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NEW ROSENBROCK W-METHODS OF ORDER 3 FOR PARTIAL DIFFERENTIAL ALGEBRAIC EQUATIONS OF INDEX 1*

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Abstract.

In this note new Rosenbrock methods for ODEs, DAEs, PDEs and PDAEs of index 1 are presented. These solvers are of order 3, have 3 or 4 internal stages, and fulfil certain order conditions to obtain a better convergence if inexact Jacobians and approximations of $\frac{\partial f}{\partial t}$ are used. A comparison with other Rosenbrock solvers shows the advantages of the new methods.

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1 Introduction.

Many complex physical phenomena can be described by the help of systems of algebraic equations, ordinary and partial differential equations. These systems are often called partial differential algebraic equations (PDAEs) and are semidiscretized in space by finite differences, volumes, and elements, i.e. the equations are transformed into a system of ordinary differential and algebraic equations. This procedure is well-known as the vertical method of lines. For our numerical experiments, it has been integrated into the finite element package MooNMD, see [JM04] for more information.

In this paper the implicit ODE or DAE

$$M\dot{u} = f(t,u), \quad u(t_0) = u_0 \tag{1.1}$$

is to be solved numerically by the help of so called Rosenbrock methods. The matrix M may be singular and the function f is given. System (1.1) has the negative property that the problem may be stiff, i.e. explicit solvers may fail when solving the system. There are several methods which are more effective for stiff ODEs and DAEs as explicit solvers:

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- The fully implicit Runge–Kutta methods (IRK methods) are a first attempt to approximate the solution of (1.1) since IRK methods have very good stability properties, but in general nonlinear equations have to be solved. A famous scheme is Radau5 (see [HW96]). In [Roc89], IRK methods are developed to solve DAEs.
- The solution of nonlinear equations can be simplified or even avoided by means of diagonally-implicit RK methods (DIRK methods), which are a special case of IRK methods, and linearly implicit RK methods (LIRK methods) like adaptive RK methods or the popular Rosenbrock–Wanner methods (ROW methods). In each step of a LIRK method, only one system of linear equations has to be solved. The price of this is that the stability properties are not so good as those of the implicit RK methods. Furthermore the Jacobian has to be computed. This approximation can be avoided if the so-called W-methods are used, which work with rather arbitrary matrices as long as stability is not important. Of course, the convergence can be accelerated if this matrix is a good approximation of the Jacobian J, for example Ostermann created Rosenbrock methods with $J = f' + \mathcal{O}(h)$ (i.e. [Ost88]). Standard books on this topic are [HW96] and [SW92]. In [SW92] one can find many hints about the classification of W-methods. DIRK methods for DAEs can be found in [Cam99].
- The LIRK methods have the disadvantage that the linear systems may be large. Thus the size of these linear systems should be reduced. This can be done with an Arnoldi process as in the code ROWMAP (see [WSP97]).
- In [HLS98], Lubich and Hochbruck use the so-called exponential integrators.
- ODEs and DAEs can also be solved numerically with (implicit) multistep methods, e.g. Petzold developed the code DASSL (i.e. [BCP96]) and Brown, Hindmarsh, and Byrne the well-known code VODE (see [BBH89]), which only solves ODEs.

In the following we concentrate on Rosenbrock methods. It is well-known that solvers for (1.1) may exhibit order reduction if they are applied to large ODE systems resulting, e.g., from the semidiscretization in space of parabolic problems. Rosenbrock methods can decrease this order reduction if some additional conditions are fulfilled. Moreover, many Rosenbrock solvers need the Jacobian and the time derivative of the right-hand side f in each time-step. In [Lan01], Lang compares Rosenbrock methods for several problems (PDEs, PDAEs of index 1 and of index 2), but all methods need an exact approximation of the Jacobian. The only exception is the order 2 method ROS2 from [VSBH99]. In this paper we propose third order Rosenbrock methods with 3 and 4 internal stages, which need only an approximation of the Jacobian. The time derivative can be neglected. Unfortunately, W-methods using an approximation of the Jacobian have some disadvantages (see [Lan01]), but if such methods are applied as usual Rosenbrock methods, i.e. the Jacobian is evaluated exactly, they are able to approximate the numerical solution very well (see [VSBH99]).

In particular, the new methods are attractive candidates for the numerical solution of the large ODE systems mentioned above. The numerical comparisons presented at the end of the paper illustrate the good qualities of the methods in both academic and more practical problems.

The paper is structured as follows. First we consider the consistency of Rosenbrock methods for several classes of problems. In Section 3 we construct three new Rosenbrock methods of order 3 with 3 internal stages. We prove that there exists no Rosenbrock method for PDAEs of index 1 with three internal stages. Therefore we develop in Section 4 new Rosenbrock W-methods with four internal stages which have different properties. Two of the methods need only three instead of four function evaluations, a third method is stiffly accurate and the last W-method is of order 4 for ODEs. In the last section we present some numerical examples.

2 Consistency and stability of Rosenbrock methods.

We start with a short overview on some stability concepts.

DEFINITION 2.1. *An ODE-solver is called non-expansive on a class $\mathcal{F}$ of explicit (i.e. $M = I$) initial value problems* (1.1) *in* $\mathbb{R}^q$*, if for an arbitrary discretization I_τ of the interval* $[t_0, \infty)$ *the inequality*

$$\|u_{m+1} - v_{m+1}\| \leq \|u_m - v_m\| \tag{2.1}$$

holds for all τ and for two approximations u_m and v_m of two different initial values u_0 and v_0 in some vectornorm in $\mathbb{R}^q$ and all problems in $\mathcal{F}$.

DEFINITION 2.2. *An ODE-solver is called A-stable, if the method is non-expansive on the class*

$$\{f \ : \ f(t,u) = \lambda u, Re\,\lambda \leq 0\}.$$

DEFINITION 2.3. *An A-stable one-step method is called strongly A-stable or L-stable if the stability function satisfies*

$$\lim_{Re\, z \to -\infty} |R_0(z)| < 1 \quad \textit{or} \quad \lim_{Re\, z \to -\infty} |R_0(z)| = 0,$$

respectively.

DEFINITION 2.4. *An s-stage Rosenbrock method is given by*

$$\begin{aligned} k_i &:= \tau\, f\Big(t_{old} + \alpha_i\, \tau, u_{old} + \sum_{j=1}^{i-1} \alpha_{ij}\, k_j\Big) \\ &\quad + \tau\, W \sum_{j=1}^{i} \gamma_{ij}\, k_j + \tau^2 \gamma_i T, \quad i = 1, \dots, s \end{aligned} \tag{2.2}$$

$$u_{new} := u_{old} + \sum_{i=1}^{s} b_i\, k_i$$

where s is the number of internal stages, α_{ij}, γ_{ij}, b_i are the parameters of the method, $W := f'(t_{old}, u_{old})$, $T := \dot{f}(t_{old}, u_{old})$, $\alpha_i := \sum_{j=1}^{i-1} \alpha_{ij}$, and $\gamma_i := \sum_{j=1}^{i-1} \gamma_{ij}$.

The parameters α_{ij}, γ_{ij}, and b_i should be chosen in such a way that certain order conditions are fulfilled to obtain a sufficient consistency order. A derivation of these conditions with Butcher series can be found in [HW96]. Here we only summarize the conditions up to the order 3 for $s = 3$:

$$\text{(2.3)} \qquad \begin{cases} \text{(A1)} & b_1 + b_2 + b_3 = 1, \\ \text{(A2)} & b_2\beta_2 + b_3\beta_3 = \frac{1}{2} - \gamma, \\ \text{(A3a)} & b_2\alpha_2^2 + b_3\alpha_3^2 = \frac{1}{3}, \\ \text{(A3b)} & b_3\beta_2\beta_{32} = \frac{1}{6} - \gamma + \gamma^2, \end{cases}$$

where we use the abbreviations $\beta_{ij} := \alpha_{ij} + \gamma_{ij}$ and $\beta_i := \sum_{j=1}^{i-1} \beta_{ij}$. We get an additional consistency condition if we set $W := f'(t_{old}, u_{old}) + \mathcal{O}(h)$ (see [SW92], [HW96], and [SW79]):

$$\text{(2.4)} \qquad \text{(B2)} \quad b_2\alpha_2 + b_3\alpha_3 = \frac{1}{2}.$$

For arbitrary matrices W we get the following order conditions (see [SW92], [HW96], and [SW79]):

$$\text{(2.5)} \qquad \begin{cases} \text{(C3a)} & b_3\alpha_{32}\alpha_2 = \frac{1}{6}, \\ \text{(C3b)} & b_3\alpha_{32}\beta_2 = \frac{1}{6} - \frac{\gamma}{2}, \\ \text{(C3c)} & b_3\beta_{32}\alpha_2 = \frac{1}{6} - \frac{\gamma}{2}. \end{cases}$$

THEOREM 2.1. *Let a consistent Rosenbrock method of order 3 with 3 internal steps be given. The method is consistent of order 3 with $J = f' + \mathcal{O}(h)$ and $T = 0$, if and only if the conditions* (B2) *and* (C3c) *are fulfilled.*

PROOF. The proof runs by the help of Taylor series expansions with a subsequent comparison of the coefficients which have to satisfy the conditions (A1), (A2), (A3a), (A3b), (B2), and (C3c). □

If a Rosenbrock method is applied for semidiscretized parabolic PDEs or PDAEs, the following condition should be satisfied to avoid order reduction (see [LO95] and [LV01]):

$$\text{(2.6)} \qquad b^\top B^j (2B^2 e - \alpha^2) = 0, \quad 1 \le j \le 2$$

with $B := (\beta_{ij})_{i,j=1}^s$, $\alpha^2 := (\alpha_1^2, \ldots, \alpha_s^2)^\top$, and $e := (1, \ldots, 1)^\top \in \mathbb{R}^s$. With (2.3) we can simplify (2.6) to (see [LV01])

$$\text{(2.7)} \qquad \begin{cases} \text{(D3a)} & b_3\beta_{32}\alpha_2^2 = \frac{1}{6} - \frac{2}{3}\gamma, \\ \text{(D3b)} & \gamma = \frac{1}{2} + \frac{1}{6}\sqrt{3}. \end{cases}$$

The above Rosenbrock type methods can be extended to semi-explicit DAEs of the form

$$\begin{aligned} M\,\dot u(t) &= f(t,u(t),v(t)), \quad u(t_0)=u_0, \\ 0 &= g(t,u(t),v(t)), \end{aligned} \tag{2.8}$$

where the matrices M and g_v are regular. Then the DAE (2.8) has index 1.

