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Report No. 07 (2010)

Editors:
Professors of the Institute for Mathematics, Martin-Luther-University Halle-Wittenberg.

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Implicit peer methods for large stiff ODE systems

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22.09.2010

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's 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 MOL problems show the efficiency of the methods compared to other Krylov codes.

MSC: 65L05, 65L06
Keywords. Implicit peer methods, large stiff systems, zero stability, FOM.

1 Introduction

In [7] two of the authors introduced the class of linearly-implicit parallel peer methods for the solution of stiff initial value problems

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

$f : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n$. 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 [9] implicit parallel methods were considered, in [6] sequential linearly-implicit methods were introduced. In [8] linearly-implicit parallel peer methods were

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

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

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

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

The stage values of the right-hand side are denoted by $F_{mi} = f(t_m + h_m c_i, Y_{mi})$, $i = 1, \ldots, s$. Introducing stacked vectors

$$Y_m = \begin{pmatrix} Y_{m1} \\ Y_{m2} \\ \vdots \\ Y_{ms} \end{pmatrix}, \quad F(t_m, Y_m) = \begin{pmatrix} f(t_m + c_1 h_m, Y_{m1}) \\ f(t_m + c_2 h_m, Y_{m2}) \\ \vdots \\ f(t_m + c_s h_m, Y_{ms}) \end{pmatrix}$$

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 $h_m = \sigma_m h_{m-1}$.
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

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

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 is limited to $p = s - 1$, in general. For special nodes and constant step size methods of order of convergence $p = s$ were constructed in [6]. In this paper we will consider different choices for G_m. In the most

general case, chosing 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 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.
Zero-stability is a crucial point for peer methods as the methods have a two-step character. In Section 2 we derive the order conditions and present a construction principle that ensures zero-stability for all step size sequences. In Section 3 we will 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 Section 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 Section 5 numerical results for several MOL problems are given. We compare the MATLAB implementation of our methods with the Krylov one-step codes ROWMAP [11] and EXP4 [2].

2 Order conditions and zero stability

The order conditions for peer methods can be derived by replacing Y_{mi} and $Y_{m-1,i}$ in (3) by values of the solution $y(t)$. Then, $f(t_{mi}, y(t_{mi})) = y'(t_{mi})$ and Taylor series expansions of these quantities gives

$$\begin{aligned}
y(t_m + c_i\sigma h_{m-1}) &= \sum_{l=0}^{p} \frac{(c_i\sigma h_{m-1})^l}{l!} y^{(l)}(t_m) + \mathcal{O}(h_{m-1}^{p+1}),\\
y(t_{m-1} + c_i h_{m-1}) &= \sum_{l=0}^{p} \frac{((c_i-1)h_{m-1})^l}{l!} y^{(l)}(t_m) + \mathcal{O}(h_{m-1}^{p+1}),\\
\sigma h_{m-1} y'(t_m + c_i\sigma h_{m-1}) &= \sum_{l=1}^{p} \sigma h_{m-1} \frac{(c_i\sigma h_{m-1})^{l-1}}{(l-1)!} y^{(l)}(t_m) + \mathcal{O}(h_{m-1}^{p+1}).
\end{aligned}$$

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

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

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

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

For constant step sizes, Eq. (5) simplifies to

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

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

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

and hence

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

where the matrices are given by

$$\begin{gathered} (V_0)_{i,j} = c_i^{j-1} \ , \quad (V_1)_{i,j} = (c_i - 1)^{j-1} \ , \quad F_{i,j} = \delta_{i,j+1}, \\ S = \mathrm{diag}(1, \sigma, \sigma^2, \ldots, \sigma^{s-1}) \quad \text{and} \quad D = \mathrm{diag}(1, 2, \ldots, s). \end{gathered} \tag{9}$$

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 question theoretically. It is easily verified for special matrix families, only. Our construction of the methods in the next section will use one such family. Now, convergence follows analogously to [6].

