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Superconvergent explicit two-step peer methods

Rüdiger Weiner[a,*], Bernhard A. Schmitt[b], Helmut Podhaisky[a], Stefan Jebens[c]

[a] *Institut für Mathematik, Universität Halle, D-06099 Halle, Germany*
[b] *Fachbereich Mathematik und Informatik, Universität Marburg, D-35032 Marburg, Germany*
[c] *Institut für Troposphärenforschung Leipzig, Germany*

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Abstract

We consider explicit two-step peer methods for the solution of nonstiff differential systems. By an additional condition a subclass of optimally zero-stable methods is identified that is superconvergent of order $p = s + 1$, where s is the number of stages. The new condition allows us to reduce the number of coefficients in a numerical search for good methods. We present methods with 4–7 stages which are tested in FORTRAN90 and compared with DOPRI5 and DOP853. The results confirm the high potential of the new class of methods.

MSC: 65L05; 65L06

Keywords: Explicit peer methods; Nonstiff ODE systems; Zero stability; Stability region; Superconvergence

1. Introduction

In a series of papers, e.g. [9,10,7], linearly implicit and implicit two-step peer methods for the solution of

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

have been considered. The new feature of peer methods is that they possess several stages like Runge–Kutta-type methods, but all of these stages have the same properties and no extraordinary solution variable is used. These methods combine the positive features of both Runge–Kutta and multi-step methods having good stability properties and showing no order reduction for very stiff systems. In numerical tests on parallel computers they were rather efficient, e.g. [14,12], and also in sequential computing environments they were competitive with standard codes [7].

In [15] corresponding explicit methods were introduced and tests with parallel explicit two-step peer methods were performed in [11]. Numerical comparisons of 6-stage methods of order 6 in [15] have shown that peer methods are competitive with ODE45 [8].

* Corresponding author.
E-mail addresses: weiner@mathematik.uni-halle.de (R. Weiner), schmitt@mathematik.uni-marburg.de (B.A. Schmitt), podhaisky@mathematik.uni-halle.de (H. Podhaisky), jebens@mail.tropos.de (S. Jebens).

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Explicit two-step peer methods are a special subclass of general linear methods [3], of course. They are also included in the concept of AB-methods of Butcher [2] and in the more general class of A-methods [1]. In [15] we have given order conditions for explicit two-step peer methods, for more general methods such conditions have been derived in [6].

Up to now we have considered methods where the order of convergence p is equal to the order of consistency and the number of stages s. The construction of efficient methods with respect to different competing aims (stability region, small error constants) is quite difficult due to the relatively large number of free parameters. In this paper an additional condition is introduced by which order of convergence $p = s + 1$ may be obtained even for variable stepsizes. It also reduces the number of free parameters and facilitates the parameter search. This additional condition corresponds to the concept of quasi-consistency of Skeel [13]. Quasi-consistency of order p is less stringent than consistency of order p. For constant stepsizes Skeel proved that quasi-consistency of order p is sufficient for convergence of order p.

The paper is organized as follows: In Section 2 a short overview on explicit two-step peer methods is given and the conditions for consistency of order p are stated.

In Section 3 we discuss the convergence of two-step explicit peer methods and consider methods having a special coefficient matrix B. By the concept of quasi-consistency of Skeel [13] we formulate an additional condition for the coefficients of the method that ensures order of convergence $p = s + 1$ for variable stepsizes for an s-stage method of order of consistency $p = s$. This additional condition must be satisfied for all stepsize ratios. Since the property of a method having an order of convergence higher than the order of consistency is called superconvergence in many areas of numerical mathematics we prefer this notion over the rather special definition of quasi-consistency.

In Section 4 we identify a special subclass of methods where the conditions of superconvergence can be explicitly solved with respect to some of the parameters. This allows us to reduce the number of free coefficients and can be incorporated in a numerical search algorithm. In fact, we present particular methods with 4–7 stages.

Results of numerical tests are given in Section 5. First, we illustrate the theoretical results on superconvergence for a special variable grid. Then we compare the peer methods with DOPRI5 and DOP853 on accepted test problems from the literature. The numerical tests show the potential of these new peer methods.

2. Explicit two-step peer methods

Explicit two-step peer methods for problem (1) as introduced in [15] read

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

where $t_{m,i} = t_m + c_i h_m$ and the values $Y_{m,i}$ are approximations to the exact solution $y(t_m + c_i h_m)$. We will use the notation

$$Y_m = (Y_{m,i})_{i=1}^{s} \in \mathbb{R}^{sn}, \quad F(Y_m) = (f(Y_{m,i}))_{i=1}^{s}, \quad A = (a_{ij}), \quad B = (b_{ij}), \quad R = (r_{ij}).$$

In general, the coefficients B, A, R will depend on the stepsize ratio

$$\sigma_m = h_m / h_{m-1}. \tag{2}$$

In order to avoid clumsy tensor product notation we will consider scalar autonomous equations in the following. Then the methods can be written in the compact form

$$Y_m = B_m Y_{m-1} + h_m A_m F(Y_{m-1}) + h_m R_m F(Y_m). \tag{3}$$

Furthermore, when it is clear from the context we will drop the index "m" for simplicity of notation.