DEFINITION 2.5. *An s-stage Rosenbrock method for problem* (2.8) *is given by*

$$\begin{pmatrix} t^{(i)} \\ u^{(i)} \\ v^{(i)} \end{pmatrix} := \begin{pmatrix} t_{old} \\ u_{old} \\ v_{old} \end{pmatrix} + \sum_{j=1}^{i-1} \alpha_{ij} \begin{pmatrix} \tau \\ k_j \\ l_j \end{pmatrix},$$

$$\begin{pmatrix} u_{new} \\ v_{new} \end{pmatrix} := \begin{pmatrix} u_{old} \\ v_{old} \end{pmatrix} + \sum_{i=1}^{s} b_i \begin{pmatrix} k_i \\ l_i \end{pmatrix},$$

$$\begin{pmatrix} M\,k_i \\ 0 \end{pmatrix} := \tau \begin{pmatrix} f\left(t^{(i)},u^{(i)},v^{(i)}\right) \\ g\left(t^{(i)},u^{(i)},v^{(i)}\right) \end{pmatrix} + \tau W \sum_{j=1}^{i} \gamma_{ij} \begin{pmatrix} k_j \\ l_j \end{pmatrix} + \tau^2\,\gamma_i\,T, \tag{2.9}$$

where

$$W := \begin{pmatrix} f_u(t_{old},u_{old},v_{old}) & f_v(t_{old},u_{old},v_{old}) \\ g_u(t_{old},u_{old},v_{old}) & g_v(t_{old},u_{old},v_{old}) \end{pmatrix},$$

$$T := \begin{pmatrix} \dot f(t_{old},u_{old},v_{old}) \\ \dot g(t_{old},u_{old},v_{old}) \end{pmatrix}.$$

The parameters of the method are α_{ij}, γ_{ij}, and b_i.

To obtain convergence, the Rosenbrock method should fulfil certain order conditions for both the ODE and the algebraic part. These consistency properties can again be derived via Butcher series technique (see [HW96]).

For a third-order method with 3 internal steps we get the algebraic condition

$$\text{(E3)} \qquad b_2\omega_{22}\alpha_2^2 + b_3(\omega_{32}\alpha_2^2 + \omega_{33}\alpha_3^2) \;=\; 1, \tag{2.10}$$

where $(\omega_{ij})_{i,j=1}^{s} = B^{-1}$. From [LV01] we know the following result.

LEMMA 2.2. *A Rosenbrock method which satisfies* (A1)–(A3b) *and* (D3a)–(D3b) *fulfils* (E3)*, too.*

PROOF. See [LV01]. □

The stability function of (2.3) is given by

$$R_0(z) = 1 + zb^\top (I - zB)^{-1} e,$$

in particular for $s = 3$ we obtain with (A1), (A2), and (A3b)

$$R_0(z) = \frac{(-1-18\gamma^2+6\gamma^3+9\gamma)z^3 + (-18\gamma^2-3+18\gamma)z^2 + (18\gamma-6)z - 6}{6(-1+z\,\gamma)^3}.$$

A Rosenbrock method with 3 internal stages, i.e. $s = 3$, is L-stable if and only if

$$-1 - 18\,\gamma^2 + 6\,\gamma^3 + 9\,\gamma = 0. \tag{2.11}$$

3 Methods of order 3 with 3 internal stages.

3.1 An L-stable method for ODEs with $J = f_u + \mathcal{O}(h)$ and $T = 0$.

A Rosenbrock method applied on ODEs with $J = f_u + \mathcal{O}(h)$ and $T = 0$ should satisfy the order conditions (A1), (A2), (A3a), (A3b), (B2), and (C3c). Moreover we choose γ such that the scheme becomes L-stable, i.e. we add equation (2.11) and have $\gamma \approx 0.436$. The method should need only two function evaluation, i.e. we have $\alpha_{21} = \alpha_{31}$, $\alpha_{32} = 0$. Finally we set $b_3 = \frac{1}{2}$ and $\hat{b}_3 = \frac{5}{36}$. Our order conditions simplify to

$$\begin{aligned} b_1 + b_2 &= \tfrac{1}{2}, & \beta_{32}\alpha_2 &= \tfrac{1}{3} - \gamma, \\ 2b_2\beta_2 + \beta_3 &= 1 - 2\gamma, & \beta_2\beta_{32} &= \tfrac{1}{3} - 2\gamma + 2\gamma^2, \\ (2b_2 + 1)\alpha_2 &= 1, & \hat{b}_1 + \hat{b}_2 &= \tfrac{31}{36}, \\ (2b_2 + 1)\alpha_2^2 &= \tfrac{2}{3}, & \hat{b}_2\beta_2 + \tfrac{5\beta_3}{36} &= \tfrac{1}{2} - \gamma. \end{aligned}$$

This system of equations can easily be solved and the solution can be found in Table 3.1. We call our new L-stable method ROS3w, where w stands for methods which need only an approximation of J. The embedded method is of order 2, fulfils (A1) and (A2), and is strongly A-stable with $R(\infty) \approx 0.69$.

Table 3.1: Set of coefficients for ROS3w.

γ = 4.358665215084590e-01e	
α_{21} = 6.666666666666666e-01e	γ_{21} = 3.635068368900681e-01e
α_{31} = 6.666666666666666e-01e	γ_{31} = −8.996866791992636e-01e
α_{32} = 0.000000000000000e+00e	γ_{32} = −1.537997822626885e-01e
b_1 = 2.500000000000000e-01e	$\hat{b}_1$ = 7.467047032740110e-01e
b_2 = 2.500000000000000e-01e	$\hat{b}_2$ = 1.144064078371002e-01e
b_3 = 5.000000000000000e-01e	$\hat{b}_3$ = 1.388888888888889e-01e

Next we ask for a method satisfying the above order conditions as well as condition (C3a) and (C3b). The answer is negative.

LEMMA 3.1. *It is impossible to create a Rosenbrock method which satisfies* (A1), ..., (A3b), (C3a), *and* (C3b).

PROOF. From (C3a) we have

$$\alpha_{32} = \frac{1}{6b_3\alpha_2}.$$

Inserting into (C3b) yields

$$\frac{\beta_2}{6\alpha_2} = \frac{1}{6} - \frac{\gamma}{2}$$

and

$$\beta_2 = \alpha_2(1 - 3\gamma).$$

It follows with (A3b)

$$b_3\beta_{32}\alpha_2 = \frac{\frac{1}{6} - \gamma + \gamma^2}{1 - 3\gamma}.$$

Together with (C3a) we get $\gamma = \frac{1}{2}$. Then (A3b) and (C3b) imply that $\alpha_{32} = \beta_{32}$, but this is a contradiction to (C3a) and (C3c). □

3.2 An L-stable method for index 1 DAEs with $J = f_u + \mathcal{O}(h)$ and $T = 0$.

For index 1 DAEs the condition (E3) should be fulfiled, i.e. we have the consistency conditions (A1), (A2), (A3a), (A3b), (B2), (C3c), and (E3). Moreover γ is determined by equation (2.11), i.e. $\gamma \approx 0.436$ and our scheme becomes L-stable. The free parameters are b_2, $\hat{b}_2$, and α_{32}. First we note that (E3) can be simplified to

$$\gamma b_2\alpha_2^2 + b_3(\gamma\alpha_3^2 - \beta_{32}) = \gamma^2$$

using $(\omega_{ij})_{i,j=1}^3 = B^{-1}$. With (B2) we get the order condition

$$b_3\beta_{32}\alpha_2^2 = \frac{1}{3}\gamma - \gamma^2. \tag{3.1}$$

Dividing (3.1) by (C3c) leads to

$$\alpha_2 = \frac{\frac{1}{3}\gamma - \gamma^2}{\frac{1}{6} - \frac{\gamma}{2}} \approx 0.87.$$

With (B2) and (A3a) we can determine b_3 and α_3. The remaining coefficients can be determined easily and are given in Table 3.2, The embedded method is strongly A-stable with $R(\infty) \approx 0.28$. We call the method ROS3Dw, where D stands for DAE of index one.

Table 3.2: Set of coefficients for ROS3Dw.

γ = 4.3586652150845900e-01	
α_{21} = 8.7173304301691801e-01	γ_{21} = 4.7532138161945031e-01
α_{31} = 3.8213294371763229e-01	γ_{31} = −9.7712149572940343e-01
α_{32} = 0.0000000000000000e+00	γ_{32} = −1.0731056295754648e-01
b_1 = 1.1863142804796199e-01	$\hat{b}_1$ = 3.6180340134778349e-01
b_2 = 3.3333333333333333e-01	$\hat{b}_2$ = 2.5000000000000000e-01
b_3 = 5.4803523861870473e-01	$\hat{b}_3$ = 3.8819659865221651e-01

3.3 A method for index 1 PDAEs with $J = f_u + \mathcal{O}(h)$ and $T = 0$.

We start with the following result.

LEMMA 3.2. *For $s = 3$ there is no L-stable Rosenbrock method of order 3, which fulfils the PDE conditions* (D3a)–(D3b).

PROOF. An L-stable method satisfies

$$6\gamma^3 - 18\gamma^2 + 9\gamma - 1 = 0$$

but (D3b) is not a root of this equation. □

LEMMA 3.3. *For $s = 3$, there exists no Rosenbrock method of order 3 which satisfies* (A1), (A2), (B2), (A3a), (A3b), (C3c), (D3a), (D3b), *and* $\alpha_{21} \leq 1$.

PROOF. Using (D3b) we find $b_3\beta_{32}\alpha_2^2 \neq 0$ in (D3a) and $b_3\beta_{32}\alpha_2 \neq 0$ in (C3c). Dividing (D3a) by (C3c) leads to

$$\alpha_2 = \frac{\frac{1}{6} - \frac{2}{3}\gamma}{\frac{1}{6} - \frac{1}{2}\gamma} = \frac{1 - 4\gamma}{1 - 3\gamma} = 2\left(\frac{1}{2} + \frac{1}{6}\sqrt{3}\right) = 2\gamma.$$
□

LEMMA 3.4. *For $s = 3$, a Rosenbrock method of order 3 which fulfils* (A1), (A2), (B2), (A3a), (A3b), (C3c), (D3a), *and* (D3b) *cannot satisfy* (C3b).

