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NEW ROSENBROCK METHODS OF ORDER 3 FOR PDAEs OF INDEX 2

JOACHIM RANG and LUTZ ANGERMANN

Institute for Scientific Computing
University of Technology at Braunschweig
Hans-Sommer-Straße 65
D-38106 Braunschweig, Germany

Institute of Mathematics
University of Technology at Clausthal
Erzstraße 1, D-38768 Clausthal-Zellerfeld, Germany

Abstract

Motivated by solving the incompressible Navier-Stokes equations, the authors develop new Rosenbrock methods for index 2 PDAEs. Based on a well-known set of order conditions, solvers of order 3 with 4 internal stages are constructed. In particular, the methods allow the use of inexact Jacobians and approximations of $\partial f / \partial t$. This leads to an important advantage in the robustness of the solvers with respect to the practical computation of these terms. At the end of the paper, five test problems of different severity and complexity are presented. They show the performance of the new methods in comparison with other Rosenbrock-solvers.

1. Introduction

In computational fluid dynamics, the Navier-Stokes system for incompressible fluids represents one of the central mathematical models.

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For its numerical solution, very often the vertical methods of lines (MOL) is applied, i.e., the system is first discretized in space. Then a major computational task consists in the numerical integration of the resulting huge MOL-DAE system. Within this framework, two aspects are important. On the one hand, it is well-known that standard integrators may exhibit order reduction if they are applied to huge ODE or DAE systems resulting, e.g., from the semidiscretization in space of parabolic equations or PDAEs. Rosenbrock methods enable to decrease this order reduction provided some additional conditions are fulfilled [8]. On the other hand, it is also well-known [1, 19] that the MOL-DAE Navier-Stokes system has the index 2.

These two aspects, but also the fundamental need in the development of solvers which lead additionally to a good balance between high accuracy, stability, computational robustness and moderate costs, motivated the construction of new Rosenbrock methods for index 2 PDAEs.

Concerning the literature, the following sources are in a close relationship to the present paper. The method ROWDA2IND [9] is a method for DAEs of index 2 and most of the other methods, for example ROS3P [7], ROS3Pw, ROS34PW2 [12] or RODASP [15] are schemes for solving PDAEs of index 1.

This work can be regarded as a continuation of the papers [12] and [5], where Rosenbrock methods were considered which meet only one of the two requirements. Here, we propose some new Rosenbrock methods for PDAEs of index 2. The new methods are of order 3 and have 4 internal stages.

In addition, they principally allow the use of inexact Jacobians and approximations of $\partial f / \partial t$. In our numerical applications, this feature is not used explicitly because W-methods using an approximation of the Jacobian exhibit some disadvantages [6]. However, if such methods are applied as usual Rosenbrock methods, i.e., the Jacobian is evaluated exactly, they yield very good results [18]. The benefit of this approach lies in the computational robustness of the solvers. This observation is also supported by the numerical examples from the above-mentioned papers [5, 12].

The contents of the paper are as follows: In Section 2, we outline the collection of order conditions to be satisfied. Section 3 deals with the explicit construction of four new methods. In Section 4, five test problems of different severity and complexity are presented. They show the impressive performance of the new methods in comparison with other Rosenbrock-solvers.

2. Rosenbrock Methods

Definition 1. An s-stage Rosenbrock method for the implicit ODE

$$M\dot{u} = f(t, u), \; u(t_0) = u_0, \tag{2.1}$$

with a matrix $M \in \mathbb{R}^{n,n}$ is given by

$$Mk_i := \tau f\left(t_{\text{old}} + \alpha_i \tau, \, u_{\text{old}} + \sum_{j=1}^{i-1} \alpha_{ij} k_j\right) + \tau W \sum_{j=1}^{i} \gamma_{ij} k_j + \tau^2 \gamma_i T, \; i = 1, \ldots, s,$$

$$u_{\text{new}} := u_{\text{old}} + \sum_{i=1}^{s} b_i k_i, \tag{2.2}$$

where s is the number of internal stages, τ is the time-step, α_{ij}, γ_{ij}, b_i are the parameters of the method, $W := f'(t_{\text{old}}, u_{\text{old}})$, $T := \dot{f}(t_{\text{old}}, u_{\text{old}})$, $\alpha_i := \sum_{j=1}^{i-1} \alpha_{ij}$ and $\gamma_i := \sum_{j=1}^{i-1} \gamma_{ij}$. By "·" and "′" we denote differentiation with respect to the time t and the phase space variable, respectively.

