Explicit two-step peer methods

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Abstract

We present the new class of explicit two-step peer methods for the solution of nonstiff differential systems. A construction principle for methods of order $p = s$, s the number of stages, with optimal zero-stability is given. Two methods of order $p = 6$, found by numerical search, are tested in Matlab on several representative nonstiff problems. The comparison with ODE45 confirms the high potential of the new class of methods.

Keywords. Explicit peer methods, nonstiff ODE systems, stability region, general linear methods.

1 Introduction

Many efficient methods have been developed for the numerical solution of ordinary differential equations

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

The most important classes of methods are one-step and multistep methods and efficient computer codes from each of these classes are widely available. To these belong the one-step code DOPRI5(4), which is also the basis of the MATLAB routine ODE45 [15], and the multistep code VODE [4]. The respective advantages of one-step and multistep methods are well known, cf. the text book of Hairer, Nørsett and Wanner [7]. With parallel implementation in mind the new class of peer methods has been introduced by some of the authors in a series of papers, e.g. [12], [13], [14], which concentrated on stiff problems and linearly-implicit and

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implicit two-step methods. 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 positive features of both Runge-Kutta and multistep methods having good stability properties and no order reduction for very stiff systems. In numerical tests on parallel computers they were rather efficient, e.g. [17], [14], and also in sequential computing environments they were competitive with standard codes [11].

In this paper we now discuss explicit two-step peer methods for nonstiff problems and concentrate on non-parallel methods. "Classical" explicit two-step Runge-Kutta schemes have been considered for instance by Jackiewicz/Zennaro [8] and Tracogna/Welfert [16], and in the context of general linear methods by Jackiewicz/Tracogna [9] and Wright [18]. Numerical results of certain parallel explicit two-step methods are given in [5].

The paper is organized as follows: In Section 2 we formulate the new class of explicit two-step peer methods as special case of linearly-implicit peer methods. In this paper we discuss a general class containing parallel and sequential methods.

In Section 3 we give order results using simplifying conditions and consider stability properties. By a special choice of coefficients we ensure optimal zero-stability for arbitrary stepsize sequences and avoid some of the theoretical difficulties of linearly implicit peer methods, see [14]. We describe a strategy for the construction of zero stable methods of order $p = s$.

Section 4 is devoted to the numerical search for good methods using the remaining free coefficients. We present two methods of order $p = 6$ with 6 stages and display their stability regions. Furthermore, we discuss the implementation of the methods with stepsize control.

Numerical results of a MATLAB code for several widely accepted nonstiff test problems are reported in Section 5. Comparisons with the MATLAB code ODE45 show the efficiency of the proposed methods.

Finally we give some conclusions and an outlook for future work.

2 Derivation of the methods

We start with the linearly-implicit two-step peer methods from [14]. In each time step from t_m to $t_{m+1} = t_m + h_m$ solutions $Y_{mi} \cong y(t_{mi})$, $i = 1, \ldots, s$, are computed as approximations at the points

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

by the formula

$$(I - \gamma_i h_m T_m) Y_{mi} = \sum_{j=1}^{s} \big(b_{ij} I + h_m \gamma_{ij} T_m\big) Y_{m-1,j} + h_m \sum_{j=1}^{s} a_{ij} f\big(t_{m-1,j}, Y_{m-1,j}\big). \tag{3}$$

Here the reals $\gamma_i > 0$, $b_{ij}, \gamma_{ij}, a_{ij}$ are the parameters of the method.

For stiff problems T has to be an approximation to the Jacobian f_y. By setting $T = 0$ we obtain an explicit method, which can be applied to nonstiff systems. Obviously, the s stages of the method can be computed in parallel on s processors since information from the previous time step only is used. In this paper however we will not focus on parallel methods. Therefore, like in explicit Runge-Kutta schemes, it is natural to use also the previously computed stage values from the present step:

$$
\begin{aligned}
Y_{mi} = \sum_{j=1}^{s} b_{ij} Y_{m-1,j} + h_m \sum_{j=1}^{s} a_{ij} f(t_{m-1,j}, Y_{m-1,j}) + \sum_{j=1}^{i-1} q_{ij} Y_{m,j} \\
+ h_m \sum_{j=1}^{i-1} r_{ij} f(t_{m,j}, Y_{m,j}), \quad i = 1, ..., s.
\end{aligned}
$$

With the notations

$$
Y_m = (Y_{mi})_{i=1}^{s} \in \mathbb{R}^{sn}, \; F(Y_m) = (f(Y_{mi}))_{i=1}^{s}, \; A = (a_{ij}), \; B = (b_{ij}), \; Q = (q_{ij}), \; R = (r_{ij})
$$

the methods can be written in the compact form (for simplicity for autonomous equations)

$$
Y_m = (B \otimes I) Y_{m-1} + h_m (A \otimes I) F(Y_{m-1}) + (Q \otimes I) Y_m + h_m (R \otimes I) F(Y_m),
$$

where Q und R are strictly lower triangular matrices.

In the following, for ease of representation only, we consider scalar equations. By replacing the coefficient matrices according to

$$
B := (I - Q)^{-1} B, \quad A, R \text{ analogously}
$$

these methods simplify to

$$
Y_m = B Y_{m-1} + h_m A F(Y_{m-1}) + h_m R F(Y_m). \tag{4}
$$

Remark 1 *Sequential linearly-implicit two-step methods were considered in [11], however (4) differs from that class when $T = 0$ is used there.* $\square$

Note, that the coefficients B, A, R in (4) will in general depend on the stepsize ratio

$$
\sigma_m = h_m / h_{m-1}. \tag{5}
$$

For simplicity we drop this dependence in the notation by writing B instead of B_m and so on.

