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Report No. 03 (2016)

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# Explicit peer methods with variable nodes

Rüdiger Weiner\*     Helmut Podhaisky†     Marcel Klinge‡

## Abstract

In this paper, explicit peer methods are studied in which some of the stage values are copies of stage values from previous steps. Technically, this leads to sparse coefficient matrices and it can be regarded as being a generalization of the first-same-as-last principle known from Runge–Kutta methods. Function evaluations can be saved, but the variable step size implementation is more complex as the nodes depend on the history of previous step size changes.

Explicit peer methods up to order  $p = 6$  are constructed using constraint numerical optimization. The new methods are compared to standard methods (Dormand/Prince 5(4) and PECE as implemented in Matlab’s ode45 and ode113) in numerical experiments.

**Keywords.** explicit peer methods, variable nodes, step size control

**MSC:** 65L05

## 1 Introduction

Explicit peer methods for the solution of non-stiff initial value problems

$$y' = f(t, y), \quad y(t_0) = y_0, \quad f : [t_0, t_e] \times \mathbb{R}^n \rightarrow \mathbb{R}^n \quad (1)$$

have been introduced in [9]. In numerical tests [10] they have been shown to be very efficient and reliable methods. These methods have been successfully applied in global error control, for instance in [6]. Methods of higher order for constant step sizes have been constructed in [2]. Furthermore, special methods with favourable strong stability preserving (SSP) properties have been constructed in [5].

Explicit peer methods with  $s$  stages compute in each step  $s$  approximations to the exact solution. All these stage values have the same order, the stage order of explicit peer methods is therefore equal to their order of consistency. For the computation of the  $s$  stage values usually  $s$  function calls are necessary. In [8] methods with the FSAL-property (*first same as last*) were discussed. Here the first stage value of the new step is equal to the last of the preceding step. This allows to reduce the number of function calls to  $s - 1$ . When considering

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the SSP properties of explicit peer methods with constant step size in [5] it was observed that the effective SSP coefficient is maximal for methods of very special structure. In these methods the FSAL-property is generalized by copying more than one stage value from the last step. The number of function calls is reduced by the number of these copied stages.

In this paper we generalize this principle to variable step sizes. We derive explicit peer methods with  $s$  stages of order  $p = s$  which require only  $s_e < s$  evaluations of the right-hand side in each step. The outline of the paper is as follows:

In Section 2 we recall the definition of explicit peer methods and summarize known results about order and stability. We generalize the copying of stage values from the preceding step to save function calls to the case of variable step sizes. We derive order conditions and prove that under some natural conditions numerical approximations exist for all step size sequences.

In Section 3 we construct specific methods by numerically optimizing stability and accuracy properties. The optimization is done with respect to stability and superconvergence. Numerical tests on standard non-stiff problems for some of the methods obtained are given in Section 4. Finally, we draw some conclusions and give an outlook for future work.

## 2 Explicit peer methods with variable nodes

Explicit peer methods for problem (1) as introduced in [9] read

$$Y_{m,i} = \sum_{j=1}^s b_{ij} Y_{m-1,j} + h_m \sum_{j=1}^s a_{ij} f(t_{m-1,j}, Y_{m-1,j}) + h_m \sum_{j=1}^{i-1} r_{ij} f(t_{m,j}, Y_{m,j}), \quad i = 1, \dots, s. \quad (2)$$

Here  $b_{i,j}$ ,  $a_{i,j}$ ,  $c_i$  and  $r_{ij}$ ,  $i, j = 1, \dots, s$  are the parameters of the method. At each step  $s$  stage values  $Y_{m,i}$ ,  $i = 1, \dots, s$  are computed approximating the exact solution  $y(t_{m,i})$  where  $t_{m,i} = t_m + c_i h_m$ . The nodes  $c_i$  are assumed to be pairwise distinct, we always assume  $c_s = 1$ . The coefficients of the method (2) depend, in general, on the step size ratio  $\sigma_m = h_m/h_{m-1}$ . Defining matrices  $B_m = (b_{i,j})_{i,j=1,\dots,s}$ ,  $A_m = (a_{i,j})$ ,  $R_m = (r_{i,j})$  and vectors  $Y_m = (Y_{m,i})_{i=1}^s \in \mathbb{R}^{sn}$  and  $F_m = (f(t_{m,i}, Y_{m,i}))_{i=1}^s$  leads to the compact form

$$Y_m = (B_m \otimes I) Y_{m-1} + h_m (A_m \otimes I) F_{m-1} + h_m (R_m \otimes I) F_m,$$

where  $R_m$  is strictly lower triangular. Like multistep methods peer methods also need  $s$  starting values  $Y_{0,i}$ . We collect here some results from [9].

Conditions for the order of consistency of explicit peer methods can be derived by considering the residuals  $\Delta_{m,i}$  obtained when the exact solution is put into the method

$$\Delta_{m,i} := y(t_{m,i}) - \sum_{j=1}^s b_{ij} y(t_{m-1,j}) - h_m \sum_{j=1}^s a_{ij} y'(t_{m-1,j}) - h_m \sum_{j=1}^{i-1} r_{ij} y'(t_{m,j}), \quad i = 1, \dots, s.$$

**Definition 1** *The peer method (2) is consistent of order  $p$  if*

$$\Delta_{m,i} = \mathcal{O}(h_m^{p+1}), \quad i = 1, \dots, s. \quad \square$$

In contrast to explicit Runge-Kutta methods, all stage values of peer methods are approximations of order  $p$  to the solution  $y(t_m + c_i h_m)$ , i.e., the stage order is equal to the order. This makes these methods advantageous for instance for MOL problems when space and time step sizes are reduced simultaneously, cf. [5]. By Taylor series expansion follows, cf. [9]

**Theorem 1** *A peer method (2) has the consistency order  $p$  iff*

$$AB(l) := c_i^l - \sum_{j=1}^s b_{ij} \frac{(c_j - 1)^l}{\sigma_m^l} - l \sum_{j=1}^s a_{ij} \frac{(c_j - 1)^{l-1}}{\sigma_m^{l-1}} - l \sum_{j=1}^{i-1} r_{ij} c_j^{l-1} = 0, \quad i = 1, \dots, s, \quad (3)$$

is satisfied for  $l = 0, \dots, p$ .  $\square$

The condition (3) for  $l = 0$  is referred to as *preconsistency*. It takes the form

$$B\mathbb{1} = \mathbb{1}. \quad (4)$$

**Definition 2** *A peer method (2) is zero stable if there is a constant  $K > 0$ , so that for all  $m, k \geq 0$  holds*

$$\|B_{m+k} \cdots B_{m+1} B_m\| \leq K. \quad \square \quad (5)$$

For a zero stable peer method of order of consistency  $p$  follows by standard arguments convergence of order  $p$ .

