Explicit multi-step peer methods for special second order differential equations

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Abstract

The construction of s-stage explicit two- and three-step peer methods of order $p = 2s$ and $p = 3s$ is considered for the solution of non-stiff second order initial value problems where the right-hand side does not depend on y'. By additional conditions superconvergence of order $p + 1$ can be achieved. Further criteria for good methods are large stability intervals and small error constants. Numerical tests of these peer methods in MATLAB and comparisons with a Runge-Kutta-Nyström method show the efficiency of the proposed methods.

Keywords. Explicit peer methods, non-stiff second order ODE systems, parallel methods for ODEs, Runge-Kutta-Nyström methods

1 Introduction

In this paper we consider explicit two- and three-step peer methods for the solution of second order differential equations where the right-hand side does not depend on y'. Second order differential equations appear in many applications particularly in physical problems. For problems with negligible friction, like celestial mechanics problems, one

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often has to solve those special second order differential equations.
Explicit peer methods for the solution of first order differential equations demonstrated their efficiency in [1], [8], [9] and [7]. The peer property means that all stages of the method have similar properties, for instance, the same order. Hence, these methods may easily provide dense output. A subclass of these methods also allows parallel implementation. In this paper we will consider peer methods for second order equations.

This paper is organized as follows: In Section 2 we formulate the classes of explicit two- and three-step peer methods.
In Section 3 we consider the theory of multi-step peer methods, addressing order conditions, stability and convergence. We construct methods which are optimally zero stable and present a condition for superconvergence.
Implementation issues are discussed in Section 4, for instance, how to avoid regularity difficulties which arise in the implementation of high order peer methods.
In Section 5 we present eight peer methods and their properties like error constants and stability intervals. We test these peer methods on widely accepted test problems and compare them with a Runge-Kutta-Nyström method.
Finally we give some conclusions and an outlook for future work.

2 Formulation of the methods

Explicit two-step peer methods for first order problems were considered in [1] and [8], in parallel form also in [9] and [7]. The second order differential equation

$$y'' = f(t, y),\ t \in [t_0, t_e], \qquad y(t_0) = y_0 \in \mathbb{R}^n,\ y'(t_0) = y'_0 \in \mathbb{R}^n \tag{1}$$

may be replaced by a system of first order. Applying a standard peer method to this first order system we obtain

$$\begin{pmatrix} Y_m \\ Z_m \end{pmatrix} = \begin{pmatrix} B & 0 \\ 0 & B \end{pmatrix} \begin{pmatrix} Y_{m-1} \\ Z_{m-1} \end{pmatrix} + h_m \begin{pmatrix} A & 0 \\ 0 & A \end{pmatrix} \begin{pmatrix} Z_{m-1} \\ F_{m-1} \end{pmatrix} + h_m \begin{pmatrix} R & 0 \\ 0 & R \end{pmatrix} \begin{pmatrix} Z_m \\ F_m \end{pmatrix}.$$

The method uses time steps of length $h_m = t_m - t_{m-1}$ and its s stages are associated with solution values at offstep points $t_{mi} = t_m + h_m c_i$, $i = 1, \ldots, s$. We used the notations

$$\begin{aligned} &Y_m := (Y_{mi})_{i=1}^s \in \mathbb{R}^{s\times n} && \text{with} && Y_{mi} \approx y(t_{mi}), \\ &Z_m := (Z_{mi})_{i=1}^s \in \mathbb{R}^{s\times n} && \text{with} && Z_{mi} \approx y'(t_{mi}), \\ &F_m := (f(t_{mi}, Y_{mi}))_{i=1}^s \in \mathbb{R}^{s\times n} \end{aligned}$$

and $A, B, R \in \mathbb{R}^{s\times s}$ where R is a strictly lower triangular matrix. Putting Z_m into the equation for Y_m we obtain the equivalent formulation

$$\begin{aligned} Y_m &= BY_{m-1} + h_m(A+RB)Z_{m-1} + h_m^2 RAF_{m-1} + h_m^2 R^2 F_m \\ Z_m &= BZ_{m-1} + h_m AF_{m-1} + h_m RF_m \end{aligned}$$

Evidently, we can gain additional degrees of freedom in this scheme by considering a partitioned method of the form

$$\begin{aligned} Y_m &= BY_{m-1} + h_m AZ_{m-1} + h_m^2 QF_{m-1} + h_m^2 RF_m, \\ Z_m &= \qquad\quad \widehat{B}Z_{m-1} + h_m\widehat{Q}F_{m-1} + h_m\widehat{R}F_m \end{aligned}$$

with $A = (a_{ij})$, $B = (b_{ij})$, $Q = (q_{ij})$, $R = (r_{ij})$, $\widehat{Q} = (\widehat{q}_{ij})$, $\widehat{B} = (\widehat{b}_{ij})$, $\widehat{R} = (\widehat{r}_{ij}) \in \mathbb{R}^{s\times s}$. With a strictly lower triangular matrix R an explicit method is obtained.

Remark 1:
This formulation of peer methods has more degrees of freedom than the formulation of peer methods for first order differential equations: The matrices Q, $\widehat{Q}$, $\widehat{B}$ and $\widehat{R}$ are independent of A, B and R, R has $s-1$ non-zero entries more than R^2 has. The most important advantage is the fact that the matrix $\widehat{R}$ can be dense because Z_m is not needed to compute F_m.

Remark 2:
The choice $R = 0$ leads to parallel methods where the s stages for Y_m and those for Z_m can be computed in parallel. However, we did not consider the case $\hat{R} = 0$ leading to methods with $2s$ parallel stages. So, the sequential methods use more information only in the computation of Y_m and we expect that parallel methods (in a sequential implementation) perform almost as well as sequential methods.

In this paper we will also consider the generalization to partitioned three-step peer methods

$$Y_m = BY_{m-1} + h_m AZ_{m-1} + h_m^2 PF_{m-2} + h_m^2 QF_{m-1} + h_m^2 RF_m, \tag{2}$$

$$Z_m = \qquad\quad \widehat{B}Z_{m-1} + h_m\widehat{P}F_{m-2} + h_m\widehat{Q}F_{m-1} + h_m\widehat{R}F_m. \tag{3}$$

This is the general form for theoretical investigations but in Section 5 we will also present two-step peer methods with $P = \widehat{P} = 0$.

3 Order and stability

Consistency of the peer methods is discussed by considering the local residuals obtained by substituting the exact solution y into the method:

$$\begin{aligned}
\triangle_{mi} &:= y(t_{mi}) - \sum_{j=1}^{s} b_{ij} y(t_{m-1,j}) - h_m \sum_{j=1}^{s} a_{ij} y'(t_{m-1,j}) - h_m^2 \sum_{j=1}^{s} p_{ij} y''(t_{m-2,j}) \\
&\quad - h_m^2 \sum_{j=1}^{s} q_{ij} y''(t_{m-1,j}) - h_m^2 \sum_{j=1}^{i-1} r_{ij} y''(t_{mj}), \\
\widehat{\triangle}_{mi} &:= y'(t_{mi}) - \sum_{j=1}^{s} \widehat{b}_{ij} y'(t_{m-1,j}) - h_m \sum_{j=1}^{s} \widehat{p}_{ij} y''(t_{m-2,j}) - h_m \sum_{j=1}^{s} \widehat{q}_{ij} y''(t_{m-1,j}) \\
&\quad - h_m \sum_{j=1}^{s} \widehat{r}_{ij} y''(t_{mj}), \qquad\qquad i = 1, \ldots, s.
\end{aligned}$$

Definition 1 *A peer method has order of consistency p, if*

$$\max_i \triangle_{mi} = \mathcal{O}(h_m^{p+1}) \qquad \text{and} \qquad \max_i \widehat{\triangle}_{mi} = \mathcal{O}(h_m^{p+1}).$$

Taylor expansion at t_m leads to the following theorem.