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

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

In contrast to Runge–Kutta methods, all stage values of peer methods are of equal importance. We therefore define

Definition 1. The peer method (3) is consistent of order p if

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

Here we collect some results from [15]:

Method (3) has order of consistency p if the conditions $AB(l) = 0$ with

$$AB_i(l) := c_i^l - \sum_{j=1}^{s} b_{ij} \frac{(c_j - 1)^l}{\sigma^l} - l \sum_{j=1}^{s} a_{ij} \frac{(c_j - 1)^{l-1}}{\sigma^{l-1}} - l \sum_{j=1}^{i-1} r_{ij} c_j^{l-1}, \quad i = 1, \ldots, s, \tag{4}$$

are satisfied for $l = 0, \ldots, p$. Especially order of consistency $p = s$ leads to the matrix equations

$$B\mathbb{1} = \mathbb{1}, \quad \mathbb{1} = (1, \ldots, 1)^{\mathrm{T}}, \tag{5}$$

$$A = (CV_0 D^{-1} - RV_0) S V_1^{-1} - \frac{1}{\sigma} B(C - I) V_1 D^{-1} V_1^{-1}, \tag{6}$$

with the diagonal matrices

$$D = \mathrm{diag}(1, \ldots, s), \qquad S = \mathrm{diag}(1, \sigma, \ldots, \sigma^{s-1}), \qquad C = \mathrm{diag}(c_1, \ldots, c_s),$$

and the two Vandermonde matrices

$$V_0 = \left(c_i^{j-1}\right)_{i,j=1}^{s}, \qquad V_1 = \left((c_i - 1)^{j-1}\right)_{i,j=1}^{s}.$$

3. Superconvergence

As in [15] we will consider here only methods with a constant coefficient matrix

$$B = \mathbb{1} v^{\mathrm{T}} + Q W Q^{-1}. \tag{7}$$

However, its form is more general with

$$v = \begin{pmatrix} \widetilde{v} \\ 1 - \widetilde{v}^{\mathrm{T}} \mathbb{1} \end{pmatrix}, \qquad W = \begin{pmatrix} \widetilde{W} & -\widetilde{W}\mathbb{1} \\ 0^{\mathrm{T}} & 0 \end{pmatrix},$$

$$Q = \begin{pmatrix} (I - \mathbb{1}\tilde{v}^{\mathrm{T}})\widetilde{Q} & (1 + \tilde{v}^{\mathrm{T}}\widetilde{Q}\mathbb{1})\mathbb{1} - \widetilde{Q}\mathbb{1} \\ -\tilde{v}^{\mathrm{T}}\widetilde{Q} & 1 + \tilde{v}^{\mathrm{T}}\widetilde{Q}\mathbb{1} \end{pmatrix},$$

and $\widetilde{W}$ is strictly upper triangular, $\widetilde{Q}$ is regular. With this choice, B has the eigenvalues

$$\lambda_1 = 1, \qquad \lambda_2 = \cdots = \lambda_s = 0,$$

a property which we call *optimal zero stability*. It holds

Lemma 1. *Let B be given by (7). Then, the method is optimally zero stable and has the properties*

$$B\mathbb{1} = \mathbb{1}, \qquad B^j = \mathbb{1} v^{\mathrm{T}} \quad \textit{for } j \geq s - 1. \tag{8}$$

Proof. By ansatz (7) the equations

$$Q\mathbb{1} = \mathbb{1}, \qquad W\mathbb{1} = 0 \quad \text{and} \quad v^{\mathrm{T}} Q = e_s^{\mathrm{T}}.$$

are satisfied. This implies

$$B = Q(\mathbb{1} e_s^{\mathrm{T}} + W) Q^{-1},$$

i.e. B has only one simple non-zero eigenvalue which is one and its eigenvector is $\mathbb{1}$. So the method is optimally zero stable and the first-order condition $B\mathbb{1} = \mathbb{1}$ is satisfied. Due to $v^{\mathrm{T}}\mathbb{1} = 1$, $WQ^{-1}\mathbb{1} = W\mathbb{1} = 0$ and the nilpotency of W it is straightforward to obtain the second property

$$B^j = \mathbb{1}v^{\mathrm{T}} \quad \text{for } j \geq s-1. \quad \blacksquare$$

In the following we will consider the convergence of explicit peer methods. We denote by

$$\varepsilon_m := Y(t_m) - Y_m$$

the global error at timestep m to the exact solution $Y(t_m) := (y(t_{m,i}))_{i=1}^s$. The method converges with order p if $\varepsilon_m = \mathcal{O}(h^p)$, where $h = \max_m h_m$. Under rather general additional assumptions order of convergence p follows from order of consistency p. For the case of constant stepsizes Skeel [13] introduced the concept of quasi-consistency. He proved that a quasi-consistent fixed-stepsize method of order $p+1$ is also convergent of order $p+1$. The assumption of quasi-consistency of order $p+1$ is less stringent than consistency of the same order. It requires consistency of order p and an additional condition. Formulated for our methods this additional condition reads

$$E\Delta_m = \mathcal{O}(h_m^{p+1}),$$

where the matrix E is known here by Lemma 1,

$$E = \lim_{l\to\infty} B^l = \mathbb{1}v^{\mathrm{T}}.$$

We will show that this condition together with order of consistency $p = s$ implies convergence of order $p = s+1$ for explicit two-step peer methods also with variable stepsizes. This improvement of the order of convergence over the order of consistency will be called *superconvergence*. The following theorem states conditions for superconvergence of order $p = s+1$.

Theorem 1. *Let* $h := \max_m h_m$, $\max_m \sigma_m \leq \sigma_{\max}$, $\varepsilon_0 = \mathcal{O}(h_0^s)$. *Let B be a matrix of form (7), let the strictly lower triangular matrix R_m be uniformly bounded for $\sigma \leq \sigma_{\max}$, and*

$$A_m = \left(CV_0S_m - R_mV_0DS - \frac{1}{\sigma}B(C-I)V_1\right)D^{-1}V_1^{-1}.$$

Then the method is convergent of order $p = s$.
If in addition $\varepsilon_0 = \mathcal{O}(h_0^{s+1})$ and

$$v^{\mathrm{T}}AB(s+1) = 0 \tag{9}$$

hold then we have superconvergence of order $p = s+1$ with errors $\varepsilon_m = \mathcal{O}(h^{s+1})$.