PROOF. Using (D3b) we find $b_3\beta_{32}\alpha_2^2 \neq 0$ in (D3a). Consequently, $\beta_2 = 0$ in (A3b) due to (D3b). But this is a contradiction to (C3b). □

THEOREM 3.5. *There exists no W-method of order 3 with 3 internal steps.*

PROOF. It follows from Lemma 3.1. □

In the following a Rosenbrock method is constructed which fulfils the following conditions: (A1), (A2), (A3a), (A3b), (B2), (C3c), (D3a), and (D3b). Here, the free parameters are $\hat{b}_2$, α_{31}, and α_{32}. The remaining coefficients can be determined as in the previous sections and are listed in Table 3.3. The method and the embedded method are strongly A-stable with $R(\infty) = \sqrt{3} - 1 \approx 0.73$. The method is called ROS3Pw, where P stands for parabolic problems.

Table 3.3: Set of coefficients for ROS3Pw.

γ	=	7.8867513459481287e-01			
α_{21}	=	1.5773502691896257e+00	γ_{21}	=	−1.5773502691896257e+00
α_{31}	=	5.0000000000000000e-01	γ_{31}	=	−6.7075317547305480e-01
α_{32}	=	0.0000000000000000e+00	γ_{32}	=	−1.7075317547305482e-01
b_1	=	1.0566243270259355e-01	$\hat{b}_1$	=	−1.7863279495408180e-01
b_2	=	4.9038105676657971e-02	$\hat{b}_2$	=	3.3333333333333333e-01
b_3	=	8.4529946162074843e-01	$\hat{b}_3$	=	8.4529946162074843e-01

4 Methods of order 3 with 4 internal stages.

In the last section we have shown that there exists no Rosenbrock W-method of order 3 with 3 internal stages. In the following we consider Rosenbrock W-methods with four internal stages and start with some order conditions.

4.1 Order conditions.

The order conditions in the case $s = 4$ read as (see [HW96])

$$\begin{cases} \text{(A1)} & b_1 + b_2 + b_3 + b_4 = 1, \\ \text{(A2)} & b_2\beta_2 + b_3\beta_3 + b_4\beta_4 = \frac{1}{2} - \gamma, \\ \text{(A3a)} & b_2\alpha_2^2 + b_3\alpha_3^2 + b_4\alpha_4^2 = \frac{1}{3}, \\ \text{(A3b)} & b_3\beta_{32}\beta_2 + b_4(\beta_{42}\beta_2 + \beta_{43}\beta_3) = \frac{1}{6} - \gamma + \gamma^2, \\ \text{(B2)} & b_2\alpha_2 + b_3\alpha_3 + b_4\alpha_4 = \frac{1}{2}, \\ \text{(C3a)} & b_3\alpha_{32}\alpha_2 + b_4(\alpha_{42}\alpha_2 + \alpha_{43}\alpha_3) = \frac{1}{6}, \\ \text{(C3b)} & b_3\alpha_{32}\beta_2 + b_4(\alpha_{42}\beta_2 + \alpha_{43}\beta_3) = \frac{1}{6} - \frac{\gamma}{2}, \\ \text{(C3c)} & b_3\beta_{32}\alpha_2 + b_4(\beta_{42}\alpha_2 + \beta_{43}\alpha_3) = \frac{1}{6} - \frac{\gamma}{2}. \end{cases}$$

LEMMA 4.1. *The conditions for PDEs* (2.6) *can be simplified by the help of* (A1), (A2), (A3a), *and* (A3b) *to*

$$\begin{cases} \text{(D3a)} & b_4\beta_{32}\beta_{43}\alpha_2^2 = 2\gamma^4 - 2\gamma^3 + \frac{1}{3}\gamma^2, \\ \text{(D3b)} & b_3\beta_{32}\alpha_2^2 + b_4\big(\beta_{42}\alpha_2^2 + \beta_{43}\alpha_3^2\big) = 2\gamma^3 - 3\gamma^2 + \frac{2}{3}\gamma, \\ \text{(D3c)} & b_4\beta_{43}\beta_{32}\beta_{21} = 0. \end{cases}$$

REMARK 4.1. *The expressions* $b_3\beta_{32}\alpha_2^2 + b_4(\beta_{42}\alpha_2^2 + \beta_{43}\alpha_3^2)$ *and* $b_4\beta_{43}\beta_{32}\beta_{21}$ *are known as part of the order conditions for 4th-order Rosenbrock methods (see* [HW96]*).*

The algebraic order condition reads as

$$\text{(E3)}\quad b_2\omega_{22}\alpha_2^2 + b_3\big(\omega_{32}\alpha_2^2 + \omega_{33}\alpha_3^2\big) + b_4\big(\omega_{42}\alpha_2^2 + \omega_{43}\alpha_3^2 + \omega_{44}\alpha_4^2\big) = 1.$$

LEMMA 4.2. *A Rosenbrock method which satisfies* (A1)–(A3b) *and* (D3a)–(D3c) *fulfils* (E3)*, too.*

PROOF. Invert B and use (A3a), (D3a), and (D3b) to get (E3). □

A Rosenbrock method of order 3 with 4 internal steps is L-stable if

$$b_4\beta_{43}\beta_{32}\beta_{21} = -\gamma^4 + 3\gamma^3 - \frac{3}{2}\gamma^2 + \frac{1}{6}\gamma. \tag{4.1}$$

LEMMA 4.3. *A Rosenbrock method which satisfies* (A1)–(A3b) *and* (D3a)–(D3c) *is L-stable if the condition*

$$\gamma^4 - 3\gamma^3 + \frac{3}{2}\gamma^2 - \frac{1}{6}\gamma = 0 \tag{4.2}$$

is satisfied, i.e. $\gamma \approx 0.44$.

PROOF. From (D3c) and (4.1) it follows (4.2) which has the solutions

$$\gamma \in \{2.41, 0.16, 0.44\}.$$

The method can only be L-stable if $\gamma = .43586$ (see [HW96]). □

LEMMA 4.4. *Let a Rosenbrock method which satisfies* (A1)–(A3b) *and* (D3a)–(D3c) *be given. The embedded method satisfying* (A1) *and* (A2) *is L-stable, too, if*

$$\hat{b}_4 = \frac{1}{\beta_3 \beta_{43}} \left[\gamma^3 - 2\gamma^2 + \frac{1}{2}\gamma \right]. \tag{4.3}$$

PROOF. We start with the expression

$$\lim_{z\to\infty} \left(1 + z b^\top (I - zB)^{-1} e\right) = 0.$$

Inserting the definitions of b and B leads to

$$\begin{aligned} -\gamma^3(b_1 + b_2 + b_3 + b_4) + \gamma^2(b_2\beta_2 + b_3\beta_3 + b_4\beta_4) + \gamma^4 \\ + b_4\beta_{21}\beta_{32}\beta_{43} - \gamma(b_3\beta_{32}\beta_2 + b_4(\beta_{42}\beta_2 + \beta_{43}\beta_3)) = 0. \end{aligned}$$

Moreover (D3a) and (D3c) imply $\beta_2 = 0$. With (A1) and (A2) we obtain the above statement. □

4.2 Two L-stable W-methods for PDAEs with 3 function evaluations.

In this section Rosenbrock W-methods are described which need only 3 function evaluations. First we note that it is impossible to create a method using only two function evaluations.

LEMMA 4.5. *There exists no Rosenbrock W-method of order 3 with 4 internal stages which fulfils* (A1)–(C3c) *and* $\alpha_{21} = \alpha_{31} = \alpha_{41},\ \alpha_{32} = \alpha_{42} = \alpha_{43} = 0$.

PROOF. This follows from (C3a). □

In what follows we need the fact that $\alpha_{21} \neq 0$ and $\alpha_{43} \neq 0$.

LEMMA 4.6. *There exists no L-stable Rosenbrock W-method of order 3 with 4 internal stages which fulfils* (A1)–(C3c) *and* $\alpha_{21} = 0$.

PROOF. We consider condition (D3a). Inserting $\alpha_{21} = 0$ yields

$$2\gamma^4 - 2\gamma^3 + \frac{1}{3}\gamma^2 = 0,$$

but this is a contradiction to the L-stability. □

LEMMA 4.7. *There exists no L-stable Rosenbrock W-method of order 3 with 4 internal stages which fulfils* (A1)–(C3c) *and* $\alpha_{43} = 0$.

PROOF. We consider condition (C3b). Since (D3a) and (D3c) imply $\beta_2 = 0$ we get $\frac{1}{6} - \frac{\gamma}{2} = 0$, but this is a contradiction to the L-stability. □

These two lemmas imply that it is possible to create L-stable W-methods only if $\alpha_{31} = \alpha_{32} = 0$ or $\alpha_{31} = \alpha_{21}$ and $\alpha_{32} = 0$. We start with the case $\alpha_{31} = \alpha_{32} = 0$.

We choose the free coefficients of the first method ROS34PW1a as follows: $\alpha_{31} = \alpha_{32} = 0$, $\alpha_{42} := \frac{1}{6\alpha_2}$, $\alpha_{43} = \frac{1}{2}$, $b_3 = \frac{1}{4}$ and $\hat{b}_4$ as in (4.3). Note that $\alpha_3 = 0$. First, (D3a) and (D3c) imply $\beta_2 = 0$. The coefficient α_{21} can be determined with (C3c) and (D3b). We obtain $\alpha_{21} = (2\gamma^3 - 3\gamma^2 + 2/3\gamma)/(1/6 - \gamma/2)$. From (C3a) we get b_4 and with (B2) and (A3a) we get α_4 and b_2. The remaining coefficients can be determined easily and are given below in Table 4.1. The letters in ROS34PW1a have the following meanings: 34 stands for order 3 with 4 internal stages, W for W-method and 1a is an internal number.

Table 4.1: Set of coefficients for ROS34PW1a.