It remains to find appropriate coefficients c, B, A and R such that the method has high order and good stability properties. In linearly-implicit two-step methods (3) optimal damping at infinity was ensured by the choice $\Gamma = -A$ and the other coefficients were chosen to give order $p = s - 1$, uniform zero-stability and $L(\alpha)$-stability with large α, see [14]. For explicit methods we will now follow a different strategy. At first, by prescribing a special structure for B being independent of σ, we guarantee zero-stability. Then, we determine the other coefficients with respect to high order and a relatively large stability region.

3 Order and stability

Analogously to [14] the accuracy of the method may be analyzed in a standard way by considering the residuals Δ_{mi} obtained when the exact solution is put into the method:

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

With the simplifying condition $AB(q)$

$$\begin{aligned} \mathbf{AB(q)}: \quad c_i^l - \sum_{j=1}^{s} b_{ij}\frac{(c_j-1)^l}{\sigma^l} - l\sum_{j=1}^{s} a_{ij}\frac{(c_j-1)^{l-1}}{\sigma^{l-1}} - l\sum_{j=1}^{i-1} r_{ij}c_j^{l-1} = 0, \\ l = 0,...,q-1,\ i = 1,...,s, \end{aligned} \tag{6}$$

using Taylor expansion we obtain analogously to [12] the following theorem.

Theorem 1 *Let $AB(p+1)$ be satisfied. Then it holds $\Delta_{mi} = \mathcal{O}(h_m^p)$, i.e. the method is of order p.* $\square$

For a method of order $p \geq s-1$ the coefficients therefore have to satisfy

$$\begin{aligned} \begin{pmatrix} 1 & c_1 & \cdots & c_1^s \\ \vdots & & & \vdots \\ 1 & c_s & \cdots & c_s^s \end{pmatrix} - B \begin{pmatrix} 1 & c_1-1 & \cdots & (c_1-1)^s \\ \vdots & & & \vdots \\ 1 & c_s-1 & \cdots & (c_s-1)^s \end{pmatrix} \widehat{S}^{-1} \\ - A \begin{pmatrix} 0 & 1 & \cdots & (c_1-1)^{s-1} \\ \vdots & & & \vdots \\ 0 & 1 & \cdots & (c_s-1)^{s-1} \end{pmatrix} \widehat{D} \begin{pmatrix} 0 & 0 \\ 0 & S^{-1} \end{pmatrix} - R \begin{pmatrix} 0 & 1 & \cdots & c_1^{s-1} \\ \vdots & & & \vdots \\ 0 & 1 & \cdots & c_s^{s-1} \end{pmatrix} \widehat{D} = \beta e_{s+1}^T, \end{aligned} \tag{7}$$

with the matrices

$$D = \mathrm{diag}(1,...,s),\ \widehat{D} = \mathrm{diag}(0,1,...,s),\ S = \mathrm{diag}(1,\sigma,...,\sigma^{s-1}),\ \widehat{S} = \mathrm{diag}(1,\sigma,...,\sigma^s).$$

The vector $\beta \in \mathbb{R}^s$ is arbitrary, however, for $\beta = 0$ we have order $p = s$. From (7) we obtain a method of order $p \geq s-1$ if

$$B\mathbb{1} = \mathbb{1}, \quad \mathbb{1} = (1,...,1)^T, \tag{8}$$

$$A = (CV_0D^{-1} - RV_0 - \frac{1}{s}\beta e_s^T)SV_1^{-1} - \frac{1}{\sigma}B(C-I)V_1D^{-1}V_1^{-1}, \tag{9}$$

where we use the notations

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

Absolute stability is discussed with the test equation

$$y' = \lambda y, \quad \Re\lambda \leq 0. \tag{10}$$

Application of method (4) with constant stepsize h yields

$$Y_m = (I - zR)^{-1}(B + zA)Y_{m-1} =: M(z)Y_{m-1}, \quad z = h\lambda, \tag{11}$$

which defines the stability matrix $M(z)$. The boundary of the stability region is characterized by $\varrho(M(z)) = 1$, where ϱ means the spectral radius of the matrix.

A necessary condition for convergence of the method is zero stability, which means that the spectral radius of $M(0)$ is equal to one and all eigenvalues on the unit circle are simple, cf. [12]. These are restrictions on the coefficient B since (11) yields

$$M(0) = B.$$

For an explicit two-step peer method of order $p = s$ many free parameters are left to obtain zero stability and other features. In order to restrict our search for good methods the following choices are made.

1. We set $c_s = 1$ and use Y_{ms} as approximation for $y(t_{m+1})$, the other nodes are to the left, $c_i < 1$, $i = 1, ..., s - 1$.

2. B is chosen as a constant matrix, i.e. independent of the stepsize ratio, with the following properties

   (a) $B\mathbb{1} = \mathbb{1}$ according to (8),

   (b) Analogously to Adams methods we will consider methods with optimal zero stability such that $B = M(0)$ has the eigenvalues

   $$\lambda_1 = 1, \quad \lambda_2 = ... = \lambda_s = 0. \tag{12}$$

3. We define A by (9) with $\beta = 0$:

   $$A = (CV_0D^{-1} - RV_0)SV_1^{-1} - \frac{1}{\sigma}B(C - I)V_1D^{-1}V_1^{-1}. \tag{13}$$

With these choices the method has order $p = s$ and we avoid the difficulties associated with long products of different matrices, cf. [14]. In fact, since $B_m \equiv B$ is constant there exists a constant $K < \infty$ such that for any stepsize sequence holds

$$\|B_{m+k} \cdots B_{m+1}B_m\| = \|B^{k+1}\| \leq K, \quad m, k \geq 0.$$

The method is therefore convergent of order $p = s$ also for variable stepsizes.

