Rosenbrock-type 'Peer' two-step methods

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

Abstract

It is well-known that one-step Rosenbrock methods may suffer from order reduction for very stiff problems. By considering two-step methods we construct s-stage methods where all stage values have stage order $s-1$. The proposed class of methods is stable in the sense of zero-stability for arbitrary stepsize sequences. Furthermore there exist L(α)-stable methods with large α for $s = 4 \dots 8$. Using the concept of *effective order* we derive methods having order s for constant stepsizes. Numerical experiments show an efficiency superior to RODAS for more stringent tolerances.

Key words: Stiff ODEs, Rosenbrock methods, general linear methods, peer method

1 Introduction

Efficient software for solving initial value problems for stiff ordinary differential equations

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

is often based on Rosenbrock-type methods [4]. However, these methods may suffer from order reduction due to their low stage order. We overcome this

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drawback by extending the class of two-step peer W-methods introduced in [8] using actual stages, as well. These two-step Rosenbrock type methods have s stage values $Y_{m,i}$ computed by the scheme

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

for a timestep $t_m \to t_{m+1}$, where $F_{m,i} := f(t_m + c_i h_m, Y_{m,i})$ and $\gamma > 0$. This kind of scheme was originally proposed in [8] as a parallel method with $g_{ij} = 0$. The values $Y_{m,i}$ are approximations to the solution $y(t)$ at points $t_{mi} = t_m + h_m c_i$. Since they all have essentially the same characteristics we call them 'peer' variables. The matrix T_m is supposed to be an approximation to the Jacobian $f_y(t_m, y(t_m))$ for stability reasons. However, the order conditions are derived independent of the matrix T_m in the sense of W-methods. The computational cost for the scheme (1) consists mainly of s function evaluations and the solution of s linear systems all having the same coefficient matrix $I - h_m\gamma T_m$.

For scalar problems we can rewrite the scheme (1) for the vectors $(Y_{m,i})_{i=1}^{s}$ and obtain

$$(I - hGT_m)Y_m = B_m Y_{m-1} + h_m A_m (F_{m-1} - T_m Y_{m-1}).$$

The coefficients b_{ij}, a_{ij} and g_{ij} have been collected in matrices B_m, A_m and $G = (g_{ij}) + \gamma I$. The index m here indicates that all matrices may depend on the stepsize ratio $\sigma_m = h_m/h_{m-1}$ of two consecutive steps. In principle, matrix G could depend on σ_m as well, but as justified by the result in Lemma 2, we restrict ourselves to a constant matrix G. A generalization of this notation for nonscalar problems is straightforward using Kronecker products, cf. [11].

Considering the linear scalar test equation $y' = \lambda y$ and using the exact Jacobian $T_m = \lambda$ the method (1) assumes the simple form

$$Y_m = M(z)Y_{m-1}, \quad M(z) = (I - zG)^{-1}B_m, \quad (2)$$

where $z = \lambda h$. In contrast to one-step methods the factor $M(z)$ is a matrix which we call the stability matrix of the method (1). Note, that $M(z)$ may change with the step index through B_m. For $|h\lambda| \to \infty$ we obtain the limit $Y_m \to 0$ independent of the previous stage values Y_{m-1} and the stepsize ratio σ_m. This follows from the property $M(\infty) = 0$ which is automatically satisfied for peer methods (1). We call this strong damping property at infinity *stiff accuracy* [7,8]. Recently, it has been shown that stiff accuracy contradicts stability for non-constant stepsizes for singly-implicit parallel peer methods of high order, where G is a diagonal matrix with constant entries, $G = \gamma I$, cf. [8]. A possible remedy for this situation is to allow different values on the diagonal, $G = \mathrm{diag}(\gamma_1, \ldots, \gamma_s)$, see [10,11] for details. This version is suited for parallel implementation with s processors since s different linear systems have to be solved per step. Although the family of peer methods was initially constructed having parallel computers in mind we often observed that peer methods were competitive with existing sequential methods on non-parallel computers, too. So it is natural to study non-parallel extensions (1) of peer methods where constant values $g_{ii} = \gamma$ on the diagonal are required. But now, an additional sequential coupling between the stages is allowed, i.e. $g_{ij} \neq 0$ for $i > j$. The methods obtained are stiffly accurate for all components and unconditionally stable, i.e. stable for all stepsize patterns, and require only one LU-decomposition per step.