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 shown to be very efficient in [6] we will 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 $Q_m = V_1^{-1} B_m V_1$ and 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

$$\mathrm{tril}(Q_m - e_1 e_1^\top) = 0 \ . \tag{10}$$

From the representation (8) of B_m follows

$$Q_m = P \left(I - V_0^{-1} G_m V_0 D F^\top \right) S \tag{11}$$

with the Pascal matrix $P = \left(\binom{j-1}{i-1}\right)_{i,j=1,\ldots,s}$ since $P = V_1^{-1} V_0$. Obviously, the condition (10) is not affected by the diagonal matrix S which can be omitted. Now, with (11) the condition (10) can be written as a linear system for the matrix G_m in the form

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

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 will be used in the following sections to construct methods of higher order of convergence $p = s$.

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 with a maximal order $p = s$ we will use all degrees of freedom in the method by using a lower triangular matrix G_m with 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 will use the remaining s parameters to obtain order $p = s$ of consistency. The additional condition (5) for z^s reads

$$\begin{pmatrix} c_1^s \\ \vdots \\ c_s^s \end{pmatrix} = B_m \begin{pmatrix} \left(\frac{c_1-1}{\sigma_m}\right)^s \\ \vdots \\ \left(\frac{c_s-1}{\sigma_m}\right)^s \end{pmatrix} + G_m \begin{pmatrix} sc_1^{s-1} \\ \vdots \\ sc_s^{s-1} \end{pmatrix}. \tag{13}$$

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* (13)*. 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 (13) imply that G_m will depend on σ 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. The 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* (13) *for $\sigma = 1$. 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 will 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.
A 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

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

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

$$\operatorname{tril}(V_1^{-1} G V_0 D F^\top) = \operatorname{tril}(V_1^{-1} G_0 V_0 D F^\top + \gamma P D F^\top) = \operatorname{tril}(V_1^{-1} G_0 V_0 D F^\top) \stackrel{!}{=} I - e_1 e_1^\top.$$

Hence, the matrices B_0, B_1 and G_0 are uniquely determined by the nodes (c_i). In a second step γ has to be chosen in a certain way which will be 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* [10], [5], *superconvergence* [12] or *effective order*, [1]. In [6] 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

$$Y_m = y(t_m + ch) - E h^s y^{(s)}(t_m) + \mathcal{O}(h^{s+1}). \tag{14}$$

Substituting (14) into (3) leads to the modified order condition

$$\exp(cz) - E z^s = B\left(\exp((c-1)z) - E z^s\right) + zG \exp(cz) + \mathcal{O}(z^{s+1}). \tag{15}$$

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

$$\frac{c^s}{s!} - E = B\left(\frac{(c-1)^s}{s!} - E\right) + G\frac{c^{s-1}}{(s-1)!}. \tag{16}$$

So, E must satisfy the rank-deficient linear system

$$(I - B_0 - \gamma B_1) E = r_0 + \gamma r_1, \tag{17}$$

with

$$r_0 = \frac{c^s}{s!} - G_0 \frac{c^{s-1}}{(s-1)!} - B_0 \frac{(c-1)^s}{s!}, \tag{18}$$

$$r_1 = -\frac{c^{s-1}}{(s-1)!} - B_1 \frac{(c-1)^s}{s!}. \tag{19}$$

Of course, equation (17) 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) *which is consistent of order* $s-1$ *and zero-stable is convergent of order* s *for constant step sizes if and only if* γ *is a root of the polynomial*

$$p(\gamma) = \det\Big(I - B_0 - \gamma B_1 + (r_0 + \gamma r_1)e_s^\top\Big). \tag{20}$$

Proof. Multiplying Eq. (17) from the left by V_1^{-1} yields the system

$$V_1^{-1}(I-B)V_1 V_1^{-1}E = V_1^{-1}(r_0 + \gamma r_1). \tag{21}$$

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 extended 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, (21) has a solution if and only if $V_1^{-1}(r_0+\gamma r_1) \in \mathrm{image}(V_1^{-1}(I-B)V_1)$ and this is equivalent to M being singular, i.e.

$$0 = \det(M) = \det((r_0+\gamma r_1)\mathbf{1}^\top + I - B_0 - \gamma B_1) = p(\gamma).$$

