Explicit parallel two-step peer methods

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Abstract

The construction of s-stage explicit parallel two-step peer methods for the solution of non-stiff initial value problems with optimal zero stability and order $p = s$ is considered. By an additional condition superconvergence of order $p = s + 1$ can be achieved. Further criteria for good methods are large stability regions and small error constants. Corresponding parameter sets have been obtained using the differential evolution genetic algorithm. Numerical tests of the parallel peer methods in MATLAB and comparisons with ODE45 show the efficiency of the proposed methods already in a sequential implementation.

Keywords. Explicit peer methods, nonstiff ODE systems, stability region, parallel methods for ODEs.

1 Introduction

Many efficient methods have been developed for the numerical solution of nonstiff ordinary differential equations. 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, which is also the basis of the MATLAB routine ODE45 [10], and the multistep code VODE [2]. The respective advantages of one-step and multistep methods are well known, cf. the text book of Hairer, Nørsett and Wanner [4].
With parallel implementation in mind the class of peer methods has been introduced by some of the authors in a series of papers, e.g. [7], [8], [9],

which concentrated on stiff problems and linearly-implicit and implicit two-step methods. Peer methods possess several stages like Runge-Kutta-type methods, but their new feature is that all of these stages have the same properties and no extraordinary solution variable is used.
In [12] sequential explicit peer methods for nonstiff problems were introduced. Numerical tests have shown their efficiency compared e.g. with ODE45. "Classical" explicit two-step Runge-Kutta schemes have been considered for instance by Jackiewicz/Zennaro [5] and Tracogna/Welfert [11], and in the context of general linear methods by Jackiewicz/Tracogna [6] and Wright [13].
In this paper we will focus on parallel explicit peer methods. We present a special strategy to derive optimally zero-stable methods with s stages and order $p = s$. For $s = 6$ we construct parallel methods of order $p = 6$ which are superconvergent of order $p = 7$ for constant stepsizes. To show the potential of these methods they are compared in a sequential implementation with a sequential explicit peer method from [12] and with ODE45.
The paper is organized as follows: In Section 2 we formulate the class of explicit two-step peer methods.
In Section 3 we give order results and consider stability properties. By a special choice of the coefficients we ensure optimal zero stability. Under additional assumptions we prove superconvergence of order $p = s + 1$.
In Section 4 we describe how the search for the remaining coefficients is performed by genetic algorithms to find good methods with $s = 6$ stages. We present two methods found by this search and their stability regions and error coefficients. These methods are of order $p = 6$ for variable and $p = 7$ for constant stepsizes.
Section 5 is devoted to the numerical results of a MATLAB code for several widely accepted non-stiff test problems. Comparisons with the MATLAB code ODE45 show the efficiency of the methods.
Finally we give some conclusions and an outlook for future work.

2 Formulation of the methods

We consider the numerical solution of non-stiff initial value problem

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

We will always assume that f is smooth with bounded derivatives. Introducing stage approximations

$$Y_{mi} \approx y(t_m + c_i h_m)$$

to the analytical solution y at off-step points $t_m + c_i h_m$ of a grid $t_0, t_1 = t_0 + h_0, \ldots$ we discuss s-stage explicit two-step peer methods from [12] defined by

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

Collecting the stages and function values as rows of $s \times n$ matrices

$$Y_m = (Y_{mi})_{i=1}^{s} \in \mathbb{R}^{s \times n}, \; F(Y_m) = (f(Y_{mi}))_{i=1}^{s},$$

and introducing the coefficient matrices

$$A = (a_{ij}),\; B = (b_{ij}),\; R = (r_{ij})$$

we can write the methods in the compact form

$$Y_m = BY_{m-1} + h_m AF(Y_{m-1}) + h_m RF(Y_m). \tag{1}$$

Note that in general the matrices A, B, R depend on the stepsize ratio $\sigma_m = h_m / h_{m-1}$.