So far peer methods have been considered with constant nodes  $c_i$ , i.e. the nodes are independent of  $\sigma_m$ . For constant step sizes in [5] explicit peer methods have been constructed which have good SSP-properties and use less than  $s$  function calls per step. We now drop this restriction of constant step sizes in order to save function calls also for variable step sizes.

Henceforth we consider nodes depending on the time step, denoted by  $c_{m,i}$  and with  $t_{m,i} = t_m + c_{m,i} h_m$ . We also assume  $c_{m,s} = 1$  for all  $m$ . Analogous to [9] we use Taylor series expansion and obtain for a sufficiently smooth solution  $y(t)$ :

$$\begin{aligned} y(t_{m,i}) &= y(t_m + c_{m,i} h_m) = \sum_{l=0}^p \frac{c_{m,i}^l h_m^l}{l!} y^{(l)}(t_m) + \mathcal{O}(h_m^{p+1}), \\ y(t_{m-1,i}) &= y(t_{m-1} + c_{m-1,i} h_{m-1}) = y(t_m + (c_{m-1,i} - 1) h_{m-1}) \\ &= y\left(t_m + \frac{(c_{m-1,i} - 1) h_m}{\sigma_m}\right) = \sum_{l=0}^p \frac{(c_{m-1,i} - 1)^l h_m^l}{l! \sigma_m^l} y^{(l)}(t_m) + \mathcal{O}(h_m^{p+1}), \\ y'(t_{m,i}) &= y'(t_m + c_{m,i} h_m) = \sum_{l=0}^p \frac{c_{m,i}^l h_m^l}{l!} y^{(l+1)}(t_m) + \mathcal{O}(h_m^{p+1}), \\ y'(t_{m-1,i}) &= y'\left(t_m + \frac{(c_{m-1,i} - 1) h_m}{\sigma_m}\right) = \sum_{l=0}^p \frac{(c_{m-1,i} - 1)^l h_m^l}{l! \sigma_m^l} y^{(l+1)}(t_m) + \mathcal{O}(h_m^{p+1}). \end{aligned}$$

By putting these expansions into the residuals  $\Delta_{m,i}$  it holds

$$\begin{aligned} \Delta_{m,i} = & \left(1 - \sum_{j=1}^s b_{ij}\right) y(t_m) + \sum_{l=1}^p \left\{ c_{m,i}^l - \sum_{j=1}^s b_{ij} \frac{(c_{m-1,j} - 1)^l}{\sigma_m^l} \right. \\ & \left. - l \sum_{j=1}^s a_{ij} \frac{(c_{m-1,j} - 1)^{l-1}}{\sigma_m^{l-1}} - l \sum_{j=1}^{i-1} r_{ij} c_{m,j}^{l-1} \right\} \frac{h_m^l}{l!} y^{(l)}(t_m) + \mathcal{O}(h_m^{p+1}). \end{aligned} \quad (6)$$

With Definition 1, the following theorem is valid for variable nodes.

**Theorem 2** *A peer method (2) has consistency order  $p$  iff*

$$\begin{aligned} AB_i(l) := & c_{m,i}^l - \sum_{j=1}^s b_{ij} \frac{(c_{m-1,j} - 1)^l}{\sigma_m^l} - l \sum_{j=1}^s a_{ij} \frac{(c_{m-1,j} - 1)^{l-1}}{\sigma_m^{l-1}} - l \sum_{j=1}^{i-1} r_{ij} c_{m,j}^{l-1} = 0, \\ & i = 1, \dots, s, \quad l = 0, \dots, p \end{aligned} \quad (7)$$

holds.  $\square$

**Definition 3** *A peer method (2) is said to have  $n_s$  shifted stages and  $s_e = s - n_s$  effective stages if*

$$e_i^\top A_m = e_i^\top R_m = (0, \dots, 0), \quad e_i^\top B_m = e_{i+1}^\top, \quad i = 1, \dots, n_s, \quad (8)$$

and

$$c_{m,i} = \frac{c_{m-1,i+1} - 1}{\sigma_m}, \quad i = 1, \dots, n_s, \quad (9)$$

$$\text{with } c_{0,i} = c_{0,i+1} - 1 \text{ for } i = 1, \dots, n_s. \quad \square \quad (10)$$

From property (8) follows  $Y_{m,i} = Y_{m-1,i+1}$ ,  $i = 1, \dots, n_s$ . The node condition (9) shows the dependence of the nodes on the step size ratio. Together with the choice of constant nodes for the effective stages, i.e.  $c_{m,i} = c_{m-1,i} = c_i$ ,  $i = n_s + 1, \dots, s$ , this allows to reduce the number of function evaluations per step to  $s_e$ .

Because of the structure property (8) there are no free parameters of the coefficients of the peer method for the shifted stages. But one easily proves that the order conditions are satisfied for the shifted values.