Theorem 1 *A peer method has order of consistency p, if*

$$\begin{aligned}
AB(k) &= 0, \qquad k = 0, 1, \ldots, p, \\
\widehat{AB}(k) &= 0, \qquad k = 0, 1, \ldots, p
\end{aligned}$$

where

$$\begin{aligned}
AB_i(k) &:= c_i^k - \sum_{j=1}^{s} b_{ij} \frac{(c_j - 1)^k}{\sigma^k} - k \sum_{j=1}^{s} a_{ij} \frac{(c_j - 1)^{k-1}}{\sigma^{k-1}} - k(k-1) \sum_{j=1}^{s} p_{ij} \frac{(\frac{c_j - 1}{\hat{\sigma}} - 1)^{k-2}}{\sigma^{k-2}} \\
&\quad - k(k-1) \sum_{j=1}^{s} q_{ij} \frac{(c_j - 1)^{k-2}}{\sigma^{k-2}} - k(k-1) \sum_{j=1}^{i-1} r_{ij} c_j^{k-2}, \\
\widehat{AB}_i(k) &:= c_i^k - \sum_{j=1}^{s} \widehat{b}_{ij} \frac{(c_j - 1)^k}{\sigma^k} - k \sum_{j=1}^{s} \widehat{p}_{ij} \frac{(\frac{c_j - 1}{\hat{\sigma}} - 1)^{k-1}}{\sigma^{k-1}} - k \sum_{j=1}^{s} \widehat{q}_{ij} \frac{(c_j - 1)^{k-1}}{\sigma^{k-1}} \\
&\quad - k \sum_{j=1}^{s} \widehat{r}_{ij} c_j^{k-1}, \qquad\qquad i = 1, \ldots, s.
\end{aligned}$$

An important source of difficulties for the rest of the paper is the dependence of these conditions on the two step size ratios

$$\sigma := \frac{h_m}{h_{m-1}}, \quad \widehat{\sigma} := \frac{h_{m-1}}{h_{m-2}}$$

for three-step methods.
The collected order conditions $AB(k) = 0$, $\widehat{AB}(k) = 0$, $k = 0, \ldots, p$ can be written in compact matrix form. With the aim of obtaining order $p \leq 3s$ we introduce the diagonal matrices $C = \mathrm{diag}(c_1, \ldots, c_s) \in \mathbb{R}^{s\times s}$, $D = \mathrm{diag}(1, 2, \ldots, p)$, $S = \mathrm{diag}(1, \sigma, \ldots, \sigma^{p-1}) \in \mathbb{R}^{p\times p}$, and the rectangular $s \times p$-matrices

$$V_0 = \begin{pmatrix} 1 & c_1 & \cdots & c_1^{p-1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & c_s & \cdots & c_s^{p-1} \end{pmatrix}, \qquad \widehat{V}_0 = \begin{pmatrix} 0 & 1 & \cdots & c_1^{p-2} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 1 & \cdots & c_s^{p-2} \end{pmatrix},$$

$$V_1 = \begin{pmatrix} 1 & c_1 - 1 & \cdots & (c_1 - 1)^{p-1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & c_s - 1 & \cdots & (c_s - 1)^{p-1} \end{pmatrix}, \qquad \widehat{V}_1 = \begin{pmatrix} 0 & 1 & \cdots & (c_1 - 1)^{p-2} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 1 & \cdots & (c_s - 1)^{p-2} \end{pmatrix},$$

$$V_2 = \begin{pmatrix} 1 & \frac{1}{\hat{\sigma}}(c_1 - 1) - 1 & \cdots & \left(\frac{1}{\hat{\sigma}}(c_1 - 1) - 1\right)^{p-1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & \frac{1}{\hat{\sigma}}(c_s - 1) - 1 & \cdots & \left(\frac{1}{\hat{\sigma}}(c_s - 1) - 1\right)^{p-1} \end{pmatrix},$$

$$\widehat{V}_2 = \begin{pmatrix} 0 & 1 & \cdots & \left(\frac{1}{\hat{\sigma}}(c_1 - 1) - 1\right)^{p-2} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 1 & \cdots & \left(\frac{1}{\hat{\sigma}}(c_s - 1) - 1\right)^{p-2} \end{pmatrix}.$$

The first conditions $AB(0) = \widehat{AB}(0) = 0$ are very simple

$$\begin{aligned} B\mathbb{1} &= \mathbb{1}, \\ \widehat{B}\mathbb{1} &= \mathbb{1}, \end{aligned} \tag{4}$$

where $\mathbb{1} = (1, \ldots, 1)^T$. The other conditions $1 \le k \le p \le 3s$ lead to the matrix equations

$$\begin{pmatrix} A & Q & P \end{pmatrix} \begin{pmatrix} V_1 D S^{-1} \\ \sigma \widehat{V}_1 D(D-I) S^{-1} \\ \sigma \widehat{V}_2 D(D-I) S^{-1} \end{pmatrix} = C V_0 - \frac{1}{\sigma} B(C-I) V_1 S^{-1} - R \widehat{V}_0 D(D-I)$$

$$\begin{pmatrix} \widehat{Q} & \widehat{R} & \widehat{P} \end{pmatrix} \begin{pmatrix} V_1 D S^{-1} \\ V_0 D \\ V_2 D S^{-1} \end{pmatrix} = C V_0 - \frac{1}{\sigma} \widehat{B}(C-I) V_1 S^{-1}$$

Note, that DS^{-1} is a common right factor on the left hand side of these equations. Depending on the required order of the methods we have to discuss the regularity of parts of the matrices

$$\widehat{V} := \begin{pmatrix} V_1 \\ \widehat{V}_1(D-I) \\ \widehat{V}_2(D-I) \end{pmatrix} \in \mathbb{R}^{3s \times p}, \tag{5}$$

$$V := \begin{pmatrix} V_1 \\ V_0 S \\ V_2 \end{pmatrix} \in \mathbb{R}^{3s \times p}. \tag{6}$$

Order $p = s$ can be obtained by solving for the matrices A and $\widehat{Q}$, if V_1 is regular. For order $p = 2s$ we additionally need Q and $\widehat{R}$ and the regularity of the first two blocks in (5,6). And for order $p = 3s$ all matrices A, Q, P, $\widehat{Q}$, $\widehat{R}$ and $\widehat{P}$ are used by requiring the regularity of the full matrices $V, \widehat{V}$. In the next section we will see how to reduce the computational effort and avoid possible singularities. More information on the Vandermonde structure of the matrices $V, \widehat{V}$ follows in Section 4.
Applying the peer method with constant step size to the test equation

$$y'' = -\omega^2 y$$

gives the recursion

$$\begin{pmatrix} Y_{m-1} \\ Y_m \\ hZ_m \end{pmatrix} = M(z) \begin{pmatrix} Y_{m-2} \\ Y_{m-1} \\ hZ_{m-1} \end{pmatrix}$$

with $z := ih\omega$ and the stability matrix

$$M(z) := \begin{pmatrix} 0 & I & 0 \\ z^2(I - z^2R)^{-1}P & (I - z^2R)^{-1}(B + z^2Q) & (I - z^2R)^{-1}A \\ z^2\widehat{P} + z^4\widehat{R}(I - z^2R)^{-1}P & z^2\widehat{Q} + z^2\widehat{R}(I - z^2R)^{-1}(B + z^2Q) & \widehat{B} + z^2\widehat{R}(I - z^2R)^{-1}A \end{pmatrix}.$$

So

$$M(0) = \begin{pmatrix} 0 & I & 0 \\ 0 & B & A \\ 0 & 0 & \hat{B} \end{pmatrix} \tag{7}$$

has block triangular form and its eigenvalues are those of B, $\widehat{B}$ and zero with multiplicity s. In analogy to the definition of zero stability of general linear methods for second order problems in [6] we define zero stability for peer methods.

Definition 2 *A peer method is zero stable, if the eigenvalues λ of B and $\hat{\lambda}$ of $\hat{B}$ satisfy the following conditions:*

$$|\lambda| \leq 1 \qquad \text{and} \qquad \{|\lambda| = 1 \quad \Rightarrow \quad \lambda \text{ is simple,}\}$$

$$|\widehat{\lambda}| \leq 1 \qquad \text{and} \qquad \{|\widehat{\lambda}| = 1 \quad \Rightarrow \quad \widehat{\lambda} \text{ is simple.}\}$$

We note that this condition is weaker than power boundedness of $M(0)$ since one is an eigenvalue of $M(0)$ with multiplicity 2 due to (4).

