Linearly-implicit two-step methods and their implementation in Nordsieck form

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Dedicated to Prof. Alan Feldstein, on the occasion of his 70$^{\text{th}}$ birthday.

Abstract

We consider the Nordsieck representation of well-known linearly-implicit two-step methods in order to facilitate stepsize changes. They are treated as implicit methods with one Newton step with a special predictor. A new predictor with better accuracy is discussed. Methods with 4–7 stages are tested and compared with RODAS. The numerical results show the potential of the Nordsieck implementation of the methods.

Key words: Linearly-implicit two-step methods, peer-method, general linear methods, Nordsieck representation

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1 Introduction

Linearly-implicit one-step methods are widely used for the solution of stiff initial value problems

$$y' = f(t, y), \quad y(t_0) = y_0. \tag{1.1}$$

They combine good stability properties with a cheap implementation. There exist efficient and reliable one-step codes, e.g. RODAS [4] with LU-decomposition

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and ROWMAP [12] using Krylov-techniques for the solution of large problems arising from semi-discretization of parabolic equations. However, there are some drawbacks of these methods

- There is in general no potential of parallelism across the method.
- For very stiff systems there occurs an order reduction.
- Methods of high order require in general the computation of the exact Jacobian in each step.

These drawbacks can be overcome by linearly-implicit two-step methods. These methods were recently introduced and investigated in a series of papers by the authors, e.g. [7], [13], [10]. Their main characterizations are:

- There exist parallel methods, where all stage values can be computed in parallel.
- The order and stage order of an s-stage method is $p \geq s-1$, even if not the exact Jacobian is used. There is no order reduction.
- There exist A-, L-stable and stiffly accurate methods.

In extensive numerical tests these methods gave excellent results, especially for larger problems. However, compared with one-step methods their implementation is more difficult. This is mainly due to the fact, that the coefficients depend on the ratio of two consecutive steps. Until now we have recomputed the coefficients of the methods for the current stepsize ratio in each step. For large systems this is not expensive compared with the overall costs, but for small systems this work may considerably influence the efficiency of the methods.

In this paper we therefore will follow another approach. We consider the methods in the framework of general linear methods (GLM). General linear methods were introduced and extensively investigated by Butcher and co-authors, e.g. [1]. In detail we will consider the Nordsieck representation of linearly-implicit two-step methods. To do this, we write our methods as implicit two-step Nordsieck methods and perform then one simplified Newton-iteration with special starting values to obtain well-known classes of linearly-implicit two-step methods. We see the main advantages in the following

- The Nordsieck form allows a cheap stepsize change by a simple scaling with the diagonal matrix of the powers of the stepsize ratio.
- The consideration of implicit methods at the beginning gives more theoretical insight for stability and accuracy investigations. The previously proposed linearly-implicit methods can be obtained with a single Newton iteration using particular starting values, and it becomes very natural to study different predictors which lead to different linearly-implicit versions of the same underlying implicit method.
- The Nordsieck form seems to be a suitable approach to implement the meth-

ods with order control in the future.

In Section 2 we derive the Nordsieck form of the linearly-implicit parallel and sequential two-step methods from [7] and [8]. For two 3-stage methods the corresponding coefficients are given.

In Section 3 linearly-implicit two-step peer-methods are considered. They are transformed into Nordsieck form and interpreted as the result of one Newton step of implicit peer-methods. We discuss a new predictor for the Newton step and give examples of special methods.

In Section 4 we give numerical results on some well-known test problems for the methods with the new predictor. A comparison with RODAS shows the efficiency of the methods, especially for stringent tolerances. The superiority of the new predictor is illustrated.

For simplicity of notation we formulate the methods in this paper for scalar equations and we restrict to autonomous problems. The extension to systems and nonautonomous problems is straightforward.

2 PTSW-methods in Nordsieck form

The implicit version of the s-stage stiffly accurate parallel two-step W-methods (PTSW-methods) considered in [7] can be written as General Linear Method in autonomous form as

$$\begin{pmatrix} Y_m \\ y_{m+1} \\ h_m F(Y_m) \end{pmatrix} = \begin{pmatrix} \gamma I_s & \mathbb{1} & U \\ \gamma e_s^T & 1 & e_s^T U \\ I_s & 0 & 0 \end{pmatrix} \begin{pmatrix} h_m F(Y_m) \\ y_m \\ h_m F(Y_{m-1}) \end{pmatrix} \tag{2.1}$$

Here y_m is the numerical approximation to $y(t_m)$ and $F(Y_m)$ denotes the vector $(f(Y_{m1}), ..., f(Y_{ms}))^T$. The computation of the stage values Y_{mi}, $i = 1, ..., s$, which are approximations to $y(t_m + c_i h_m)$, can be done in parallel on s processors.