Explicit two-step peer methods can be written as special general linear methods [3],

$$\begin{pmatrix} Y_m \\ y^{[m]} \end{pmatrix} = \begin{pmatrix} R & B & A \\ R & B & A \\ I & 0 & 0 \end{pmatrix} \begin{pmatrix} hF_m \\ y^{[m-1]} \end{pmatrix},$$

by some replication of variables:

$$y^{[m]} = \begin{pmatrix} Y_m \\ hF_m \end{pmatrix}.$$

Stability investigations of general linear methods are very difficult, already for constant stepsizes, since the stability matrix possesses s eigenvalues. This was the reason why Butcher and Wright [2] and Butcher [3] have introduced the concept of *inherent Runge-Kutta stability* (IRKS), which guarantees that the stability matrix has only one non-zero eigenvalue $\lambda_1(z)$. This eigenvalue is similar to the stability function of a Runge-Kutta method and in particular it approximates the exponential function

$$\lambda_1(z) = e^z + \mathcal{O}(z^{p+1}).$$

By restricting the order to $p = s-1$ Wright [18] derives explicit general linear methods with inherent Runge-Kutta stability for nonstiff systems. However, in our opinion IRKS may be rather restrictive, since it may be possible to obtain larger stability regions for general matrices $M(z)$. Furthermore, there is no construction principle available for $p = s$.

Example. For $s = 3, p = 2$ the stability function of an explicit Runge-Kutta method with optimal stability interval on the real axis is [6], p.130,

$$R_0(z) = 1 + z + \frac{1}{2}z^2 + \frac{1}{16}z^3.$$

Its stability interval is $\approx [-6.4, 0]$. In contrast, the explicit two-step peer method with 3 stages of order 2 with the coefficients

$$\begin{aligned}
&c = (-0.52272085472056641, 0.27365754138645715, 1)^T,\\
&\beta = (-0.17809611978032626000, 0.44446116339508443000, 2.96349836247717029000)^T,
\end{aligned} \tag{14}$$

$$r_{21} = -0.09159413232682273, \quad r_{31} = -0.57457711150669493, \quad r_{32} = 0.50989353951662779,$$

$$B = \begin{pmatrix} 0.07371534039303789 & 0.35335840725111239 & 0.57292625235584972 \\ -0.01537801647775663 & -0.07371534039303789 & 1.08909335687079452 \\ 0 & 0 & 1 \end{pmatrix}$$

has the stability region given in Figure 1, reaching as far as ≈ -21.15 on the real axis.

Hence we will consider methods with order $p = s$ and will not require IRKS.

Now, as remaining parameters we have the nodes $c_1, ..., c_{s-1}$, the lower triangular matrix R and some freedom in the matrix B. A very simple choice

$$B = \mathbb{1}e_s^T$$

which clearly satisfies (8) was considered in [1]. For this choice holds $B(C - I) = 0$ because of $c_s = 1$ and the expression for A simplifies to

$$A = (CV_0D^{-1} - RV_0)SV_1^{-1}.$$

This fact can also be exploited in the implementation. As we will see below, the vector

$$Z_m := h_m D^{-1} V_1^{-1} F(Y_m) \tag{15}$$

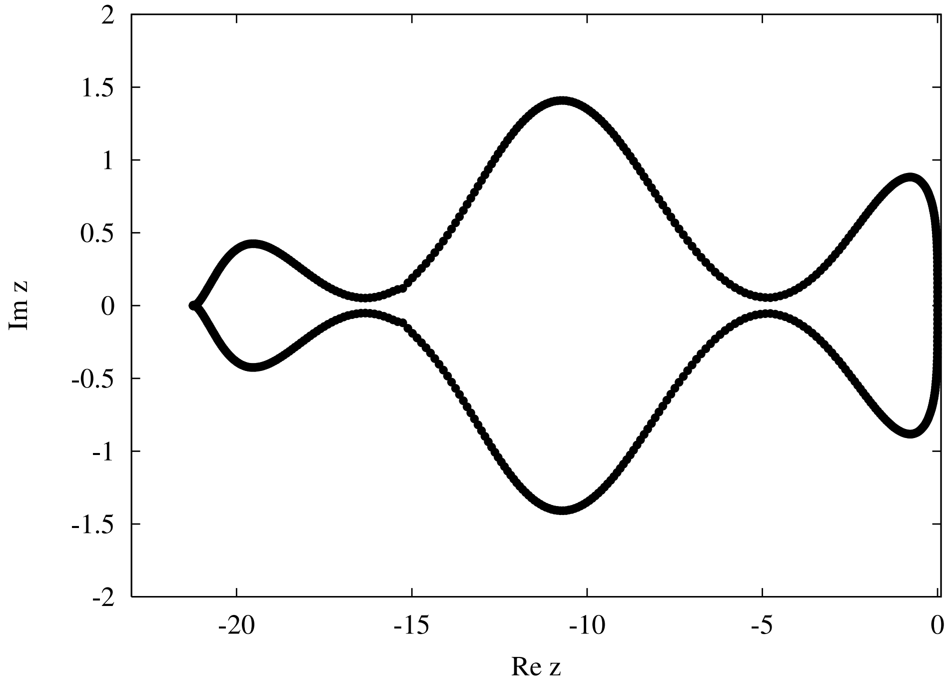

Figure 1: Stability region of method (14).

has a certain meaning and with $y_{m+1} = Y_{ms}$ we may write the time step in the form

$$\begin{pmatrix} Y_m \\ y_{m+1} \\ Z_m \end{pmatrix} = \underbrace{\begin{pmatrix} R & \mathbb{1} & CV_0 - RV_0D \\ e_s^T R & 1 & e_s^T(CV_0 - RV_0D) \\ D^{-1}V_1^{-1} & 0 & 0 \end{pmatrix}}_{=:\mathcal{N}} \begin{pmatrix} h_m F(Y_m) \\ y_m \\ \sigma_m S Z_{m-1} \end{pmatrix}. \tag{16}$$