**Lemma 1** *Let a peer method (2) satisfy (8) and (9). Then condition (7) holds for all shifted stages  $i = 1, \dots, n_s$  and for all  $l = 0, 1, \dots$   $\square$*

With the diagonal matrices

$$\begin{aligned} D &= \text{diag}(1, \dots, s), \quad C = \text{diag}(c_{m-1,i}), \quad S_m = \text{diag}(1, \sigma_m, \dots, \sigma_m^{s-1}), \\ \widehat{C} &= \text{diag}\left(\frac{c_{m-1,2} - 1}{\sigma_m}, \dots, \frac{c_{m-1,n_s+1} - 1}{\sigma_m}, c_{n_s+1}, \dots, c_s\right), \end{aligned}$$

with the Vandermonde matrix

$$V_1 = \left( (c_{m-1,i} - 1)^{j-1} \right)_{i,j=1}^s$$

and with

$$K_0 = \begin{pmatrix} 1 & \frac{c_{m-1,2}-1}{\sigma_m} & \cdots & \frac{(c_{m-1,2}-1)^{s-1}}{\sigma_m^{s-1}} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & \frac{c_{m-1,n_s+1}-1}{\sigma_m} & \cdots & \frac{(c_{m-1,n_s+1}-1)^{s-1}}{\sigma_m^{s-1}} \\ 1 & c_{n_s+1} & \cdots & c_{n_s+1}^{s-1} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & c_s & \cdots & c_s^{s-1} \end{pmatrix}$$

the conditions (7) for  $l = 1, \dots, s$  for the order of consistency  $p = s$  lead to

$$A_m = \left( \widehat{C}K_0D^{-1} - R_mK_0 \right) S_mV_1^{-1} - \frac{1}{\sigma_m}B_m(C - I)V_1D^{-1}V_1^{-1}. \quad (11)$$

**Theorem 3** *A peer method (2) satisfying (8), (9), preconsistency (4) and (11) has order of consistency  $p = s$ .  $\square$*

Theorem 3 and Lemma 1 show that the construction of peer methods with  $s$  stages of order  $p = s$  is possible if the matrix  $V_1$  is nonsingular. In this case the special structure of the method can be used for all step size sequences, which reduces the number of function calls in each step to  $s_e$ . In the cited papers always constant, pairwise distinct nodes have been considered, so that  $V_1$  is always invertible. For variable nodes this has to be checked. The following theorem gives a sufficient condition for the regularity of  $V_1$  so that the coefficient matrix  $A_m$  is uniquely defined for all step size ratios.

**Theorem 4** *Let the peer method (2) with  $s$  stages and  $n_s$  shifted stages be given. Let  $c_s = 1$  and let  $c_i$ ,  $i = n_s + 1, \dots, s$  be pairwise distinct and constant for all  $m$  and satisfy*

$$0 < c_i < 1 \text{ for } i = n_s + 1, \dots, s - 1. \quad (12)$$

*Assume that the node condition (9) holds. Then the nodes  $c_{m,i}$  are pairwise distinct.*

**Proof 1** *We prove by induction over  $m$  that the shifted nodes are nonpositive and pairwise distinct. By assumption (12) using (9), (10) follows immediately that*

$$c_{1,1}, c_{1,2}, \dots, c_{1,n_s} \leq 0,$$

*and that they are pairwise distinct, the statement holds for  $m = 1$ . Suppose the result is true until  $m - 1$ , i.e.*

$$c_{m-1,1}, c_{m-1,2}, \dots, c_{m-1,n_s} \leq 0 \quad (13)$$

*and the shifted nodes are pairwise distinct. Then from (9) follows*

$$c_{m,i} = \frac{c_{m-1,i+1} - 1}{\sigma_m} \neq \frac{c_{m-1,i+2} - 1}{\sigma_m} = c_{m,i+1}, \quad i = 1, \dots, n_s - 1$$

*and  $c_{m,i} \leq 0$  for  $i = 1, \dots, n_s$ . Because the constant nodes  $c_{n_s+1}, \dots, c_s$  are assumed to be positive the statement follows.  $\blacksquare$*

**Remark 1** Equation (3) for order  $p$  is equivalent to the condition that

$$P(c_i) = \sum_{j=1}^s b_{ij}P(c_j - 1) + \sum_{j=1}^s a_{ij}P'(c_j - 1) + \sum_{j=1}^{i-1} r_{ij}P'(c_j) \quad (14)$$

holds for all polynomials  $P(t)$  of degree  $p$ . Choosing integrals of Lagrange basis polynomials,  $P_k(t) = \int_0^t L_k(s) ds$ ,  $k = 1, \dots, s$ , where  $L_k(t) = \prod_{\substack{l=1 \\ l \neq k}}^s (t - c_l + 1)(c_k - c_l)^{-1}$ , yields an explicit representation for the coefficients  $a_{ik}$ , namely

$$a_{ik} = \int_0^{c_i} L_k(t) dt - \sum_{j=1}^s b_{ij} \int_0^{c_j-1} L_k(t) dt - \sum_{j=1}^{i-1} r_{ij} L_k(c_j).$$

Equation (14) can also conveniently be written in the form

$$\exp(cz) = B \exp((c-1)z) + Az \exp((c-1)z) + Rz \exp(cz) + \mathcal{O}(z^{p+1})$$

with the exponentials evaluated componentwise.  $\square$

### 3 Construction of special methods

In this section we describe the construction of peer methods of order  $p = s$  with the special structure defined by Definition 3. Furthermore we require superconvergence of order  $p = s + 1$  for constant step sizes. We have used the interior point algorithm of `fmincon` from the optimization toolbox in MATLAB and we have considered constant step sizes in the optimization with the aim of finding sufficiently large stability regions and small error coefficients. For the construction of suitable methods we use the following strategy:

- special structure (8) for the constant coefficient matrices  $B$  and  $R$ ,
- $c_s = 1$  and  $c_1, \dots, c_{n_s}$  by the node condition (9) for  $\sigma = 1$ ,
- $A_m$  defined by (11) for  $\sigma = 1$ .

For pairwise distinct nodes  $0 < c_{n_s+1}, \dots, c_{s-1} < 1$  we perform a random walk search. For each fixed set of the nodes we compute the remaining coefficients of  $B, R$  with `fmincon` with respect to the following restrictions:

1.  $b_{i,j} \geq 0$  and  $B\mathbb{1} = \mathbb{1}$  (preconsistency)
2. superconvergence, i.e. we require

$$e_s^\top (I - B + \mathbb{1}e_s^\top)^{-1} AB(s+1) \leq 1.e-14,$$

3.  $\|AB(s+1)\|_\infty \leq 10^{-2}$ .