PTSW-methods pass $s+1$ quantities between two steps: the 'master' variable y_m approximating the solution and s 'slave' variables $h_m f(Y_{mi})$ approximating the derivative of the solution at node points. This guarantees zero-stability and allows to achieve order $p = s$ with s stages.

Application to the test equation $y' = \lambda y$ yields with $z = h_m\lambda$

$$\begin{pmatrix} y_{m+1} \\ h_m F(Y_m) \end{pmatrix} = M(z) \begin{pmatrix} y_m \\ h_m F(Y_{m-1}) \end{pmatrix}$$

with

$$M(z) = \begin{pmatrix} 1 & e_s^T U \\ 0 & 0 \end{pmatrix} + \frac{z}{1-\gamma z} \begin{pmatrix} \gamma e_s^T \\ I_s \end{pmatrix} \begin{pmatrix} \mathbb{1} & U \end{pmatrix}.$$

Stiff accuracy, which is characterized by $c_s = 1$ and the special coefficients in the second row of (2.1), gives $Y_{ms} = y_{m+1}$ and the first row in the stability matrix vanishes for $z \to \infty$ giving $y_{m+1} = 0$. If we, in addition, require for the spectral radius $\rho(U) = 0$, we have $\rho(M(\infty)) = 0$, a desirable property for very stiff systems. Corresponding L-stable methods were considered in [5].

The order conditions are obtained by Taylor series expansion and can be written for order $p = s$ as

$$\exp(cz) = \gamma z \exp(cz) + \mathbb{1} + Uz \exp(\frac{c-1}{\sigma_m} z) + \mathcal{O}(z^{s+1}),$$

with

$$\exp(cz) = \Big(\exp(c_1 z), ..., \exp(c_s z) \Big)^T$$

and $\sigma_m = h_m / h_{m-1}$. Order s is achieved for

$$U = (CV_0 - \gamma V_0 D) D^{-1} S_m V_1^{-1}, \tag{2.2}$$

where we use the notations

$$\begin{aligned} &V_0 = \Big(c_i^{j-1} \Big),\ V_1 = \Big((c_i - 1)^{j-1} \Big),\ C = \operatorname{diag}(c_i), \\ &D = \operatorname{diag}(1, 2, ..., s),\ S_m = \operatorname{diag}(1, \sigma_m, ..., \sigma_m^{s-1}). \end{aligned} \tag{2.3}$$

Equation (2.1) can then be written as

$$\begin{pmatrix} Y_m \\ y_{m+1} \\ h_m D^{-1} V_1^{-1} F(Y_m) \end{pmatrix} =$$

$$\begin{pmatrix} \gamma I & \mathbb{1} & CV_0 - \gamma V_0 D \\ \gamma e_s^T & 1 & e_s^T (CV_0 - \gamma V_0 D) \\ D^{-1} V_1^{-1} & 0 & 0 \end{pmatrix} \begin{pmatrix} I & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \sigma_m S_m \end{pmatrix} \begin{pmatrix} h_m F(Y_m) \\ y_m \\ h_{m-1} D^{-1} V_1^{-1} F(Y_{m-1}) \end{pmatrix}$$

With the *Nordsieck vector*

$$y^{[m]} = \begin{pmatrix} y_m \\ h_{m-1} D^{-1} V_1^{-1} F(Y_{m-1}) \end{pmatrix} \tag{2.4}$$

and with the $(s+1)$-dimensional diagonal matrix

$$\widetilde{S}_m = \mathrm{diag}(1, \sigma_m, ..., \sigma_m^s)$$

we finally obtain the implicit PTSW-method in Nordsieck form

$$\begin{pmatrix} Y_m \\ y^{[m+1]} \end{pmatrix} = \underbrace{\left(\begin{array}{c|cc} \gamma I & \mathbb{1} & CV_0 - \gamma V_0 D \\ \hline \gamma e_s^T & 1 & e_s^T(CV_0 - \gamma V_0 D) \\ D^{-1}V_1^{-1} & 0 & 0 \end{array}\right)}_{=:\mathcal{N}} \begin{pmatrix} I & 0 \\ 0 & \widetilde{S}_m \end{pmatrix} \begin{pmatrix} h_m F(Y_m) \\ y^{[m]} \end{pmatrix} \tag{2.5}$$

The Nordsieck vector $y^{[m]}$ contains approximations to the scaled derivatives

$$y^{[m]} \approx \begin{pmatrix} y(t_m) \\ h_{m-1} y'(t_m) \\ \vdots \\ \frac{h_{m-1}^s}{s!} y(s)(t_m) \end{pmatrix}, \quad \text{and} \quad \widetilde{S}_m y^{[m]} \approx \begin{pmatrix} y(t_m) \\ h_m y'(t_m) \\ \vdots \\ \frac{h_m^s}{s!} y^{(s)}(t_m) \end{pmatrix}, \tag{2.6}$$

as it is seen by substituting exact values $Y_{m-1,i} = y(t_{m-1} + c_i h_{m-1})$ into (2.4).