Definition 3 *The stability interval of a peer method is defined by*

$$S := \{z \in i\mathbb{R} : \rho(M(x)) \leq 1 \quad \forall_{x \in i\mathbb{R}} |x| \leq |z|\}.$$

We now come to the main convergence result and we denote the global errors by

$$\begin{aligned} \varepsilon_m &:= Y(t_m) - Y_m \qquad \text{with} \qquad Y(t_m) := (y(t_{mi}))_{i=1}^s \\ \widehat{\varepsilon}_m &:= Z(t_m) - Z_m \qquad \text{with} \qquad Z(t_m) := (y'(t_{mi}))_{i=1}^s \end{aligned}$$

Definition 4 *A peer method has order of convergence p, if there is a constant C with*

$$\begin{aligned} ||\varepsilon_m|| &\leq Ch^p, \\ ||\widehat{\varepsilon}_m|| &\leq Ch^p \end{aligned}$$

where $h := \max_m h_m$.

Theorem 2 *Let the following conditions for the peer method* (2) *be satisfied.*

- *The peer method has order of consistency p.*
- *The peer method is zero stable.*

- *The initial values have order p, i.e.* $\varepsilon_0 = \mathcal{O}(h_0^p)$, $\varepsilon_1 = \mathcal{O}(h_1^p)$, $\widehat{\varepsilon}_0 = \mathcal{O}(h_0^p)$ *and* $\widehat{\varepsilon}_1 = \mathcal{O}(h_1^p)$.
- $\widehat{\sigma}, \sigma \in (1-\delta, 1+\delta)$ *for a sufficiently small* $\delta > 0$ *and the matrices* B, $\widehat{B}$ *and* R *are constant.*

Then this peer method has order of convergence p.

Proof: For simplicity of notation we consider the scalar case. With the notation

$$F\big(Y(t_m)\big) := \Big(f\big(t_{mi}, y(t_{mi})\big)\Big)_{i=1}^{s}$$

the local residuals are given by

$$\begin{aligned}
\triangle_m &= Y(t_m) - BY(t_{m-1}) - h_m A_m Z(t_{m-1}) - h_m^2 P_m F\big(Y(t_{m-2})\big) - h_m^2 Q_m F\big(Y(t_{m-1})\big) \\
&\quad - h_m^2 R F\big(Y(t_m)\big), \\
\widehat{\triangle}_m &= Z(t_m) - \widehat{B} Z(t_{m-1}) - h_m \widehat{P}_m F\big(Y(t_{m-2})\big) - h_m \widehat{Q}_m F\big(Y(t_{m-1})\big) - h_m \widehat{R}_m F\big(Y(t_m)\big)
\end{aligned}$$

and therefore in the m-th the global errors in y and y' satisfy

$$\begin{aligned}
\varepsilon_m &= Y(t_m) - Y_m \\
&= Y(t_m) - BY_{m-1} - h_m A_m Z_{m-1} - h_m^2 P_m F_{m-2} - h_m^2 Q_m F_{m-1} - h_m^2 R F_m \\
&= B\varepsilon_{m-1} + h_m A_m \widehat{\varepsilon}_{m-1} + h_m^2 P_m \Big(F\big(Y(t_{m-2})\big) - F_{m-2}\Big) \\
&\quad + h_m^2 Q_m \Big(F\big(Y(t_{m-1})\big) - F_{m-1}\Big) + h_m^2 R \Big(F\big(Y(t_m)\big) - F_m\Big) + \triangle_m, \\
\widehat{\varepsilon}_m &= Z(t_m) - Z_m \\
&= Z(t_m) - \widehat{B} Z_{m-1} - h_m \widehat{P}_m F_{m-2} - h_m \widehat{Q}_m F_{m-1} - h_m \widehat{R}_m F_m \\
&= \widehat{B}\widehat{\varepsilon}_{m-1} + h_m \widehat{P}_m \Big(F\big(Y(t_{m-2})\big) - F_{m-2}\Big) + h_m \widehat{Q}_m \Big(F\big(Y(t_{m-1})\big) - F_{m-1}\Big) \\
&\quad + h_m \widehat{R}_m \Big(F\big(Y(t_m)\big) - F_m\Big) + \widehat{\triangle}_m.
\end{aligned}$$

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

$$f\big(t_{mi}, y(t_{mi})\big) - F_{mi} = J_{mi}\varepsilon_{mi}$$

with

$$J_{mi} := \int_0^1 f_y\Big(y(t_{mi}) + \theta\big(Y_{mi} - y(t_{mi})\big)\Big) d\theta.$$

Therefore it holds:

$$\begin{aligned}
P_m\Big(F\big(Y(t_{m-2})\big) - F_{m-2}\Big) &= G_m\varepsilon_{m-2} && \text{with} && G_m := P_m\mathrm{diag}_i(J_{m-2,i})\\
Q_m\Big(F\big(Y(t_{m-1})\big) - F_{m-1}\Big) &= H_m\varepsilon_{m-1} && \text{with} && H_m := Q_m\mathrm{diag}_i(J_{m-1,i})\\
R\Big(F\big(Y(t_m)\big) - F_m\Big) &= K_m\varepsilon_m && \text{with} && K_m := R\,\mathrm{diag}_i(J_{mi})\\
\widehat{P}_m\Big(F\big(Y(t_{m-2})\big) - F_{m-2}\Big) &= \widehat{G}_m\varepsilon_{m-2} && \text{with} && \widehat{G}_m := \widehat{P}_m\mathrm{diag}_i(J_{m-2,i})\\
\widehat{Q}_m\Big(F\big(Y(t_{m-1})\big) - F_{m-1}\Big) &= \widehat{H}_m\varepsilon_{m-1} && \text{with} && \widehat{H}_m := \widehat{Q}_m\mathrm{diag}_i(J_{m-1,i})\\
\widehat{R}_m\Big(F\big(Y(t_m)\big) - F_m\Big) &= \widehat{K}_m\varepsilon_m && \text{with} && \widehat{K}_m := \widehat{R}_m\mathrm{diag}_i(J_{mi})
\end{aligned}$$

This leads to the recursion

$$\begin{aligned}
\varepsilon_m &= B\varepsilon_{m-1} + h_{m-1}\sigma_m A_m\widehat{\varepsilon}_{m-1} + h_{m-2}^2\sigma_{m-1}^2\sigma_m^2 G_m\varepsilon_{m-2} + h_{m-1}^2\sigma_m^2 H_m\varepsilon_{m-1} + h_m^2 K_m\varepsilon_m + \triangle_m\\
\widehat{\varepsilon}_m &= \widehat{B}\widehat{\varepsilon}_{m-1} + h_{m-2}\sigma_{m-1}\sigma_m\widehat{G}_m\varepsilon_{m-2} + h_{m-1}\sigma_m\widehat{H}_m\varepsilon_{m-1} + h_m\widehat{K}_m\varepsilon_m + \widehat{\triangle}_m
\end{aligned}$$

By repeated substitution we obtain

$$\begin{aligned}
\varepsilon_m &= B^m\varepsilon_0 + \sum_{j=0}^{m-2} h_{m-1-j}B^j\sigma_{m-j}A_{m-j}\widehat{\varepsilon}_{m-1-j} + \sum_{j=0}^{m-2} h_{m-2-j}^2 B^j\sigma_{m-1-j}^2\sigma_{m-j}^2 G_{m-j}\varepsilon_{m-2-j}\\
&\quad + \sum_{j=0}^{m-2} h_{m-1-j}^2 B^j\sigma_{m-j}^2 H_{m-j}\varepsilon_{m-1-j} + \sum_{j=0}^{m-2} h_{m-j}^2 K_{m-j}\varepsilon_{m-j} + \sum_{j=0}^{m-2} B^j\triangle_{m-j}\\
\widehat{\varepsilon}_m &= \widehat{B}^m\widehat{\varepsilon}_0 + \sum_{j=0}^{m-2} h_{m-2-j}\widehat{B}^j\sigma_{m-1-j}\sigma_{m-j}\widehat{G}_{m-j}\varepsilon_{m-2-j} + \sum_{j=0}^{m-2} h_{m-1-j}\widehat{B}^j\sigma_{m-j}\widehat{H}_{m-j}\varepsilon_{m-1-j}\\
&\quad + \sum_{j=0}^{m-2} h_{m-j}\widehat{K}_{m-j}\varepsilon_{m-j} + \sum_{j=0}^{m-2}\widehat{B}^j\widehat{\triangle}_{m-j}
\end{aligned}$$