Proof. For simplicity of notation we again consider the case $n = 1$. Since the method is consistent of order s, the initial errors are of order s and the stepsize increase is bounded, order of convergence $p = s$ follows by standard arguments.

Now let (9) be satisfied in addition. For the global error we have the equation

$$\begin{aligned}\varepsilon_m &= Y(t_m) - Y_m = Y(t_m) - BY_{m-1} - h_mA_mF(Y_{m-1}) - h_mR_mF(Y_m)\\ &= B\varepsilon_{m-1} + h_mA_m(F(Y(t_{m-1})) - F(Y_{m-1})) + h_mR_m(F(Y(t_m)) - F(Y_m)) + h_m\Delta_m.\end{aligned}$$

Differences of function values can be replaced with the mean value theorem by

$$f(Y_{m-1,i}) - f(y(t_{m-1,i})) = -J_{mi}\varepsilon_{m-1,i}$$

where

$$J_{mi} := \int_0^1 f_y(y(t_{m-1,i}) + \theta(Y_{m-1,i} - y(t_{m-1,i})))\mathrm{d}\theta, \quad i = 1,\ldots,s.$$

We obtain the vector equation

$$A_m(F(Y(t_{m-1})) - F(Y_{m-1})) = G_m\varepsilon_{m-1} \quad \text{with } G_m := A_m\mathrm{diag}(J_{mi})$$

and analogously

$$R_m(F(Y(t_m)) - F(Y_m)) = H_m\varepsilon_m \quad \text{with } H_m := R_m\mathrm{diag}(J_{m+1,i}).$$

So, the error recursion becomes

$$\varepsilon_m = B\varepsilon_{m-1} + h_{m-1}\sigma_m G_m \varepsilon_{m-1} + h_m H_m \varepsilon_m + h_m \Delta_m.$$

By repeated substitution we obtain

$$\varepsilon_m = B^m \varepsilon_0 + \sum_{j=0}^{m-1} h_{m-j-1}\sigma_{m-j} B^j G_{m-j}\varepsilon_{m-j-1} + \sum_{j=0}^{m-1} h_{m-j} B^j H_{m-j}\varepsilon_{m-j} + \sum_{j=0}^{m-1} h_{m-j} B^j \Delta_{m-j}. \tag{10}$$

Using assumption (9) on the last term leads to

$$\begin{aligned}\sum_{j=0}^{m-1} h_{m-j} B^j \Delta_{m-j} &= \sum_{j=s-1}^{m-1} h_{m-j} B^j \Delta_{m-j} + \sum_{j=0}^{s-2} h_{m-j} B^j \Delta_{m-j} \\ &= \mathbb{1} v^{\mathrm{T}} \sum_{j=s-1}^{m-1} h_{m-j}\Delta_{m-j} + \mathcal{O}(h^{s+1}) = \mathcal{O}(h^{s+1}), \end{aligned} \tag{11}$$

since v^{T} eliminates the $\mathcal{O}(h^s)$ contribution. The matrices $\sigma_m A_m$ and R_m are uniformly bounded for $\sigma_m \le \sigma_{\max}$ and there is a constant c such that

$$\|\sigma_{m-j} B^j G_{m-j}\| \le c, \quad \|B^j H_{m-j}\| \le c, \; t_0 \le t_j \le t_m \le t_e.$$

This yields

$$\begin{aligned}&\left\| \sum_{j=0}^{m-1} B^j \sigma_{m-j} G_{m-j} h_{m-j-1}\varepsilon_{m-j-1} + \sum_{j=0}^{m-1} B^j H_{m-j} h_{m-j}\varepsilon_{m-j} \right\| \\ &\quad \le c h_0 \|\varepsilon_0\| + 2c \sum_{j=1}^{m-1} h_j \|\varepsilon_j\| + c h_m \|\varepsilon_m\|.\end{aligned}$$

So, from order s of convergence $\varepsilon_m = \mathcal{O}(h^s)$, $\varepsilon_0 = \mathcal{O}(h_0^{s+1})$ and with (11) it follows from (10)

$$\|\varepsilon_m\| \le 2c \sum_{j=1}^{m-1} h_j \|\varepsilon_j\| + \mathrm{d}h^{s+1}, \quad m \ge 1. \tag{12}$$

We will use the following relation which holds for any sequence X_l:

$$1 + \sum_{j=1}^{m-1} \left(X_{m-j} \prod_{l=1}^{m-j-1} (1 + X_l) \right) = \prod_{l=1}^{m-1} (1 + X_l). \tag{13}$$

Using this equation allows us to prove the inequality

$$\|\varepsilon_m\| \le \prod_{l=1}^{m-1} (1 + 2c h_l) \mathrm{d}h^{s+1}$$

with $X_l = 2c h_l$ by induction.

For $m = 1$ inequality (12) means $\|\varepsilon_1\| \le \mathrm{d}h^{s+1}$ and therefore the assertions hold here.

Now let the inequality be satisfied for $j \le m-1$, $\|\varepsilon_j\| \le \prod_{l=1}^{j-1}(1 + 2c h_l)\mathrm{d}h^{s+1}$. Then, (12) gives

$$\begin{aligned}\|\varepsilon_m\| &\le 2c \sum_{j=1}^{m-1} h_j \|\varepsilon_j\| + \mathrm{d}h^{s+1} \\ &\le \left(1 + 2c \sum_{j=1}^{m-1} h_j \prod_{l=1}^{j-1} (1 + 2c h_l) \right) \mathrm{d}h^{s+1}\end{aligned}$$

$$= \prod_{l=1}^{m-1}(1+2ch_l)\mathrm{d}h^{s+1} \quad \text{by (13)}$$

$$\leq \prod_{l=1}^{m-1} \mathrm{e}^{2ch_l}\mathrm{d}h^{s+1} \leq \mathrm{e}^{2c(t_e-t_0)}\mathrm{d}h^{s+1}.$$

This means superconvergence of order $p = s + 1$. ■

Remark 1. (9) is only one additional condition. However, it must be satisfied for all $\sigma \leq \sigma_{\max}$. □

4. A special class of methods

In the following we construct methods having order of convergence $p = s+1$. We will incorporate condition (9) in a search for efficient explicit two-step peer methods and so decrease the number of free parameters. The complicated relations between the parameters simplify considerably for the special case $v = e_s$ in (7).