The main advantage of two-step methods (1) over traditional Rosenbrock methods is the possibility of having high stage order. And since s quantities are passed from step to step instead of just one single approximation to $y(t_m)$, continuous output of high order is available, as well, with no extra costs.

Peer methods like (1) can be derived from implicit general linear methods (see [3] and the references therein) by considering certain predictors and taking just one Newton step. Conversely, we can formulate an implicit version of the family of methods proposed in this article as it is described for parallel peer methods in [9]. However, for many stiff problems the single iteration seems to be an appropriate choice since it preserves the order and the linear stability properties at fairly low costs.

This paper is organized as follows. In Section 2 we derive the order conditions of the methods. In Section 3 we propose a construction to ensure unconditional stability. Further, we employ the concept of *effective order* and derive methods having order s for constant stepsizes and order $s-1$ for variable stepsizes. We derive methods up to $s = 8$ stages. Numerical results are reported in Section 4.

2 Order conditions and linear stability

A compact representation of the local order conditions uses a formal variable z where z^k stands for $h_m^k y^{(k)}(t_m)$, cf. [1,3]. Since G is a triangular matrix the following simplifying assumptions are slightly more general than the conditions given in [8]. They are

$$AB(p+1): \quad \exp(cz) = (B_m + zA_m)\exp((c-1)z/\sigma_m) + \mathcal{O}(z^{p+1}), \tag{3}$$

$$G(p): \quad G\exp(cz) = A_m \exp((c-1)z/\sigma_m) + \mathcal{O}(z^{p+1}), \tag{4}$$

where $\exp(cz)$ and similar terms are evaluated in components, e.g. $\exp(cz) = [\exp(c_1 z), \dots, \exp(c_s z)]^T$. This notation is also used in the following lemma.

Lemma 1 *The conditions AB($p+1$) and G(p) ensure that the local residual vector δ_m of the scheme* (1) *defined by*

$$(I - h_m G T_m)\delta_m = y(t_m + ch_m) - h_m G T_m y(t_m + ch_m) - B_m y(t_{m-1} + ch_{m-1}) \\ - h_m A_m \left(y'(t_{m-1} + ch_{m-1}) - T_m y(t_{m-1} + ch_{m-1})\right) \quad (5)$$

is of order p, $\delta_m = \mathcal{O}(h_m^{p+1})$, independent of T_m.

PROOF. We substitute $t_{m-1} + ch_{m-1} = t_m + (c-1)h_m/\sigma_m$ and expand all quantities in the residual δ_m in Taylor series around t_m, treating terms without T_m and with T_m separately. Substituting $h_m^k y^{(k)}(t_m) = z^k$ it is seen that all terms up to order p vanish if the conditions AB($p+1$) and G(p) hold. $\square$

Defining the global errors $\Delta_m = y(t_m + ch_m) - Y_m$ and assuming that f satisfies a Lipschitz-condition we get the following error recursion

$$\Delta_m = M(h_m T_m)\Delta_{m-1} + \mathcal{O}(h_m \|\Delta_{m-1}\|) + \delta_m. \quad (6)$$

Before we state the convergence result we recall from [8] that a peer method is called *stable* if

$$\|B_{m+l} B_{m+l-1} \cdots B_{m+1} B_m\| \le L \quad (7)$$

holds for some constant $L < \infty$ and for all m and $l \ge 0$. Since $M(0) = B_m$, for constant stepsizes the condition (7) corresponds to the zero–stability of multistep methods.

We can use the convergence theory for multistep methods (cf. [4]) and obtain the following theorem similar to [8].