By assumption the matrices $\sigma_j A_j$, $\sigma_{j-1}^2\sigma_j^2 P_j$, $\sigma_j^2 Q_j$, $\sigma_{j-1}\sigma_j\widehat{P}_j$, $\sigma_j\widehat{Q}_j$ and $\widehat{R}_j$ with $\sigma_j \in (1-\delta, 1+\delta)$ are uniformly bounded. Since the matrices B and $\widehat{B}$ are also power bounded there is a constant $c > 0$ such that we have for all $0 \le j \le m-2$:

$$\begin{aligned}
&||B^j\sigma_{m-j}A_{m-j}|| \le c, \quad ||B^j\sigma_{m-1-j}^2\sigma_{m-j}^2 G_{m-j}|| \le c, \quad ||B^j\sigma_{m-j}^2 H_{m-j}|| \le c, \quad ||K_{m-j}|| \le c,\\
&||\widehat{B}^j\sigma_{m-1-j}\sigma_{m-j}\widehat{G}_{m-j}|| \le c, \quad ||\widehat{B}^j\sigma_{m-j}\widehat{H}_{m-j}|| \le c, \qquad ||\widehat{K}_{m-j}|| \le c.
\end{aligned}$$

Using this fact leads to the inequalities

$$||\sum_{j=0}^{m-2} h_{m-1-j}B^j\sigma_{m-j}A_{m-j}\widehat{\varepsilon}_{m-1-j}|| \leq ch_1||\widehat{\varepsilon}_1|| + c\sum_{j=2}^{m-1} h_j||\widehat{\varepsilon}_j||,$$

$$||\sum_{j=0}^{m-2} h_{m-2-j}^2B^j\sigma_{m-1-j}^2\sigma_{m-j}^2G_{m-j}\varepsilon_{m-2-j}|| \leq ch_0^2||\varepsilon_0|| + ch_1^2||\varepsilon_1|| + c\sum_{j=2}^{m-2} h_j^2||\varepsilon_j||,$$

$$||\sum_{j=0}^{m-2} h_{m-1-j}^2B^j\sigma_{m-j}^2H_{m-j}\varepsilon_{m-1-j}|| \leq ch_1^2||\varepsilon_1|| + c\sum_{j=2}^{m-1} h_j^2||\varepsilon_j||,$$

$$||\sum_{j=0}^{m-2} h_{m-j}^2K_{m-j}\varepsilon_{m-j}|| \leq c\sum_{j=2}^{m-1} h_j^2||\varepsilon_j|| + ch_m^2||\varepsilon_m||,$$

$$||\sum_{j=0}^{m-2} h_{m-2-j}\widehat{B}^j\sigma_{m-1-j}\sigma_{m-j}\widehat{G}_{m-j}\varepsilon_{m-2-j}|| \leq ch_0||\varepsilon_0|| + ch_1||\varepsilon_1|| + c\sum_{j=2}^{m-2} h_j||\varepsilon_j||,$$

$$||\sum_{j=0}^{m-2} h_{m-1-j}\widehat{B}^j\sigma_{m-j}\widehat{H}_{m-j}\varepsilon_{m-1-j}|| \leq ch_1||\varepsilon_1|| + c\sum_{j=2}^{m-1} h_j||\varepsilon_j||,$$

$$||\sum_{j=0}^{m-2} h_{m-j}\widehat{K}_{m-j}\varepsilon_{m-j}|| \leq c\sum_{j=2}^{m} h_j||\varepsilon_j||.$$

Since the peer method has order of consistency p and is zero stable, it holds

$$||\sum_{j=0}^{m-2} B^j\triangle_{m-j}|| = c\sum_{j=2}^{m}\mathcal{O}(h_j^{p+1}) = \mathcal{O}(h^p)\sum_{j=2}^{m}\mathcal{O}(h_j) = \mathcal{O}(h^p)$$

$$||\sum_{j=0}^{m-2} \widehat{B}^j\widehat{\triangle}_{m-j}|| = c\sum_{j=2}^{m}\mathcal{O}(h_j^{p+1}) = \mathcal{O}(h^p)\sum_{j=2}^{m}\mathcal{O}(h_j) = \mathcal{O}(h^p)$$

By using these inequalities and the fact that the initial values have order p we obtain

$$\Big(1 - ch_m^2\Big)||\varepsilon_m|| \leq 3c\sum_{j=2}^{m-1} h_j^2||\varepsilon_j|| + c\sum_{j=2}^{m-1} h_j||\widehat{\varepsilon}_j|| + dh^p.$$

For sufficiently small step sizes the final relations for the global errors are

$$
\begin{aligned}
||\varepsilon_m|| &\leq \widehat{c}\sum_{j=2}^{m-1} h_j^2||\varepsilon_j|| + \widehat{c}\sum_{j=2}^{m-1} h_j||\widehat{\varepsilon}_j|| + \widehat{d}h^p, \\
||\widehat{\varepsilon}_m|| &\leq 3c\sum_{j=2}^{m} h_j||\varepsilon_j|| + dh^p, \\
&\leq \widehat{c}\sum_{j=2}^{m} h_j||\varepsilon_j|| + \widehat{d}\,h^p.
\end{aligned}
$$

We note that now the error $\widehat{\varepsilon}_m$ is explicitly bounded by ε_j and $\widehat{d}$ only and may be used to replace $\widehat{\varepsilon}_j$ in the estimate for ε_m:

$$
\begin{aligned}
||\varepsilon_m|| &\leq \widehat{c}\sum_{j=2}^{m-1} h_j^2||\varepsilon_j|| + \widehat{c}\sum_{j=2}^{m-1} h_j||\widehat{\varepsilon}_j|| + \widehat{d}h^p \\
&\leq \widehat{c}\sum_{j=2}^{m-1} h_j^2||\varepsilon_j|| + \widehat{c}^2\sum_{j=2}^{m-1} h_j\sum_{k=2}^{j} h_k||\varepsilon_k|| + \widetilde{d}h^p \\
&= \widehat{c}\sum_{j=2}^{m-1} h_j^2||\varepsilon_j|| + \widehat{c}^2\sum_{k=2}^{m-1} h_k\sum_{j=k}^{m-1} h_j||\varepsilon_k|| + \widetilde{d}h^p \\
&= \widehat{c}\sum_{j=2}^{m-1} h_j||\varepsilon_j||\Big(h_j + \widehat{c}\sum_{k=j}^{m-1} h_k\Big) + \widetilde{d}h^p \\
&\leq \widehat{c}\sum_{j=2}^{m-1} h_j||\varepsilon_j||\Big((1+\widehat{c})(t_e - t_0)\Big) + \widetilde{d}h^p \\
&\leq \widetilde{c}\sum_{j=2}^{m-1} h_j||\varepsilon_j|| + \widetilde{d}h^p
\end{aligned}
\tag{8}
$$

For $X_j \in \mathbb{R}$ the relation

$$
1 + \sum_{j=2}^{m-1} X_j \prod_{k=2}^{j-1}(1+X_k) = \prod_{k=2}^{m-1}(1+X_k)
$$

is verified easily. Using this identity with $X_k := \widetilde{c}h_k$ we will prove the inequality

$$||\varepsilon_m|| \leq \prod_{k=2}^{m-1}(1+X_k)\widetilde{d}h^p \tag{9}$$

by induction. We start the induction for $m = 2$ with (8), i.e.

$$||\varepsilon_2|| \leq \widetilde{d}h^p.$$

Now using (9) for $2 \leq j \leq m-1$ with $m \geq 3$ we get at step m:

$$\begin{aligned}
||\varepsilon_m|| &\leq \sum_{j=2}^{m-1} \widetilde{c}h_j||\varepsilon_j|| + \widetilde{d}h^p \\
&\leq \left(1 + \sum_{j=2}^{m-1} \widetilde{c}h_j \prod_{k=2}^{j-1}(1+X_k)\right)\widetilde{d}h^p \\
&= \prod_{k=2}^{m-1}(1+X_k)\widetilde{d}h^p
\end{aligned}$$