Theorem 2. *Let $c_s = 1$ and B given by (7) with $v = e_s$. Let R be constant and*

$$\sum_{i=1}^{s-1} r_{si}c_i^{l-1} = \frac{1}{l}, \quad l = 2, \ldots, s+1. \tag{14}$$

Then under the conditions of Theorem 1 the explicit two-step peer method is superconvergent of order $p = s + 1$.

Proof. With the notation $\mathbf{c}^l = (c_1^l, \ldots, c_s^l)^{\mathrm{T}}$, $c_s = 1$ and $v = e_s$ condition (9) reads

$$e_s^{\mathrm{T}}\left[\mathbf{c}^{s+1} - \frac{1}{\sigma^{s+1}}B(\mathbf{c}-\mathbb{1})^{s+1} - \frac{s+1}{\sigma^s}A(\mathbf{c}-\mathbb{1})^s - (s+1)R\mathbf{c}^s\right] = 0.$$

Because of $e_s^{\mathrm{T}}Q = e_s^{\mathrm{T}}$ and $c_s = 1$ the term with B vanishes. Furthermore we have

$$e_s^{\mathrm{T}}A = [e_s^{\mathrm{T}}(CV_0S - RV_0DS) - \frac{1}{\sigma}e_s^{\mathrm{T}}B(C-I)V_1]D^{-1}V_1^{-1}$$
$$= e_s^{\mathrm{T}}(CV_0D^{-1} - RV_0)SV_1^{-1}.$$

The superconvergence condition thus becomes

$$0 = 1 - (s+1)e_s^{\mathrm{T}}R\mathbf{c}^s - \frac{s+1}{\sigma^s}e_s^{\mathrm{T}}(CV_0D^{-1} - RV_0)SV_1^{-1}(\mathbf{c}-\mathbb{1})^s.$$

With $e_s^{\mathrm{T}}CV_0 = \mathbb{1}^{\mathrm{T}}$ it is clearly satisfied if $1-(s+1)e_s^{\mathrm{T}}R\mathbf{c}^s = 0$ and $e_s^{\mathrm{T}}(CV_0D^{-1} - RV_0) = \mathbb{1}^{\mathrm{T}}D^{-1} - e_s^{\mathrm{T}}RV_0 = 0$ which gives the sufficient conditions

$$\sum_{i=1}^{s-1} r_{si}c_i^{l-1} = \frac{1}{l}, \quad l = 1, \ldots, s+1.$$

We now show that the condition for $l = 1$ is redundant since the first column of $(CV_0D^{-1} - RV_0)$ is multiplied by $e_1^{\mathrm{T}}V_1^{-1}(\mathbf{c}-\mathbb{1})^s = 0$. Consider the polynomial

$$\Psi(t) = \prod_{i=1}^{s}(t - c_i + 1) = t^s + \sum_{k=0}^{s-1}\psi_k t^k.$$

For $t = c_i - 1$ we have

$$0 = \Psi(c_i - 1) = (c_i - 1)^s + \sum_{k=0}^{s-1}\psi_k(c_i-1)^k.$$

The vector $\psi = (\psi_0, \ldots, \psi_{s-1})^{\mathrm{T}}$ therefore satisfies the system

$$\left(\mathbb{1}, \mathbf{c}-\mathbb{1}, \ldots, (\mathbf{c}-\mathbb{1})^{s-1}\right)\psi + (\mathbf{c}-\mathbb{1})^s = V_1\psi + (\mathbf{c}-\mathbb{1})^s = 0. \tag{15}$$

So, due to $c_s = 1$, $\psi_0 = \Psi(0) = 0$ from (15) indeed follows

$$0 = \psi_0 = e_1^{\mathrm{T}} V_1^{-1}(\mathbf{c}-\mathbb{1})^s.$$

This implies that we have only s equations for R. ■

We note that (14) is an overdetermined system for the nontrivial elements of the last row of R. Hence, it is also a restriction on the nodes c_i. For the construction of suitable methods we use the following strategy:

- $c_s = 1$, B defined by (7) with $v = e_s$.
- $A = (CV_0S - RV_0DS - \frac{1}{\sigma}B(C-I)V_1)D^{-1}V_1^{-1}$.
- $r_{s1}, \ldots, r_{s,s-1}$ and c_{s-1} by (14).

For the remaining coefficients of R, Q, W and $c_1, \ldots, c_{s-2}$ we perform a random walk search with the aim of finding sufficiently large stability regions and small error coefficients analogously to [15].

The following explicit two-step peer methods of order $p = s+1$ for $s = 4, 5, 6, 7$ were obtained by this search.