Theorem 1 *Let the error recursion* (6) *be satisfied with a local error $\delta_m = \mathcal{O}(h_m^{p+1})$. Assume further, that the method is stable, i.e.* (7), *and has bounded coefficients for stepsize ratios $\sigma_m \le \sigma_{\max}$. Then, for a sufficiently smooth solution y and accurate initial values Y_0 the method is convergent of order p, i.e. the global error Δ_m satisfies $\Delta_m = \mathcal{O}(h^p)$ with $h = \max h_m$.*

In the remaining sections we always assume that the simplifying assumptions AB(s) and G(s) hold. This implies at least order $s-1$ according to Theorem 1. It is convenient to express AB(s) and G(s) using certain $s \times s$ matrices. We define $V = (v_{ij})$, $P = (p_{ij})$, and F by

$$v_{ij} = c_i^{j-1}, \quad p_{ij} = \binom{j-1}{i-1}, \quad F = [e_2, .., e_s, 0],$$

and $S_m = \mathrm{diag}(1, \sigma_m, \ldots, \sigma_m^{s-1})$, $D = \mathrm{diag}(1, 2, \ldots, s)$. Here, e_i is the i-th unit vector. Now we find the equivalent form

$$\begin{aligned} AB(s): \qquad & V \;= B_m V P^{-1} S_m^{-1} + A_m V P^{-1} S_m^{-1} D F^T & \text{(8a)} \\ G(s): \qquad & GV = A_m V P^{-1} S_m^{-1}. & \text{(8b)} \end{aligned}$$

Once G is chosen, the matrix $A_m = GVS_m PV^{-1}$ is given by G(s) and, then, $B_m = (V - GVDF^T)S_m PV^{-1}$ by AB(s).

3 Construction of unconditionally stable methods

The objective of this section is to determine the coefficients in the lower triangular matrix G so that the method (1) is stable for arbitrary stepsize ratios $\sigma_m = h_m/h_{m-1}$. Due to the consistency condition $AB(1)$, which is $B_m \mathbb{1} = \mathbb{1}$, $\mathbb{1} := [1, \ldots, 1]^T$, we always have an eigenvalue one in $M(0) = B_m$. Now, we require that the $s-1$ other eigenvalues of B_m vanish for all σ_m. To this end we consider a matrix Q_m related to B_m by a similarity transformation, namely,

$$Q_m = PV^{-1} B_m V P^{-1} = P(I - V^{-1} GVDF^T) S_m,$$

and require that $Q_m - e_1 e_1^T$ is a strictly upper triangular matrix. Since $Qe_1 = e_1$, this condition is much more restrictive than the zero eigenvalue condition $\rho(Q_m - e_1 e_1^T) = 0$. However, this stronger condition is more appropriate for variable stepsizes since it guarantees stability (7) for arbitrary stepsize sequences. Any product $B_m \cdots B_1$ with more than $s-1$ factors can be reduced to a short product $VP^{-1} e_1 e_1^T Q_{s-1} Q_{s-2} \cdots Q_2 Q_1 PV^{-1}$ consisting of $s-1$ factors Q_k only.

Let us denote by $\mathrm{tril}(\cdot)$ the lower and $\mathrm{tril}^*(\cdot)$ the strictly lower part of a matrix, where the rest is filled with zeros. The formal definition is

$$\mathrm{tril}(X) = \sum_{\substack{i,j \\ i \ge j}} e_i^T X e_j e_i e_j^T \quad \text{and} \quad \mathrm{tril}^*(X) = \sum_{\substack{i,j \\ i > j}} e_i^T X e_j e_i e_j^T.$$

By the definition of Q_m and the linearity of $\mathrm{tril}(\cdot)$ the desired condition

$$\mathrm{tril}(Q_m - e_1 e_1^T) = 0,$$

can be satisfied by requiring

$$\mathrm{tril}(V^{-1} GVDF^T) = I - e_1 e_1^T = FF^T, \tag{9}$$

since PS_m is upper triangular. Condition (9) holds with the choice

$$\mathrm{tril}^*(V^{-1} GV) = FD^{-1}. \tag{10}$$

Introducing the strictly lower part of G as $G^* = G - \gamma I = \mathrm{tril}^*(G)$ and we can write (10) as

$$G^* V = VFD^{-1} + VU, \tag{11}$$

where U is some upper triangular matrix. We note that the matrix G^* from (11) does not depend on σ_m. It may be constructed row by row starting with zero for $s = 1$.