Obviously, for constant R the matrix $\mathcal{N}$ does not depend on the stepsize ratio σ and needs not to be recomputed. The change of stepsize is simply accomplished by scaling the vector Z_{m-1} with the diagonal matrix $\sigma_m S$. Putting the exact derivatives $y'(t_m + (c_i - 1)h_{m-1})$ for the function values $F(Y_{m-1})$ into the definition (15) we obtain

$$Z_{m-1} = h_{m-1} D^{-1} V_1^{-1} \begin{pmatrix} y'(t_m + (c_1 - 1)h_{m-1}) \\ \vdots \\ y'(t_m + (c_s - 1)h_{m-1}) \end{pmatrix} = \begin{pmatrix} h_{m-1} y'(t_m) \\ \vdots \\ \frac{h_{m-1}^s}{(s-1)!} y^{(s)}(t_m) \end{pmatrix} + \mathcal{O}(h_{m-1}^{s+1}).$$

So this is simply the Nordsieck vector at t_m with respect to the old stepsize h_{m-1} and scaling with $\sigma_m S$ in (16) adjusts the stepsize for the new timestep. We thus can interpret (16) as Nordsieck form of this special two-step peer method. In the next section we will use Z_{m-1} to compute an embedded solution for stepsize control. For a detailed discussion of the Nordsieck form of two-step peer methods see [10].

In the aforementioned thesis [1] also the choice $B = \mathbb{1} e_s^T + W$ with a strictly upper triangular matrix W satisfying $W\mathbb{1} = 0$ was discussed. A more general ansatz for B will be considered now.

4 Method search and implementation issues

We consider the case $p = s = 6$ and choose B as constant matrix in the form

$$B = \mathbb{1} e_s^T + QWQ^{-1}, \tag{17}$$

with

$$W = \begin{pmatrix} \widetilde{W} & -\widetilde{W}\mathbb{1} \\ 0^T & 0 \end{pmatrix}, \quad Q = \begin{pmatrix} \widetilde{Q} & (I - \widetilde{Q})\mathbb{1} \\ 0^T & 1 \end{pmatrix}.$$

The matrix $\widetilde{W}$ is strictly upper triangular and $\widetilde{Q}$ is regular. In fact it is sufficient to consider nonzero elements in the first upper diagonal of $\widetilde{W}$ only. With this choice (8) and (12) are satisfied. By a random walk optimization we then searched for appropriate coefficients $c_1, ..., c_{s-1}$, $\widetilde{W}$, $\widetilde{Q}$ and R. Due to the large number of free parameters this is a difficult task and the methods given below may be far from optimal. The coefficients were searched for in the neighbourhood of

$$c_i = \frac{i-1}{s-1},\ i = 1, ..., s, \quad \widetilde{W} = 0, \quad R = 0, \quad \widetilde{Q} = I.$$

As the main criterion in our random search we considered small error constants and required that the right hand side of $AB(s+2)$ should be small for some σ-interval around one. The sum of 1-norms for $\sigma = 0.8 + 0.03i,\ i = 0, ..., 21$ was used here. Among the computed methods with small error coefficients a further selection was made with respect to

1. an acceptable stability region. For simplicity only the stability interval was computed for equispaced points z along the real axis.

2. small method coefficients. In order to limit the propagation of round-off errors during computation coefficient matrices with moderate norms are required. In [14] methods with small condition of the Vandermonde matrix V_0 have shown to be advantageous. According to (16) the main source of large coefficients is the inverse $D^{-1}V_1^{-1}$. In our search we therefore also monitored the value

$$vmax = \max_{i,j} |(D^{-1}V_1^{-1})_{ij}|.$$

We present two methods found in this search. Peer1 is characterized by a smaller value $vmax$, whereas Peer2 possesses a larger stability interval.

Peer1:

$$\begin{aligned}
c_1 &= -0.01770390142245916, & c_2 &= 0.16516501573769842, & c_3 &= 0.34860715432519789,\\
c_4 &= 0.56248294653082265, & c_5 &= 0.78286213656097884, & c_6 &= 1,\\
r_{21} &= 0.61070074583568145, & r_{31} &= -0.8517020678485627, & r_{32} &= 0.61458879899440335,\\
r_{41} &= 0.45876210425592723, & r_{42} &= 0.24406335829023736, & r_{43} &= 0.56950703375000739,\\
r_{51} &= -0.22974128518503159, & r_{52} &= -0.67668748673169174, & r_{53} &= 0.30010953293359376,\\
r_{54} &= 0.52817537128029626, & r_{61} &- 0.6026613367944304, & r_{62} &= 0.18876383194059831,\\
r_{63} &- 0.19986049206166063, & r_{64} &= 0.13193964475487591, & r_{65} &= 0.51653958905093377,
\end{aligned}$$

$$
\begin{aligned}
&b_{11} = 0.00024758445881146, && b_{12} = -0.01237865517145417, && b_{13} = 0.03244372731149522,\\
&b_{14} = 0.01723705850413894, && b_{15} = -0.00143340193760978, && b_{16} = 0.96388368683531519,\\
&b_{21} = 0.00055711351843759, && b_{22} = -0.00015932594507341, && b_{23} = 0.00722949162026803,\\
&b_{24} = -0.00087094478515981, && b_{25} = 0.00911183822052122, && b_{26} = 0.98413182737100638,\\
&b_{31} = -0.00035987165554283, && b_{32} = 0.00074637700496433, && b_{33} = -0.00158995766506194,\\
&b_{34} = 0.00258730440624810, && b_{35} = -0.00460224052628880, && b_{36} = 1.00321838843568113,\\
&b_{41} = 0.00064942550979462, && b_{42} = -0.00088568943688745, && b_{43} = 0.00394739594025460,\\
&b_{44} = -0.00074302571362487, && b_{45} = 0.02698458342340990, && b_{46} = 0.97004731027705319,\\
&b_{51} = 0.00006119550695291, && b_{52} = 0.00017940331636687, && b_{53} = -0.00040544739055120,\\
&b_{54} = -0.00061214302531627, && b_{55} = 0.00224472486564561, && b_{56} = 0.99853226672690207,\\
&b_{61} = 0, && b_{62} = 0, && b_{63} = 0,\\
&b_{64} = 0, && b_{65} = 0, && b_{66} = 1.
\end{aligned}
$$