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

The condition $p(\gamma) = \det(M_0 + \gamma M_1) = 0$ with (20) corresponds to a generalized eigenvalue problem with the matrices

$$\begin{aligned} M_0 &= r_0 e_s^\top + I - B_0, \\ M_1 &= r_1 e_s^\top - B_1. \end{aligned}$$

Since M_1 is always nonsingular we have

$$p(\gamma) = \det(M_0 + \gamma M_1) = \det(-M_0 M_1^{-1} - \gamma I)\det(-M_1) \tag{22}$$

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 $-M_0M_1^{-1}$. Of course, only real positive eigenvalues are of practical interest.

4 Special methods and implementation issues

In the construction of the different types of methods described in Section 3 only the coefficients from the matrices B and G are fixed. The choice of the off-step nodes c_i is still free. Searching for good methods we have performed a random walk search varying the nodes c_i 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 $\sigma = 1$) which we denote by *err*

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

We present three types of methods:

	$s=3$	$s=4$	$s=5$
	s3	s4	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

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

1. **multi-implicit methods with the matrix G independent of σ**
   The methods are of order $p = s - 1$ for general step sizes and of order $p = s$ for constant ones. The coefficients $G_m = \mathrm{diag}(\gamma_1, \ldots, \gamma_s) + G_0$ for $\sigma = 1$ are computed from (12) and (13) 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**
   These methods have order of consistency $p = s$ also for variable step sizes. The coefficients $G_m = \mathrm{diag}(\gamma_1, \ldots, \gamma_s) + G_0$ for every σ are computed from (12) and (13). So G_m changes during the integration process and has to be recomputed with the actual step size ratio σ. The nodes, α and err of the methods used in our tests are given in Table 2.

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 coefficients $G_m = \gamma I + G_0$ for $\sigma = 1$ are computed from (12) and (22). 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).

	$s=3$	$s=4$	$s=5$
	s3-sigma	s4-sigma	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:

$$g_{11} = \frac{0.1217562008972019\sigma^2 + 0.3153257129775683\sigma + 0.1802850861272289}{\sigma^2 + 1.726541567788656\sigma + 0.4935685268285777}$$
$$g_{21} = \frac{0.3000456289599450\sigma^3 + 0.7927752380513838\sigma^2 + 0.6240378735073610\sigma + 0.1556348476255093}{\sigma^3 + 2.324869601505632\sigma^2 + 1.526606748214190\sigma + 0.2953158861619276}$$
$$g_{31} = \frac{0.3179289434446160\sigma^3 + 0.8248259206820989\sigma^2 + 0.6348921595899917\sigma + 0.1562144929255245}{\sigma^3 + 2.324869601505632\sigma^2 + 1.526606748214190\sigma + 0.2953158861619276}$$
$$g_{22} = \frac{0.1451962276213406\sigma + 0.09677526815055233}{\sigma + 0.5983280337169764}$$
$$g_{32} = \frac{0.2808957982721961\sigma + 0.1874938170231784}{\sigma + 0.5983280337169764}$$
$$g_{33} = 0.1576628564887841$$

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

We will now describe details of the implementation. The computation of each stage approximation Y_{mi} of the peer method requires the solution of the nonlinear system

$$Y_{mi} - h_m g_{ii} F_{mi} = \sum_{j=1}^{s} b_{ij} Y_{m-1,j} + h_m \sum_{j=1}^{i-1} g_{ij} F_{mj}. \tag{23}$$

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

$$0 = Y_{mi} - h_m g_{ii} F_{mi} - w_i =: g\left(Y_{mi}\right) \ . \tag{24}$$

Newton's method applied to (24) gives a sequence of linear systems of the form

$$\begin{aligned} \left(I - \delta_i T_i\right) \Delta Y_{mi}^k &= w_i - Y_{mi}^k + \delta_i f\left(Y_{mi}^k\right) \\ Y_{mi}^{k+1} &= Y_{mi}^k + \Delta Y_{mi}^k \ , \quad k = 0, 1, 2, ... \end{aligned} \tag{25}$$

where $T_i = \partial f\left(t_{mi}, Y_{mi}^k\right) / \partial y$ and $\delta_i = h_m g_{ii}$. As stopping criterion for the Newton process the condition

$$\max_{j=1,\ldots,n} \frac{\left|\Delta Y_{mi_j}^k\right|}{atol + rtol \left|Y_{m-1,i_j}\right|} \leq 0.1$$