Lemma 2 *The equation* (11) *has a unique solution G^* if the nodes c_i are pairwise distinct. The construction is possible row-wise for G^* and column-wise for U. If G^* is a solution of (11) for dimension s, then,*

$$\widehat{G}^* = \begin{bmatrix} G^* & 0 \\ g^T & 0 \end{bmatrix} \in \mathbb{R}^{s+1,s+1}$$

is the solution of (11) *with dimension $s+1$.*

PROOF. We prove the uniqueness G^* inductively. For $s = 1$ the only solution is $G^* = [0]$. Now, let $\widehat{G}^* \in \mathbb{R}^{s+1,s+1}$ be a solution of (11), that is,

$$\widehat{G}^* \widehat{V} = \widehat{X} + \widehat{V}\widehat{U}, \tag{12}$$

where we use the symbol '$\frown$' to denote the matrices of size $(s+1) \times (s+1)$, e.g. $\widehat{X} = \widehat{V}\widehat{F}\widehat{D}^{-1}$ and $\widehat{V} := (c_i^{j-1})_{i,j \le s+1}$. We partition (12) and obtain

$$\begin{bmatrix} G^* & 0 \\ g^T & 0 \end{bmatrix} \begin{bmatrix} V & * \\ v^T & * \end{bmatrix} = \begin{bmatrix} X & * \\ x^T & * \end{bmatrix} + \begin{bmatrix} V & * \\ v^T & * \end{bmatrix} \begin{bmatrix} U & * \\ 0^T & * \end{bmatrix}. \tag{13}$$

Notice that G^* is a solution of the system (11) of size s since

$$G^* V = X + VU = VFD^{-1} + VU + we_s^T, \tag{14}$$

where $w = -Xe_s$ is added since X and VFD^{-1} differ in the last column. Hence G^* is unique, by induction. The first $s-1$ column in U appear unchanged in the problem of size s and hence they are uniquely defined either, since G^* is unique. The assumption on the nodes guarantees the existence of V^{-1}. It remains to show that we can find a unique g^T from (13). From column s in (13) we see that

$$Ue_s = V^{-1}(G^* V - X)\, e_s, \tag{15}$$

and this determines the last column in U. Similarly, the last row in (13) then gives

$$g^T = \left(x^T + v^T U\right) V^{-1}, \tag{16}$$

which completes the proof. $\square$

The construction in the proof of Lemma 2 allows the successive computation of the rows of G. However, it is not really necessary to find an explicit formula for G. In a computer algebra system we can expand (11) into a linear system involving the coefficients of G^* and U and solve it directly. For reference, we report the first three rows of G^* here:

$$
\begin{aligned}
g_{21} &= c_2 - c_1, \\
g_{31} &= \frac{(c_3 - c_1)\,(2\,c_1 - 3\,c_2 + c_3)}{2\;(c_1 - c_2)} \\
g_{32} &= \frac{(c_1 - c_3)\,(c_3 - c_2)}{2\,(c_1 - c_2)} \\
g_{41} &= \frac{(c_4 - c_1)\,(6\,c_1^2 + (-9\,c_2 - 6\;c_3 + 3\,c_4)\,c_1 + c_2\,(11\,c_3 - 2\;c_4) + c_4\,(2\,c_4 - 5\,c_3))}{6\;(c_1 - c_2)\,(c_1 - c_3)} \\
g_{42} &= \frac{(c_1 - c_4)\,(c_4 - c_2)\,(3\,c_2 - 5\;c_3 + 2\,c_4)}{6\,(c_1 - c_2)\,(c_2 - c_3)} \\
g_{43} &= \frac{(c_1 - c_4)\,(c_2 - c_4)\,(c_3 - c_4)}{3\;(c_1 - c_3)\,(c_3 - c_2)}.
\end{aligned}
$$