To obtain the linearly-implicit PTSW-method in Nordsieck representation we perform one iteration with a simplified Newton method and a special starting value. In linearly-implicit PTSW-methods linear equations are solved for stage values K_m corresponding to $F(Y_m)$. With this notation and the abbreviation

$$w = y_m + h_m(CV_0 - \gamma V_0 D) S_m D^{-1} V_1^{-1} K_{m-1}$$

for known values the nonlinear system reads

$$K_m - F(h_m \gamma K_m + w) = 0.$$

Performing one iteration with iteration matrix T and a predictor $K_m^{(0)}$ yields for the i-th stage value $k_{mi} = k_{mi}^{(1)}$ the linear system

$$(I - h_m \gamma T)[k_{mi} - k_{mi}^{(0)}] = -k_{mi}^{(0)} + f(h_m \gamma k_{mi}^{(0)} + w_i).$$

Choosing

$$k_{mi}^{(0)} = -\frac{1}{\gamma} \sum_{j=1}^{s} \gamma_{ij} k_{m-1,j}$$

we obtain

$$(I - h_m\gamma T)[k_{mi} + \frac{1}{\gamma}\sum_{j=1}^{s}\gamma_{ij}k_{m-1,j}] = \frac{1}{\gamma}\sum_{j=1}^{s}\gamma_{ij}k_{m-1,j} + f(h_m\sum_{j=1}^{s}\gamma_{ij}k_{m-1,j} + w_i).$$

With

$$\Gamma = \left(\gamma_{ij}\right) = -\gamma V_0 S_m V_1^{-1}$$

and the notation

$$A = CV_0SD^{-1}V_1^{-1}$$

we finally arrive at the PTSW-methods given in [7], formula (1.2).

Remark 2.1 *The choice of* Γ *ensures for exact values* $k_{m-1,i} = y'(t_{m-1} + c_ih_{m-1})$ *the relation* $k_{mi} - k_{mi}^{(0)} = \mathcal{O}(h_m^{s+1})$.

These PTSW-methods have been successfully used for the solution of MOL-systems of high dimension on a parallel computer, cf. [7]. If we consider the implementation on a sequential computer then we can replace γI in (2.1) by a lower triangular matrix G with $g_{ii} = \gamma$ and arrive at the class of two-step W-methods considered in [8]. Their implicit version can be written as GLM in the form

$$\begin{pmatrix} Y_m \\ y_{m+1} \\ h_mF(Y_m) \end{pmatrix} = \begin{pmatrix} G & \mathbb{1} & U \\ e_s^TG & 1 & e_s^TU \\ I_s & 0 & 0 \end{pmatrix} \begin{pmatrix} h_mF(Y_m) \\ y_m \\ h_mF(Y_{m-1}) \end{pmatrix} \tag{2.7}$$

The conditions for order s read now

$$\exp(cz) = Gz\exp(cz) + \mathbb{1} + Uz\exp(\frac{c-1}{\sigma_m}z) + \mathcal{O}(z^{s+1}),$$

giving

$$U = [CV_0 - GV_0D]D^{-1}S_mV_1^{-1}.$$

Analogously to the parallel methods, we obtain the Nordsieck representation

$$\begin{pmatrix} Y_m \\ y^{[m+1]} \end{pmatrix} = \underbrace{\left(\begin{array}{c|cc} G & \mathbb{1} & CV_0 - GV_0D \\ \hline e_s^TG & 1 & e_s^T(CV_0 - GV_0D) \\ D^{-1}V_1^{-1} & 0 & 0 \end{array}\right)}_{\mathcal{N}} \begin{pmatrix} I & 0 \\ 0 & \widetilde{S}_m \end{pmatrix} \begin{pmatrix} h_mF(Y_m) \\ y^{[m]} \end{pmatrix}. \tag{2.8}$$

The derivation of the linearly-implicit method is similar to that for parallel methods. We perform one Newton step with starting value

$$k_{mi}^{(0)} = -\frac{1}{\gamma}\sum_{j=1}^{s}\gamma_{ij}k_{m-1,j} - \frac{1}{\gamma}\sum_{j=1}^{i-1}\widetilde{\gamma}_{ij}k_{m,j}.$$

Here the strictly lower triangular matrix $\widetilde{\Gamma} = \left(\widetilde{\gamma}_{ij}\right)$ is arbitrary and is chosen by implementation issues. With

$$\Gamma = \left(\gamma_{ij}\right) = -(\gamma V_0 + \widetilde{\Gamma}V_0)S_m V_1^{-1}$$

we have order s for the linearly-implicit method. With the notations

$$A = U - \Gamma, \quad \widetilde{A} = G - \gamma I - \widetilde{\Gamma}$$

we obtain the linearly-implicit methods of order $p = s$ of [8].