The objective function is the left boundary of the stability interval on the real axis. With (11) the peer methods are consistent of order  $p = s$ . As in [9] and [10] we consider constant coefficient matrices  $B$  and  $R$ . With the preconsistency and  $b_{ij} \geq 0$  the zero stability (5) follows immediately. Then convergence of order  $p$  follows in standard way. The following methods with  $s = 4, 5, 6$  stages and  $n_s = 2, 3$  shifted stages were obtained in our numerical search, they are denoted by Peers $n_s$ . Here  $c_i = c_{0,i}$ ,  $i = 1, \dots, s$ .

**Peer42:**

$$\begin{aligned}
c_1 &= -1.8021655269393027, & c_2 &= -8.0216552693930265e-1, & c_3 &= 1.9783447306069735e-1, \\
c_4 &= 1, \\
b_{11} &= 0, & b_{12} &= 1, & b_{13} &= 0, \\
b_{14} &= 0, & b_{21} &= 0, & b_{22} &= 0, \\
b_{23} &= 1, & b_{24} &= 0, & b_{31} &= 1.8295119733753218e-1, \\
b_{32} &= 1.6786110670955488e-8, & b_{33} &= 3.2985044218078528e-4, & b_{34} &= 8.1671893543417640e-1, \\
b_{41} &= 9.999999999115896e-1, & b_{42} &= 8.0926939582092916e-12, & b_{43} &= 3.1200119197275861e-14, \\
b_{44} &= 7.1711268672717985e-13, \\
r_{21} &= 0, & r_{31} &= 9.1564614760167007e-1, & r_{32} &= 1.0428807926063595e-1, \\
r_{41} &= 3.7177944377312799e-1, & r_{42} &= 9.1571058331922361e-1, & r_{43} &= 4.9997205345197546e+0.
\end{aligned}$$

**Peer52:**

$$\begin{aligned}
c_1 &= -1.6835993949514214e+0, & c_2 &= -6.8359939495142141e-1, & c_3 &= 3.1640060504857864e-1, \\
c_4 &= 6.6861286851143886e-1, & c_5 &= 1, \\
b_{11} &= 0, & b_{12} &= 1, & b_{13} &= 0, \\
b_{14} &= 0, & b_{15} &= 0, & b_{21} &= 0, \\
b_{22} &= 0, & b_{23} &= 1, & b_{24} &= 0, \\
b_{25} &= 0, & b_{31} &= 2.0401107486318123e-3, & b_{32} &= 5.4931645109554894e-1, \\
b_{33} &= 1.2691303375483114e-2, & b_{34} &= 5.5801947580191649e-3, & b_{35} &= 4.3037194002231693e-1, \\
b_{41} &= 1.3641956992647886e-2, & b_{42} &= 9.6038820598149144e-1, & b_{43} &= 2.3987171310584761e-2, \\
b_{44} &= 1.5212169608928865e-3, & b_{45} &= 4.6144875438302300e-4, & b_{51} &= 1.0305298901588130e-2, \\
b_{52} &= 7.0106889289606744e-1, & b_{53} &= 7.7603788787189328e-3, & b_{54} &= 2.8086542930327690e-1, \\
b_{55} &= 2.0348666667835275e-11, \\
r_{21} &= 0, & r_{31} &= 9.3511152530501707e-1, & r_{32} &= 7.5839418616423826e-1, \\
r_{41} &= 9.1435534264183937e-1, & r_{42} &= 3.7119962655902966e-1, & r_{43} &= 9.5415905234365583e-1, \\
r_{51} &= 7.7605011925913325e-1, & r_{52} &= 8.5321434905217208e-1, & r_{53} &= 6.3811174309270080e-1, \\
r_{54} &= 6.9476629964156711e-1.
\end{aligned}$$

**Peer53:**

$$\begin{aligned}
c_1 &= -2.7731789467332275e+0, & c_2 &= -1.7731789467332275e-1, & c_3 &= -7.7317894673322740e-1, \\
c_4 &= 2.2682105326677257e-1, & c_5 &= 1, \\
b_{11} &= 0, & b_{12} &= 1, & b_{13} &= 0, \\
b_{14} &= 0, & b_{15} &= 0, & b_{21} &= 0,
\end{aligned}$$

$$\begin{aligned}
b_{22} &= 0, & b_{23} &= 1, & b_{24} &= 0, \\
b_{25} &= 0, & b_{31} &= 0, & b_{32} &= 0, \\
b_{33} &= 0, & b_{34} &= 1, & b_{35} &= 0, \\
b_{41} &= 6.6605197574996679e-11, & b_{42} &= 1.0045553304692934e-1, & b_{43} &= 9.7360363398070666e-12, \\
b_{44} &= 4.9148223805056312e-1, & b_{45} &= 4.0806222889276489e-1, & b_{51} &= 1.0702153787220736e-6, \\
b_{52} &= 9.9909106339664955e-1, & b_{53} &= 1.3486915017490726e-6, & b_{54} &= 9.0636951837809281e-4, \\
b_{55} &= 1.4817809188069772e-7, & & & & \\
r_{21} &= 0, & r_{31} &= 0, & r_{32} &= 0, \\
r_{41} &= 7.9865080155095880e-1, & r_{42} &= 3.0013464462079181e-1, & r_{43} &= 7.7904570829856890e-1, \\
r_{51} &= 3.0583193929197805e-1, & r_{52} &= 8.2205567462641449e-1, & r_{53} &= 8.6704036134804785e-1, \\
r_{54} &= 4.9999999885035393e+0. & & & & 
\end{aligned}$$