If we require $\mathrm{AB}(s)$, $\mathrm{G}(s)$ and the stability condition (11) we still have some degrees of freedom in the nodes c and the value of γ. In the light of the convergence theorem it might be desirable to satisfy $\mathrm{AB}(s+1)$ in order to obtain global convergence of order s. But this requirement is very restrictive and does not lead to practical methods, at least, for $s = 3$ and $s = 4$ getting complex nodes c. Fortunately, $\mathrm{AB}(s+1)$ is not a crucial requirement for order s with constant stepsizes. As we explain below, using the concept of *effective order* and a carefully chosen value of γ, global order s is attainable for any set of nodes c. An obvious choice for the nodes is the equidistant points $c_i = c_1 + (i-1)h_c$, $i = 1, \dots, s$. Here, surprisingly, all parameters g_{ij} take the same value, $g_{ij} = h_c$ for $i > j$. In practice, however, we prefer the nodes

$$
c_i = -\frac{\cos\left((i - \frac{1}{2})\pi/s\right)}{\cos\left(\frac{1}{2}\pi/s\right)}, \tag{17}
$$

being the roots of stretched Chebychev polynomials. They range from $c_1 = -1$ to $c_s = 1$. The advantage of having nodes outside $[0, 1]$ is a smaller condition number of the Vandermonde matrix V, cf. [10]. Consequently, the entries in the matrices A_m and B_m are of small magnitude, which is important for robustness of the method.

The concept of *effective order* proposed by Butcher, e.g. [2], can be used for peer methods, too, at least in the case of constant stepsizes $h = h_m$. The underlying idea is that Y_m is supposed to be an approximation to $y(t_m + ch) + Eh^s/s!\, y^{(s)}(t_m)$. It is crucial that the vector E does not depend on the current step m. If new local residuals $\widetilde{\delta}_m$, defined by

$$
\begin{aligned}
(I-hGT_m)\widetilde{\delta}_m = {} & y(t_m+ch)+E\frac{h^s}{s!}y^{(s)}(t_m)-hGT_m(y(t_m+ch)+E\frac{h^s}{s!}y^{(s)}(t_m)) \\
& - B\left[y(t_{m-1}+ch)+E\frac{h^s}{s!}y^{(s)}(t_{m-1})\right] \\
& - hA\Big[f(t_{m-1}+ch, y(t_{m-1}+ch)+E\frac{h^s}{s!}y^{(s)}(t_{m-1})) \\
& - T_m(y(t_{m-1}+ch)+E\frac{h^s}{s!}y^{(s)}(t_{m-1}))\Big],
\end{aligned} \tag{18}
$$

are of order s, i.e. $\widetilde{\delta}_m=\mathcal{O}(h^{s+1})$, then the global errors $\widetilde{\Delta}_m = y(t_m+ch)+Eh^s/s!\,y^{(s)}(t_m)-Y_m$ are also of order s, $\widetilde{\Delta}_m=\mathcal{O}(h^s)$, since they obey the recursion

$$\widetilde{\Delta}_m = M(hT_m)\widetilde{\Delta}_{m-1}+\mathcal{O}(h\|\widetilde{\Delta}_{m-1}\|)+\widetilde{\delta}_m,$$

similar to (6). Assuming AB(s) and $G(s)$, i.e. order $s-1$, we have $\widetilde{\delta}_m=\mathcal{O}(h^s)$. So we only need to look at order h^s in (18). The term involving T_m vanishes already due to condition $G(s)$. Thus the additional condition for convergence of order s is that the term without T_m cancels, i.e.