Since $\prod_{k=2}^{j-1}(1+X_k) \leq \prod_{k=2}^{m-1} e^{X_k} = e^{\Sigma\tilde{c}h_k}$ the global error in the y variable has order p,

$$||\varepsilon_m|| \leq \prod_{k=2}^{m-1}(1+X_k)\widetilde{d}h^p \leq e^{\tilde{c}(t_e-t_0)}\widetilde{d}h^p =: \overline{d}h^p.$$

For the global error in the derivative y' it holds

$$\begin{aligned}
||\widehat{\varepsilon}_m|| &\leq 3c\sum_{j=2}^{m} h_j||\varepsilon_j|| + dh^p \\
&\leq \left(1 + 3c\sum_{j=2}^{m} h_j\right)\overline{d}h^p \\
&\leq \Big(1 + 3c(t_e - t_0)\Big)\overline{d}h^p.
\end{aligned}$$

This is convergence of order p. ■

Remark 3:
The assumptions of the theorem required the boundedness of the matrices σA, $\widehat{\sigma}^2\sigma^2 P$,

$\sigma^2 Q$, $\sigma\widehat{Q}$, $\widehat{\sigma}\sigma\widehat{P}$ and $\widehat{R}$ for $\widehat{\sigma}, \sigma \in (1-\delta, 1+\delta)$ with a sufficiently small $\delta > 0$ only. This is a severe restriction for practical implementations and we allow smaller and bigger step size ratios in Section 4 with additional precautions.

There are many free parameters left for a zero stable explicit three-step peer method. Our strategy to find good methods is based on choosing coefficient matrices B and $\widehat{B}$ with the following properties:

- B and $\widehat{B}$ are independent of the step size ratios $\widehat{\sigma}$ and σ.
- B and $\widehat{B}$ satisfy the preconsistency conditions $B\mathbb{1} = \mathbb{1}$ and $\widehat{B}\mathbb{1} = \mathbb{1}$.
- The method is optimally zero stable, i.e. both B and $\widehat{B}$ have only one single non-zero eigenvalue 1.

The following theorem gives a suitable ansatz which satisfies all of these aims, see [9].

Theorem 3 *Let B given by*

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

where

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

with $\widetilde{Q}$ a regular and $\widetilde{W}$ a strictly upper triangular matrix.
Then B has only the single non-zero eigenvalue 1 and furthermore it holds:

$$\begin{aligned} B\mathbb{1} &= \mathbb{1} \\ B^j &= \mathbb{1}v^T \qquad \text{for } j \geq s-1 \end{aligned}$$

Using matrices B and $\widehat{B}$ having the structure used in this theorem a peer method can even have superconvergence of order $p+1$. The vectors v and $\widehat{v}$ are the left eigenvectors of B resp. $\widehat{B}$.

Theorem 4 *Let the peer method* (2) *satisfy the following conditions:*

- *The peer method has order of consistency p.*
- *The conditions $v^T AB(p+1) = 0$ and $\widehat{v}^T\widehat{AB}(p+1) = 0$ are fulfilled.*

- *The initial values have order $p+1$, i.e. $\varepsilon_0 = \mathcal{O}(h_0^{p+1})$, $\varepsilon_1 = \mathcal{O}(h_1^{p+1})$, $\widehat{\varepsilon}_0 = \mathcal{O}(h_0^{p+1})$ and $\widehat{\varepsilon}_1 = \mathcal{O}(h_1^{p+1})$.*
- *The matrices B and $\widehat{B}$ are chosen according to Theorem 3, R is constant and $\widehat{\sigma}, \sigma \in (1-\delta, 1+\delta)$ for a sufficient small $\delta > 0$.*

Then this peer method is superconvergent of order $p+1$.

Proof: Due to $v^T AB(p+1) = 0$ we obtain

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

Analogously it holds

$$\sum_{j=0}^{m-2} \widehat{B}^j \widehat{\triangle}_{m-j} = \mathcal{O}(h^{p+1}).$$

From order of convergence p (all assumptions of Theorem 2 are satisfied) the rest of the proof is analogous to the proof of convergence with $p+1$ instead of p. ■

4 Implementation

The proof of convergence required the uniform boundedness of all step size-dependent matrices. In order to achieve this goal we must prevent three cases in practice:

- $\sigma \to 0$
- $\sigma \to \infty$
- Specific step size changes may lead to singular matrices (5) or (6).

The first two cases are avoided by bounding the step size ratios

$$0.2 \leq \sigma \leq 2$$

But this alone is not sufficient to bound the step size proposals of the step size control since repeated step rejections could lead to arbitrary small step size ratios. In this case our implementation does not only repeat the actual but also the previous step. And in the step after a failed step increase of step size is forbidden. This strategy was proposed in [4] for ROW-methods.

It is also necessary to avoid matrix singularities. For example we need the regularity of the σ-dependent matrix V in (6) which for $p = 3s$ essentially is a Vandermonde matrix with the nodes

$$\sigma c_i, \qquad c_i - 1, \qquad c_i - 1 - \widehat{\sigma}, \qquad i = 1, \ldots, s.$$

Since step size ratios are positive this matrix is regular if the nodes satisfy the condition $0 < c_i \leq 1$. Unfortunately, the conditions for the regularity of $\widehat{V}$ are not so easy to determine since it is equivalent to the regularity of the following incomplete Hermite interpolation problem:
Determine a polynom q of degree $3s - 1$ with

$$q(c_i - 1) = q_i, \qquad q'(c_i - 1) = q_{s+i}, \qquad q'(c_i - 1 - \widehat{\sigma}) = q_{2s+i} \quad \text{for } i = 1, \ldots, s.$$

For the methods presented in the next section we specify the intervals for $\widehat{\sigma}$ and σ in which both matrices are regular.

In practice we do not want to restrict the choice of the nodes c_i or the step size ratios too much (with the exception of the condition $0.2 \leq \sigma \leq 2$). So far, it is also very expensive to solve the order conditions for the coefficients A etc. in each step since the matrices V and $\widehat{V}$ depend on $\hat{\sigma}$. These two problems, singularity and expensive computations, are avoided by allowing only specific step size ratios, namely

$$\sigma \in \{0.2, 0.5, 0.8, 1, 1.2, 1.5, 2\} \tag{10}$$

The step size proposal of the step size control will be rounded to the nearest σ from the above set (10). The matrices for these values were computed once with quadruple precision and stored. For the step size ratios from this set (10) all V-matrices are regular for the methods considered in Section 5.

Figure 1 shows the influence of round-off errors on error constants which should be zero in exact arithmetic. The solid curve represents error constants for the peer method v3-s2-p6 where the step size-dependent matrices were computed for each step size on

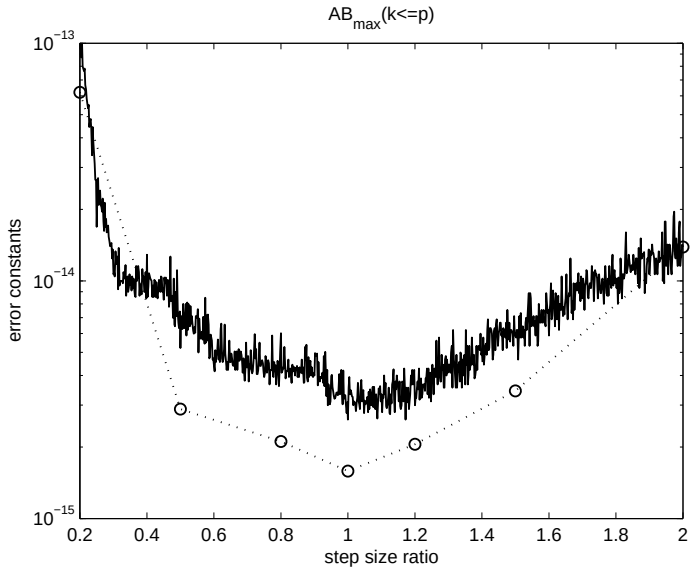

Figure 1: Influence of roundoff errors on error constants

the σ axis with a resolution of 0.002 in double precision. The dotted curve shows the same error constants for this peer method where the step size-dependent matrices were computed only for the step sizes from the set (10) with quadruple precision. The error constants were computed with double precision for both curves. Obviously the dotted curve shows less rounding errors.

The advantages of higher accuracy and of saving time outweigh the disadvantage by the restriction to only 7 distinct step size ratios. In our tests there were no big differences between a numerical solution computed with arbitrary step size ratios and a numerical solution with ratios from the set (10). The main advantage is the effort reduction. Therefore all methods presented in the next section use this kind of implementation.