Peer2:

$$
\begin{aligned}
&c_1 = -0.00181172751639972, && c_2 = 0.23040882079033181, && c_3 = 0.42697708485727196,\\
&c_4 = 0.59898194159865381, && c_5 = 0.79790762834190389, && c_6 = 1,\\
&r_{21} = 0.69822633662492034, && r_{31} = -0.92330274784826672, && r_{32} = 0.57508585182876329,\\
&r_{41} = 0.72958417504369280, && r_{42} = 0.03030801107310688, && r_{43} = 0.43687098663414830,\\
&r_{51} = -0.33065522354677321, && r_{52} = -0.62187309914873915, && r_{53} = 0.19461907769296319,\\
&r_{54} = 0.47589927912788465, && r_{61} = -0.42316357547255231, && r_{62} = 0.27274990240324287,\\
&r_{63} = -0.18671228442398832, && r_{64} = 0.00487974025256928, && r_{65} = 0.51917885691767557,\\
&b_{11} = 0.00022674290842532, && b_{12} = 0.00118055243557665, && b_{13} = -0.00548237059603823,\\
&b_{14} = 0.02108407322175899, && b_{15} = -0.01400182873640206, && b_{16} = 0.99699283076667933,\\
&b_{21} = -0.00004771568299736, && b_{22} = 0.00019067249928068, && b_{23} = 0.00770664434518127,\\
&b_{24} = -0.00689666210198479, && b_{25} = -0.01301778705831074, && b_{26} = 1.01206484799883095,\\
&b_{31} = -0.00011864014669474, && b_{32} = 0.00012542860339340, && b_{33} = 0.00016099319579623,\\
&b_{34} = -0.01944267859647398, && b_{35} = -0.00334107428971509, && b_{36} = 1.02261597123369418,\\
&b_{41} = 0.00002864604376507, && b_{42} = 0.00015588709778739, && b_{43} = 0.00004881709139124,\\
&b_{44} = -0.00046138985456025, && b_{45} = -0.01196937878432601, && b_{46} = 1.01219741840594256,\\
&b_{51} = -0.00000007590460206, && b_{52} = 0.00000431260571033, && b_{53} = 0.00008890966992158,\\
&b_{54} = -0.00000346963457253, && b_{55} = -0.00011701874894198, && b_{56} = 1.00002734201248466,\\
&b_{61} = 0, && b_{62} = 0, && b_{63} = 0,\\
&b_{64} = 0, && b_{65} = 0, && b_{66} = 1.
\end{aligned}
$$

With the matrix A computed by (13) the methods are of order $p = s = 6$. Figures 2 and 3 show the stability regions of both methods. There also exist methods with even larger stability interval. However, for the nonstiff test problems in Section 5 the larger stability interval was no advantage for these methods. The methods Peer1 and Peer2 were implemented in MATLAB and compared with the MATLAB code ODE45, [15]. ODE45 is based on the explicit Runge-Kutta (4,5) formula of Dormand/Prince [6], which is well-known as DOPRI5 from the book of Hairer, Nørsett and Wanner [7].

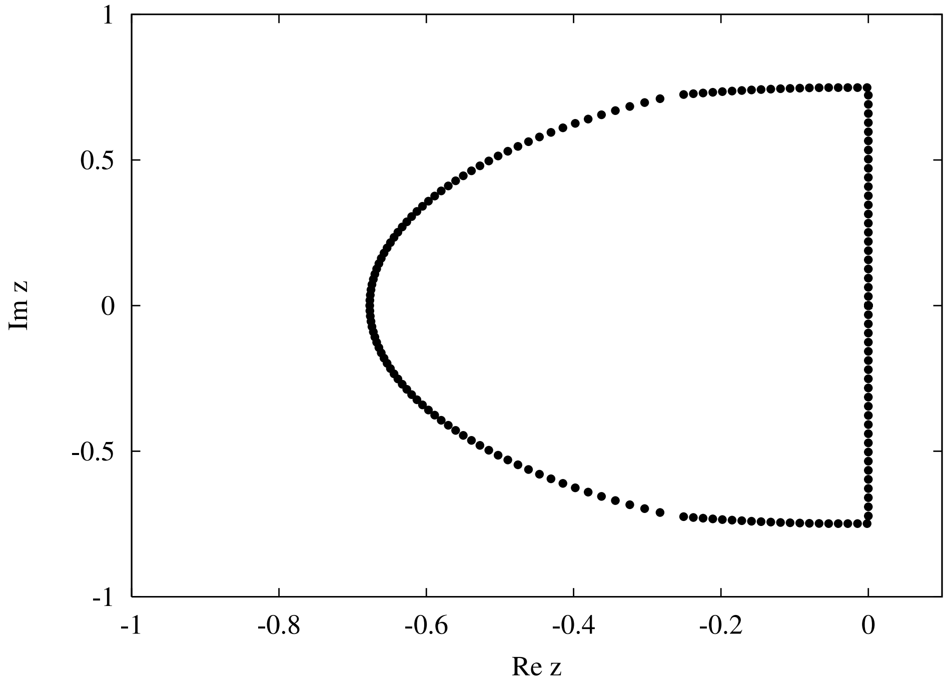

Figure 2: Stability region of method Peer1.