$$\frac{z^s}{s!}\left(c^s+E-B\left[(c-1)^s+E\right]-sA\left[(c-1)^{s-1}\right]\right)=0, \tag{19}$$

where $z^s=h^s y^{(s)}(t_m)$. Since $(I-B)$ is singular the system (19) cannot be solved for E without further restrictions. Writing (19) as

$$(I-V^{-1}BV)V^{-1}E = V^{-1}[sA(c-1)^{s-1}+B(c-1)^s-c^s],$$

and multiplying on the left by $[I-V^{-1}BV+e_1e_1^T]^{-1}$ leads to

$$(I-e_1e_1^T)V^{-1}E=[I-V^{-1}BV+e_1e_1^T]^{-1}V^{-1}[sA(c-1)^{s-1}+B(c-1)^s-c^s]. \tag{20}$$

Matrix $I-V^{-1}BV+e_1e_1^T$ is regular since $Q-e_1e_1^T$ and, consequently, $-V^{-1}BV+e_1e_1^T$ are strictly upper triangular matrices. This system (20) is solvable if and only if the first component on the right hand side vanishes. It turns out that

$$p(\gamma):=e_1^T[I-V^{-1}BV+e_1e_1^T]^{-1}V^{-1}[sA(c-1)^{s-1}+B(c-1)^s-c^s]$$

is a polynomial in γ of degree s. It is straightforward to compute $p(\gamma)$. For example, for $s=4$ we find the polynomial

$$
\begin{aligned}
p(\gamma) = {} & -24\,\gamma^4+96\,\gamma^3-108\,\gamma^2+(-8\,c_1+4\,c_2+4\,c_3+32)\,\gamma \\
& +2\,c_1^2+\frac{16\,c_1}{3}-2\,c_1\,c_2-\frac{8\,c_2}{3}-2\,c_1\,c_3+2\,c_2\,c_3-\frac{8\,c_3}{3}-1,
\end{aligned}
$$

with general nodes c. Note, that the free parameter c_4 has no influence on $p(\gamma)$. According to (20) we have global order s if $p(\gamma)=0$ holds, i.e. for fixed nodes c we find s solutions γ.

Remark 1 *An equivalent approach to guarantee* (19) *is to look at the stability matrix* $M(z)$*. Effective order* s *implies that* $M(z)$ *has one eigenvalue* $\exp(z)+\mathcal{O}(z^{s+1})$ *for* z *near to* 0*. The precise condition is*

$$M(z)\left[\exp(cz)+E\frac{z^s}{s!}\right]=\exp(z)\left[\exp(cz)+E\frac{z^s}{s!}\right]+\mathcal{O}(z^{s+1}).$$

A carefull study of the characteristic polynomial $\det(M(z)-xI)$ *finally leads to the the same polynomials* $p(\gamma)$ *as obtained above.*

The next step might be the computation of the vector E, preferably with $e_s^T E = 0$ to avoid the necessity of a finishing method, and to take care of having starting values $Y_0 = y(ch) + \frac{Eh^s}{s!}y^{(s)}(0) + \mathcal{O}(h^{s+1})$. Although this step might improve the overall accuracy of the methods it is not needed. Even when we start with $Y_0 = y(ch)+\mathcal{O}(h^{s+1})$ the global order is s. This is because $\mathcal{O}(h^s)$ errors in the initial data (or due to a missing finishing procedure) do not amplify to $\mathcal{O}(h^{s-1})$ during the integration. In our computations, we will use starting values $Y_0 = y(ch) + \mathcal{O}(h^{s+1})$.

The values of γ leading to global convergence of order s for Chebychev nodes (17) are shown in Table 1. We also computed numerically the corresponding angles α of the $L(\alpha)$ stability defined by

$$\alpha = \inf\{|\pi-\arg(z)| : \rho(M(z)) \le 1\}.$$

We see L-stable methods, i.e. $\alpha = 90°$, for all numbers of stages $s = 4,\ldots,8$. Actually, a more exhaustive computation shows that the methods are always L-stable if γ is chosen within the intervals $[0.308, 1.0464]$, $[0.2765, 1.1554]$, $[0.3447, 0.93235]$, $[0.2567, 0.8258]$ and $[0.35, 0.83]$ for $s = 4, 5, 6, 7$ and $s = 8$, respectively.