	$s=3$	$s=4$	$s=5$
	s3-single	s4-single	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

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

was used and a maximum of 10 Newton iterations was performed.
The linear systems in (25) are solved iteratively by the Krylov-method FOM with a maximal dimension of 20 for the Krylov space. The Krylov solution is accepted if the residual in (25) satisfies $res \leq ktol \cdot atol$. Here, $atol$ is the absolute tolerance for the step size control of the integration method. We used $ktol = 0.1$ 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_{mi}^0. For peer methods with strictly increasing nodes $0 \leq c_1 < c_2 \cdots < c_s = 1$ we observed the best results in our tests when the initial guess was computed by an extrapolation of the s most recent points in time. In stage i this means that Y_{mi}^0 is computed by polynomial extrapolation from the subgrid

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

using 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 performed far better than with an approximation Y_{mi}^0 extrapolated from the old stage values Y_{m-1} only. This can be seen in Figure 1 where both strategies are compared with the method $s4$ and the problem Nilidi (cf. Section 5) of dimension 40000.
Step size control is performed in a standard way, the new step size is computed by

$$h_{new} = h_m \min\left(2, \max(0.2, 0.8 \cdot \mathrm{est}^{\frac{-1}{q}})\right) \tag{26}$$

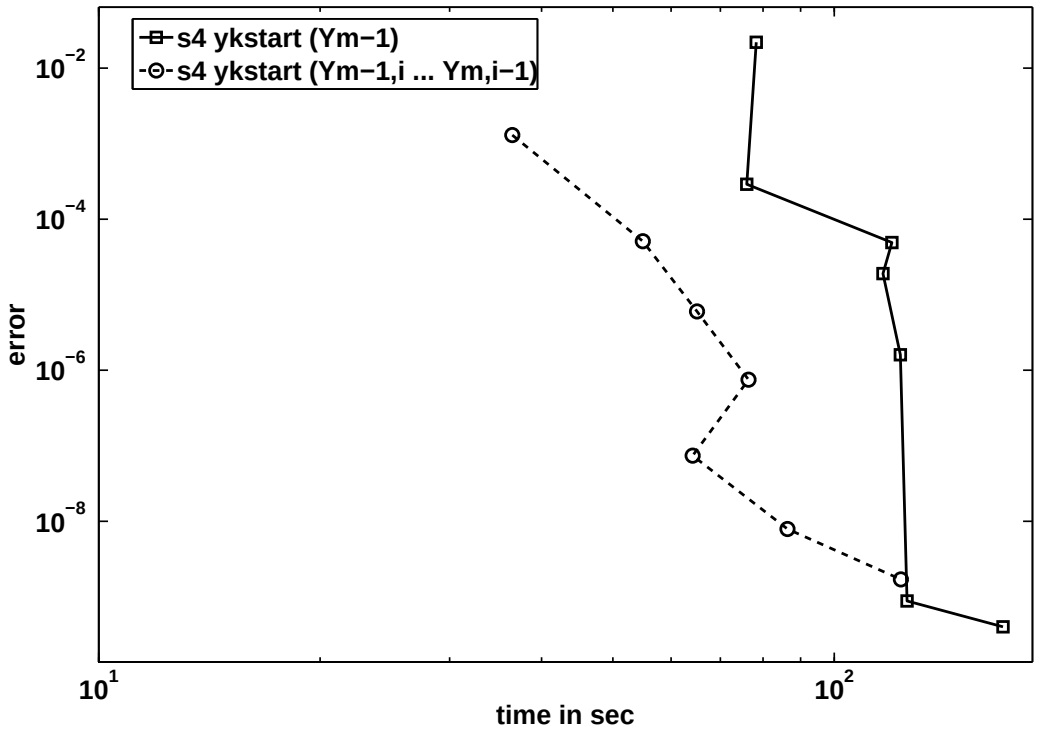

Figure 1: Comparison of two initial guess strategies

where

$$\text{est} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(\frac{p_i(t_{m+1,s}) - Y_{m+1,s_i}}{atol_i + rtol_i\,|Y_{ms_i}|}\right)^2} \tag{27}$$