By an starting procedure analogous to [8] we avoid function evaluations for $t < t_0$. Step size control is based on an embedded solution of order $2s - 2$.

5 Numerical tests

We will present the results for eight peer methods. The first set contains four two-step methods of order $2s$, where $P = \widehat{P} = 0$, and the second set four three-step methods of order $3s$. The following table gives a survey of their properties. p is the order of consistency, *interval* denotes the size of the stability interval on the positive imaginary axis. The error constants are the maximal values for y and y' with $\sigma = 1$. *regularity* gives the intervals on the axes $\sigma \times \widehat{\sigma}$ where the matrices (5) and (6) are regular. The suffix *-par* in the methods' names means that these methods are parallel methods with $R = 0$.

method	s	p	interval	$v^T AB(p+1)$	$\max AB_i(p+1)$	regularity
v2-s3-p6	3	6	0.72	$3 \cdot 10^{-5}$	$3 \cdot 10^{-1}$	$[0.52,\ 2]$
v2-s3-p6-par	3	6	0.50	$8 \cdot 10^{-16}$	$6 \cdot 10^{1}$	$[0.46,\ 1.57]$
v2-s4-p8	4	8	0.45	$3 \cdot 10^{-6}$	$3 \cdot 10^{0}$	$[0.64,\ 2]$
v2-s4-p8-par	4	8	0.53	$2 \cdot 10^{-6}$	$2 \cdot 10^{2}$	$[0.38,\ 1.65]$
v3-s2-p6	2	6	1.05	$2 \cdot 10^{-13}$	$1 \cdot 10^{0}$	$[0.17,\ 2] \times [0.17,\ 2]$
v3-s2-p6-par	2	6	0.72	$2 \cdot 10^{-12}$	$2 \cdot 10^{1}$	$(0,\ 2] \times (0,\ 2]$
v3-s3-p9	3	9	0.60	$9 \cdot 10^{-9}$	$5 \cdot 10^{0}$	$(0,\ 2] \times (0,\ 2]$
v3-s3-p9-par	3	9	0.35	$4 \cdot 10^{0}$	$2 \cdot 10^{2}$	$[0.27,\ 2] \times [0.36,\ 2]$

The peer methods are compared with RKN64 which is a 6-stage Runge-Kutta-Nyström method of order 6 using 5 function evaluations per step. Its coefficients are taken from the floppy disk attached to [2]. For step size control it uses an embedded solution of order 4. RKN64 is also used for the computation of the initial values of the peer methods.

The test examples ARES, AURO, CPEN and PLEI are from [6], Kepler and Solar are from Chapter I.2. of [5].

All methods are implemented sequentially in MATLAB. The dotted lines show the theoretical potential of the parallel methods when implemented on s processors. Here the number of function evaluations was divided by the number s of stages.