Remark 1: The formulation for non-autonomous problems is straightforward. $\square$

Remark 2: New methods are not obtained by introducing recently computed stages $\sum_{j<i} q_{ij} Y_{mj}$ in the actual timestep. This is seen by the transformations $\widetilde{A} := (I - Q)^{-1} A$, $\widetilde{B} := (I - Q)^{-1} B$ and $\widetilde{R} := (I - Q)^{-1} R$ since the method

$$Y_m = BY_{m-1} + h_m AF(Y_{m-1}) + h_m RF(Y_m) + QY_m$$

is equivalent to

$$Y_m = \widetilde{B} Y_{m-1} + h_m \widetilde{A} F(Y_{m-1}) + h_m \widetilde{R} F(Y_m). \qquad \square$$

Parallel methods are obtained by the choice $R = 0$ eliminating any reference to the stages Y_m of the actual step. In this case the s stage approximations Y_{mi}, $i = 1, \ldots, s$, and in particular the s function evaluations, can be computed in parallel on s processors. In this paper we will focus on the construction of parallel methods. For the theoretical investigations, however, we consider the general case $R \neq 0$.

3 Order and stability

The local residuals are defined by

$$h_m \triangle_{mi} := y(t_{mi}) - \sum_{j=1}^{s} b_{ij} y(t_{m-1,j}) - h_m \sum_{j=1}^{s} a_{ij} y'(t_{m-1,j})$$

$$-h_m \sum_{j=1}^{i-1} r_{ij} y'(t_{mj}), \qquad i = 1, \ldots, s.$$

Definition 1: A two-step method has order of consistency p if

$$\triangle_{mi} = \mathcal{O}(h_m^p), \qquad i = 1, \ldots, s. \qquad \square$$

In a Taylor expansion of the local residuals the following terms appear

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

$$\text{with} \quad \sigma = \sigma_m := \frac{h_m}{h_{m-1}} \qquad \text{for} \quad i = 1, \ldots, s.$$

They yield sufficient conditions for the consistency of peer methods.
Theorem 1. An explicit two-step peer method (1) has order of consistency p if the conditions

$$AB(l) = 0, \qquad l = 0, \ldots, p$$

are satisfied. $\square$
For order $p = s$ the conditions of the theorem can be conveniently cast in matrix form. With the notations $\mathbb{1} = (1, \ldots, 1)^T$, $\mathbf{c}^k = \left(c_i^k\right)_{i=1}^s$, $(\mathbf{c} - \mathbb{1})^k = \left((c_i - 1)^k\right)_{i=1}^s$,

$$D = \mathrm{diag}(1, \ldots, s), \quad \widehat{D} = \mathrm{diag}(0, 1, \ldots, s),$$

$$S = \mathrm{diag}(1, \sigma, \ldots, \sigma^{s-1}), \quad \widehat{S} = \mathrm{diag}(1, \sigma, \ldots, \sigma^s),$$

we obtain order of consistency $p = s$ if the $s \times (s+1)$ matrix system

$$\Big(\mathbb{1}, \mathbf{c}, \ldots, \mathbf{c}^s\Big) - B\Big(\mathbb{1}, \mathbf{c} - \mathbb{1}, \ldots, (\mathbf{c} - \mathbb{1})^s\Big)\widehat{S}^{-1}$$

$$-A\Big(0, \mathbb{1}, \cdots, (\mathbf{c}-\mathbb{1})^{s-1}\Big)\widehat{D}\begin{pmatrix} 0 & 0 \\ 0 & S^{-1} \end{pmatrix} - R\Big(0, \mathbb{1}, \cdots, \mathbf{c}^{s-1}\Big)\widehat{D} = 0$$

is satisfied. This system is equivalent to

$$B\mathbb{1} = \mathbb{1} \qquad \text{and}$$
$$A = (CV_0S - RV_0DS - \frac{1}{\sigma}B(C-I)V_1)D^{-1}V_1^{-1}$$

where

$$C = \mathrm{diag}(c_i), \quad V_0 = (c_i^{j-1})_{i,j=1}^{s} = \big(\mathbb{1}, \mathbf{c}, \ldots, \mathbf{c}^{s-1}\big), \quad V_1 = ((c_i-1)^{j-1})_{i,j=1}^{s}.$$

Applying the peer method with constant stepsize to the test equation $y' = \tilde{\lambda}y$ gives the recursion

$$Y_m = BY_{m-1} + zAY_{m-1} + zRY_m, \quad z = h\tilde{\lambda},$$

which can be solved for Y_m by

$$Y_m = (I - zR)^{-1}(B + zA)Y_{m-1} = M(z)Y_{m-1}. \tag{2}$$

The factor $M(z)$ is the stability matrix

$$M(z) = (I - zR)^{-1}(B + zA).$$

Considering the recursion (2) with step-dependent coefficient matrices B_m leads to severe theoretical problems concerning the uniform boundedness of its solutions even for $z = 0$. These problems are avoided with a constant matrix B.