The order is $q = s - 1$ for the methods of type 1 and 3 and $q = s$ for the methods of type 2. The error estimate (27) uses the interpolation polynomial $p(t)$ 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 type 1 and 3 and the points $(t_{m+1}, Y_{ms}), (t_{m+1,1}, Y_{m+1,1}), \ldots, (t_{m+1,s-1}, Y_{m+1,s-1})$ 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 [11] contains various ROW-methods and uses a special multiple Arnoldi process for the solution of the linear systems. We used as basic method GRK4T [4] (RM-GRK4T in the figures). EXP4 of Hochbruck, Lubich and Selhofer [2] is an exponential W-method with Krylov approximation for

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

In our tests we used 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 [2] 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 [11]

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

  Here f and the initial and the Dirichlet boundary values are determined by the exact solution

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

- **Nilidi:** The nonlinear diffusion equation [11]

$$u_t = \mathrm{e}^u(u_{xx} + u_{yy}) + u(18\mathrm{e}^u - 1), \quad (x,y) \in \Omega = [0,\pi/3]^2\,, \quad t \in [0,1]\,. \tag{28}$$

  Initial and 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

$$\begin{aligned} E_t &= \nabla\cdot(D_1\nabla E) + \sigma\left(T^4 - E\right) \\ T_t &= \nabla\cdot(D_2\nabla T) - \sigma\left(T^4 - E\right) \end{aligned} \tag{29}$$

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

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

  with $k = 5\cdot 10^{-5}$ and $Z_0 = 1$ or $Z_0 = 5$. For $Z_0 = 5$ the nonlinear source term in (29) has a jump which makes the problem computationally more difficult. The initial values and details of the discretization can be found in [3].

For all problems we used 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 were solved for seven tolerances $tol = 10^{-2}, \ldots, 10^{-8}$ with $rtol_i = atol_i = tol$. 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

$$\text{error} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(\frac{u_i - uex_i}{1 + |uex_i|}\right)^2}. \tag{30}$$

The reference solutions uex were computed with high accuracy by standard integrators. The new methods solved all problems reliably. For crude tolerances the 3-stage methods are best, for more strict tolerances the higher order methods are more efficient. 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 at the stiff Radiation problem with $Z_0 = 5$ for sharper tolerances the errors of all peer methods are at least 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.
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.
The aim of using implicit methods was 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 on the hard Radiation problem ($Z_0 = 5$) the linearly implicit peer methods failed for tolerances 10^{-2} and 10^{-3} even with an increased Krylov dimension of 50. For strict tolerances, however, the linearly-implicit peer methods gave similar results in the number of steps and accuracy, but they were slightly faster due to their simpler structure.

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 and $p = s$ for constant step sizes (type 1 and 3). Methods with $s = 3, 4, 5$ stages have been implemented 'matrix-free' using the Krylov solver FOM for the linear systems inside the Newton iteration. In numerical tests on high-dimensional MOL problems they worked reliably and efficiently with an advantage over linearly-implicit methods for crude tolerances. Due to their high stage order implicit peer methods are superior to one-step methods using Krylov techniques when high accuracy is required.