With the more general matrix B from (17) the simple Nordsieck form (16) is no longer valid, we get instead

$$\begin{pmatrix} Y_m \\ Z_m \end{pmatrix} = \begin{pmatrix} R & B & CV_0 - RV_0 D \\ D^{-1}V_1^{-1} & 0 & 0 \end{pmatrix} \begin{pmatrix} h_m F_m \\ Y_{m-1} \\ \sigma_m S Z_{m-1} \end{pmatrix} - \begin{pmatrix} 0 & 0 & B(C-I)V_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ Z_{m-1} \end{pmatrix}$$

This formula was used in our MATLAB implementation of the Peer methods. The error estimation is performed with respect to the last stage Y_{ms}. With Z_{m-1} according to (15) an embedded solution

$$\widehat{Y}_{ms} = Y_{m-1,s} + \sigma_m S \sum_{j=1}^{p-1} Z_{m-1,j}$$

of order $p-1$ is computed and used for stepsize control. The new stepsize h_{new} is computed in classical manner with the restriction $0.2h \leq h_{new} \leq 1.5h$. Note that by appropriate scaling the Taylor coefficients in Z_{m-1} can be used easily for dense output of order p.

The starting values for the peer methods are computed with a slightly modified version of DOPRI5. To avoid computations with negative stepsizes we proceed as follows: At first we compute Y_{0s} with DOPRI5 by one step with starting stepsize h_D, where h_D is

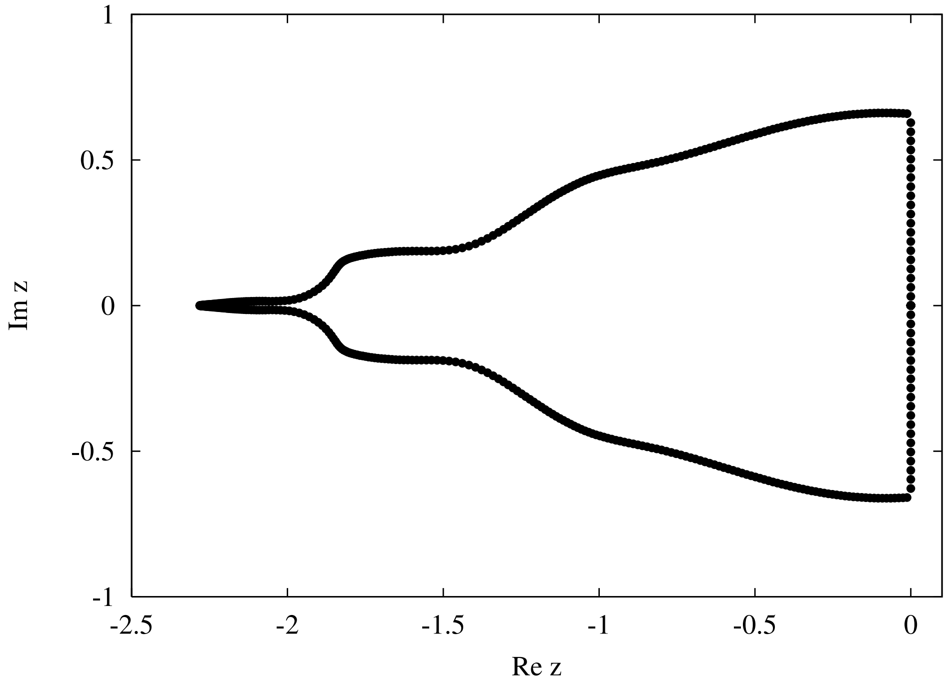

Figure 3: Stability region of method Peer2.

automatically reduced by the built-in error estimation in DOPRI5, if necessary. Then we compute approximations Y_{0i} for $y(t_0 + \delta_i h_D)$, $i = 2, ..., s-1$, without stepsize control, where

$$\delta_i = \frac{c_i - c_1}{1 - c_1},$$

and set $Y_{01} = y_0$ since c_1 is the minimal node. This means that the starting interval of the peer method does not begin at t_0 from (1), but it is shifted such that the first node $t_1 + (c_1 - 1)h_D$ coincides with the begin of the interval of integration. For the first step with the peer method starting at $t_1 = t_0 + h_D$ we set $h_1 = h_D/(1 - c_1)$. The computed values Y_{0i} are then just the needed approximations for $y(t_1 + (c_i - 1)h_1)$. Since we use the initial value as very first stage $Y_{01} = y_0$ we need only 5 computations with DOPRI5. It is possible to reduce the effort for the starting procedure by using the dense output of DOPRI5, but in our tests we did not do this to eliminate possible sources of inaccuracies.

5 Numerical results

We tested the methods Peer1 and Peer2 on several well known test examples for nonstiff systems and compared them with ODE45. The problems are the following:

ORBIT, the orbit problem from [6], 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 [7] (with same names and parameters): AREN, BRUS, LRNZ and PLEI.

We have solved these problems with $rtol = atol$ for $atol = 10^{-i}$, $i = 2, ..., 12$. In the following figures we present the number of function evaluations (FCN) and the logarithm of the obtained accuracy at the endpoint

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

where y is the numerical solution and y_{ref} a reference solution which, except for ORBIT, is computed with ODE45 and high accuracy.