Example 1 *We consider the 3-stage PTSW-method PTSWA3 of [7] with* $c = (-2.02539, -0.334697, 1)$*. It is of order 3 and L(84.8°)-stable. The Nordsieck form* (2.5) *(with 6 digits) is given by*

$$\mathcal{N} = \left(\begin{array}{ccc|cccc} 0.515546 & 0 & 0 & 1 & -2.54094 & 6.19058 & -14.6532 \\ 0 & 0.515546 & 0 & 1 & -0.850242 & 0.457125 & -0.210751 \\ 0 & 0 & 0.515546 & 1 & 0.484454 & -0.0310912 & -0.546637 \\ \hline 0 & 0 & 0.515546 & 1 & 0.484454 & -0.0310912 & -0.546637 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0.130468 & -0.670353 & 0.539885 & 0 & 0 & 0 & 0 \\ 0.0651676 & -0.147717 & 0.0825495 & 0 & 0 & 0 & 0 \end{array}\right)$$

Example 2 *The Nordsieck representation of the sequential two-step W-method TSW3A of [8] with* $c = (0.5, 1.5, 1)$ *is given by*

$$\mathcal{N} = \left(\begin{array}{ccc|cccc} 0.4 & 0 & 0 & 1 & 0.1 & -0.15 & -0.175 \\ 1.1137 & 0.4 & 0 & 1 & -0.0136991 & -0.0636991 & -0.160274 \\ 0.558962 & -0.0767954 & 0.4 & 1 & 0.117833 & -0.128576 & -0.100853 \\ \hline 0.558962 & -0.0767954 & 0.4 & 1 & 0.117833 & -0.128576 & -0.100853 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ -0.5 & 0.5 & 0 & 0 & 0 & 0 & 0 \\ 0.666667 & 0.666667 & -1.33333 & 0 & 0 & 0 & 0 \end{array}\right)$$

This method is of order 3 and L-stable.

3 Two-step peer-methods

Peer-methods compute at each integration step s solution values $Y_{mi} \approx y(t_m + c_i h_m)$ of equal importance. They have very favourable stability properties for very stiff systems, since their stability matrix vanishes at infinity, $M(\infty) = 0$. Parallel linearly-implicit methods were introduced in [10] and applied to MOL-systems in [13], methods for sequential implementation are considered in [9]. In [11] implicit versions of two-step peer-methods are investigated.

As GLM the implicit version of sequential two-step peer-methods is given by

$$\begin{pmatrix} Y_m \\ Y_m \end{pmatrix} = \begin{pmatrix} G & B \\ G & B \end{pmatrix} \begin{pmatrix} h_m F(Y_m) \\ Y_{m-1} \end{pmatrix}. \tag{3.1}$$

Here G is a lower triangular matrix with elements g_{ij} where $g_{ii} = \gamma$, $i = 1, ..., s$. For parallel methods G is a diagonal matrix $G = \operatorname{diag}(\gamma_i)$. The conditions for order $p = s - 1$ are

$$\exp(\sigma_m c z) = G\sigma_m z \exp(\sigma_m c z) + B \exp(z(c-1)) + \mathcal{O}(h^s).$$

These conditions define

$$B = (V_0 - GV_0 D F_0^T) S_m V_1^{-1}, \tag{3.2}$$

with the shift matrix $F_0 = \left(\delta_{i-1,j}\right)$. The matrix G will be defined by stability considerations. Introducing the Nordsieck vectors

$$y^{[m]} = V_1^{-1} Y_{m-1}, \quad y^{[m+1]} = V_1^{-1} Y_m$$

and considering (3.2) we can write (3.1) as

$$\begin{pmatrix} Y_m \\ y^{[m+1]} \end{pmatrix} = \underbrace{\left(\begin{array}{c|c} G & V_0 - GV_0 D F_0^T \\ \hline V_1^{-1} G & V_1^{-1}(V_0 - GV_0 D F_0^T) \end{array}\right)}_{\mathcal{N}} \begin{pmatrix} h_m F(Y_m) \\ S_m y^{[m]} \end{pmatrix}. \tag{3.3}$$

For exact values $Y_m = \left(y(t_{m-1} + c_i h_{m-1})\right)$ it holds

$$y^{[m]} = \begin{pmatrix} y(t_m) \\ h_{m-1} y'(t_m) \\ \vdots \\ \frac{h_{m-1}^{s-1}}{(s-1)!} y^{(s-1)}(t_m) \end{pmatrix} + \mathcal{O}(h_{m-1}^s).$$