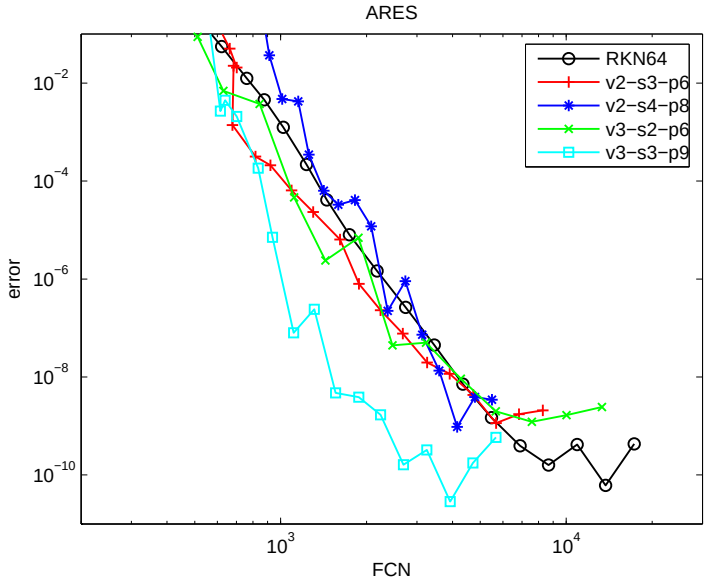

Figure 2: Sequential peer methods for the Arenstorf orbit problem

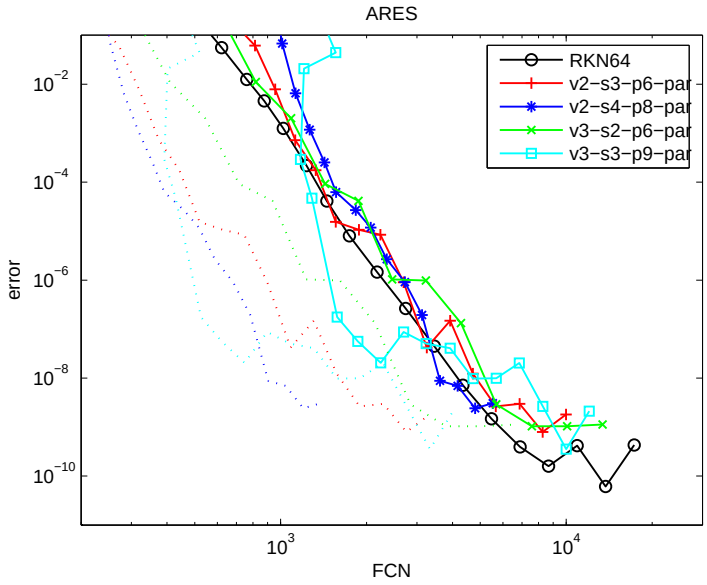

Figure 3: Parallel peer methods for the Arenstorf orbit problem

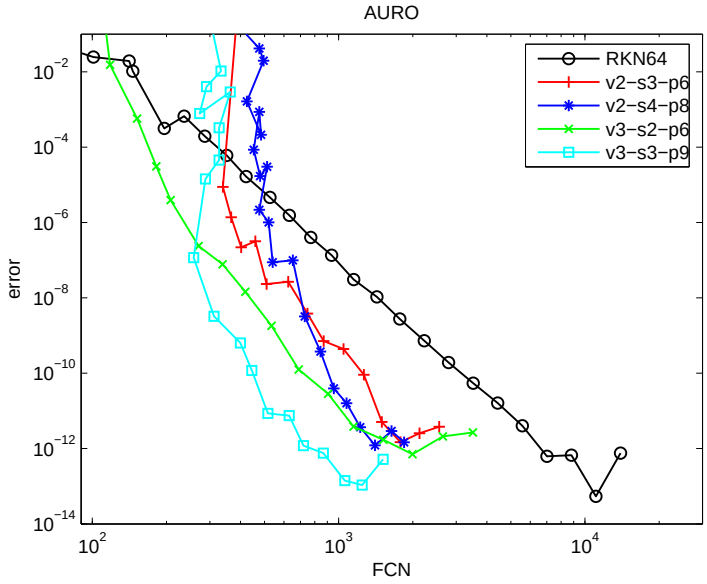

Figure 4: Sequential peer methods for the aurora borealis problem

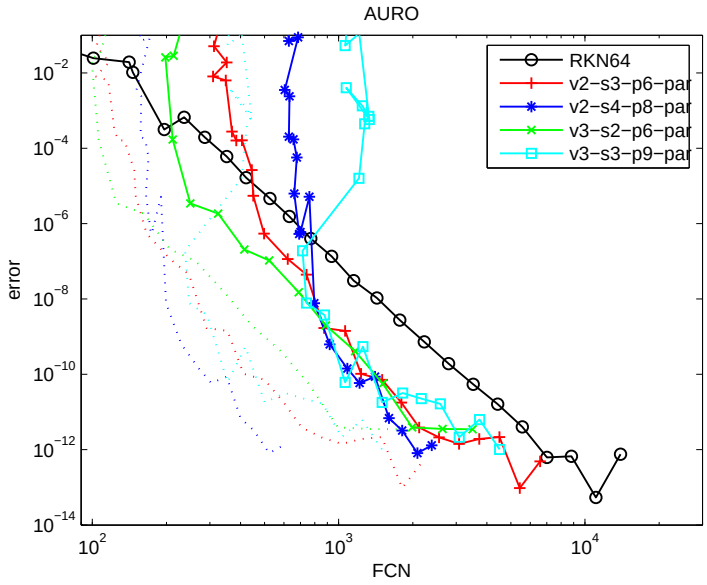

Figure 5: Parallel peer methods for the aurora borealis problem

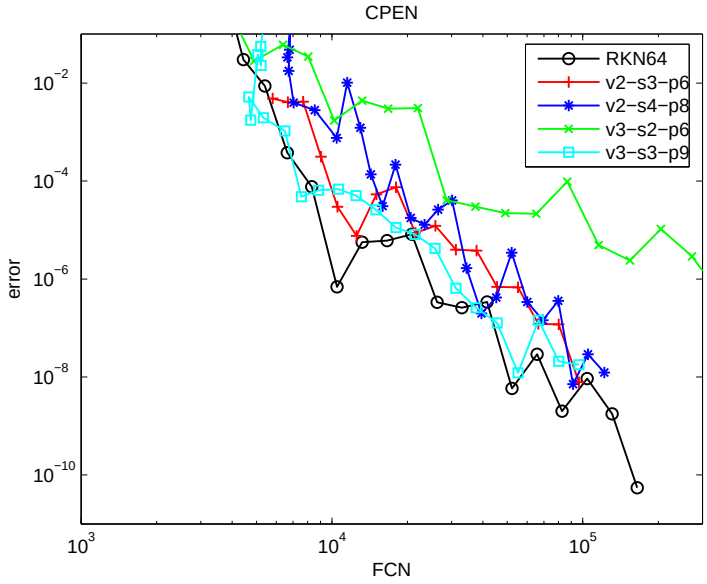

Figure 6: Sequential peer methods for the nonlinear coupled pendulum problem

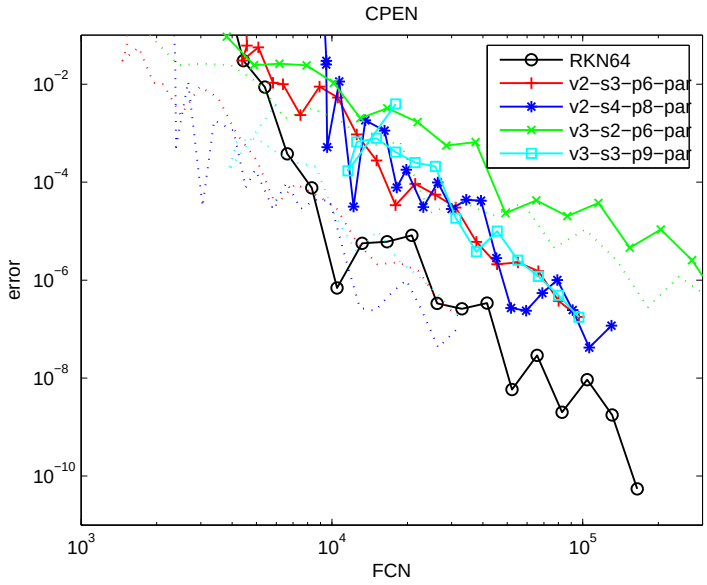

Figure 7: Parallel peer methods for the nonlinear coupled pendulum problem

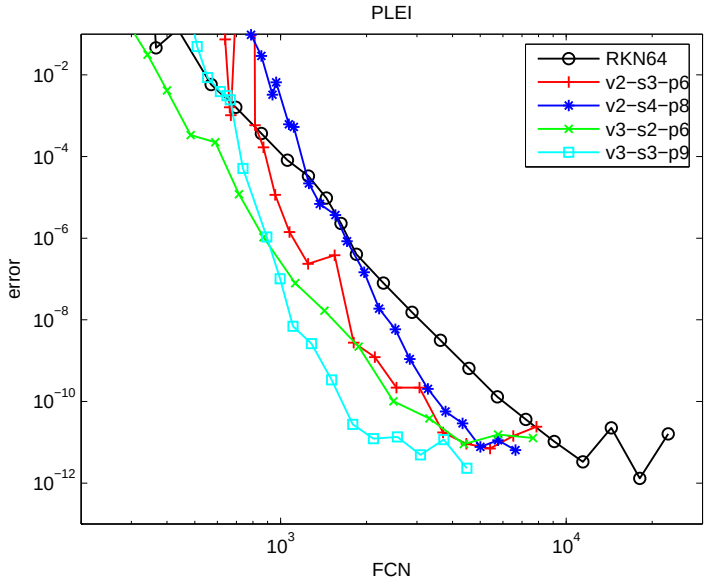

Figure 8: Sequential peer methods for the Pleiades problem

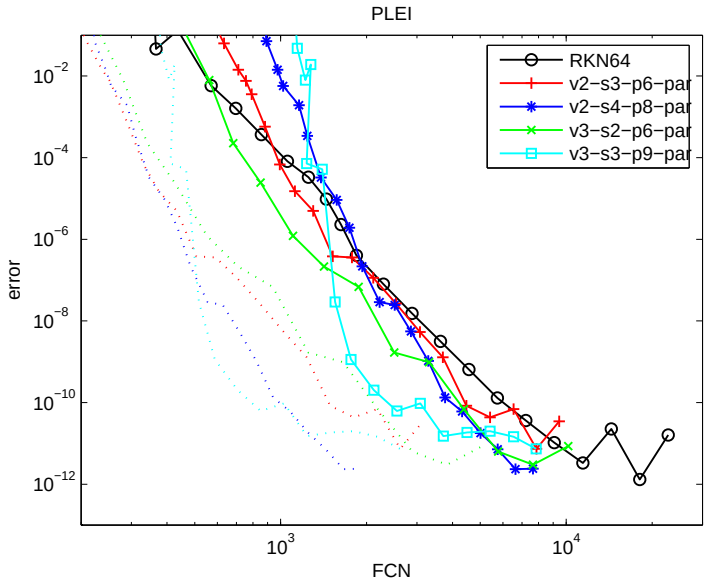

Figure 9: Parallel peer methods for the Pleiades problem

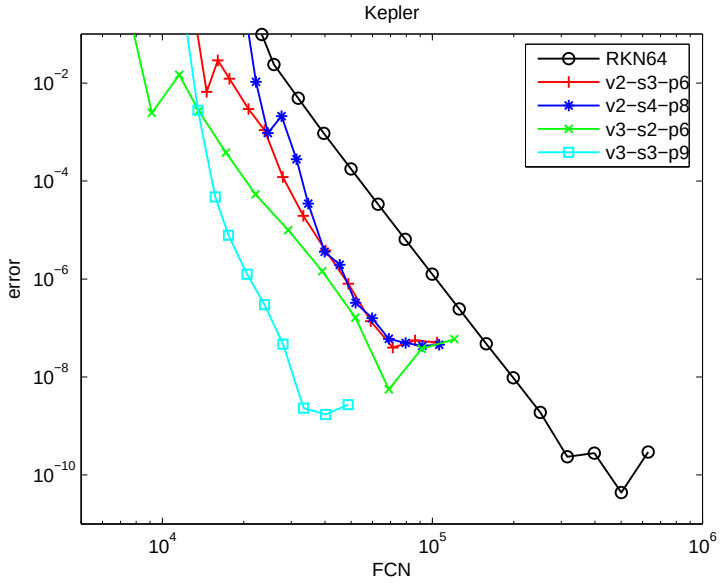

Figure 10: Sequential peer methods for the two body problem

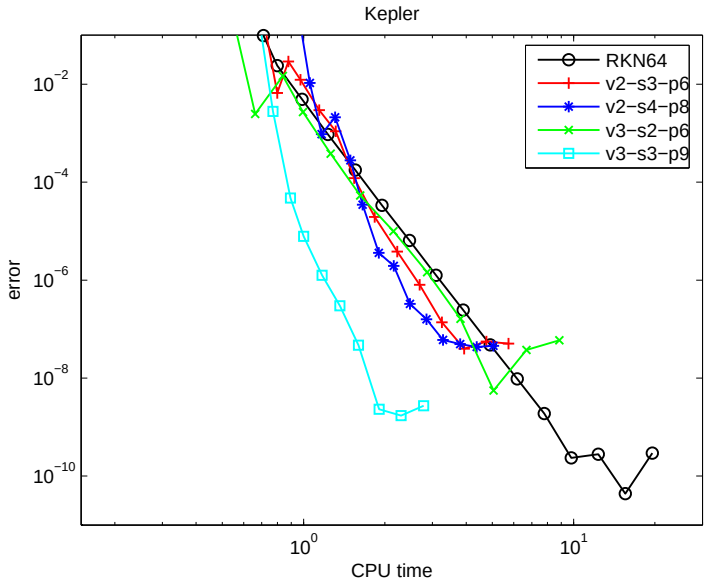

Figure 11: Sequential peer methods for the two body problem with CPU time plot

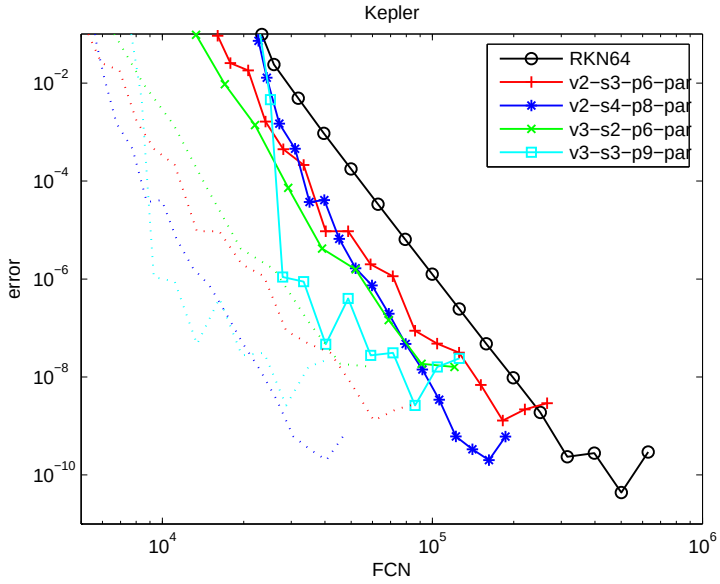

Figure 12: Parallel peer methods for the two body problem

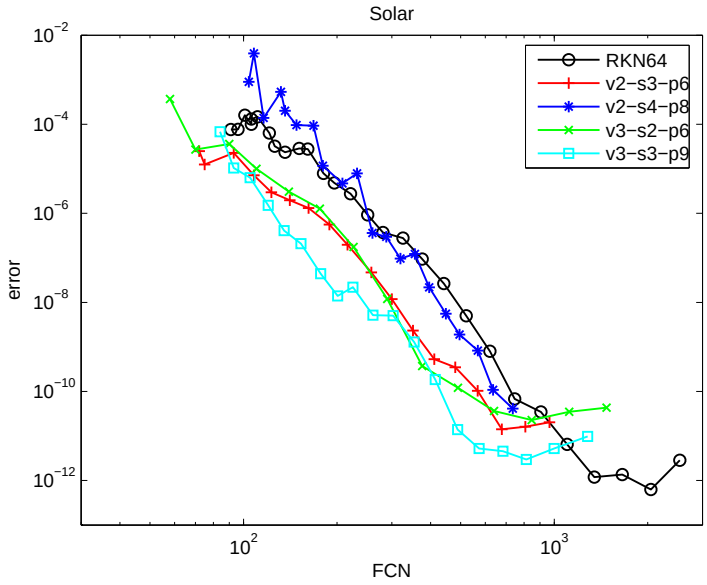

Figure 13: Sequential peer methods for the solar problem

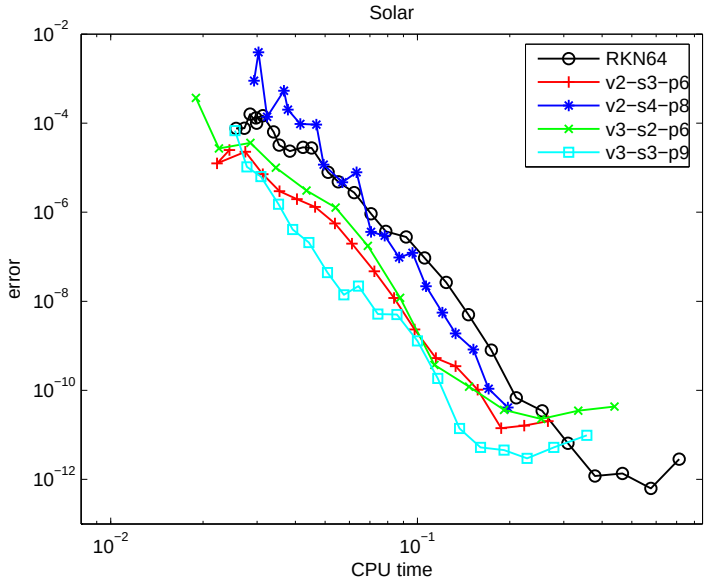

Figure 14: Sequential peer methods for the solar problem with CPU time plot

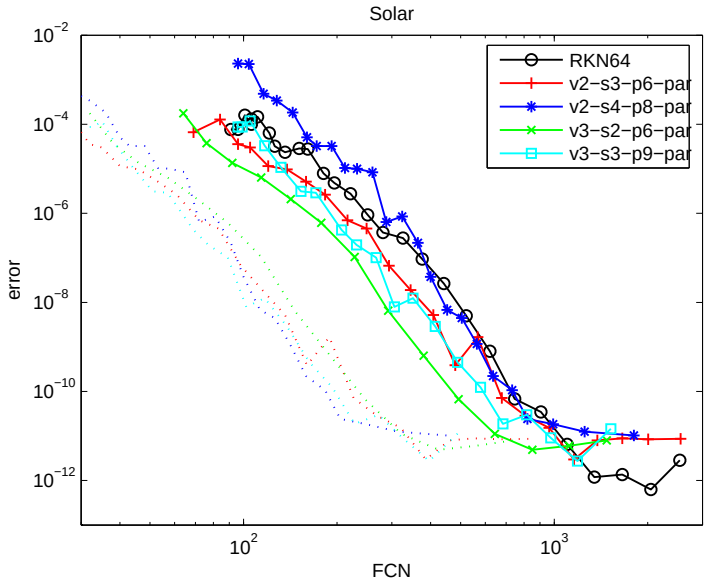

Figure 15: Parallel peer methods for the solar problem

6 Conclusions and outlook

In the numerical tests the sequential peer methods require far less function evaluations than RKN64 in all problems except CPEN. On the other hand the overhead of the peer implementation is much larger. In order to get realistic estimates we also considered the computing times for two examples (see Figures 11 and 14). Here, for a simple equation of low dimension ($n = 2$) like the Kepler problem the clear advantage of the peer methods over RKN64 on an error versus function evaluations plot (Fig.10) shrinks a lot