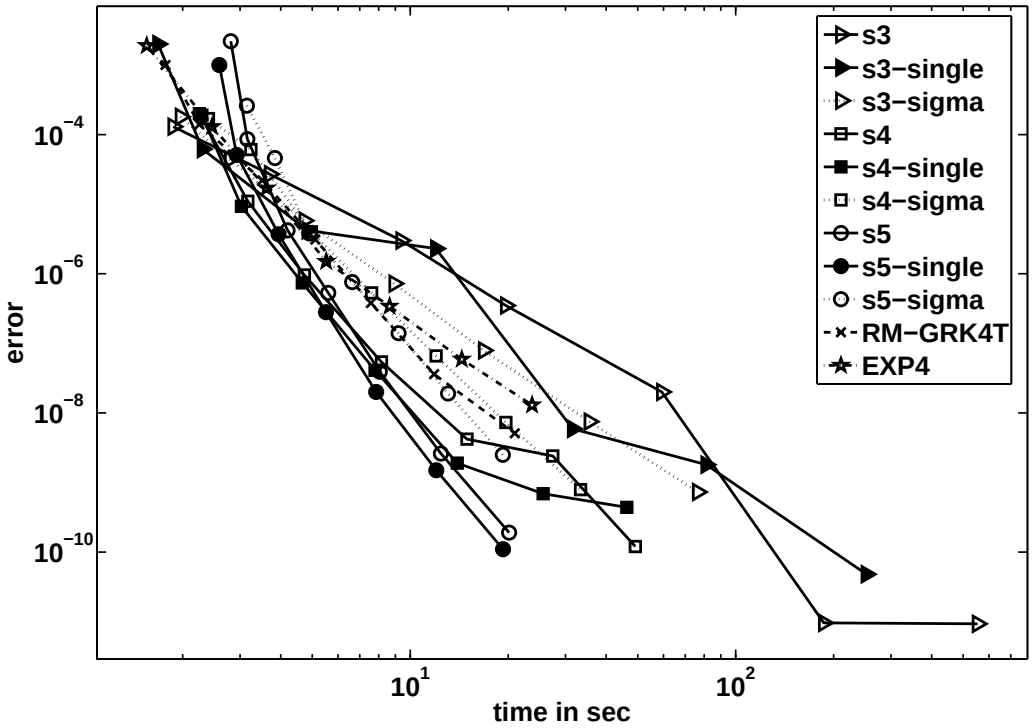

Figure 2: Results for Bruss2D, $n = 20000$

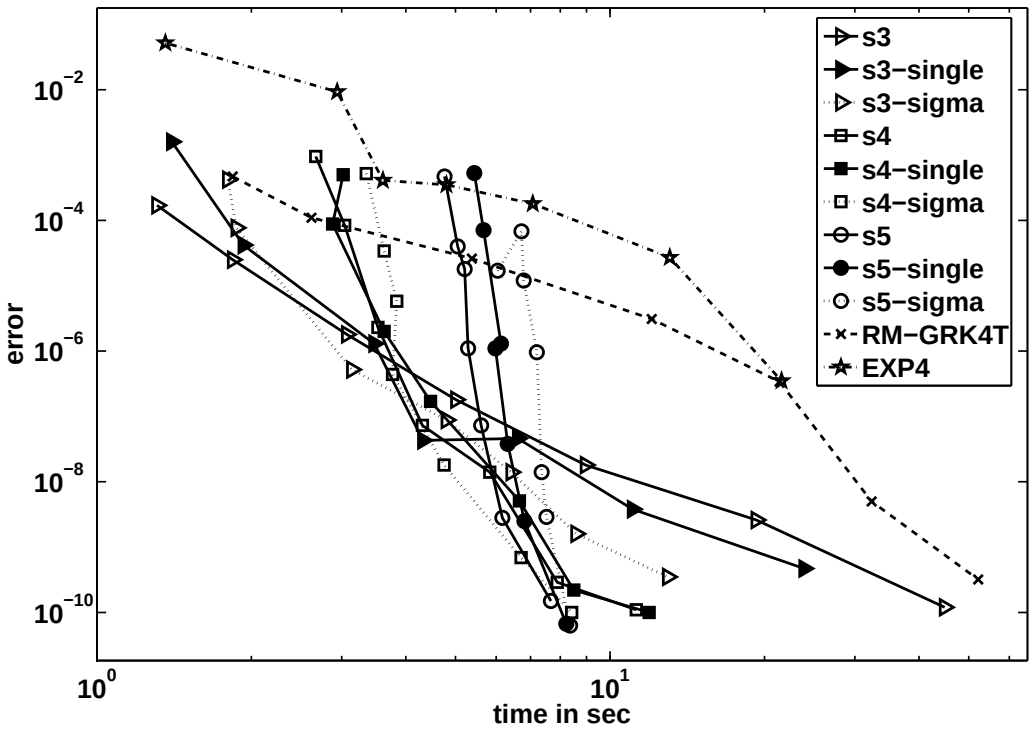

Figure 3: Results for Diffu2, $n = 10000$