Peer4:

$c_1 = -8.99579676124057740\text{e}{-1}$, $c_2 = 3.21166533529362690\text{e}{-1}$, $c_3 = 8.32246931855046760\text{e}{-1}$,
$c_4 = 1$,
$b_{11} = 1.24122229845558500\text{e}{-2}$, $b_{12} = 9.37457581037608700\text{e}{-2}$, $b_{13} = 7.03125551563550100\text{e}{-2}$,
$b_{14} = 8.23529463755328270\text{e}{-1}$, $b_{21} = 1.97908313062304530\text{e}{-1}$, $b_{22} = -3.80342030451579200\text{e}{-2}$,
$b_{23} = 2.06437692794558640\text{e}{-1}$, $b_{24} = 6.33688197188294750\text{e}{-1}$, $b_{31} = 8.64455447310573900\text{e}{-2}$,
$b_{32} = -1.24782671699802370\text{e}{-1}$, $b_{33} = 2.56219800606020700\text{e}{-2}$, $b_{34} = 1.01271514690814291$,
$b_{41} = 0$, $b_{42} = 0$, $b_{43} = 0$,
$b_{44} = 1$,
$r_{21} = 6.47346459819632580\text{e}{-1}$, $r_{31} = -8.87837183228577520\text{e}{-1}$, $r_{32} = 1.85153850645476487$,
$r_{41} = 4.34438602634850000\text{e}{-4}$, $r_{42} = 5.08504783610419040\text{e}{-1}$, $r_{43} = 4.05019328519322130\text{e}{-1}$.

Peer5:

$c_1 = 2.62539061452960590\text{e}{-1}$, $c_2 = -4.50848350565414890\text{e}{-1}$, $c_3 = 5.33427944293478510\text{e}{-1}$,
$c_4 = 8.84369578605042570\text{e}{-1}$, $c_5 = 1$,
$b_{11} = -2.64505945758810000\text{e}{-4}$, $b_{12} = 1.09262291173906480\text{e}{-1}$, $b_{13} = -6.22696731672207200\text{e}{-2}$,
$b_{14} = 9.94055581282522700\text{e}{-2}$, $b_{15} = 8.53866329810820780\text{e}{-1}$, $b_{21} = 5.17861549738358000\text{e}{-3}$,
$b_{22} = -1.20635526468584800\text{e}{-2}$, $b_{23} = 6.99088749473043000\text{e}{-3}$, $b_{24} = 7.92546307515196800\text{e}{-2}$,
$b_{25} = 9.20639418903224790\text{e}{-1}$, $b_{31} = 3.99498350696981000\text{e}{-3}$, $b_{32} = -2.38561827238057500\text{e}{-2}$,
$b_{33} = 1.67073365583257900\text{e}{-2}$, $b_{34} = 3.82292024534117800\text{e}{-2}$, $b_{35} = 9.64924660205098370\text{e}{-1}$,
$b_{41} = 2.75545576901500000\text{e}{-5}$, $b_{42} = -6.27759080522287000\text{e}{-3}$, $b_{43} = 3.20560334823196000\text{e}{-3}$,
$b_{44} = -4.37927796570849000\text{e}{-3}$, $b_{45} = 1.00742371086500925$, $b_{51} = 0$,
$b_{52} = 0$, $b_{53} = 0$, $b_{54} = 0$,
$b_{55} = 1$,
$r_{21} = -2.87779236489906900\text{e}{-1}$, $r_{31} = 9.31553531336830940\text{e}{-1}$, $r_{32} = -3.03057633677963180\text{e}{-1}$,
$r_{41} = -6.61803665041225030\text{e}{-1}$, $r_{42} = -7.16310781038366250\text{e}{-1}$, $r_{43} = 1.16888920439989306$,
$r_{51} = 2.78444244409284230\text{e}{-1}$, $r_{52} = -1.62131729090246000\text{e}{-3}$, $r_{53} = 3.33426297245164910\text{e}{-1}$,
$r_{54} = 2.80773607407724020\text{e}{-1}$.

Peer6:

$c_1 = 2.43289622316122800\text{e}{-2}$, $c_2 = 2.51877852944711690\text{e}{-1}$, $c_3 = 4.85556921458272720\text{e}{-1}$,
$c_4 = 6.84744184641423160\text{e}{-1}$, $c_5 = 9.28591728864534330\text{e}{-1}$, $c_6 = 1$,
$b_{11} = -8.51372947032340000\text{e}{-4}$, $b_{12} = 1.97294810946422400\text{e}{-2}$, $b_{13} = 2.31525283650099400\text{e}{-2}$,
$b_{14} = -8.45384663531875300\text{e}{-2}$, $b_{15} = 3.54546062306402800\text{e}{-2}$, $b_{16} = 1.00705322360992741$,
$b_{21} = 4.95051945357715000\text{e}{-3}$, $b_{22} = -1.45506352933319900\text{e}{-2}$, $b_{23} = 6.18466562244525100\text{e}{-2}$,
$b_{24} = 7.69410819192377200\text{e}{-2}$, $b_{25} = -2.21802789970720300\text{e}{-2}$, $b_{26} = 8.92992656693136640\text{e}{-1}$,