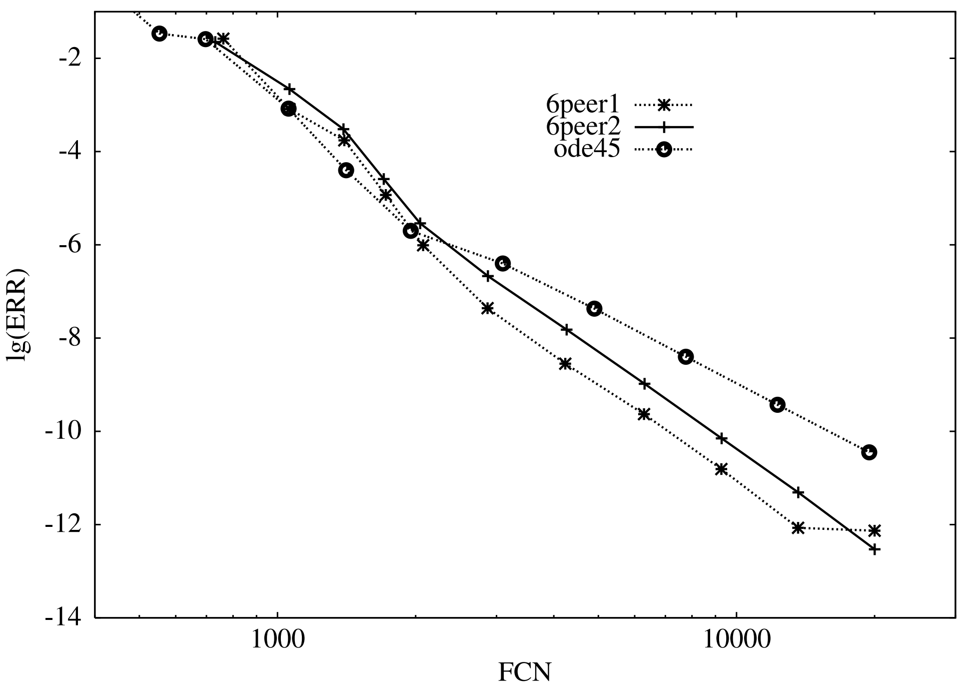

Figure 4: Results for ORBIT.

The results show that the explicit two-step peer methods compete well with ODE45. Due to their higher order (obtained with the same number of function evaluations) they perform better than ODE45 at all problems for most tolerances. Especially at LRNZ they are clearly superior. The stepsize control works well for all problems. Sometimes, for very stringent tolerances, the precision of MATLAB is not sufficient and the error levels out at certain accuracies. In computations in Delphi with extended precision up to $atol = 10^{-14}$ this behaviour was not observed.

The smaller stability region of Peer1 does not seem to be a drawback for these nonstiff problems, except for the MOL problem BRUS, where Peer2 is superior for all tolerances.

6 Conclusions

The results show that two-step peer methods are a promising class of numerical methods also for nonstiff problems. It is straightforward to derive s-stage methods of order $p = s$ with

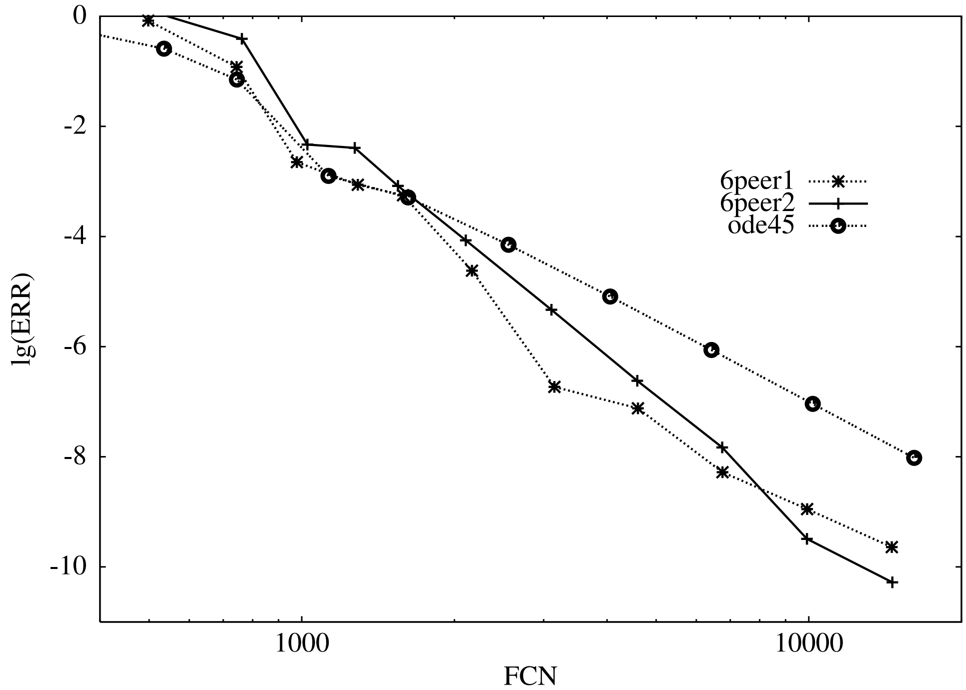

Figure 5: Results for AREN.

optimal zero-stability. However, the determination of free parameters to obtain methods with large stability region and good properties for variable stepsizes is a difficult task. By random walk search we have found two suitable methods which are competitive with established nonstiff solvers like ODE45. A more refined search may still lead to more efficient methods.

Some directions for further investigations are parallel methods ($R = 0$), methods of even higher order and finally a variable order code.

