. 5 Results for Radiation with $Z_0 = 1$, $n = 20000$

2 magnitudes smaller than those of the linearly-implicit methods with the same runtimes. We assume that this advantage of the peer methods can be attributed to their high stage order which prevents from order reduction.

The aim of using implicit methods is to improve the robustness of the methods compared to linearly-implicit peer methods which use exactly one Newton iteration in some sense. In further tests not shown here this improvement really could be observed for crude tolerances. For instance, for the hard Radiation problem ($Z_0 = 5$) the linearly implicit peer methods fail for tolerances 10^{-2} and 10^{-3} even with an in-

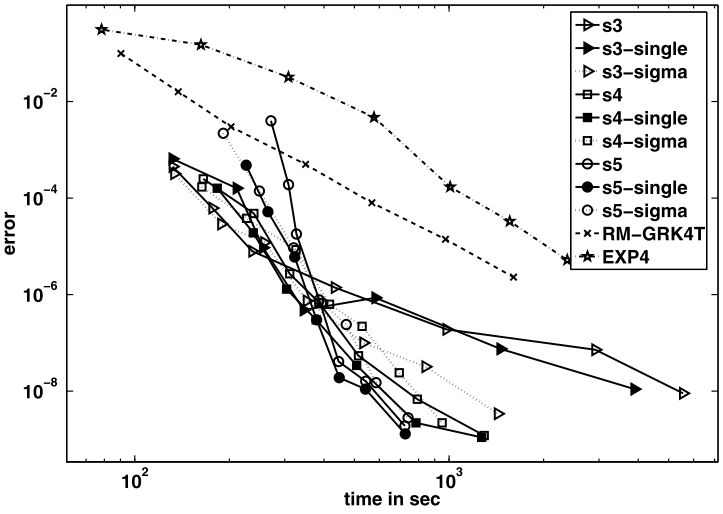

Fig. 6 Results for Radiation with $Z_0 = 5$, $n = 20000$

creased Krylov dimension of 50. For strict tolerances, however, the linearly-implicit peer methods display similar results in the number of steps and accuracy, but they are slightly faster due to their simpler structure.

The number of Newton steps depends mostly on the initial guess, if it is good then few iteration steps must be done. We think our new strategy described in Sect. 4 is applicable. By using this strategy the number of iteration steps decrease with the tolerance atol, because of the smaller step sizes.

6 Conclusions

We have constructed several s-stage optimally zero-stable implicit peer methods of three different types with $s \in \{3, 4, 5\}$. Their order of convergence is $p = s$ for variable step sizes (type 2) or $p = s - 1$ for variable step sizes and $p = s$ for constant step sizes (types 1 and 3). Methods with $s = 3, 4, 5$ stages have been implemented 'matrix-free' by using the Krylov solver FOM for the linear systems inside the Newton iteration. In numerical tests on high-dimensional MOL problems they work reliably and efficiently with an advantage over linearly-implicit methods for crude tolerances. Due to their high stage order, the implicit peer methods with $s = 4, 5$ are superior to one-step methods with Krylov techniques when high accuracy is required. The 3-stage peer methods perform well for low accuracy demands.

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