A linearly-implicit version is obtained by applying one Newton step to

$$Y_m - h_m G F(Y_m) - (V_0 - GV_0 D F_0^T) S_m y^{[m-1]} = 0.$$

With the iteration matrix $T \approx f_y(Y_{m-1,s})$, starting value $Y_m^{(0)}$ and using $(V_0 - GV_0DF_0^T)S_m y^{[m-1]} = BY_{m-1}$ one iteration step reads

$$(I - h_m GT)(Y_m - Y_m^{(0)}) = -Y_m^{(0)} + h_m GF(Y_m^{(0)}) + BY_{m-1}.$$

If we define

$$\Theta = V_0 S_m V_1^{-1}, \quad Y_m^{(0)} = \Theta Y_{m-1}, \tag{3.4}$$

we obtain

$$(I - h_m GT)Y_m = -h_m G\Theta TY_{m-1} + hGF(\Theta Y_{m-1}) + BY_{m-1}.$$

In [9] $F(\Theta Y_{m-1})$ is replaced by $\Theta F(Y_{m-1})$. This change does not affect the order $p = s - 1$ of the method. For linear autonomous ODEs both versions are equivalent. For nonlinear problems it is not clear which formulation gives better results. However, the version with $\Theta F(Y_{m-1})$ has the advantage that in the case of a rejected step the old function values can be reused. Denoting $A = G\Theta$ and using $\Theta F(Y_{m-1})$ we finally obtain

$$(I - h_m GT)Y_m = h_m A(F(Y_{m-1}) - TY_{m-1}) + BY_{m-1}.$$

Componentwise this is equivalent to

$$\begin{aligned}(I - h_m \gamma T)Y_{m,i} = &\sum_{j=1}^{s} b_{ij} Y_{m-1,j} + h_m \sum_{j=1}^{s} a_{ij} \left(F_{m-1,j} - TY_{m-1,j}\right) \\ &+ h_m T \sum_{j=1}^{i-1} g_{ij} Y_{m,j}, \quad i = 1, \ldots, s,\end{aligned}$$

which is just formula (1) in [9].

Numerical tests in [9] have shown the efficiency of these methods. However, the special choice of the predictor (3.4) may be not optimal for non-parallel methods. To predict the initial approximation Y_{0i} for the current stage i we may use, in general, all components of the input vector $y^{[m]}$ and the values $hf(Y_{m,j})$, $j = 1, \ldots, i-1$, from the current step. The predictor is then of the form

$$Y_m^{(0)} = h\widehat{A} f(Y_m) + \widehat{\Theta} y^{[m]}, \tag{3.5}$$

with a strictly lower triangular matrix $\widehat{A}$. Requiring that the predictor is of order $s - 1$, i.e., $Y_m - Y_m^{(0)} = \mathcal{O}(h^s)$, the matrix $\widehat{\Theta}$ is fully defined from $\widetilde{A}$ via the order condition

$$\exp(cz) = z\widehat{A} \exp(cz) + \widehat{\Theta} Z + O(z^s), \tag{3.6}$$

with $Z = [1, z, \frac{z^2}{2!}, \ldots, \frac{z^{s-1}}{s-1!}]^T$.

Remark 3.1 *The matrix $\widehat{A}$ may be chosen arbitrarily, for the numerical tests in Section 4 we compute it from the condition that $\|\widehat{\Theta}\|_F$ is minimized.*

We give now two examples of 4-stage linearly-implicit peer-methods, where the predictor is computed by (3.6) and Remark 3.1. These methods are also used in our numerical tests.

Example 3 *The sequential 4-stage peer-method PEER4 of [9] with nodes $c = (-1, -0.414214, 0.414214, 1)$ has the Nordsieck representation*

$$\mathcal{N} = \left(\begin{array}{cccc|cccc}
0.300748 & 0 & 0 & 0 & 1 & -1.30075 & 1.6015 & -1.90225 \\
0.585786 & 0.300748 & 0 & 0 & 1 & -1.30075 & 1.59229 & -1.98323 \\
0.414214 & 1 & 0.300748 & 0 & 1 & -1.30075 & 1.57928 & -1.84109 \\
0.252453 & 1.27614 & 0.471405 & 0.300748 & 1 & -1.30075 & 1.57008 & -1.5591 \\
\hline
0.252453 & 1.27614 & 0.471405 & 0.300748 & 1 & -1.30075 & 1.57008 & -1.5591 \\
-0.121779 & 0.111041 & 0.134293 & 0.876445 & 0 & 0 & -0.0157103 & 0.609723 \\
0.392887 & -0.760844 & -0.358114 & 0.726071 & 0 & 0 & 0 & 0.219075 \\
0.220851 & -0.248664 & -0.153705 & 0.181518 & 0 & 0 & 0 & 0
\end{array}\right)$$

The method is of order 3 for variable and of order 4 for constant stepsizes. It is stiffly accurate with $M(\infty) = 0$ and $L(89.9°)$-stable. In contrast to [9] where the predictor (3.4) *is used, we consider in our tests*

$$\widehat{A} = \begin{pmatrix}
0 & 0 & 0 & 0 \\
-0.22485 & 0 & 0 & 0 \\
-0.30047 & 0.69344 & 0 & 0 \\
0.19526 & -0.43689 & 1.2416 & 0
\end{pmatrix}, \quad \widehat{\Theta} = \begin{pmatrix}
1 & -1.0000 & 1.0000 & -1.0000 \\
1 & -0.18936 & -0.27814 & 0.60350 \\
1 & 0.021248 & 0.14509 & 0.61556 \\
1 & 0 & 0 & 0
\end{pmatrix}$$