Definition 2. A peer method with constant coefficient matrix B is zero stable if

$$\exists L > 0 \quad \forall m \geq 0 \qquad \|B^m\| < L. \qquad \square$$

The boundedness in Definition 2 holds if the method has optimal zero stability, which means that the eigenvalues of $M(0) = B$ are given by

$$\lambda_1 = 1, \quad \lambda_2 = \ldots = \lambda_s = 0. \tag{3}$$

Definition 3. The stability region of the peer method is defined by

$$S := \{z \in \mathbb{C} : \rho(M(z)) < 1\}. \qquad \square$$

There are many free parameters left for a zero stable explicit two-step peer method of order $p = s$. Our strategy to find good methods is based on chosing coefficient matrices B with the following properties:

- B is fixed and independent of the stepsize ratio σ.
- B satisfies the order condition $B\mathbb{1} = \mathbb{1}$.
- The method is optimally zero stable, i.e. B has the eigenvalues (3).

Theorem 2. Let B given by

$$B = \mathbb{1}v^T + QWQ^{-1} \tag{4}$$

where

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

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

and $\widetilde{W}$ is strictly upper triangular, $\widetilde{Q}$ regular.
Then, the method is optimally zero stable and has the properties

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

Proof. By ansatz the equations

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

are satisfied. This implies

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

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 $v^T\mathbb{1} = 1$, $WQ^{-1}\mathbb{1} = W\mathbb{1} = 0$ and the nilpotency of W it is straightforward to obtain the second property

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

The following theorem states conditions for convergence of order $p = s$ and for superconvergence of order $p = s+1$. For simplicity of notation we consider the case $n = 1$. We denote by

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

the global error at timestep m to the exact solution $Y(t_m) := (y(t_{mi}))_{i=1}^s$.
Theorem 3. Let $h := \max_m h_m$, $\max_m \sigma_m \le \sigma_{max}$, $\varepsilon_0 = \mathcal{O}(h_0^s)$. Let B be a fixed matrix of the form (4) and the strictly lower triangular matrices R_m be uniformly bounded for $\sigma \le \sigma_{max}$, and

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

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

$$v^T AB(s+1) = 0 \tag{5}$$

hold then we have superconvergence of order $p = s+1$, i.e. $\|\varepsilon_m\| \le dh^{s+1}$.
Proof. 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.
Let now in addition (5) be satisfied. For the global error we have the equation

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

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

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

So we obtain the vector equation

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

and analogously

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

So, the error recursion becomes

$$\varepsilon_m = B\varepsilon_{m-1} + h_{m-1}\sigma_mG_m\varepsilon_{m-1} + h_mH_m\varepsilon_m + h_m\Delta_m.$$

By repeated substitution we obtain

$$\begin{aligned}\varepsilon_m =& B^m\varepsilon_0 + \sum_{j=0}^{m-1} h_{m-j-1}\sigma_{m-j}B^j G_{m-j}\varepsilon_{m-j-1} \\ &+ \sum_{j=0}^{m-1} h_{m-j}H_{m-j}\varepsilon_{m-j} + \sum_{j=0}^{m-1} h_{m-j}B^j\Delta_{m-j}. \end{aligned} \tag{6}$$

Using assumption (5) in the last term leads to

$$\begin{aligned}\sum_{j=0}^{m-1} h_{m-j}B^j\Delta_{m-j} &= \sum_{j=s-1}^{m-1} h_{m-j}B^j\Delta_{m-j} + \sum_{j=0}^{s-2} h_{m-j}B^j\Delta_{m-j} \\ &= \mathbb{1}v^T \sum_{j=s-1}^{m-1} h_{m-j}\Delta_{m-j} + \mathcal{O}(h^{s+1}) = \mathcal{O}(h^{s+1}). \end{aligned} \tag{7}$$

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

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

This yields

$$\begin{aligned}\|\sum_{j=0}^{m-1} B^j\sigma_{m-j}G_{m-j}h_{m-j-1}\varepsilon_{m-j-1} + \sum_{j=0}^{m-1} B^j H_{m-j}h_{m-j}\varepsilon_{m-j}\| \\ \le ch_0\|\varepsilon_0\| + 2c\sum_{j=1}^{m-1} h_j\|\varepsilon_j\| + ch_m\|\varepsilon_m\|.\end{aligned}$$