$b_{31} = -2.46589698388427000\text{e}{-3}$, $b_{32} = -2.07218672492735600\text{e}{-2}$, $b_{33} = 1.69524118278705000\text{e}{-3}$,
$b_{34} = 1.18422016941148500\text{e}{-1}$, $b_{35} = 1.21153318895049660\text{e}{-1}$, $b_{36} = 7.81917187214172620\text{e}{-1}$,
$b_{41} = 8.70851738235150000\text{e}{-4}$, $b_{42} = -2.36502913707016000\text{e}{-3}$, $b_{43} = 8.52945331260661000\text{e}{-3}$,
$b_{44} = 1.25533214496212000\text{e}{-2}$, $b_{45} = -7.48660279979864000\text{e}{-3}$, $b_{46} = 9.87898005436405840\text{e}{-1}$,
$b_{51} = 8.79356192977100000\text{e}{-5}$, $b_{52} = 3.24333836530330000\text{e}{-4}$, $b_{53} = 2.45178978725498000\text{e}{-3}$,
$b_{54} = -8.58561299346010000\text{e}{-4}$, $b_{55} = 1.15344560795608000\text{e}{-3}$, $b_{56} = 9.96841056448306910\text{e}{-1}$,
$b_{61} = 0$, $b_{62} = 0$, $b_{63} = 0$,
$b_{64} = 0$, $b_{65} = 0$, $b_{66} = 1$,
$r_{21} = 6.86997418552900210\text{e}{-1}$, $r_{31} = -7.73392658570786480\text{e}{-1}$, $r_{32} = 6.18300837055176990\text{e}{-1}$,
$r_{41} = 6.92115070787555020\text{e}{-1}$, $r_{42} = 6.27662870962438100\text{e}{-2}$, $r_{43} = 4.63817671654442790\text{e}{-1}$,
$r_{51} = -3.35202109833644230\text{e}{-1}$, $r_{52} = -5.82580694920580360\text{e}{-1}$, $r_{53} = 1.94317812328683670\text{e}{-1}$,
$r_{54} = 5.79365767854102430\text{e}{-1}$, $r_{61} = 1.93473224012620830\text{e}{-1}$, $r_{62} = 2.74078532142707980\text{e}{-1}$,
$r_{63} = 1.65985529861765190\text{e}{-1}$, $r_{64} = 2.65210898143553500\text{e}{-1}$, $r_{65} = 1.76677905728075980\text{e}{-1}$.

Peer7:

$c_1 = -3.96806284491904080\text{e}{-1}$, $c_2 = -7.99724867279874160\text{e}{-1}$, $c_3 = 1.37943162980955080\text{e}{-1}$,
$c_4 = 3.63189713406609370\text{e}{-1}$, $c_5 = 6.20037580579519270\text{e}{-1}$, $c_6 = 9.16353684788949000\text{e}{-1}$,
$c_7 = 1$,
$b_{11} = -1.38009671018635700\text{e}{-2}$, $b_{12} = 7.02291591478891200\text{e}{-2}$, $b_{13} = -2.46992200467653980\text{e}{-1}$,
$b_{14} = 3.83759826512140300\text{e}{-2}$, $b_{15} = -4.48248847962380000\text{e}{-4}$, $b_{16} = 1.22241906392661880\text{e}{-1}$,
$b_{17} = 1.03039436822571490$, $b_{21} = 5.04644319416500000\text{e}{-5}$, $b_{22} = -3.21288194210241000\text{e}{-3}$,
$b_{23} = 1.24658243781360410\text{e}{-1}$, $b_{24} = 1.70463395762737100\text{e}{-2}$, $b_{25} = 3.82712857344034200\text{e}{-2}$,
$b_{26} = 1.67302902388694700\text{e}{-2}$, $b_{27} = 8.06456258179253750\text{e}{-1}$, $b_{31} = 7.10308189494710000\text{e}{-4}$,
$b_{32} = 2.92709375337501000\text{e}{-3}$, $b_{33} = 1.29658446422970000\text{e}{-2}$, $b_{34} = 7.82568690295340000\text{e}{-4}$,
$b_{35} = -5.10341195119284600\text{e}{-2}$, $b_{36} = 3.33580394359931700\text{e}{-2}$, $b_{37} = 1.00029026480047323$,
$b_{41} = 1.38726791823451000\text{e}{-3}$, $b_{42} = 4.79030956797505000\text{e}{-3}$, $b_{43} = 1.82618678939080200\text{e}{-2}$,
$b_{44} = -1.17179472008287000\text{e}{-3}$, $b_{45} = -1.67590523989876000\text{e}{-2}$, $b_{46} = -4.46229569525919900\text{e}{-2}$,
$b_{47} = 1.03811435869154488$, $b_{51} = 1.51883446616300000\text{e}{-5}$, $b_{52} = 2.75033637127845000\text{e}{-3}$,
$b_{53} = 1.55986314652173500\text{e}{-2}$, $b_{54} = 3.22340070781964000\text{e}{-3}$, $b_{55} = -9.21560681384200000\text{e}{-5}$,
$b_{56} = -5.38266509292824000\text{e}{-3}$, $b_{57} = 9.83887264272089590\text{e}{-1}$, $b_{61} = -2.09679522602340000\text{e}{-4}$,
$b_{62} = 3.29842409450230000\text{e}{-4}$, $b_{63} = 1.07557824557508600\text{e}{-2}$, $b_{64} = 2.46826954337116000\text{e}{-3}$,
$b_{65} = 4.66907860438599000\text{e}{-3}$, $b_{66} = 5.31195518989027000\text{e}{-3}$, $b_{67} = 9.76674751319753830\text{e}{-1}$,
$b_{71} = 0$, $b_{72} = 0$, $b_{73} = 0$,
$b_{74} = 0$, $b_{75} = 0$, $b_{76} = 0$,
$b_{77} = 1$,
$r_{21} = 9.83223692944738900\text{e}{-2}$, $r_{31} = -4.77251042367424820\text{e}{-1}$, $r_{32} = 8.89832876886939630\text{e}{-1}$,
$r_{41} = -2.18433801131322980\text{e}{-1}$, $r_{42} = 1.61584562678006478$, $r_{43} = 9.01777803616132580\text{e}{-1}$,
$r_{51} = 3.17718610520241780\text{e}{-1}$, $r_{52} = 1.36309594030026349$, $r_{53} = -1.36903252629912459$,
$r_{54} = 9.89591604222077890\text{e}{-1}$, $r_{61} = -1.57995220503071320\text{e}{-1}$, $r_{62} = -7.33415705393999840\text{e}{-1}$,
$r_{63} = -1.45644480922142974$, $r_{64} = -8.17448090456891800\text{e}{-1}$, $r_{65} = 1.04337486670236103$,
$r_{71} = 1.40986205345731000\text{e}{-3}$, $r_{72} = -8.60057818504400000\text{e}{-5}$, $r_{73} = 2.61901308120309790\text{e}{-1}$,
$r_{74} = 1.73994530235014030\text{e}{-1}$, $r_{75} = 3.39536081702410240\text{e}{-1}$, $r_{76} = 2.08047411502428190\text{e}{-1}$.