Example 4 *PEER4A is a peer-method in Nordsieck form with the nodes $c = (-1, -\frac{1}{2}, \frac{1}{2}, 1)$. It is of order 3 and L-stable. The Nordsieck matrix $\mathcal{N}$ is given by*

$$\mathcal{N} = \left(\begin{array}{cccc|cccc}
\frac{6}{19} & 0 & 0 & 0 & 1 & -\frac{25}{19} & \frac{31}{19} & -\frac{37}{19} \\
\frac{81}{152} & \frac{6}{19} & 0 & 0 & 1 & -\frac{205}{152} & \frac{31}{19} & -\frac{149}{76} \\
\frac{419}{1064} & \frac{121}{133} & \frac{6}{19} & 0 & 1 & -\frac{1191}{1064} & \frac{31}{19} & -\frac{1051}{532} \\
\frac{816}{2527} & \frac{2568}{2527} & \frac{144}{361} & \frac{6}{19} & 1 & -\frac{2663}{2527} & \frac{31}{19} & -\frac{263}{133} \\
\hline
\frac{816}{2527} & \frac{2568}{2527} & \frac{144}{361} & \frac{6}{19} & 1 & -\frac{2663}{2527} & \frac{31}{19} & -\frac{263}{133} \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
\frac{5741}{15162} & -\frac{3662}{7581} & -\frac{148}{361} & \frac{16}{19} & 0 & -\frac{4969}{15162} & 0 & \frac{1}{133} \\
\frac{206}{1083} & -\frac{124}{1083} & -\frac{56}{361} & \frac{4}{19} & 0 & -\frac{142}{1083} & 0 & 0
\end{array}\right)$$

We use the predictor defined by

$$\widehat{A} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ -\frac{61}{216} & 0 & 0 & 0 \\ -\frac{307}{624} & \frac{149}{156} & 0 & 0 \\ \frac{1}{9} & -\frac{1}{6} & \frac{19}{18} & 0 \end{pmatrix}, \quad \widehat{\Theta} = \begin{pmatrix} 1 & -1 & 1 & -1 \\ 1 & -\frac{47}{216} & -\frac{17}{54} & \frac{13}{18} \\ 1 & \frac{23}{624} & \frac{23}{104} & \frac{23}{26} \\ 1 & 0 & 0 & 0 \end{pmatrix}.$$

The method PEER4A has – similarly to PTSW- and TSW-methods but in contrast to PEER4 and all other previously proposed peer-methods – the specially chosen row $\left[\begin{array}{cccc|cccc} 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{array}\right]$ in the method's array. This corresponds to the *first stage as last stage* or FSAL property of Runge-Kutta methods and enforces the second component of the Nordsieck vector to be the *exact* scaled derivative of the first component, i.e. $y_2^{[m+1]} = h_m f(y_1^{[m]})$. This FSAL property is in particiular advantageous for estimating higher order errors, e.g. $y^{(p+2)}(t_m)$, and therefore for variable order implementations [2]. The construction of peer-methods with $s > 4$ and FSAL is subject of current work.

Remark 3.2 *Method PEER4A was found by requiring that* $T^{-1}(M(0)-e_1e_1^T)T$ *is a strictly upper triangular matrix with* $T = [e_1, e_4, e_2, e_3]$*. This leads, together with the condition* $e_2^T(V_1^{-1})e_s = \frac{1}{\gamma}$ *to ensure the FSAL property, to a linear system for the elements of the matrix* G*. Choosing* T *as a permutation matrix guarantees unconditional zero stability,* $\|\prod_m S_m M(0)\| < C$*, and generalizes the work in [9] where* $T = I$ *was used. Investigations of unconditional zero stability for general linear methods with inherent Runge-Kutta stability can be found in [3].*

4 Numerical Experiments

We have tested the sequential s-stage peer-methods, $s = 4, 5, 6, 7$, of [9] in Nordsieck form and with the new predictor (3.6) on the following examples

- HIRES as described in [4],
- OREGO as described in [4] with $t_e = 360$,
- PLATE as described in [4],
- KREISS as proposed in [6] (for details see also [5]).

The last problem is characterized by a strongly varying Jacobian. PLATE requires an angle of A(α)-stability of $\alpha \approx 71°$.

The local truncation errors are estimated based on an embedded method of order $s-2$. The stepsize $h_m = \sigma_m h_{m-1}$ is allowed to vary in every step with a ratio in the range $\sigma_m \in (0, 1.5]$. The matrix $I - h_m \gamma T_m$ is generated and decomposed into LU factors in every step, where T_m is computed using finite differences.