**Peer62:**

$$\begin{aligned}
c_1 &= -1.8424747772679322e+0, & c_2 &= -8.4247477726793218e-1, & c_3 &= 1.5752522273206779e-1, \\
c_4 &= 4.9258529919492555e-1, & c_5 &= -2.7057802272382603e-1, & c_6 &= 1, \\
b_{11} &= 0, & b_{12} &= 1, & b_{13} &= 0, \\
b_{14} &= 0, & b_{15} &= 0, & b_{16} &= 0, \\
b_{21} &= 0, & b_{22} &= 0, & b_{23} &= 1, \\
b_{24} &= 0, & b_{25} &= 0, & b_{26} &= 0, \\
b_{31} &= 3.2313254028305205e-2, & b_{32} &= 6.0136081924997954e-2, & b_{33} &= 3.4065568037978169e-4, \\
b_{34} &= 2.4583718993830062e-1, & b_{35} &= 2.7063840627312874e-2, & b_{36} &= 6.3430897780070361e-1, \\
b_{41} &= 8.5859313577844362e-2, & b_{42} &= 1.8631921931642929e-2, & b_{43} &= 2.6016551239587354e-1, \\
b_{44} &= 1.7896715388634141e-1, & b_{45} &= 3.0876673251922432e-1, & b_{46} &= 1.4760936568907340e-1, \\
b_{51} &= 3.1414875301815824e-2, & b_{52} &= 2.0672825905290726e-1, & b_{53} &= 9.8504452608241519e-2, \\
b_{54} &= 3.5345309355455143e-2, & b_{55} &= 5.5982958923421984e-2, & b_{56} &= 5.7202414475815833e-1, \\
b_{61} &= 8.6739619485816688e-1, & b_{62} &= 2.2720361605980909e-2, & b_{63} &= 5.2812310752888295e-2, \\
b_{64} &= 2.5115017356787128e-2, & b_{65} &= 9.7949839962663317e-3, & b_{66} &= 2.2161131429910445e-2, \\
r_{21} &= 0, & r_{31} &= 9.2549206179788002e-1, & r_{32} &= 8.5748585237134178e-1, \\
r_{41} &= 6.3852181023379495e-1, & r_{42} &= 2.2333887960478063e-1, & r_{43} &= 1.3693042055158124e+0, \\
r_{51} &= 6.6190594557383708e-1, & r_{52} &= -4.6153823570452340e-1, & r_{53} &= -4.2875988351834293e-1, \\
r_{54} &= 4.1048820930102585e-2, & r_{61} &= 6.0582123606194549e-1, & r_{62} &= 6.2605873010288726e-1, \\
r_{63} &= 5.1988364008583876e-1, & r_{64} &= 1.7643266031476210e+0, & r_{65} &= 1.0648736694704959e+0,
\end{aligned}$$

**Peer63:**

$$\begin{aligned}
c_1 &= -2.77756778549973837e+0, & c_2 &= -1.77756778549973837e+0, & c_3 &= -7.7756778549973837e-1, \\
c_4 &= 2.2243221450026163e-1, & c_5 &= 6.1036825784909732e-1, & c_6 &= 1, \\
b_{11} &= 0, & b_{12} &= 1, & b_{13} &= 0, \\
b_{14} &= 0, & b_{15} &= 0, & b_{16} &= 0, \\
b_{21} &= 0, & b_{22} &= 0, & b_{23} &= 1, \\
b_{24} &= 0, & b_{25} &= 0, & b_{26} &= 0, \\
b_{31} &= 0, & b_{32} &= 0, & b_{33} &= 0,
\end{aligned}$$

$b_{34} = 1,$	$b_{35} = 0,$	$b_{36} = 0,$
$b_{41} = 4.7097962387189697e-2,$	$b_{42} = 2.2800617212884015e-2,$	$b_{43} = 5.0113763486760873e-2,$
$b_{44} = 1.3528050524309280e-4,$	$b_{45} = 1.0759535807070014e-1,$	$b_{46} = 7.7225701833722216e-1,$
$b_{51} = 3.2849719579764891e-1,$	$b_{52} = 2.4765591686882551e-2,$	$b_{53} = 1.4514439937780071e-1,$
$b_{54} = 3.1339118561839734e-2,$	$b_{55} = 4.7020167245230027e-1,$	$b_{56} = 5.2022123527752227e-5,$
$b_{61} = 8.8689631497310562e-1,$	$b_{62} = 1.6997897210738463e-2,$	$b_{63} = 8.1609844111232482e-2,$
$b_{64} = 1.4339569170406654e-2,$	$b_{65} = 1.5557355715756718e-4,$	$b_{66} = 8.0097735919452129e-7,$
$r_{21} = 0,$	$r_{31} = 0,$	$r_{32} = 0,$
$r_{41} = 4.6628908892256105e-1,$	$r_{42} = 7.6380535674398486e-1,$	$r_{43} = 1.1173272476300462e+0,$
$r_{51} = -1.2027178017536724e+0,$	$r_{52} = 2.3847420650102588e-1,$	$r_{53} = 1.2069120086254363e+0,$
$r_{54} = 1.0993062702019800e+0,$	$r_{61} = 3.8549573688369415e-1,$	$r_{62} = -1.4724668354196908e+0,$
$r_{63} = 1.4834234905947858e+0,$	$r_{64} = 5.5037599923757796e-1,$	$r_{65} = 8.5263043096934754e-1.$

Figure 1 shows the stability regions of the methods.