γ = 4.358665215084590e-01e	
α_{21} = 2.218787467653286e+00e	γ_{21} = −2.218787467653286e+00e
α_{31} = 0.000000000000000e+00e	γ_{31} = −9.461966143940745e-02e
α_{32} = 0.000000000000000e+00e	γ_{32} = −7.913526735718213e-03e
α_{41} = 1.208587690772214e+00e	γ_{41} = −1.870323744195384e+00e
α_{42} = 7.511610241919324e-02e	γ_{42} = −9.624340112825115e-02e
α_{43} = 5.000000000000000e-01e	γ_{43} = 2.726301276675511e-01e
b_1 = 3.285609536316354e-01e	$\hat{b}_1$ = −2.500000000000000e-01e
b_2 = −5.785609536316354e-01e	$\hat{b}_2$ = 0.000000000000000e+00e
b_3 = 2.500000000000000e-01e	$\hat{b}_3$ = 2.500000000000000e-01e
b_4 = 1.000000000000000e+00e	$\hat{b}_4$ = 1.000000000000000e+00e

For our second method we set $\alpha_{31} = \alpha_{21}$, $\alpha_{32} = 0$, $\alpha_{42} = 0$, $\alpha_{43} = 1/10$, $b_3 = 1/4$ and $\hat{b}_4$ as in (4.3). Note that $\alpha_2 = \alpha_3$. Again we have $\beta_2 = 0$. From (C3c) and (D3b) we obtain $\alpha_2 = (2\gamma^3 - 3\gamma^2 + 2/3\gamma)/(1/6 - \gamma/2)$. The remaining coefficients can be determined in same way as for ROS34PW1a. They are given below in Table 4.2.

Table 4.2: Set of coefficients for ROS34PW1b.

γ = 4.358665215084590e-01e	
α_{21} = 2.218787467653286e+00e	γ_{21} = −2.218787467653286e+00e
α_{31} = 2.218787467653286e+00e	γ_{31} = −2.848610224639349e+00e
α_{32} = 0.000000000000000e+00e	γ_{32} = −5.267530183845237e-02e
α_{41} = 1.453923375357884e+00e	γ_{41} = −1.128167857898393e+00e
α_{42} = 0.000000000000000e+00e	γ_{42} = −1.677546870499461e-01e
α_{43} = 1.000000000000000e-01e	γ_{43} = 5.452602553351021e-02e
b_1 = 5.495647928937977e-01e	$\hat{b}_1$ = −1.161024191932427e-03e
b_2 = −5.507258170857301e-01e	$\hat{b}_2$ = 0.000000000000000e+00e
b_3 = 2.500000000000000e-01e	$\hat{b}_3$ = 2.500000000000000e-01e
b_4 = 7.511610241919324e-01e	$\hat{b}_4$ = 7.511610241919324e-01e

4.3 A stiffly accurate W-method for PDAEs.

DEFINITION 4.1. *A Rosenbrock method satisfying*

$$\beta_{si} = b_i, \quad i = 1, \ldots, s, \quad \textit{and} \quad \alpha_s = 1 \tag{4.4}$$

is called stiffly accurate.

Methods which satisfy the condition (4.4) yield asymptotically exact results for the problem $\dot{u} = \lambda(u - \varphi(t)) + \dot{\varphi}(t)$. The order conditions can be written as follows

$$\left\{\begin{array}{lrcl}
\text{(A1')} & b_1 + b_2 + b_3 & = & 1 - \gamma, \\
\text{(A2')} & b_2\beta_2 + b_3\beta_3 & = & \frac{1}{2} - 2\gamma + \gamma^2, \\
\text{(A3a)} & b_2\alpha_2^2 + b_3\alpha_3^2 & = & \frac{1}{3} - \gamma, \\
\text{(A3b')} & b_3\beta_{32}\beta_2 & = & \frac{1}{6} - \frac{3}{2}\gamma + 3\gamma^2 - \gamma^3, \\
\text{(B2')} & b_2\alpha_2 + b_3\alpha_3 & = & \frac{1}{2} - \gamma, \\
\text{(C3a')} & b_3\alpha_{32}\alpha_2 + \gamma(\alpha_{42}\alpha_2 + \alpha_{43}\alpha_3) & = & \frac{1}{6}, \\
\text{(C3b')} & b_3\alpha_{32}\beta_2 + \gamma(\alpha_{42}\beta_2 + \alpha_{43}\beta_3) & = & \frac{1}{6} - \frac{\gamma}{2}, \\
\text{(C3c')} & b_3\beta_{32}\alpha_2 & = & \frac{1}{6} - \gamma + \gamma^2, \\
\text{(D3a')} & b_3\beta_{32}\alpha_2^2 & = & 2\gamma^3 - 2\gamma^2 + \frac{1}{3}\gamma, \\
\text{(D3c')} & b_3\beta_{32}\beta_2 & = & 0.
\end{array}\right.$$

Note that the condition (D3a) and (D3b) are equivalent if the Rosenbrock method is stiffly accurate. The free parameters of our method are $\alpha_{42} := 0$ and $\alpha_{43} := 1$. First $\beta_2 = 0$ (by (D3c')) and α_2 can determined by (D3a') and (C3c'). From (C3b') we get β_3 and from (A2') b_3. Using the conditions (B2') and (A3a') yields b_2 and α_3. The remaining coefficients of ROS34PW2 can be computed easily and are listed in Table 4.3. The embedded method is strongly A-stable with $R(\infty) \approx 0.48$.

Table 4.3: Set of coefficients for ROS34PW2.

γ	=	4.3586652150845900e-01			
α_{21}	=	8.7173304301691801e-01	γ_{21}	=	−8.7173304301691801e-01
α_{31}	=	8.4457060015369423e-01	γ_{31}	=	−9.0338057013044082e-01
α_{32}	=	−1.1299064236484185e-01	γ_{32}	=	5.4180672388095326e-02
α_{41}	=	0.0000000000000000e+00	γ_{41}	=	2.4212380706095346e-01
α_{42}	=	0.0000000000000000e+00	γ_{42}	=	−1.2232505839045147e+00
α_{43}	=	1.0000000000000000e+00	γ_{43}	=	5.4526025533510214e-01
b_1	=	2.4212380706095346e-01	$\hat{b}_1$	=	3.7810903145819369e-01
b_2	=	−1.2232505839045147e+00	$\hat{b}_2$	=	−9.6042292212423178e-02
b_3	=	1.5452602553351020e+00	$\hat{b}_3$	=	5.0000000000000000e-01
b_4	=	4.3586652150845900e-01	$\hat{b}_4$	=	2.1793326075422950e-01

4.4 A W-method for PDAEs satisfying 4-th order conditions for ODEs.

From [HW96] we get the following 4-th order conditions for ODEs

$$\begin{cases} \text{(A4a)} & b_3\beta_{32}\alpha_2^2 + b_4(\beta_{42}\alpha_2^2 + \beta_{43}\alpha_3^2) = \frac{1}{12} - \frac{\gamma}{3}, \\ \text{(A4b)} & b_4\beta_{43}\beta_{32}\beta_{21} = \frac{1}{24} - \frac{\gamma}{2} + \frac{3}{2}\gamma^2 - \gamma^3, \\ \text{(A4c)} & b_2\alpha_2^3 + b_3\alpha_3^3 + b_4\alpha_4^3 = \frac{1}{4}, \\ \text{(A4d)} & b_3\alpha_3\alpha_{32}\beta_2 + b_4\alpha_4(\alpha_{42}\beta_2 + \alpha_{43}\beta_3) = \frac{1}{8} - \frac{\gamma}{3}. \end{cases}$$

It follows with (D3b) and (D3c) that

$$\frac{1}{24} - \frac{\gamma}{2} + \frac{3}{2}\gamma^2 - \gamma^3 = 0, \tag{4.5}$$

hence we have $\gamma \approx 1.06857$.

LEMMA 4.8. *A Rosenbrock W-method satisfying* (A1)–(D3c), (A4a), *and* (A4b) *cannot be L-stable.*

PROOF. This follows from (4.1) and (4.5). □

LEMMA 4.9. *Let a Rosenbrock W-method satisfying* (A1)–(A4d) *be given. There exists no embedded method of order 3.*

PROOF. Let us assume that an embedded method of order 3 exists. Then this embedded method satisfies condition (A1)–(A3b). From [HW96] we know that these equations form the linear system

$$\begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & \beta_2 & \beta_3 & \beta_4 \\ 0 & \alpha_2^2 & \alpha_3^2 & \alpha_4^2 \\ 0 & 0 & \beta_{32} & \beta_{42}\beta_2 + \beta_{43}\beta_3 \end{pmatrix} \begin{pmatrix} \hat{b}_1 \\ \hat{b}_2 \\ \hat{b}_3 \\ \hat{b}_4 \end{pmatrix} = \begin{pmatrix} 1 \\ \frac{1}{2} - \gamma \\ \frac{1}{3} \\ \frac{1}{6} - \gamma + \gamma^2 \end{pmatrix}. \tag{4.6}$$

If the matrix (4.6) is regular, it follows $\hat{b}_i = b_i$, $i = 1, \ldots, 4$ and the approximation $\hat{u}$ cannot be used for step size control. Therefore it has to be required that the matrix in (4.6) is singular, i.e.

$$\big(\beta_2\alpha_4^2 - \beta_4\alpha_2^2\big)\beta_{32}\beta_2 = \big(\beta_2\alpha_3^2 - \beta_3\alpha_2^2\big)(\beta_{42}\beta_2 + \beta_{43}\beta_3).$$

From the previous sections we know $\beta_2 = 0$, hence the singularity condition simplifies to

$$\beta_3\alpha_2^2\beta_{43}\beta_3 = 0.$$

It follows $\beta_3 = 0$, $\alpha_2 = 0$ or $\beta_{43} = 0$. But this is a contradiction to (4.5), (A3b), (C3b), and (D3a). □

As free parameters we choose $\alpha_3 = 2\alpha_4$, $\alpha_2 = 4\alpha_4$, and $\alpha_{32} = \frac{3}{4}$. Again we have $\beta_2 = 0$. Then we determine the coefficients b_2, b_3, and b_4 by (A2a), (B2), and (A4c). The conditions (C3c), (D3a), and (D3b) can be used to obtain β_{32}, β_{42}, and β_{43}. Note that this system of equations is nonlinear and is not uniquely solvable. The computation of the remaining coefficients is straight forward. The embedded method satisfies (A1), (A2), (B2) and $\hat{b}_4 = 0$. The coefficients of ROS34PW3 are listed in Table 4.4. The method is strongly A-stable with $R(\infty) \approx 0.63$, and the embedded method with $R(\infty) \approx 0.43$, resp.

Table 4.4: Set of coefficients for ROS34PW3.