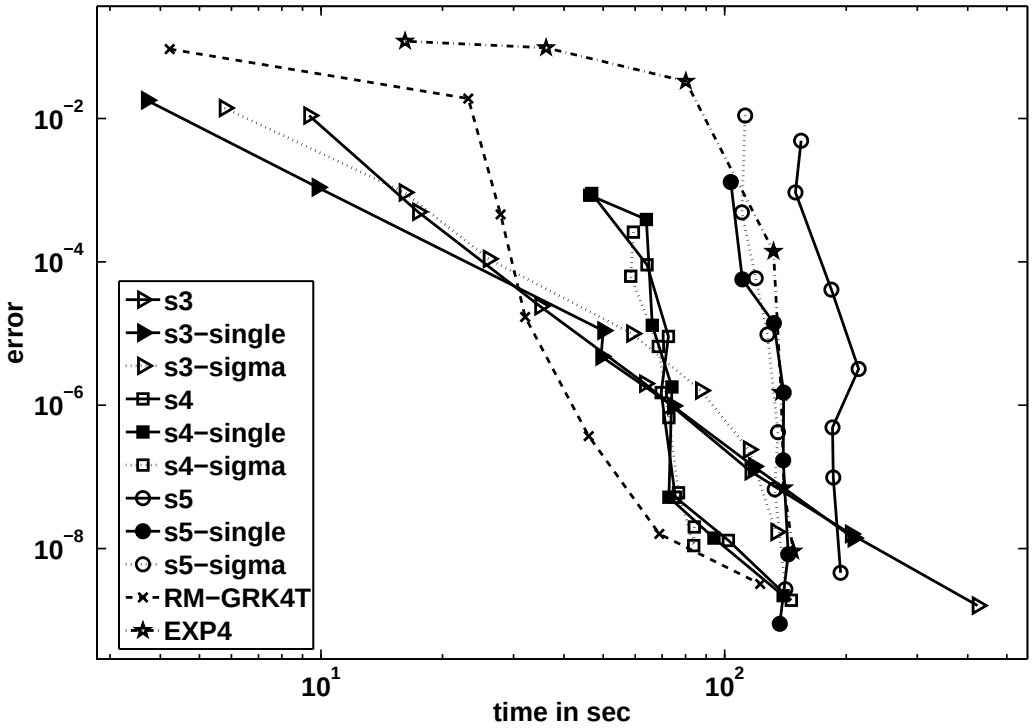

Figure 4: Results for Nilidi, $n = 40000$

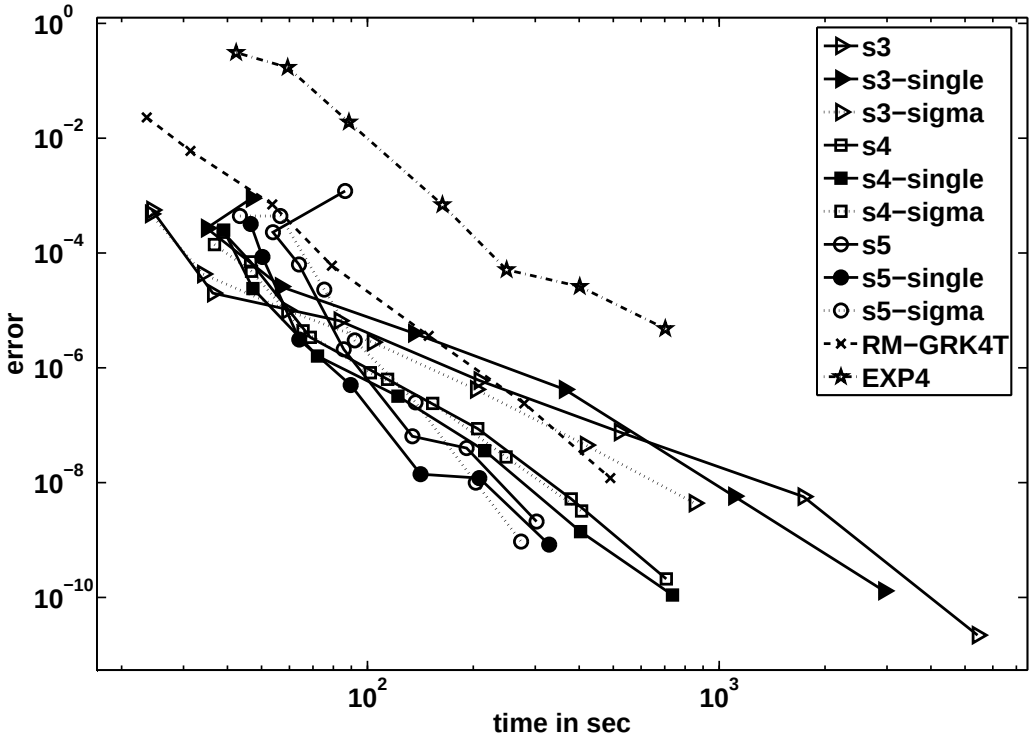

Figure 5: Results for Radiation with $Z_0 = 1$, $n = 20000$