We display the obtained accuracy at the end point of the integration vs. the computing time in the Figures 4.1–4.4. For comparison we include the results for the state of the art code RODAS. RODAS performs six function evaluations and solves six linear systems per step. Hence, its implementation costs are approximately the same as for our six-stage method.

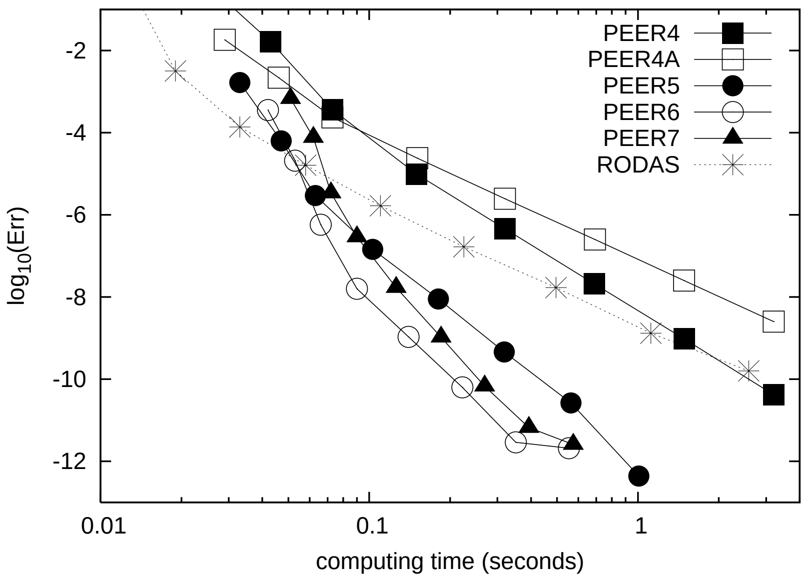

Fig. 4.1. Work-precision diagram for OREGO

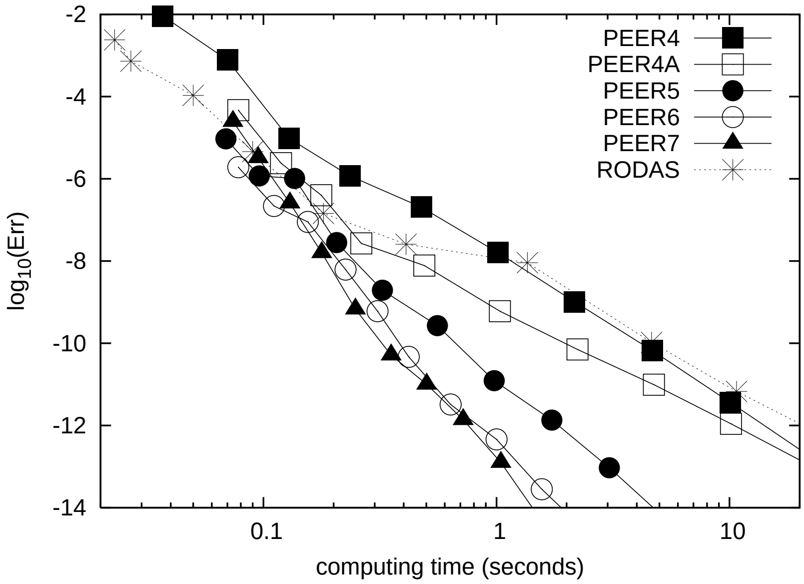

Fig. 4.2. Work-precision diagram for PLATE

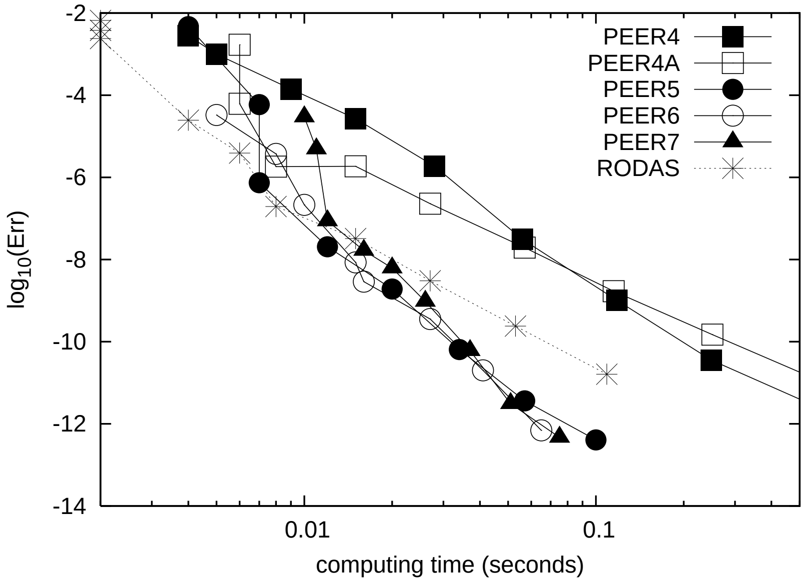

Fig. 4.3. Work-precision diagram for HIRES

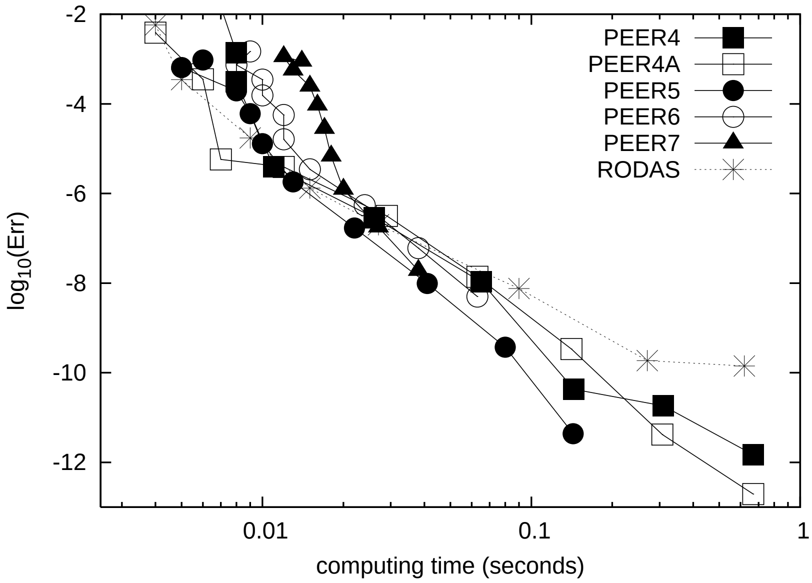

Fig. 4.4. Work-precision diagram for KREISS

The figures illustrate the efficiency of the peer-methods in Nordsieck implementation. For all test-problems we see a similar behavior: for crude tolerances RODAS is very competitive and for more severe tolerances the higher order peer-methods become superior. PLATE with eigenvalues of the Jacobian with large imaginary part offers no difficulty for the peer-methods.

In our tests we did not yet exploit the fact that the order of the methods does not depend on the matrix T. In contrast to RODAS we therefore can keep the Jacobian fixed for some steps, what may reduce the computing time substantially. The development of a suitable strategy of re-computation of the