γ = 1.0685790213016289e+00	
α_{21} = 2.5155456020628817e+00	γ_{21} = −2.5155456020628817e+00
α_{31} = 5.0777280103144085e-01	γ_{31} = −8.7991339217106512e-01
α_{32} = 7.5000000000000000e-01	γ_{32} = −9.6014187766190695e-01
α_{41} = 1.3959081404277204e-01	γ_{41} = −4.1731389379448741e-01
α_{42} = −3.3111001065419338e-01	γ_{42} = 4.1091047035857703e-01
α_{43} = 8.2040559712714178e-01	γ_{43} = −1.3558873204765276e+00
b_1 = 2.2047681286931747e-01	$\hat{b}_1$ = 3.1300297285209688e-01
b_2 = 2.7828278331185935e-03	$\hat{b}_2$ = −2.8946895245112692e-01
b_3 = 7.1844787635140066e-03	$\hat{b}_3$ = 9.7646597959903003e-01
b_4 = 7.6955588053404989e-01	$\hat{b}_4$ = 0.0000000000000000e+00

5 Comparison of Rosenbrock methods and numerical results.

All examples are solved numerically by the help of the FEM-package MooNMD3.0 (see [JM04]) on a uniform spatial grid consisting of 1024 quadrangles, i.e. $h = 2^{-5}$. We compare our new methods with other well-known Rosenbrock methods such as ROS3P, ROWDAIND2, RODAS3, RODAS, and RODASP. An overview of the selected Rosenbrock methods can be found in Table 5.1.

We apply these schemes to a PDE, an index-1 PDAE and the Navier–Stokes equations with different right-hand sides. For the definition of the index of linear PDAEs we refer to the paper [RA05]. In [Ran04] can be found a discussion about the perturbation index of the Navier–Stokes equations and its semi-discretized version which has index 2. Note, that we make a pressure correction after each time step of our computations. Hence it seems appropriate to solve the Navier–Stokes equations with index-1 schemes. The calculations at the end of this section confirm this rating.

The global error $\underline{\epsilon}$ is measured in the discrete L_2-norm ($\|\underline{\epsilon}\|_{l_2(N)}$), and the numerically observed temporal order of convergence is computed by

$$q_{num} = \log_2 \left(\frac{\|\underline{\epsilon}\|_{l_2(N)}}{\|\underline{\epsilon}\|_{l_2(2N)}} \right).$$

In this section, the letter J is used to denote a time interval.

EXAMPLE 5.1. Let $\Omega := (0,1)^2$, $J := (0,1)$, and consider the PDE system

$$\left\{ \begin{array}{rcll} \dot{u} - \Delta u + v &=& f_1, & \text{in } J \times \Omega, \\ \dot{v} - \Delta v - \lambda v &=& f_2, & \text{in } J \times \Omega. \end{array} \right. \tag{5.1}$$

Table 5.1: Properties of the selected Rosenbrock methods.

name	s	p	index 1	index 2	PDEs	$R(\infty)$	stiffly acc.	reference
ROS3P	3	3	yes	no	yes	0.73	no	[LV01]
ROWDAIND2	3	3	yes	yes	no	0	yes	[LR90]
ROS3w	3	3	yes	no	no	0	no	see Sect. 3.1
ROS3Dw	3	3	yes	no	no	0	no	see Sect. 3.2
ROS3Pw	3	3	yes	no	yes	0.73	no	see Sect. 3.3
ROS34PW2	4	3	yes	no	yes	0	yes	see Sect. 4.3
ROS34PW3	4	4	yes	no	yes	0.63	no	see Sect. 4.4
RODAS3	3	3	yes	no	no	0	yes	[SGG+97]
RODAS	6	4	yes	no	no	0	yes	[HW96]
RODASP	6	4	yes	no	yes	0	yes	[Ste95]

The prescribed solution has the form

$$u(t,x,y) = t^2(1-x)(1-y)xy,$$
$$v(t,x,y) = 10 - (10+t)e^{-t}(1-x)(1-y)xy.$$

In the numerical tests, we have used homogeneous Dirichlet boundary conditions at the whole boundary. The initial conditions and the functions f_1 and f_2 are chosen such that $(u,v)^\top$ is the closed form solution of (5.1). The computations were carried out with $\lambda = -10$, bilinear finite elements and time steps $\tau_N = \frac{1}{10 \cdot 2^N}$ with $N = 0, 1, \ldots, 5$. Note that for any t the solution can be represented exactly by the discrete functions.

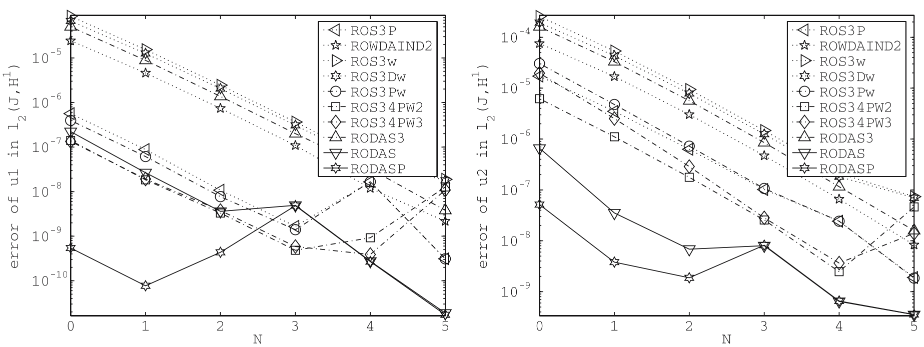

Figure 5.1: Example 5.1, global error vs. time step $\tau_N = 1/10 \cdot 2^N$.

The results are presented in Figure 5.1, Table A.1, and Table A.2. First we note that RODASP gave the best results since it is a fourth order method designed for parabolic problems. Considering the second component RODAS gave very good results, too. The best schemes with order 3 are ROS34PW2 and ROS34PW3.

EXAMPLE 5.2. We consider the PDE (5.1) with the solution

$$u(t,x,y) = t^2(2-x)(2-y)xy,$$
$$v(t,x,y) = 10-(10+t)e^{-t}(2-x)(2-y)xy.$$

The right-hand side $(f_1, f_2)^\top$, the Dirichlet boundary conditions, and the initial conditions are taken from the exact solution. As in the previous example, we set $\lambda = -10$. The problem is solved with bilinear continuous finite elements and a sequence of time steps $\tau_N = \frac{1}{10 \cdot 2^N}$ with $N = 0, 1, \ldots, 5$ (see Figure 5.2, Table A.3, and Table A.4).

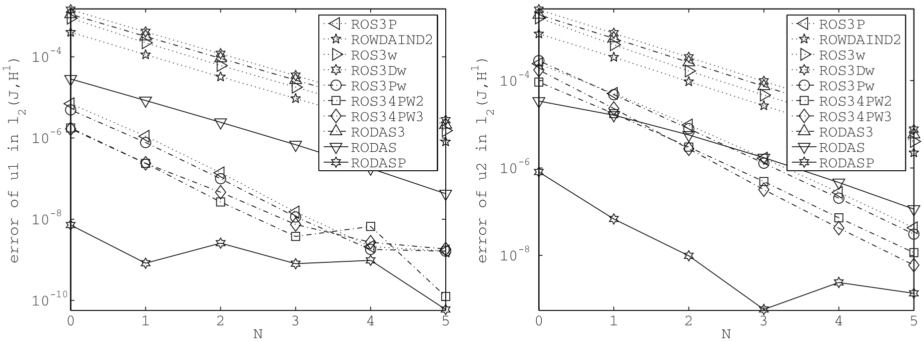

Figure 5.2: Example 5.2, global error vs. time step $\tau_N = 1/10 \cdot 2^N$.

It can be observed that the 4th-order method RODASP gave the best results. The numerically observed order of convergence for the methods satisfying the conditions for the PDE (ROS3P, ROS3Pw, and the ROS34PW-family) drops down to approximately $2.5 \cdots 3$ (see Table A.3 and Table A.4). The remaining third order methods (ROWDAIND2, ROS3w, ROS3Dw, RODAS3, and RODAS) have more severe order reduction. Their numerically observed order of convergence drops down to approximately $1.75 \cdots 2$. This is due to the fact that the problem includes time-dependent Dirichlet boundary conditions. A discussion about these phenomena can be found in [LO95].

EXAMPLE 5.3. Let again $\Omega := (0,1)^2$, $J := (0,1)$, and consider the PDAE

$$\left\{ \begin{aligned} \dot{u} - \Delta u - \Delta v + xu_x + yu_y - u + v &= f_1, \quad \text{in } \Omega, \\ -\Delta u - \Delta v + u^2 + v^2 &= f_2, \quad \text{in } \Omega. \end{aligned} \right. \tag{5.2}$$

Note that (5.2) has the perturbation index $\mathfrak{i}_p = 1$. The Dirichlet boundary conditions, the initial condition and the functions f_1 and f_2 are taken from the exact solution

$$u(t,x,y) = (2x+y)\sin t,$$
$$v(t,x,y) = (x+3y)\cos t.$$

We solve (5.2) by the help of linear continuous finite elements and a sequence of time steps $\tau_N = \frac{1}{10\cdot 2^N}$ with $N = 0, 1, \ldots, 5$. Since the solution is linear in x and y, the semidiscretization is exact. The Jacobian is computed exactly. The global error and the numerical order of convergence are presented in Figure 5.3, Table A.5, and Table A.6.

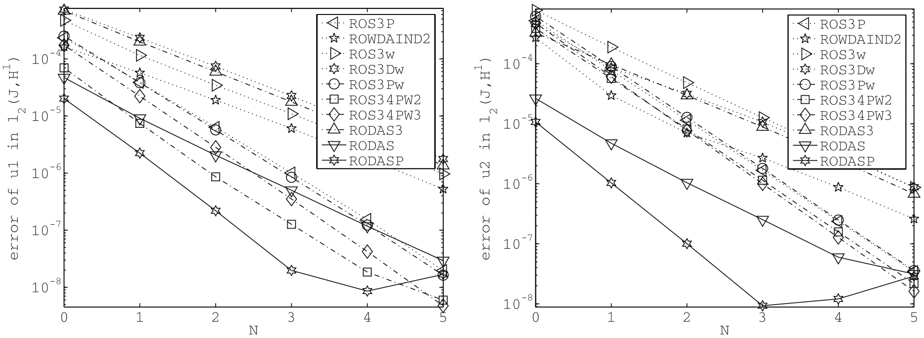

Figure 5.3: Example 5.3, global error vs. time step $\tau_N = 1/10 \cdot 2^N$.