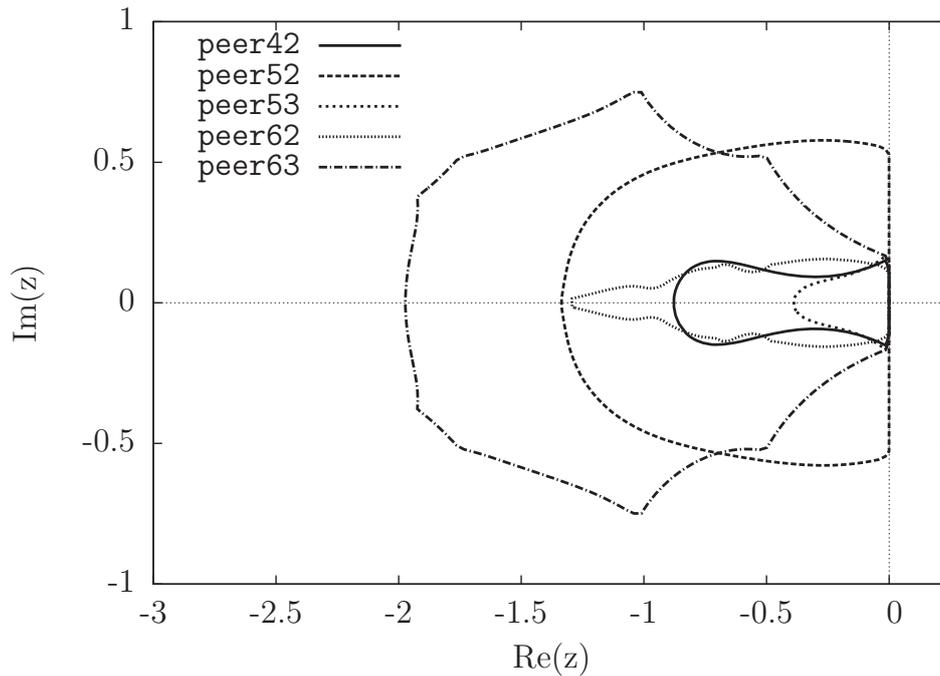


Figure 1: Stability region of explicit peer methods.

## 4 Numerical tests

We have implemented the methods in MATLAB. The starting values were computed with `ode45`, for step size control we estimated the  $(s + 1)$ -st derivative. We exploit the special structure (8) and (9) so that only  $s_e$  function evaluations per step are computed.

First, we want to illustrate the superconvergence of the constructed peer methods for constant step sizes. We consider the orbit problem [1], [3]

$$\begin{aligned}y_1' &= y_3 \\y_2' &= y_4 \\y_3' &= -\frac{y_1}{(y_1^2 + y_2^2)^{\frac{3}{2}}} \\y_4' &= -\frac{y_2}{(y_1^2 + y_2^2)^{\frac{3}{2}}}\end{aligned}$$

with initial values from the exact solution  $y(t) = (\cos t, \sin t, -\sin t, \cos t)^\top$  for  $t \in [0, 1]$ . Figure 2 shows the considered step sizes  $h$  and the logarithm of the obtained error

$$err = \max_{i=1, \dots, n} \frac{|Y_{m,s,i} - y_{ref,i}|}{1 + |y_{ref,i}|}$$

at the endpoint  $t_e = 1$ , where  $Y_{m,s}$  is the numerical solution and  $y_{ref}$  the exact solution. For better illustration we added lines with slopes corresponding to orders  $p = 5, 6, 7$ . For the constructed peer methods with  $s = 4, 5, 6$  the expected orders of superconvergence  $p = 5, 6, 7$  for constant step sizes can clearly be observed.

In the tests with step size control we compare our methods with `ode23`, `ode45` and `ode113` from the MATLAB ODE-suite [7]. As test problems we used the following standard test examples for nonstiff initial value problems: KEPL, the orbit problem from [3] with  $y_0 = (1 - \varepsilon, 0, 0, \sqrt{\frac{1+\varepsilon}{1-\varepsilon}})^\top$ ,  $\varepsilon = 0.9$  and  $t_e = 20$ . The reference solution is described there as well. The other test problems are taken from [4] with same parameters and denoted by the same names as in [4]: AREN, BRUS, LRNZ and PLEI. Reference solutions were computed with `ode45` and high accuracy. We have solved these problems with  $rtol = atol$  for  $atol = 10^{-i}$ ,  $i = 1, \dots, 12$ . In the Figures 3–7 we present the number of function evaluations and the logarithm of the obtained errors.

The results show that the new methods due to their higher order are superior to `ode23` and that the 5- and 6-stage methods are more efficient than `ode45`. For stringent tolerances the Adams method `ode113` has by far the lowest number of function evaluations, which is due to the order control up to  $p = 13$ . However, compared with the other methods the achieved accuracy of `ode113` differs more strongly from the prescribed tolerance.

The step size control in the peer methods works well. As predicted, the shift strategy worked also for variable step sizes for all occurring values of  $\sigma_m$ . For the Brusselator problem for crude tolerances the drawback of the small stability regions of `peer42` and `peer53` can be observed.

## 5 Conclusions

We have presented a special class of explicit peer methods. The methods are characterized by having shifted stages, which allow to reduce the number of function calls. While this property has been used before only for constant step sizes, the proposed methods work

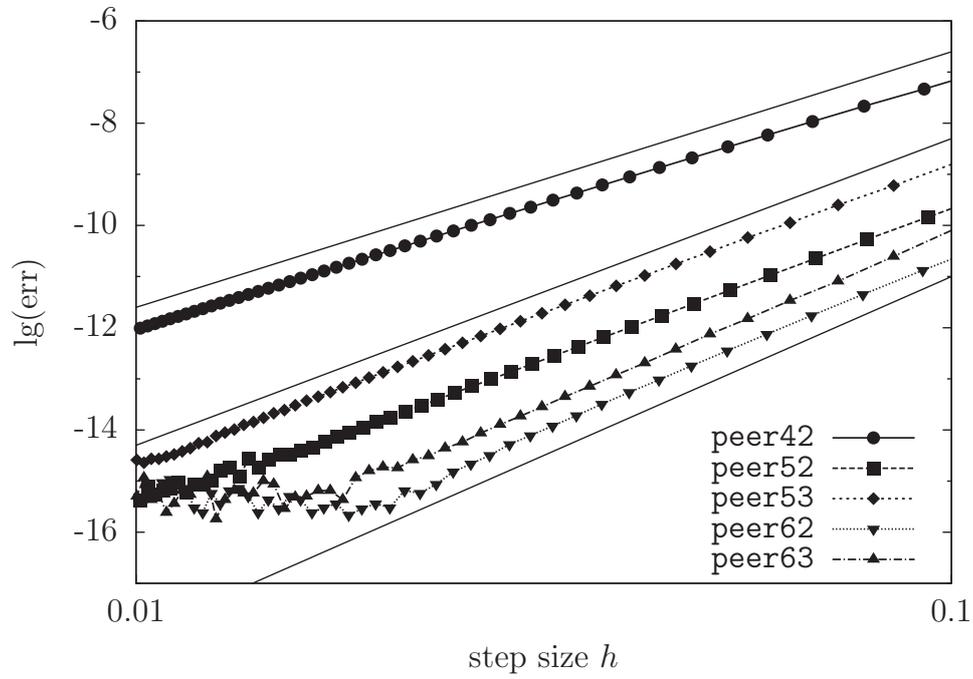


Figure 2: Order test for the orbit problem.