From order of convergence s, i.e. $\varepsilon_m = \mathcal{O}(h^s)$, $\varepsilon_0 = \mathcal{O}(h_0^{s+1})$ and with (7) follows from (6)

$$\|\varepsilon_m\| \le 2c\sum_{j=1}^{m-1} h_j\|\varepsilon_j\| + dh^{s+1}, \quad m \ge 1. \tag{8}$$

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

$$1 + \sum_{j=1}^{m-1} X_{m-j} \prod_{l=1}^{m-j-1}(1+X_l) = \prod_{l=1}^{m-1}(1+X_l) \tag{9}$$

Using this equation allows us to prove the inequality

$$\|\varepsilon_m\| \le \prod_{l=1}^{m-1}(1+2ch_l)dh^{s+1}$$

with $X_l = 2ch_l$ by induction.
For $m = 1$ (8) means $\|\varepsilon_1\| \le dh^{s+1}$ and therefore the assertions holds here.
Now let the inequality be satisfied for $j \le m-1$, $\|\varepsilon_j\| \le \prod_{l=1}^{j-1}(1+2ch_l)dh^{s+1}$.
Then, (8) gives

$$\begin{aligned}
\|\varepsilon_m\| &\le 2c\sum_{j=1}^{m-1} h_j\|\varepsilon_j\| + dh^{s+1} \\
&\le \Big(1 + 2c\sum_{j=1}^{m-1} h_j \prod_{l=1}^{j-1}(1+2ch_l)\Big)dh^{s+1} \\
&= \prod_{l=1}^{m-1}(1+2ch_l)dh^{s+1} \quad \text{by (9)} \\
&\le \prod_{l=1}^{m-1} e^{2ch_l}dh^{s+1} \le e^{2c(t_e-t_0)}dh^{s+1}.
\end{aligned}$$

This means superconvergence of order $p = s+1$. ■
So, an alternative to requiring all s conditions AB(s+1) for global order $s+1$ is the equation (5) which is only one additional restriction for the coefficients. The following example gives a class of methods which fulfill the assumptions of Theorem 3 for arbitrary stepsize ratios σ even with a constant matrix R.
Example 1. Consider the simple case $B = \mathbb{1}e_s^T$, i.e. $v = e_s$. With the choice $c_s = 1$ we have $B(C-I) = 0$ and A simplifies to

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

The superconvergence condition (5) becomes

$$\begin{aligned}
0 &= 1 - \frac{s+1}{\sigma^s}e_s^T A(\mathbf{c}-\mathbb{1})^s - (s+1)e_s^T Rc^s \\
&= 1 - \frac{s+1}{\sigma^s}e_s^T (CV_0D^{-1} - RV_0)SV_1^{-1}(\mathbf{c}-\mathbb{1})^s - (s+1)e_s^T Rc^s
\end{aligned}$$

For constant R this is satisfied if (after multiplying with σ^s) the coefficients at σ^l vanish for $l = 0, ..., s$. One immediately obtains the sufficient condition

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

We note that the first s equations here, $e_s^T R V_0 D = \mathbb{1}^T$, lead to a trivial last row of A. A closer look shows that the condition for σ^0 is redundant due to

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

This property can be derived as follows. The system

$$\Big(1, \mathbf{c} - \mathbb{1}, \ldots, (\mathbf{c} - \mathbb{1})^{s-1}\Big)\psi + (\mathbf{c} - \mathbb{1})^s = V_1 \psi + (\mathbf{c} - \mathbb{1})^s = 0$$

is satisfied by the coefficient vector $(\psi_0, \ldots, \psi_{s-1})^T$ of the polynomial $t^s + \sum_{k=0}^{s-1} \psi_k t^k = \prod_{i=1}^{s} (t - c_i + 1)$ which vanishes at $t = 0$ since $c_s = 1$. Hence, $0 = \psi_0 = e_1^T V_1^{-1} (c - \mathbb{1})^s$.
We finally arrive at the following conditions for superconvergence of order $p = s + 1$:

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

For $s = 2$ we obtain $r_{21} = 3/4$, $c_1 = 2/3$. For larger s there is more freedom to choose the coefficients. $\square$
It is not clear if there exist parallel methods which satisfy (5) for variable stepsizes ($\sigma \neq 1$). However, in the next section we will present parallel methods which fulfill (5) for $\sigma = 1$ and therefore are superconvergent for constant stepsizes. We expect that these methods will have advantages also in the case of slowly changing stepsizes, e.g. for stringent tolerances. This is confirmed by our numerical results in Section 5.