First we note that RODASP is again the best method. This is due to fact that it is a fourth order scheme. For the u_2-component it can be observed that the method RODAS yield very good results, too, especially for large step sizes. Again the methods for semidiscretized PDEs give better results as the methods for DAEs.

Example 5.4. Let $J := (0, 1)$ and $\Omega := (0, 1)^2$. We consider the Navier–Stokes equations

$$\begin{aligned} \dot{u} - Re^{-1}\Delta u + (u \cdot \nabla)u + \nabla p &= f \quad \text{in } J \times \Omega, \\ \nabla \cdot u &= 0 \quad \text{in } J \times \Omega, \\ u &= g \quad \text{on } J \times \partial\Omega, \\ u(0, x) &= u_0 \quad x \in \Omega, \end{aligned} \tag{5.3}$$

where Re denotes the positive Reynolds number. The right-hand side f, the initial condition u_0 and the non-homogeneous Dirichlet boundary conditions are chosen such that

$$\begin{aligned} u_1(t, x, y) &= t^3 y^2, \\ u_2(t, x, y) &= t^2 x, \\ p(t, x, y) &= tx + y - (t + 1)/2 \end{aligned}$$

is the solution of (5.3). Moreover we set $Re = 1$. We used the Q_2/P_1^{disc}-discretization on a uniform mesh which consists of squares with an edge length $h = 1/64$ and solved the problem with variable time step sizes. The Jacobian is computed exactly. Note that for any t the solution can be represented exactly by the discrete functions. Hence, all occurring errors will result from the temporal discretization. During the calculations we have to deal with 33 282 d.o.f. for the velocity and 11 288 d.o.f. for the pressure. After each time step a pressure correction is done.

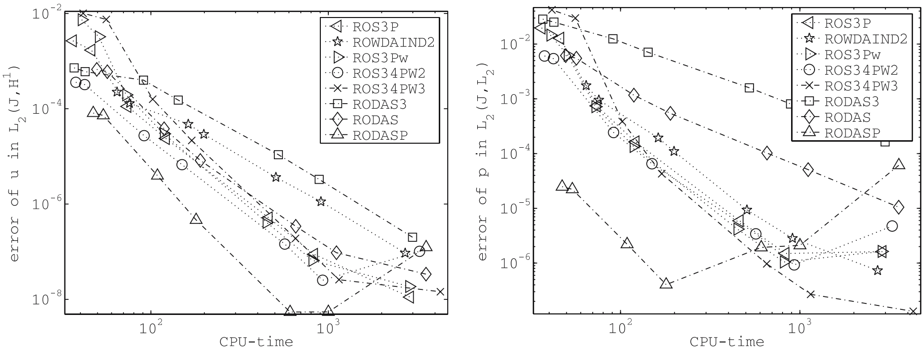

Figure 5.4: Example 5.4, global error vs. CPU-time.

The numerical results are presented in Figure 5.4. Considering the velocity error u it can be observed that for large tolerances RODASP is the best scheme. For small tolerances all methods are able to reduce the global error to approximately 10^{-7} or 10^{-8}. Only the schemes RODAS3 and ROWDAIND2 have little problems for medium tolerances.

Let us now consider the pressure error. Here we get a different impression. RODASP gives only for large tolerances the best results. For small tolerances ROS34PW3 is the best method. Bad results are obtained with the schemes RODAS3 and RODAS. Both methods do not have not the full order 3. The method ROWDAIND2 gives very good results for small tolerances, too. The methods ROS3P and ROS3Pw give nearly the same good results.

Example 5.5. We consider the Navier–Stokes equations (5.3) with Dirichlet boundary conditions on the whole boundary and with the solution

$$\begin{aligned} u_1(t,x,y) &= t^3 y^2, \\ u_2(t,x,y) &= \exp(-50t)x, \\ p(t,x,y) &= (10+t)\exp(-t)(x+y-1). \end{aligned}$$

The computations were carried out with $Re = 1$, a spatial grid consisting of squares of edge length $h = 1/32$, and variable time step sizes. This gives 8 450 velocity d.o.f. and 3 072 pressure d.o.f. for the Q_2/P_1^{disc} finite element discretization.

Note, that the component u_2 decreases very fast to zero. Therefore it is not surprising that the methods have great problems to solve the problem at least for large tolerances. The numerical results are shown in Figure 5.5. Again RODASP give fine results. Bad results are again obtained with RODAS3. The best results are obtained with ROS34PW3 for both components.

Example 5.6. The following problem can be found in [Cho68] and has the solution

$$u_1 = -\cos(n\pi x)\sin(n\pi y)\exp(-2n^2\pi^2 t/\hat{\tau}),$$

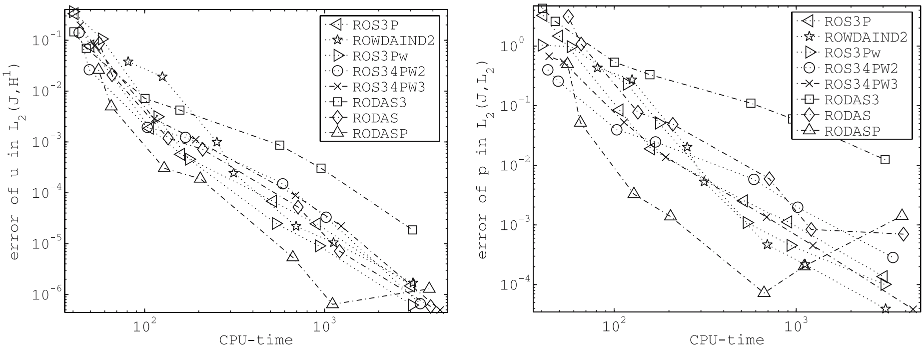

Figure 5.5: Example 5.5, global error vs. CPU-time.

$$u_2 = \sin(n\pi x)\cos(n\pi y)\exp(-2n^2\pi^2 t/\hat{\tau}),$$
$$p = -\tfrac{1}{4}(\cos(2n\pi x) + \cos(2n\pi y))\exp(-4n^2\pi^2 t/\hat{\tau}).$$

For the relaxation time $\hat{\tau} = Re = 1000$, this is a solution of the Navier–Stokes equations (5.3) consisting of an array of opposite-signed vortices which decay exponentially as $t \to \infty$.

In the numerical tests, we have used Dirichlet boundary conditions on the whole boundary. The right hand side f, the initial condition u_0 and the non-homogeneous Dirichlet boundary conditions are chosen such that $(u_1, u_2, p)^\top$ is the closed form solution of (5.3) for a given set of parameters. We will present computations for the relaxation time $\hat{\tau} = 1$, the vortex configuration $n = 4$, the final time $\bar{t} = 1$ with different Reynolds numbers on a fixed spatial grid. The grid consisted of squares with edge length $h = 1/64$. On this grid, the Q_2/P_1^{disc} finite element discretization possesses 33 282 d.o.f. for the velocity and 12 288 d.o.f. for the pressure. Moreover the problem is solved with variable step sizes.

The results are presented in Figure 5.6. The velocity error in $l_2(J, H^1(\Omega))$ is reduced to the discretization error in space by all methods. The best results for the pressure error $l_2(J, L_2(\Omega))$ are obtained with ROWDAIND2, ROS3P,

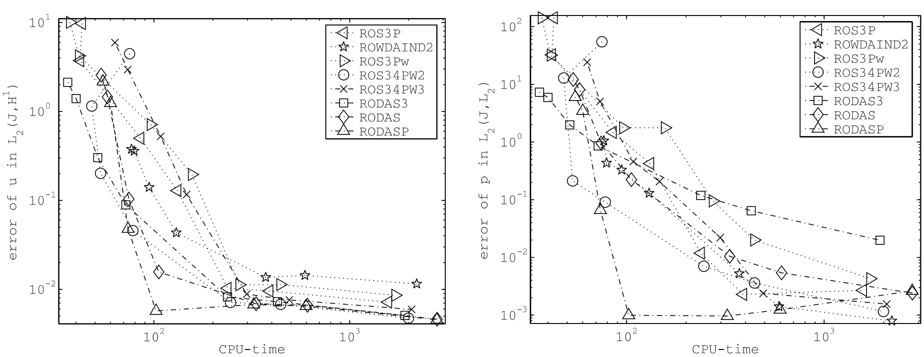

Figure 5.6: Example 5.6, global error vs. CPU-time.

ROS34PW2, ROS34PW3 and RODASP. The worst results were obtained with RODAS3 and ROS3Pw.

EXAMPLE 5.7. The flow around a cylinder which will be considered was defined as a benchmark problem in [ST96] and studied numerically in detail in [Joh04]. Figure 5.7 presents the flow domain. The right-hand side of the Navier–Stokes equations (5.3) is $f = 0$, the final time is $\bar{t} = 8$ and the inflow and outflow boundary conditions are given by

$$u(t,0,y) = u(t,2.2,y) = 0.41^{-2}\sin(\pi t/8)(6y(0.41-y),0)\ m\ s^{-1},\ 0 \le y \le 0.41.$$

On all other boundaries, the no-slip condition $u = 0$ is prescribed. The Reynolds number of the flow, based on the mean inflow, the diameter of the cylinder and the prescribed viscosity $\nu = 10^{-3}\,m^2\,s^{-1}$, is $0 \le Re(t) \le 100$.

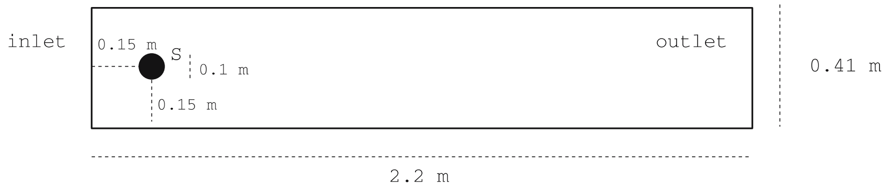

Figure 5.7: Example 5.7, the channel with the cylinder.

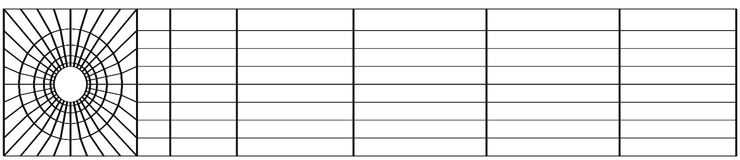

Figure 5.8: Example 5.7, the coarsest grid (level 0).