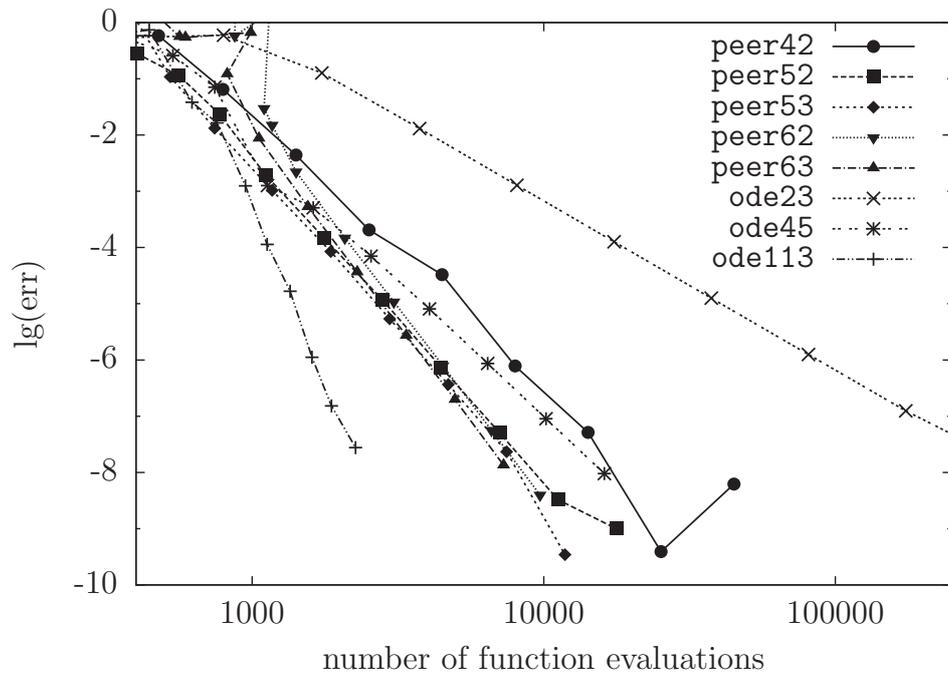


Figure 3: Results for AREN.

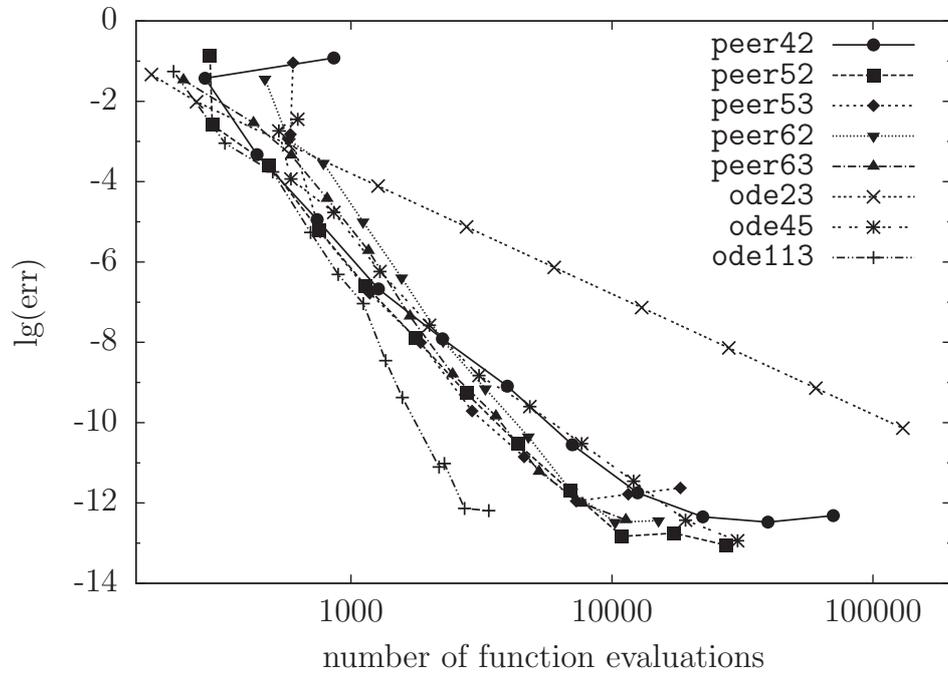


Figure 4: Results for BRUS.