4 Method search

We investigate parallel methods where $R = 0$ with $s = 6$ stages. By setting $c_6 = 1$ the last stage Y_{ms} is an approximation of $y(t_{m+1})$. Now the remainig 45 coefficients have to be chosen:

$$c_1, \ldots, c_5, \quad v_1, \ldots, v_5, \quad \widetilde{W}, \quad \widetilde{Q}$$

The main criterion in our search is a small value of the coefficient $v^T AB(s+1)$ for $\sigma = 1$ because the equation $v^T AB(s+1) = 0$ would guarantee us superconvergence of order 7 for constant stepsizes. Another criterion is a large stability region. We test the stability of the methods on some simple curves in the complex plane to ensure well shaped and sufficiently large stability regions. Another criterion is concerned with the growth of round-off errors which is less severe if the method coefficients are small. The main source of large coefficients is the term $D^{-1}V_1^{-1}$ in the matrix A. Therefore a small value $vmax$ defined by

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

is another objective of our search.
Due to the complicated dependence of our criteria from the method parameters the optimization of the free parameters is a difficult task. We decided to use a random walk strategy called Differential Evolution, see [1]. This method is a genetic algorithm: It takes random linear combinations of parent parameter sets to create new child sets by

$$B_{\text{child}} = B_{\text{parent1}} + r(B_{\text{parent2}} - B_{\text{parent3}}),$$

where we used

$$0.6 < r < 0.9.$$

Then the new parameter set is compared with one old parameter set (which does not have to be one of the parent sets) and the child set replaces this old set if it fulfills the aims better than the old one.
In the numerical tests we will compare two parallel methods found by this strategy with a sequential two-step peer method (Peer1 from [12]) and DOPRI5. The parallel methods Peer2 and Peer3 have the following coefficients:
Peer2:

$$\begin{array}{llll}
c_1 = 0.6118248815846032, & c_2 = 1.0734784354567433, & c_3 = 1.7733348046756701, \\
c_4 = 1.9723174701317718, & c_5 = 1.4155260278449762, & c_6 = 1, \\
b_{11} = -0.0002018014618169, & b_{12} = 0.0163046148021061, & b_{13} = -0.0128515448163182, \\
b_{14} = 0.0026210658256846, & b_{15} = 0.0037912816867902, & b_{16} = 0.9903363839635542, \\
b_{21} = 0.0000544024471988, & b_{22} = 0.0002461809574527, & b_{23} = 0.0041283950478615, \\
b_{24} = 0.0010819600004067, & b_{25} = -0.0064960842108611, & b_{26} = 1.0009851457579413, \\
b_{31} = -0.0001328308941648, & b_{32} = 0.0002658525002543, & b_{33} = -0.0003998575435093,
\end{array}$$

$b_{34} = -0.0145129321795745$, $b_{35} = 0.0102211440356485$, $b_{36} = 1.0045586240813458$,
$b_{41} = 0.0001957981480035$, $b_{42} = -0.0001497912121220$, $b_{43} = 0.0001414730364895$,
$b_{44} = -0.0001814296594351$, $b_{45} = -0.0178068457426533$, $b_{46} = 1.0178007954297175$,
$b_{51} = -0.0000076319822224$, $b_{52} = 0.0001817796323311$, $b_{53} = -0.0001755381239482$,
$b_{54} = -0.0000406141572347$, $b_{55} = 0.0005369077073085$, $b_{56} = 0.9995050969237656$,
$b_{61} = 0$, $b_{62} = 0$, $b_{63} = 0$,
$b_{64} = 0$, $b_{65} = 0$, $b_{66} = 1$.