The coarsest grid (level 0) is presented in Figure 5.8. All computations have been carried out on level 3 of the spatial grid refinement resulting in 107 712 velocity d.o.f. and 39 936 pressure d.o.f. The time step was chosen to be $\tau = 0.01$.

The characteristic values of the flow are the drag coefficient $c_d(t)$ and the lift coefficient $c_l(t)$ at the cylinder. These coefficients can be computed by

$$\begin{aligned} c_d(t) &= -20\,[(u_t, v_d) + (\nu\nabla u, \nabla v_d) + ((u\cdot\nabla)u, v_d) - (p, \cdot\nabla v_d)] \\ c_l(t) &= -20\,[(u_t, v_l) + (\nu\nabla u, \nabla v_l) + ((u\cdot\nabla)u, v_l) - (p, \cdot\nabla v_l)] \end{aligned}$$

for all functions $v_d \in (H^1(\Omega))^2$ with $(v_d)|_S = (1,0)^\top$ and v_d vanishes on all other boundaries and for all test functions $v_l \in (H^1(\Omega))^2$ with $(v_l)|_S = (0,1)^\top$ and v_l vanishes on all other boundaries, respectively. Another benchmark value in [ST96] is the difference of the pressure between the front and the back at the cylinder at the final time $p(8,0.15,0.2) - p(8,0.25,0.2)$. Reference values for this difference and the maximal values of the drag and the lift coefficient are given in [Joh04].

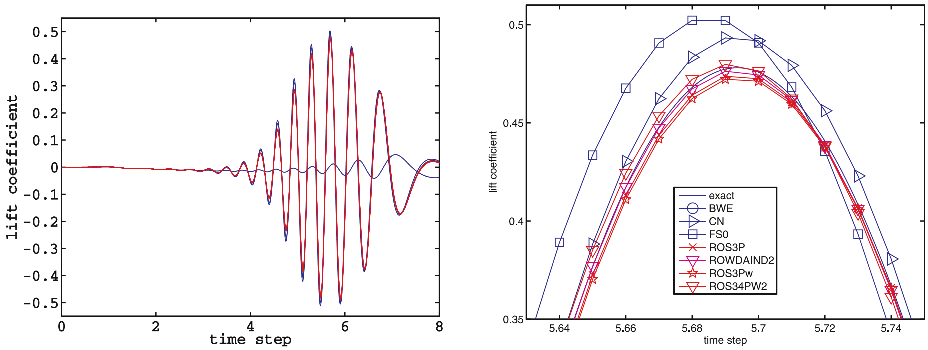

Figure 5.9: Example 5.7, lift coefficient and zoom around the maximal lift value.

The computations were done with the Backward Euler scheme (BWE), the Crank–Nicolson scheme (CN), the fractional-step-θ-scheme (FS), ROS3P, ROWDAIND2, ROS3Pw, ROS34PW2, and ROS34PW3. The other Rosenbrock methods used in the previous examples are neglected since the computing effort is too high or the accuracy is too small. We compare our Rosenbrock schemes with BWE, CN and FS since these methods are often used to solve this problem. For more informations about the schemes the reader is referred to [Emm01].

Figure 5.9 shows the lift and drag coefficients and the pressure difference as functions of time. In all graphs, also the reference curve from [Joh04] is given. We see that BWE produced the most inaccurate results. This is the only method which is, for this time step length, unable to generate the correct oscillations in the lift coefficient. From the zoom of lift coefficient curve (right in Figure 5.9) it becomes obvious that all methods are relatively close the reference curve. The best results were obtained by the Rosenbrock methods.

In Table 5.2 the pressure difference at time $t = 8$ is given. We present the value itself, its deviation from the reference value given in [Joh04] and the rel-

Table 5.2: Pressure difference at $t = 8$, $\Delta p_{ref} = -0.1116$ from [Joh04].

method	Δp	$\Delta p - \Delta p_{ref}$	$\left\lvert \frac{\Delta p - \Delta p_{ref}}{\Delta p_{ref}} \right\rvert * 100\%$
BWE	−1.17553e-01	−5.9531e-03	5.53e+00
CN	−1.10304e-01	1.2956e-03	1.16e+00
FS	−1.10170e-01	1.4301e-03	1.28e+00
ROS3P	−1.11683e-01	−8.3245e-05	7.46e-02
ROWDAIND2	−1.11750e-01	−1.4972e-04	1.34e-01
ROS3Pw	−1.11653e-01	−5.2525e-05	4.71e-02
ROS3PW2	−1.11570e-01	3.0263e-05	2.71e-02
ROS3PW3	−1.11572e-01	2.7619e-05	2.47e-02

ative error. The best result are obtained with ROS3PW2 and ROS3PW3. All Rosenbrock methods produce quite accurate results which are much better than the results obtained with the implicit θ-schemes. Also for this value, the results from BWE are the most inaccurate. One reason is probably the damping which is introduced by the BWE.

As an illustrative conclusion, we present Figure 5.10 as an extension of Figure V.1 from the book by Lang (see [Lan01, p. 57]) which shows a suggestion

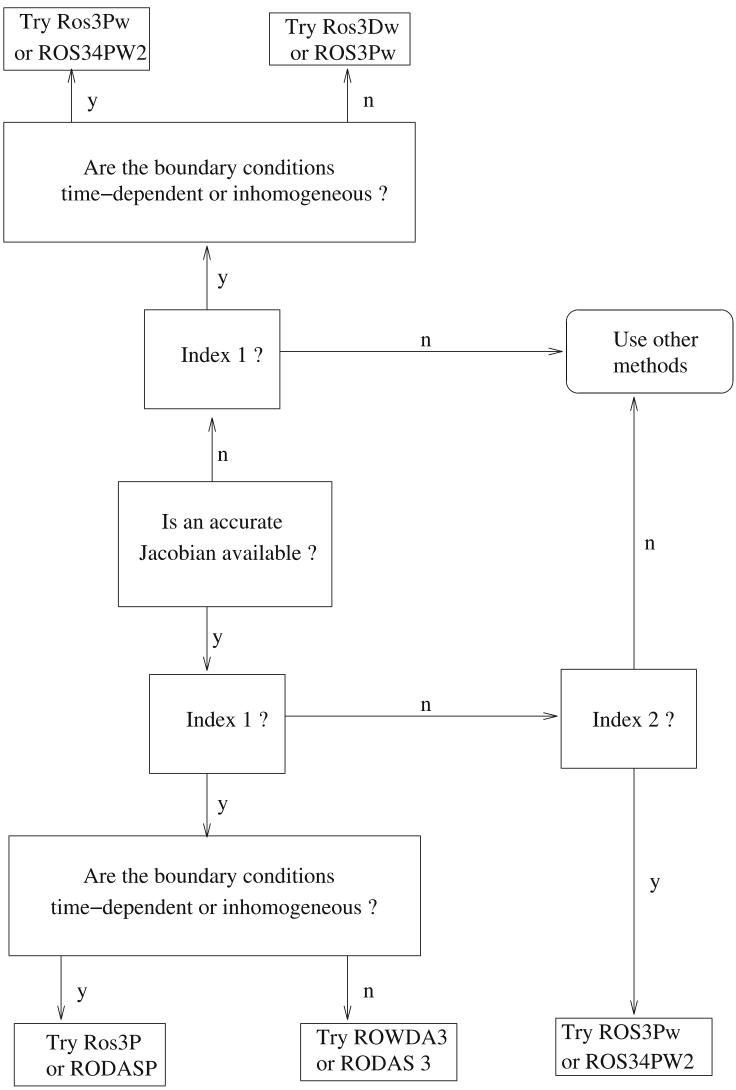

Figure 5.10: Suggestions for the selection of Rosenbrock methods.

for the selection of Rosenbrock methods. A main difference between both figures is the point that Figure 5.10 does not know the "index-0" case since a perturbation index is used. Moreover the authors would like to suggest the W-methods ROS3Pw and ROS34PW2 for solving MOL-DAEs of index 2. Last but not least ROS2 may be a rather inaccurate scheme to solve problems where an exact evaluation of the Jacobian is not possible. A better choice may be the W-methods ROS3Dw, ROS3Pw, and ROS34PW2. In the books by Brenan, Campbell and Petzold [BCP96] and by Hairer, Lubich and Roche [HLR89] can be found schemes which are able to solve problems of index 3.

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A Numerically observed temporal order of convergence.

A.1 Example 5.1.

Table A.1: u-component of Example 5.1. Error and numerical order of convergence.

	τ	$\frac{1}{10}$	$\frac{1}{20}$	$\frac{1}{40}$	$\frac{1}{80}$	$\frac{1}{160}$
ROS3P	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	5.64e-07	8.77e-08	1.07e-08	1.66e-09	1.66e-08
	q_{num}		2.68	3.03	2.69	−3.32
ROWDAIND2	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	2.44e-05	4.59e-06	7.39e-07	1.09e-07	1.19e-08
	q_{num}		2.41	2.63	2.77	3.19
ROS3w	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	8.62e-05	1.53e-05	2.45e-06	3.64e-07	5.27e-08
	q_{num}		2.49	2.65	2.75	2.79
ROS3Dw	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	6.77e-05	1.26e-05	2.05e-06	3.08e-07	4.48e-08
	q_{num}		2.42	2.62	2.74	2.78
ROS3Pw	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	3.97e-07	6.13e-08	7.73e-09	1.40e-09	1.66e-08
	q_{num}		2.69	2.99	2.46	−3.57
ROS34PW2	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	1.40e-07	1.84e-08	3.31e-09	4.82e-10	9.23e-10
	q_{num}		2.93	2.47	2.78	−0.94
ROS34PW3	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	1.33e-07	1.92e-08	3.76e-09	5.85e-10	3.89e-10
	q_{num}		2.80	2.35	2.68	0.59
RODAS3	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	4.99e-05	8.83e-06	1.37e-06	2.00e-07	3.23e-08
	q_{num}		2.50	2.68	2.78	2.63
RODAS	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	2.23e-07	2.66e-08	3.27e-09	9.39e-09	3.34e-10
	q_{num}		3.07	3.03	−1.52	4.81
RODASP	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	5.42e-10	7.70e-11	4.35e-10	4.84e-09	2.69e-10
	q_{num}		2.82	−2.50	−3.48	4.17

Table A.2: v-component of Example 5.1. Error and numerical order of convergence.