on an error versus CPU time plot (Fig.14). This difference decreases for more complicated systems like the Solar test ($n = 18$, Fig.13, Fig.14). Since the peer methods perform well even for these very simple test equations on error versus CPU time plots we think that for more realistic problems the greater overhead of the peer methods is a negligible disadvantage compared to RKN64.
The numerical solutions are not very accurate for very sharp tolerances for all considered methods due to the limited precision in the double format. The complicated computation of the coefficients of the peer methods makes them more sensitive to rounding errors than RKN64. Therefore the achievable accuracy is in general better for RKN64 than for the peer methods. This behaviour changes when a higher machine precision is used.
The best sequential peer method is *v3-s3-p9* and the best parallel method *v2-s4-p8-par*. The latter one is more efficient than RKN64 even in a sequential implementation showing the potential of these peer methods.
The search for good coefficient sets is a difficult problem due to the very different aims. We think that the methods from the tests are by far not optimal yet but they show the potential of the considered class of methods.
A point for further investigations are fast solvers for the Vandermonde systems with the matrices (6,5), see [3]. Here it might help to extend the scheme (2) by additional terms with Z_{m-2}. Another interesting field may be four-step peer methods. Using the matrices B and $\widehat{B}$ from Theorem 3 results like zero stability and superconvergence carry over and with the additional coefficients methods of order $4s$ are possible.
Our numerical tests here give only a first impression on the potential of parallel peer methods, tests on parallel computers are planned. Such parallel tests were performed in [7] for first order differential equations showing that the speed-up can be nearly s if the evaluation of the right-hand side is expensive.

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