Peer3:

$c_1 = -1.5059380428823135$, $c_2 = 1.8868474949714833$, $c_3 = 1.4970866313843472$,
$c_4 = 1.1159258232229363$, $c_5 = -0.1970136127048126$, $c_6 = 1$,
$b_{11} = -0.0225785693967892$, $b_{12} = 0.0013253766595541$, $b_{13} = -0.0036530922022752$,
$b_{14} = -0.0142699859919805$, $b_{15} = -0.0044014437941312$, $b_{16} = 1.0435777147256222$,
$b_{21} = 1.7214162000456492$, $b_{22} = 0.0224962010656484$, $b_{23} = 0.1996960330718455$,
$b_{24} = 0.0612836240529984$, $b_{25} = 0.2234734056129229$, $b_{26} = -1.2283654638490646$,
$b_{31} = 0.2508149083793880$, $b_{32} = -0.0418880552349988$, $b_{33} = -0.0028929498879621$,
$b_{34} = 0.1407936710151073$, $b_{35} = -0.0836831719273983$, $b_{36} = 0.7368555976558639$,
$b_{41} = 0.0074550750188110$, $b_{42} = -0.0071762422454037$, $b_{43} = -0.0118722084841789$,
$b_{44} = -0.0041355648188329$, $b_{45} = -0.0366243529130506$, $b_{46} = 1.0523532934426554$,
$b_{51} = -0.0002922158511566$, $b_{52} = 0.0178989600408910$, $b_{53} = -0.0014837042405599$,
$b_{54} = -0.1241240433452149$, $b_{55} = 0.0071108830379358$, $b_{56} = 1.1008901203581045$,
$b_{61} = 0$, $b_{62} = 0$, $b_{63} = 0$,
$b_{64} = 0$, $b_{65} = 0$, $b_{66} = 1$.

These methods have the following properties (for $\sigma = 1$):

method	s	order	$v^T AB(\text{s+1})$	max $\lvert AB_i(s+1)\rvert$	v_{max}
Peer2	6	7	0	24.7	48.6
Peer3	6	7	0	$1{\cdot}10^{-11}$	7.2

The stability regions are given in Figure 1.

5 Numerical tests

We tested the methods Peer2 and Peer3 on several well known test examples for nonstiff systems in a sequential implementation and compared them with the sequential methods Peer1 from [12] and ODE45 [10] in MATLAB. The problems are the following:

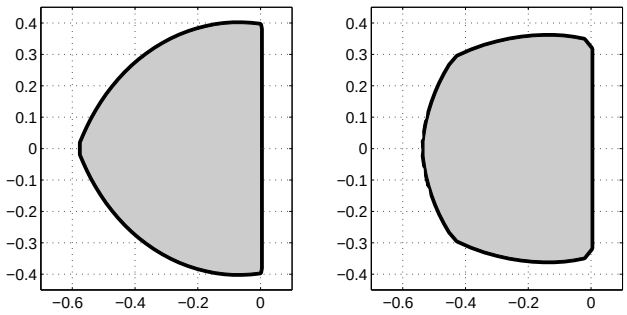

Figure 1: Stability region of Peer2 (left) and Peer3 (right).

ORBIT, the orbit problem from [3], 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 [4] (with same names and parameters): AREN, BRUS, LRNZ and PLEI.
The starting values are computed with DOPRI5, for a detailed description of the starting procedure see [12].
The stepsize control of the peer methods is realized by error estimation with an embedded solution $\widehat{Y}$ of order $s - 1$:

$$err = \max_k \frac{|Y_{ms}^{(k)} - \widehat{Y}_{ms}^{(k)}|}{atol + rtol \cdot \max\{|Y_{ms}^{(k)}|, |\widehat{Y}_{ms}^{(k)}|\}}$$

$$h_{m+1} = \min\{amax, \max\{amin, a \cdot (\frac{1}{err})^{\frac{1}{s}}\}\} \cdot h_m$$

Stepsize increase is bounded by $amax = 1.5$. The other parameters are $a = 0.85$, $amin = 0.2$, $atol = rtol$. For the numerical tests we used the tolerances

$$rtol = 10^{-k} \qquad k = 3, \ldots, 13.$$

In the following figures we present the number of function evaluations (FCN) and the logarithm of the obtained accuracy at the endpoint