Jacobian, and an order control will be the topic of future work.

The comparison of PEER4 and PEER4A with the FSAL property shows an advantage of PEER4A for crude tolerances. For more stringent tolerances PEER4 becomes more efficient. This is due to the fact, that for constant stepsizes PEER4 is of order 4 and gives better accuracy when the stepsize changes are small for stringent tolerances.

We also compared the new predictor with the old one (3.4). In all tests the new predictor gave better results, the typical behavior is illustrated by Figure 4.5 for the Oregonator. Especially for crude tolerances a considerable gain of accuracy can be observed.

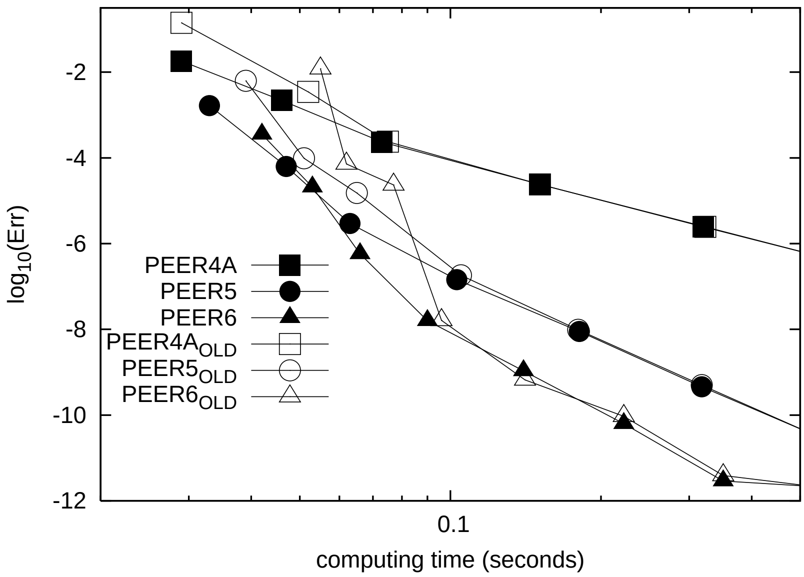

Fig. 4.5. Comparison of the two predictors for OREGO

5 Conclusions

This paper describes the efficient implementation of linearly-implicit two-step methods by using the Nordsieck representation. For some recently constructed methods the Nordsieck form is computed and examples are given. By considering the methods as a result of one Newton step in implicit two-step methods a new choice for the predictor is derived. The numerical experiments show an efficiency superior to RODAS for more stringent tolerances. The new predictor performs superior to the old one used in [9].

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