5. Numerical tests

At first we want to illustrate the superconvergence for a special variable grid. We consider the two-body problem ([3], (201d))

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

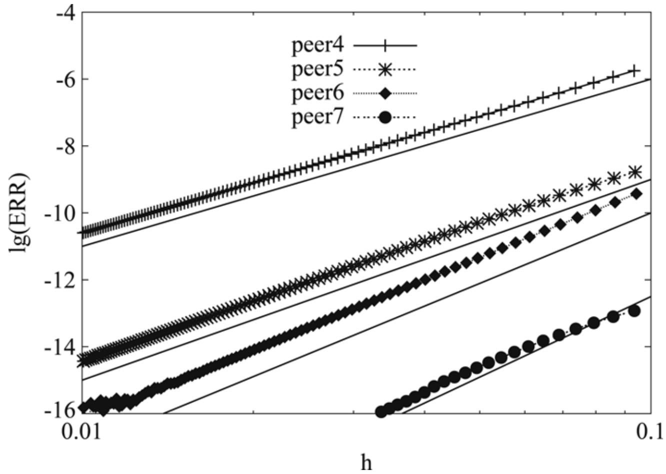

Fig. 1. Errors for an alternating grid.

$$y_4' = -\frac{y_2}{(y_1^2 + y_2^2)^{\frac{3}{2}}}$$

for $0 \leq t \leq 3\pi$ and with initial values from the exact solution $y(t) = (\cos t, \sin t, -\sin t, \cos t)^{\mathrm{T}}$. We applied alternating stepsizes h and $0.8h$, i.e. $\sigma_{2i+1} = 0.8$, $\sigma_{2i} = 1.25$. The norm of the error at the endpoint is displayed in Fig. 1. For illustration we added lines with slopes corresponding to orders 5, 6, 7, 8. For the methods with $s = 4, 5, 6$ the predicted orders $p = 5, 6, 7$ can be seen clearly. For $s = 7$ order $p = 8$ can be seen only in a small range of stepsizes since all errors are near machine precision.

For the tests with automatic stepsize control we have implemented the methods Peer4–Peer7 in FORTRAN90 and compared them on accepted test problems with the state of the art codes DOPRI5 and DOP853, cf. [5]. The details of implementation (e.g. computation of starting values, Nordsieck form) for the peer methods are the same as in [15].

The test problems are the ORBIT problems from [4], p. 86, with $e = 0.9$ and $t_e = 20$. The reference solution is described there as well. The other test problems are taken from [5] (with same names and parameters): AREN, BRUS, EULR, LRNZ and PLEI.

We have solved these problems with $rtol = atol$ for $atol = 10^{-i}$, $i = 3, \ldots, 14$. In the following figures we present the number of function evaluations (FCN) and the logarithm of the obtained accuracy at the endpoint

$$ERR = \max_{i=1,\ldots,n} \frac{|y_i - y_{\mathrm{ref},i}|}{1 + |y_{\mathrm{ref},i}|},$$

where y is the numerical solution and y_{ref} a reference solution which, except for ORBIT, is computed with DOP853 and high accuracy.

Figs. 2–7 show the expected behaviour of the peer methods, the predicted order $p = s + 1$ can be observed by comparing the slope of the curves with those of DOPRI5 and DOP853.

For some prescribed tolerance $atol$ the peer methods give more accurate results than the DOPRI codes. This leads to a bend in the figures for sharp tolerances when the errors come near double precision accuracy. This effect also appears for DOPRI but at still more stringent tolerances. In order to demonstrate this we also included in the figure for PLEI (Fig. 7) the results with $atol = 10^{-15}$, 10^{-16} for DOP853 and DOPRI5.

6. Conclusions

By deriving the condition for superconvergence we could extract a special class of explicit two-step peer methods having order of convergence $p = s + 1$ for all stepsize ratios. Some particular methods with 4–7 stages have been implemented and tested with good performance. Peer4 is comparable with DOPRI5, Peer5 is more efficient for most tolerances and problems. For crude tolerances DOP853 is more efficient than the higher-order peer methods. This is probably due to its larger stability region and a suboptimal choice of the starting stepsize for the peer methods. But for medium tolerances Peer6 and Peer7 are comparable with DOP853.

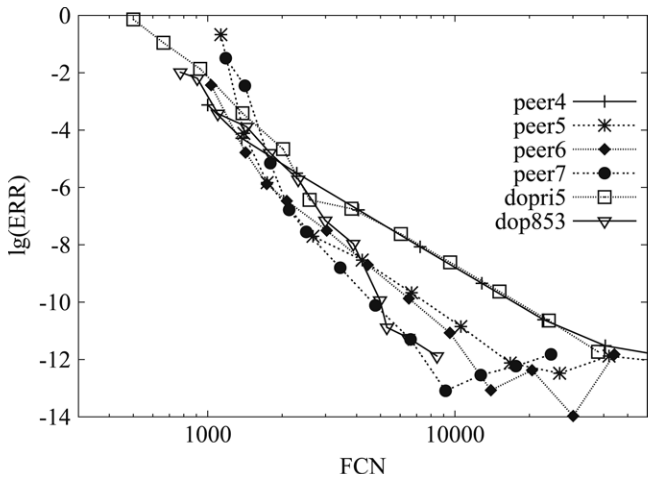

Fig. 2. Results for ORBIT.