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

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

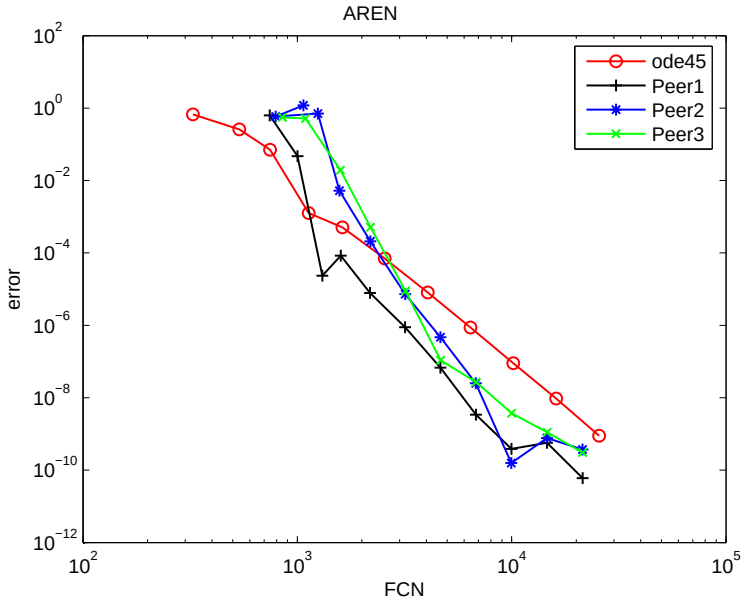

Figure 2: Results for AREN.

The results show the efficiency of the new parallel methods already in a sequential implementation. The sequential method Peer1 performs slightly better than the parallel methods, especially for crude tolerances. The relative performance of the parallel peer methods varies with the test problem but for stringent tolerances they are at least comparable to ODE45. The mild stiffness of the Brusselator shows up in Figure 3 where the smaller stability region slows down the parallel methods and here also the largest difference between Peer2 and Peer3 is observed. On the other hand, at the Lorenz attractor the peer methods clearly outperform ODE45.

6 Conclusions

We considered parallel zero stable 6-stage peer methods with order of consistency $p = s = 6$ and used the free parameters to obtain superconvergence of order $p = s + 1 = 7$ for constant stepsizes and large stability regions. By a parameter search with the Differential Evolution algorithm we found 2 suitable methods. Numerical results on several standard test problems show

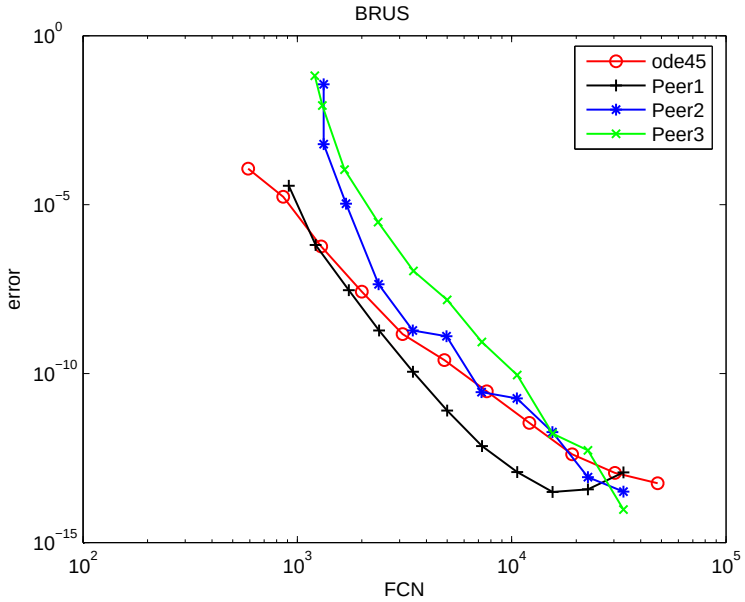

Figure 3: Results for BRUS.

the efficiency of these peer methods. Even in a sequential implementation the parallel peer methods perform better than ODE45 at high tolerances. Forthcoming tests on a parallel computer will show what performance can be expected in parallel implementations. Due to the highly parallel structure of the peer methods we expect a speed-up nearly s on problems with expensive right-hand sides.