4 Numerical tests

We have implemented the family of peer methods (1) fully defined by (8), (17), (11) with γ chosen from Table 1 in a manner similar to the one described in [11]. 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 difference. 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 $\sigma_m \in [0, 1.5]$. We present results for the following examples

- HIRES as described in [4],
- PLATE as described in [4],
- KREISS as proposed in [6] (for details see also [5]).

	s	γ	α
	4	0.25978983545051426	88.5°
*	4	0.30074836217942170	89.9°
	4	1.03888182868010988	90.0°
	5	0.16872684142585724	0.0°
*	5	0.26036881402181763	89.3°
	5	0.56147312920978467	90°
	6	0.14382407007209353	52.8°
*	6	0.19942255252118767	85.4°
	6	0.34763568282211337	90°
	7	0.12308525270799290	0.0°
	7	0.16150016158249455	75.3°
*	7	0.24256912841054176	89.4°
	7	0.58711723028670171	90°
	8	0.10363109465902397	0.0°
	8	0.13953918433758174	71.2°
*	8	0.18481054336428444	85.4°
	8	0.39345299165596424	90°

Table 1
List of γ-values and the corresponding numerically computed angles α of L(α) stability. The star marks those methods which are used in the numerical experiments.

The last problem is characterized by a strongly varying Jacobian. We display the obtained accuracy at the end point of the integration vs. the number of steps in the Figures 1-3. For comparison we include the results for RODAS [4], a code based on a six-stage fourth order Rosenbrock method. 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. However, in contrast to RODAS, we can re-use old Jacobian matrices or even LU factors of them in peer methods without having any order reductions. And this can lead to a substantial gain of efficiency, very strongly depending on the particular problem, of course. We do not exploit this advantage here.

We see for all three test-problems a similar behavior: for crude tolerances RODAS is very competitive and for more severe tolerances the peer methods become superior.

Some of the difficulties of our implementation for crude tolerances are due to the relatively small initial stepsize which we have chosen for a reliable computation of the starting values using the RADAU code.