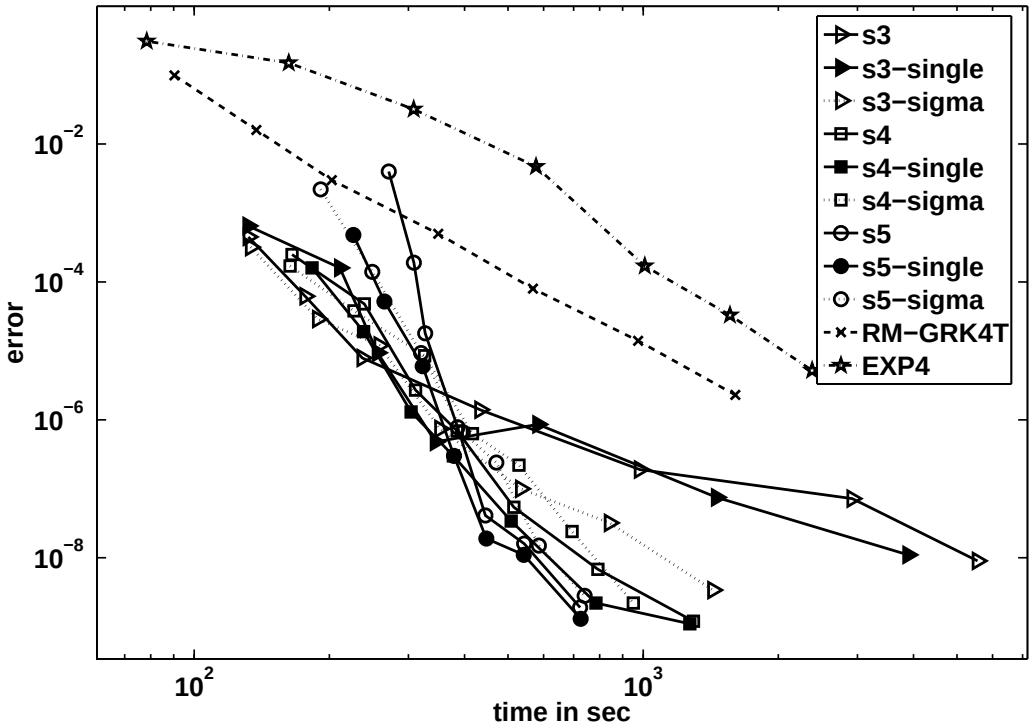

Figure 6: Results for Radiation with $Z_0 = 5$, $n = 20000$

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