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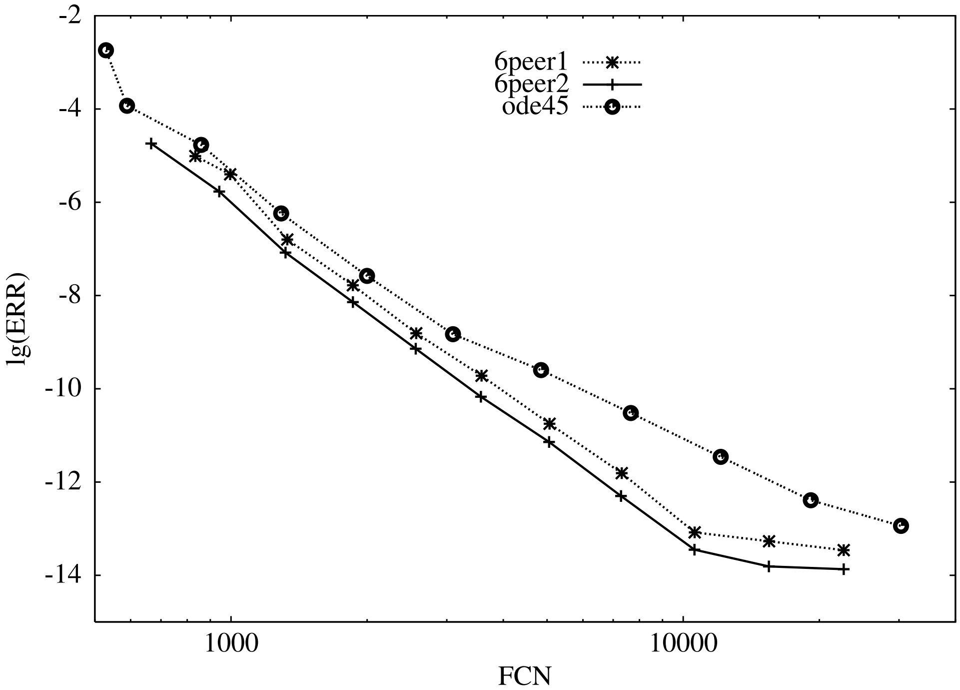

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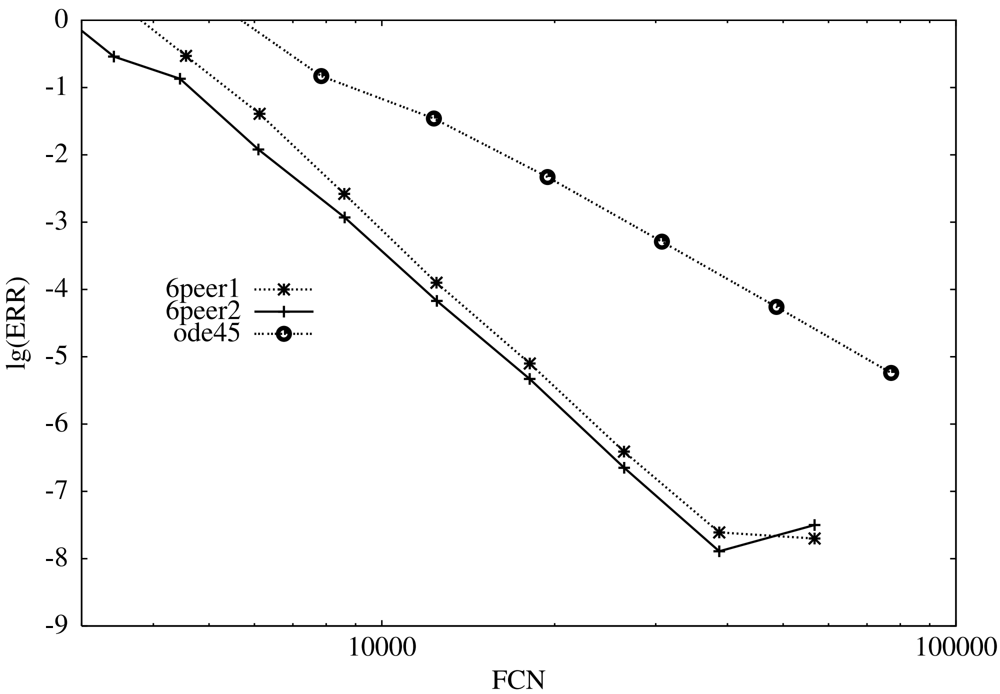

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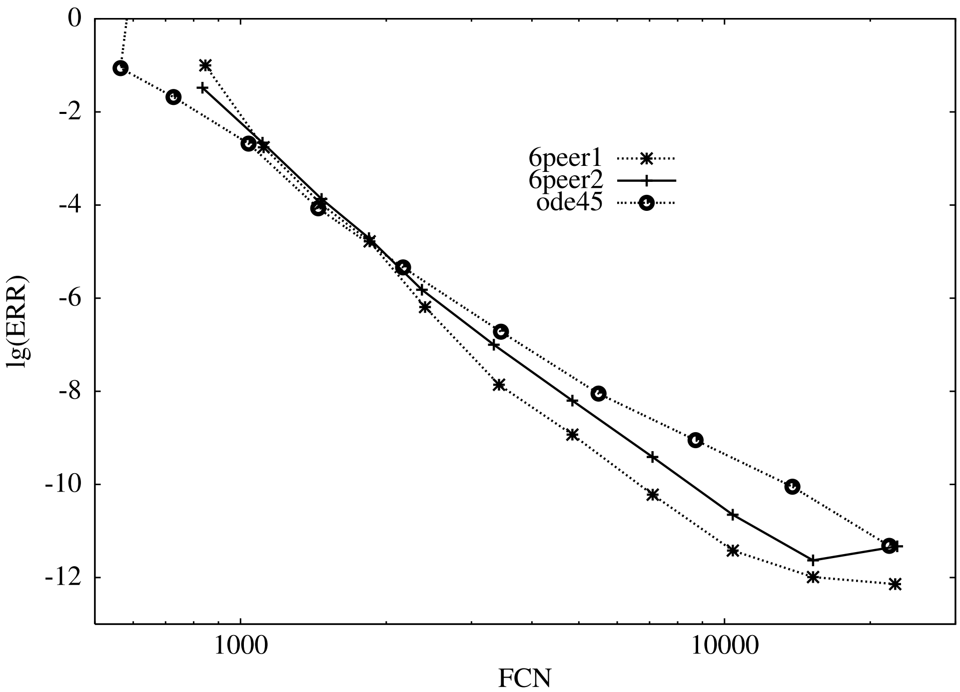

Figure 8: Results for PLEI.