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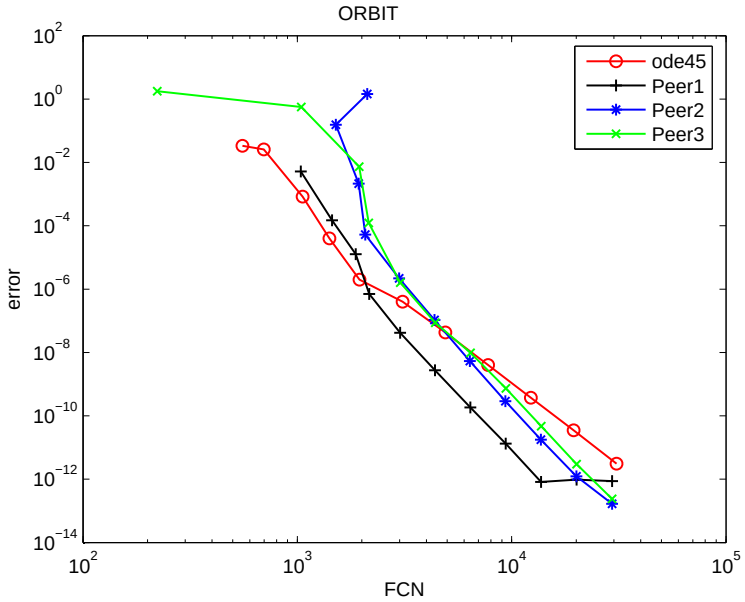

Figure 4: Results for ORBIT.

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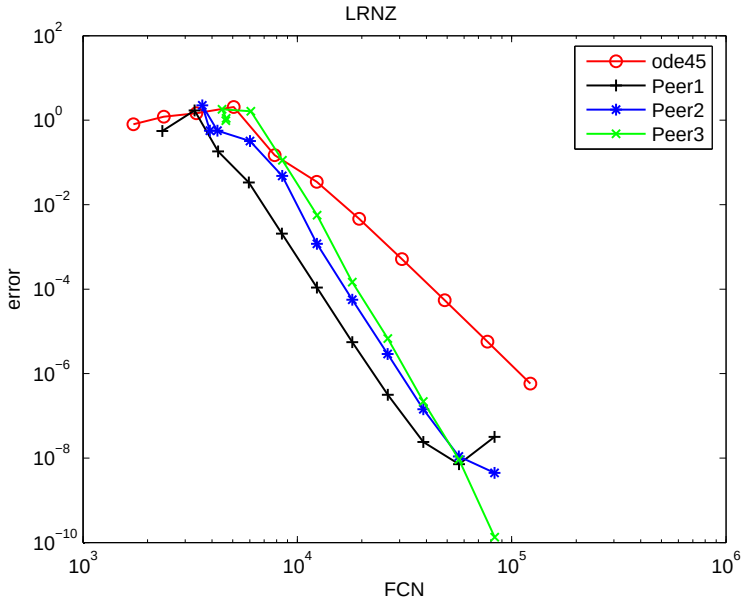

Figure 5: Results for LRNZ.

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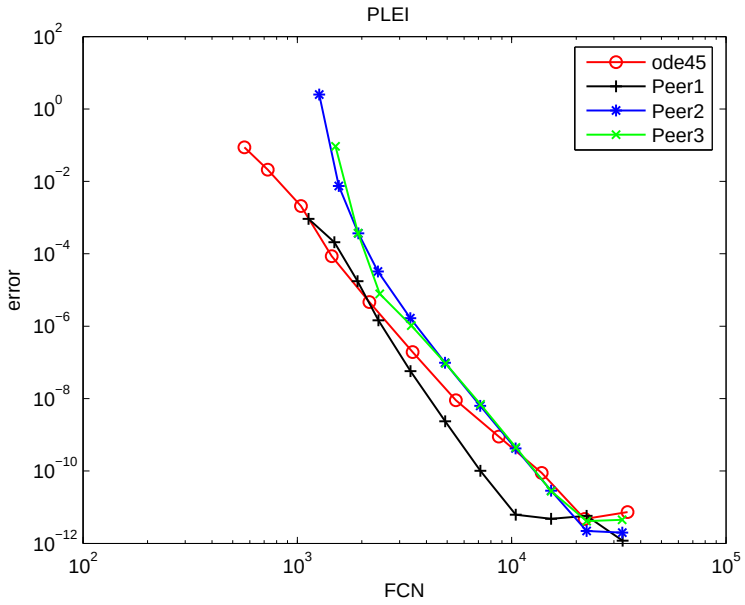

Figure 6: Results for PLEI.