	τ	$\frac{1}{10}$	$\frac{1}{20}$	$\frac{1}{40}$	$\frac{1}{80}$	$\frac{1}{160}$
ROS3P	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	1.72e-05	3.51e-06	6.28e-07	1.02e-07	2.43e-08
	q_{num}		2.30	2.48	2.63	2.07
ROWDAIND2	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	7.58e-05	1.70e-05	3.03e-06	4.71e-07	6.60e-08
	q_{num}		2.16	2.49	2.69	2.83
ROS3w	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	2.57e-04	5.37e-05	9.42e-06	1.47e-06	2.12e-07
	q_{num}		2.26	2.51	2.68	2.79
ROS3Dw	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	1.94e-04	4.33e-05	7.87e-06	1.25e-06	1.82e-07
	q_{num}		2.16	2.46	2.66	2.78
ROS3Pw	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	3.05e-05	4.77e-06	7.25e-07	1.07e-07	2.43e-08
	q_{num}		2.67	2.72	2.76	2.14
ROS34PW2	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	6.22e-06	1.11e-06	1.77e-07	2.56e-08	2.48e-09
	q_{num}		2.49	2.64	2.79	3.37
ROS34PW3	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	1.97e-05	2.52e-06	2.88e-07	2.83e-08	3.66e-09
	q_{num}		2.96	3.13	3.35	2.95
RODAS3	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	1.61e-04	3.32e-05	5.65e-06	8.52e-07	1.16e-07
	q_{num}		2.28	2.55	2.73	2.88
RODAS	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	6.60e-07	3.57e-08	6.51e-09	1.33e-08	5.29e-09
	q_{num}		4.21	2.45	−1.03	1.33
RODASP	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	5.15e-08	3.82e-09	1.88e-09	8.19e-09	6.55e-10
	q_{num}		3.76	1.02	−2.13	3.64

A.2 Example 5.2.

Table A.3: u-component of Example 5.2. Error and numerical order of convergence.

	τ	$\frac{1}{10}$	$\frac{1}{20}$	$\frac{1}{40}$	$\frac{1}{80}$	$\frac{1}{160}$
ROS3P	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	6.99e-06	1.10e-06	1.39e-07	1.51e-08	2.12e-09
	q_{num}		2.66	2.99	3.21	2.83
ROWDAIND2	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	4.02e-04	1.12e-04	3.21e-05	9.37e-06	2.76e-06
	q_{num}		1.84	1.81	1.78	1.76
ROS3w	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	8.93e-04	2.21e-04	6.10e-05	1.79e-05	5.27e-06
	q_{num}		2.01	1.86	1.77	1.76
ROS3Dw	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	1.44e-03	4.10e-04	1.18e-04	3.44e-05	9.89e-06
	q_{num}		1.81	1.79	1.78	1.80
ROS3Pw	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	4.93e-06	7.72e-07	9.95e-08	1.14e-08	1.81e-09
	q_{num}		2.68	2.96	3.13	2.65
ROS34PW2	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	1.77e-06	2.37e-07	2.66e-08	3.77e-09	6.65e-09
	q_{num}		2.90	3.16	2.82	−0.82
ROS34PW3	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	1.69e-06	2.38e-07	4.63e-08	7.45e-09	2.72e-09
	q_{num}		2.83	2.36	2.64	1.45
RODAS3	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	1.11e-03	3.17e-04	9.15e-05	2.66e-05	7.65e-06
	q_{num}		1.81	1.79	1.78	1.80
RODAS	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	2.85e-05	8.39e-06	2.44e-06	6.84e-07	1.78e-07
	q_{num}		1.76	1.78	1.84	1.95
RODASP	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	7.19e-09	8.26e-10	2.58e-09	8.03e-10	9.73e-10
	q_{num}		3.12	−1.64	1.68	−0.28

Table A.4: v-component of Example 5.2. Error and numerical order of convergence.

	τ	$\frac{1}{10}$	$\frac{1}{20}$	$\frac{1}{40}$	$\frac{1}{80}$	$\frac{1}{160}$
ROS3P	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	2.44e-04	5.10e-05	9.66e-06	1.68e-06	2.76e-07
	q_{num}		2.26	2.40	2.52	2.61
ROWDAIND2	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	1.18e-03	3.45e-04	9.51e-05	2.67e-05	7.73e-06
	q_{num}		1.78	1.86	1.83	1.79
ROS3w	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	2.73e-03	6.64e-04	1.67e-04	4.66e-05	1.38e-05
	q_{num}		2.04	1.99	1.84	1.75
ROS3Dw	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	4.19e-03	1.22e-03	3.42e-04	9.66e-05	2.75e-05
	q_{num}		1.78	1.83	1.82	1.81
ROS3Pw	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	2.86e-04	4.76e-05	7.94e-06	1.29e-06	2.03e-07
	q_{num}		2.58	2.59	2.62	2.67
ROS34PW2	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	9.29e-05	1.76e-05	3.02e-06	4.89e-07	7.23e-08
	q_{num}		2.40	2.54	2.63	2.76
ROS34PW3	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	1.75e-04	2.30e-05	2.76e-06	3.19e-07	4.20e-08
	q_{num}		2.93	3.06	3.11	2.92
RODAS3	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	3.21e-03	9.30e-04	2.62e-04	7.44e-05	2.12e-05
	q_{num}		1.79	1.83	1.82	1.81
RODAS	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	3.40e-05	1.62e-05	5.70e-06	1.72e-06	4.66e-07
	q_{num}		1.07	1.51	1.72	1.89
RODASP	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	8.10e-07	6.81e-08	9.79e-09	5.78e-10	2.40e-09
	q_{num}		3.57	2.80	4.08	−2.05

A.3 Example 5.3.

Table A.5: u-component of Example 5.3. Error and numerical order of convergence.

	τ	$\frac{1}{10}$	$\frac{1}{20}$	$\frac{1}{40}$	$\frac{1}{80}$	$\frac{1}{160}$
ROS3P	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	2.35e-04	3.89e-05	6.34e-06	1.01e-06	1.55e-07
	q_{num}		2.59	2.62	2.65	2.70
ROWDAIND2	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	1.64e-04	5.71e-05	1.90e-05	6.05e-06	1.82e-06
	q_{num}		1.52	1.59	1.65	1.73
ROS3w	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	4.75e-04	1.16e-04	3.46e-05	1.09e-05	3.32e-06
	q_{num}		2.03	1.74	1.66	1.72
ROS3Dw	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	7.33e-04	2.34e-04	7.40e-05	2.25e-05	6.45e-06
	q_{num}		1.65	1.66	1.72	1.80
ROS3Pw	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	2.52e-04	3.83e-05	5.71e-06	8.45e-07	1.23e-07
	q_{num}		2.72	2.74	2.76	2.78
ROS34PW2	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	6.99e-05	7.44e-06	8.59e-07	1.27e-07	1.85e-08
	q_{num}		3.23	3.11	2.76	2.78
ROS34PW3	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	1.73e-04	2.23e-05	2.83e-06	3.52e-07	4.23e-08
	q_{num}		2.96	2.98	3.01	3.06
RODAS3	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	6.97e-04	2.00e-04	5.96e-05	1.77e-05	5.02e-06
	q_{num}		1.80	1.75	1.75	1.82
RODAS	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	4.71e-05	9.14e-06	2.06e-06	5.01e-07	1.18e-07
	q_{num}		2.37	2.15	2.04	2.09
RODASP	$\|\underline{\epsilon}\|_{l_2(J,H^1)}$	2.02e-05	2.24e-06	2.19e-07	1.98e-08	8.59e-09
	q_{num}		3.17	3.36	3.47	1.20

Table A.6: v-component of Example 5.3. Error and numerical order of convergence.

	τ	$\frac{1}{10}$	$\frac{1}{20}$	$\frac{1}{40}$	$\frac{1}{80}$	$\frac{1}{160}$
ROS3P	$\|\|\underline{\epsilon}\|\|_{l_2(J,H^1)}$	5.22e-04	7.79e-05	1.15e-05	1.67e-06	2.36e-07
	q_{num}		2.75	2.76	2.78	2.82
ROWDAIND2	$\|\|\underline{\epsilon}\|\|_{l_2(J,H^1)}$	2.72e-04	2.96e-05	7.03e-06	2.69e-06	8.76e-07
	q_{num}		3.20	2.08	1.38	1.62
ROS3w	$\|\|\underline{\epsilon}\|\|_{l_2(J,H^1)}$	7.80e-04	1.89e-04	4.85e-05	1.27e-05	3.32e-06
	q_{num}		2.04	1.97	1.94	1.93
ROS3Dw	$\|\|\underline{\epsilon}\|\|_{l_2(J,H^1)}$	4.58e-04	8.59e-05	3.16e-05	1.06e-05	3.17e-06
	q_{num}		2.41	1.44	1.57	1.75
ROS3Pw	$\|\|\underline{\epsilon}\|\|_{l_2(J,H^1)}$	6.16e-04	9.01e-05	1.28e-05	1.81e-06	2.49e-07
	q_{num}		2.77	2.81	2.83	2.86
ROS34PW2	$\|\|\underline{\epsilon}\|\|_{l_2(J,H^1)}$	3.89e-04	5.71e-05	8.18e-06	1.15e-06	1.58e-07
	q_{num}		2.77	2.80	2.84	2.86
ROS34PW3	$\|\|\underline{\epsilon}\|\|_{l_2(J,H^1)}$	4.76e-04	6.09e-05	7.76e-06	9.97e-07	1.28e-07
	q_{num}		2.97	2.97	2.96	2.96
RODAS3	$\|\|\underline{\epsilon}\|\|_{l_2(J,H^1)}$	3.27e-04	9.68e-05	2.96e-05	8.85e-06	2.51e-06
	q_{num}		1.76	1.71	1.74	1.82
RODAS	$\|\|\underline{\epsilon}\|\|_{l_2(J,H^1)}$	2.64e-05	4.74e-06	1.04e-06	2.52e-07	5.97e-08
	q_{num}		2.48	2.18	2.05	2.08
RODASP	$\|\|\underline{\epsilon}\|\|_{l_2(J,H^1)}$	1.07e-05	1.03e-06	1.01e-07	9.30e-09	1.21e-08
	q_{num}		3.37	3.36	3.43	−0.38

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