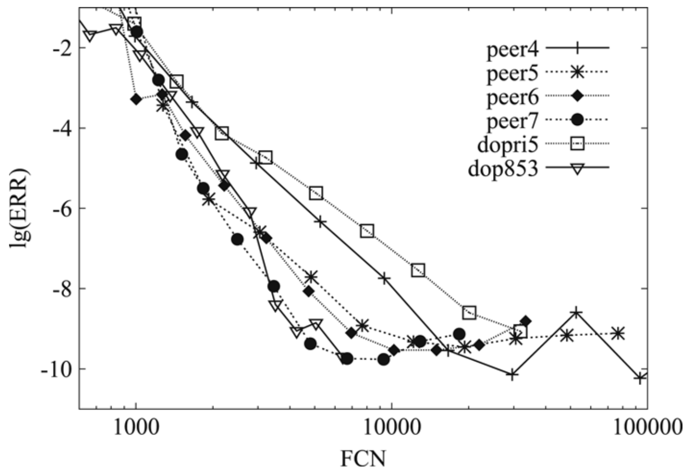

Fig. 3. Results for AREN.

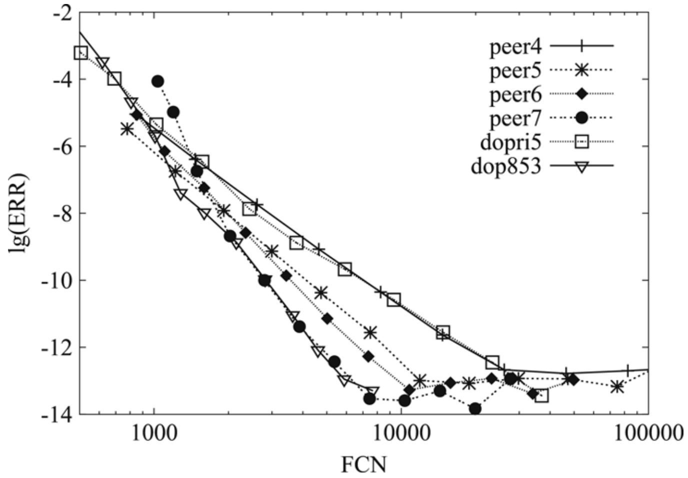

Fig. 4. Results for BRUS.

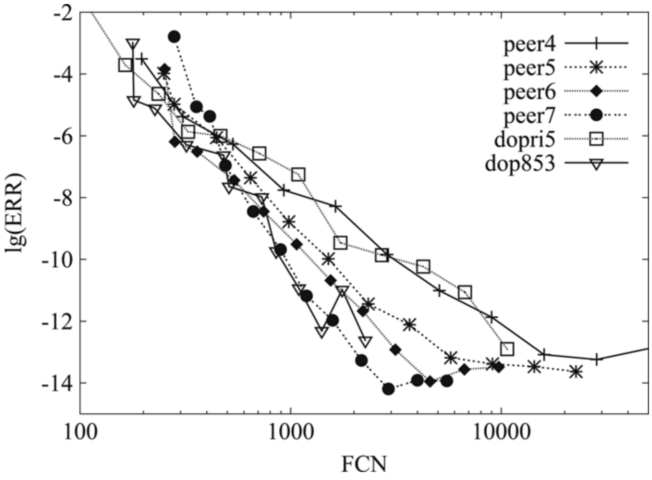

Fig. 5. Results for EULR.

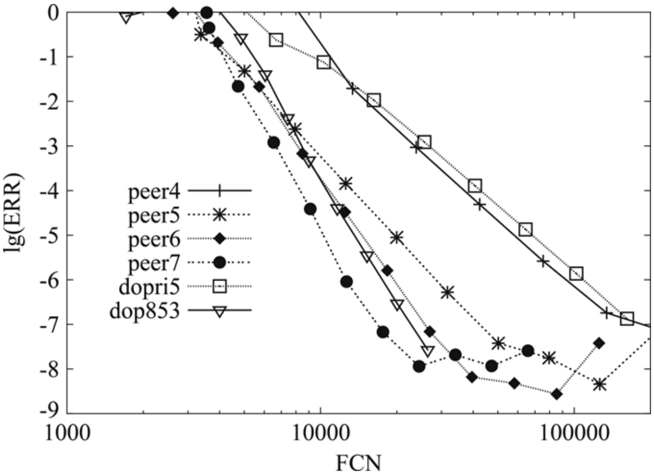

Fig. 6. Results for LRNZ.

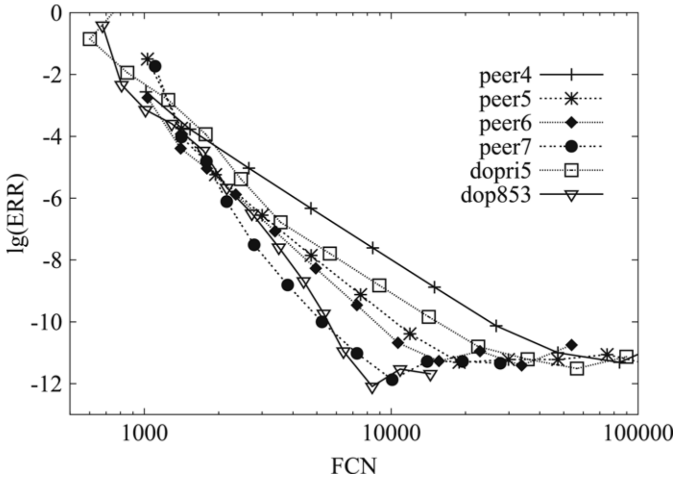

Fig. 7. Results for PLEI.

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