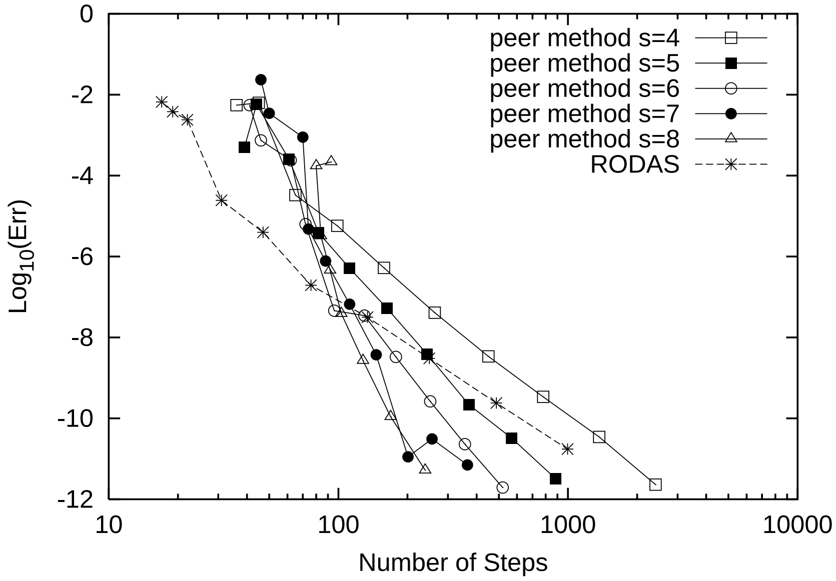

Fig. 1. Results for HIRES

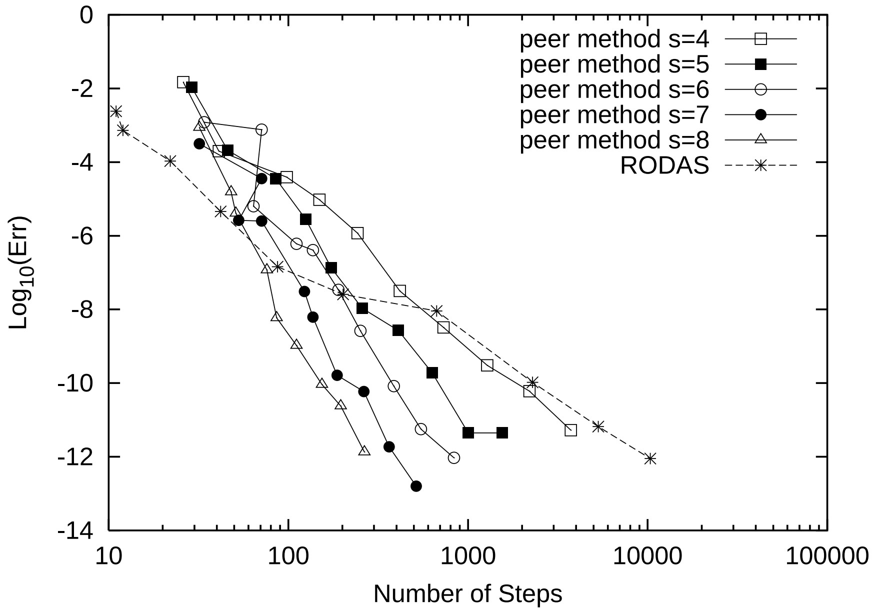

Fig. 2. Results for PLATE

5 Conclusions

This paper describes the construction of stable two-step Rosenbrock-methods with $s = 4 \ldots 8$ stages of order $s-1$ suitable for stiff problems. The advantages of passing all stage values Y_m from step to step are obvious: full stage order is obtained and no exact Jacobian is required for the order conditions. Loss of stability for varying stepsize is avoided by a certain structural restriction on the stability matrix $M(0)$ yielding a uniformly bounded matrix family under mild restrictions on the stepsize sequence. The numerical experiments show

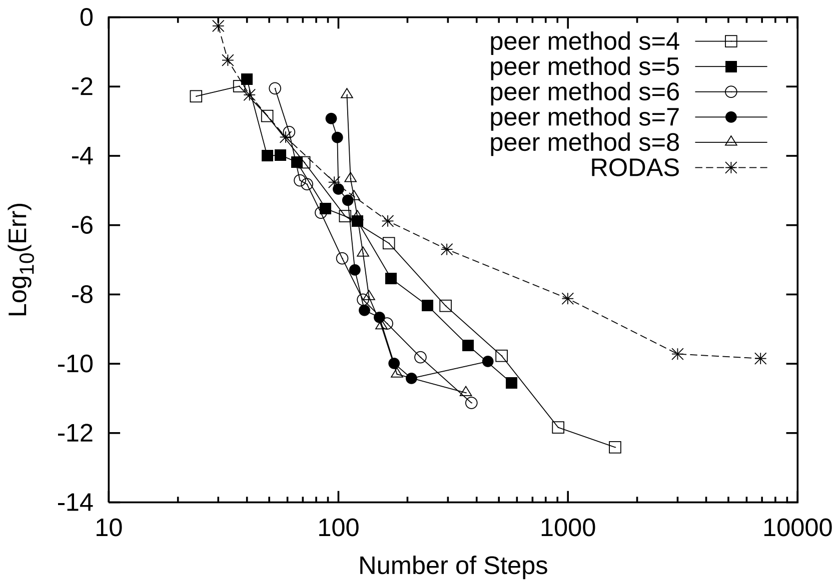

Fig. 3. Results for KREISS

an efficiency superior to RODAS for more stringent tolerances.

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