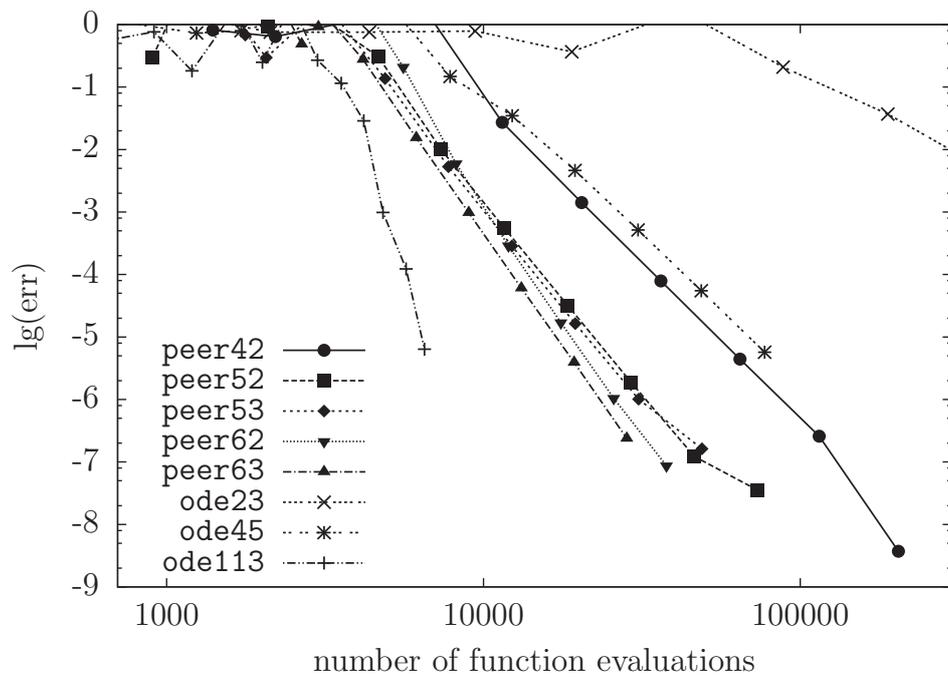


Figure 5: Results for LRNZ.

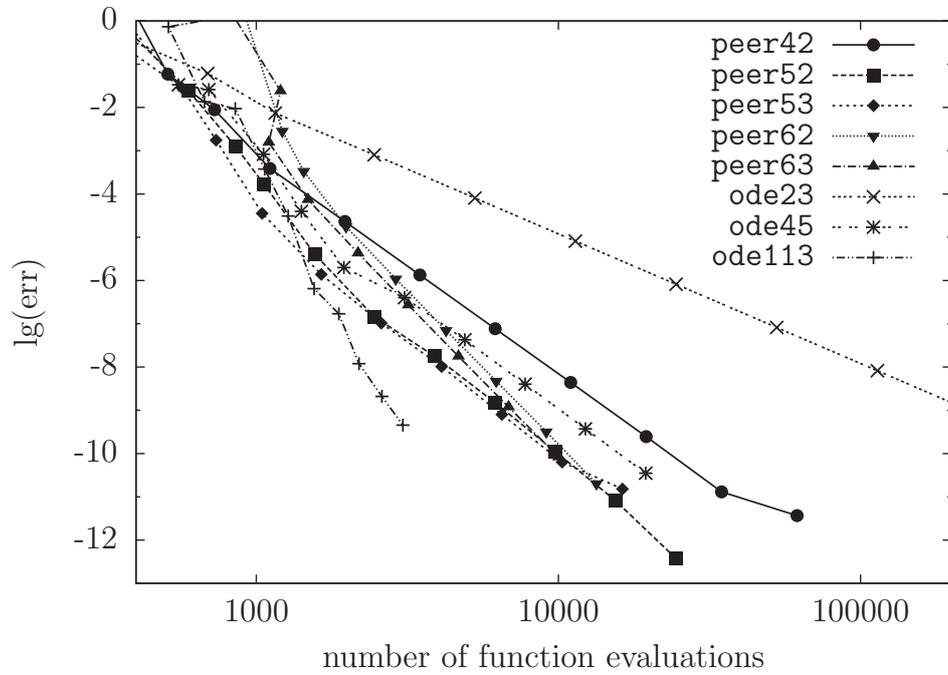


Figure 6: Results for KEPL.

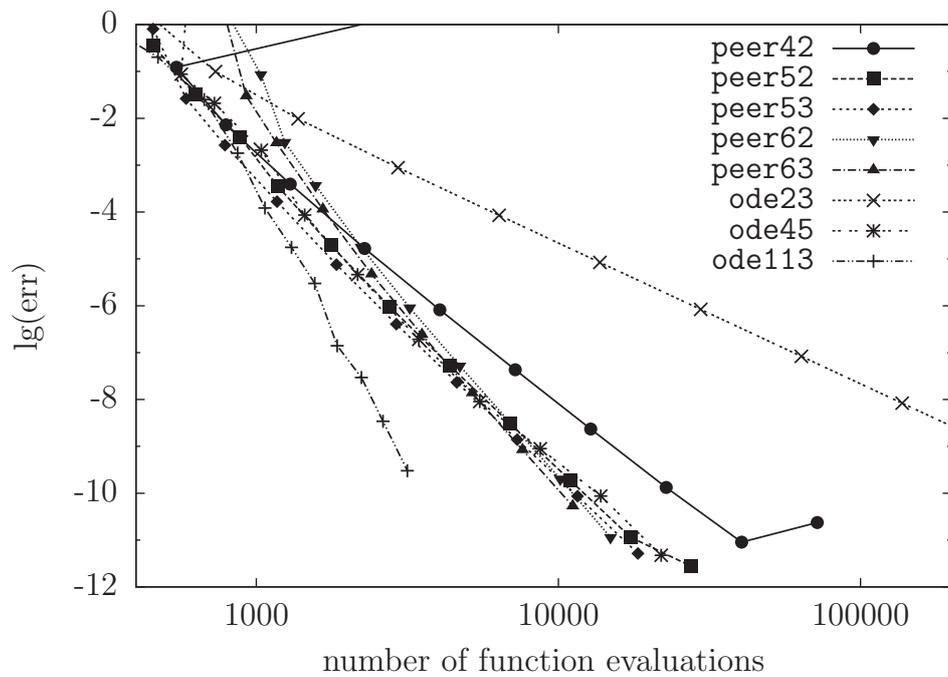


Figure 7: Results for PLEI.

also with variable step sizes allowing an usual step size control. The numerical results are promising. Methods with shifted stages and constant step size have shown to have favorable SSP-properties. So we assume that for such problems the new methods with variable step sizes may be of interest. This will be a topic of future work.

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## Reports of the Institutes 2016

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