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 by the use of Butcher series can be found in [2, Sect. IV.7]. Here, we only summarize the conditions up to the order 3:

$$\begin{cases} \text{(A1)} & \sum b_i = 1 \\ \text{(A2)} & \sum b_i \beta_i = \frac{1}{2} - \gamma \\ \text{(A3a)} & \sum b_i \alpha_i^2 = \frac{1}{3} \\ \text{(A3b)} & \sum b_i \beta_{ij} \beta_j = \frac{1}{6} - \gamma + \gamma^2, \end{cases} \tag{2.3}$$

where we have used the abbreviations $\beta_{ij} := \alpha_{ij} + \gamma_{ij}$ and $\beta_i := \sum_{j=1}^{i-1} \beta_{ij}$. If we choose $W := f'(t_{\text{old}}, u_{\text{old}}) + \mathcal{O}(h)$, we get an additional consistency condition [17]:

$$\text{(B2)} \quad \sum b_i \alpha_i = \frac{1}{2}. \tag{2.4}$$

For arbitrary matrices $W \in \mathbb{R}^{n,n}$, we get the following order conditions [17]:

$$\begin{cases} \text{(C3a)} & \sum b_i \alpha_{ij} \alpha_j = \frac{1}{6} \\ \text{(C3b)} & \sum b_i \alpha_{ij} \beta_j = \frac{1}{6} - \frac{\gamma}{2} \\ \text{(C3c)} & \sum b_i \beta_{ij} \alpha_j = \frac{1}{6} - \frac{\gamma}{2}. \end{cases} \tag{2.5}$$

If a Rosenbrock method is applied to semidiscretized PDEs or PDAEs, the following condition should be satisfied to avoid order reduction [8]:

$$b^{\top} B^j (2B^2 e - \alpha^2) = 0, \quad 1 \leq j \leq s - 1, \tag{2.6}$$

where

$$b := (b_1, \ldots, b_s)^{\top}, \; B := (\beta_{ij})_{i,j=1}^{s}, \; \alpha^2 := (\alpha_1^2, \ldots, \alpha_s^2)^{\top}$$

and $e := (1, \ldots, 1)^{\top} \in \mathbb{R}^s$.

To obtain convergence, the Rosenbrock method should fulfill certain order conditions for both the ODE and the algebraic part. These consistency properties can be derived again via the Butcher series technique [2, 13].

For a third-order method, we get the condition

$$\text{(E3)} \sum b_i \omega_{ij} \alpha_j^2 = 1, \tag{2.7}$$

where ω_{ij} are the entries of the inverse B^{-1}.

From [9], we know that a Rosenbrock method should satisfy certain order conditions if the method is applied to an index-2 DAE, i.e.,

$$\begin{cases} \text{(F3a)} & \sum b_i \omega_{ij} \omega_{jk} \alpha_k^2 = 2 \\ \text{(F3b)} & \sum b_i \alpha_i \alpha_{ij} \omega_{jk} \omega_{kl} \alpha_l^2 = \dfrac{2}{3} \\ \text{(F3c)} & \sum b_i \omega_{ij} \alpha_j \alpha_{jk} \omega_{kl} \omega_{lm} \alpha_m^2 = 2. \end{cases} \tag{2.8}$$

If u_2 appears non-linearly in the semi-explicit DAE,

$$\begin{cases} \dot{u}_1 = f_1(u_1, u_2) \\ 0 = f_2(u_1), \end{cases}$$

then the condition

$$\text{(G3)} \sum b_i \alpha_{ij} \omega_{jk} \omega_{kl} \alpha_l^2 \alpha_{lm} \omega_{mn} \omega_{nr} \alpha_r^2 = \frac{4}{3} \tag{2.9}$$

has to be satisfied [9].

The stability function of (22) is given by

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

3. Construction of Methods

We start with the following result:

Lemma 1. *There exists no Rosenbrock method of order* 3 *with* 3 *internal stages which satisfies* (23), (26), (F3b) *and* (F3c).

Proof. In the case $s = 3$, the condition (26) simplifies to

$$\begin{cases} \text{(D3a)} & b_3 \beta_{32} \alpha_2^2 = \dfrac{1}{6} - \dfrac{2}{3} \\ \text{(D3b)} & \gamma = \dfrac{1}{2} + \dfrac{1}{6}\sqrt{3}. \end{cases} \tag{3.10}$$

The inverse of B is given by

$$B^{-1} = (\omega_{ij})_{i,j=1}^{3} = \begin{pmatrix} \dfrac{1}{\gamma} & 0 & 0 \\ \dfrac{-\beta_{21}}{\gamma^2} & \dfrac{1}{\gamma} & 0 \\ -\dfrac{-\beta_{21}\beta_{32} + \gamma\beta_{31}}{\gamma^3} & \dfrac{-\beta_{32}}{\gamma^2} & \dfrac{1}{\gamma} \end{pmatrix}.$$

First, we consider the conditions (F3b) and (F3c). We get

$$\frac{2}{3} = \sum_{i,j,k,l}^{3} b_i \alpha_i \alpha_{ij} \omega_{jk} \omega_{kl} \alpha_l^2 = b_3 \alpha_3 \alpha_{32} \omega_{22}^2 \alpha_2^2 = \frac{1}{\gamma^2} b_3 \alpha_3 \alpha_{32} \alpha_2^2,$$

$$2 = \sum_{i,j,k,l}^{3} b_i \omega_{ij} \alpha_j \alpha_{jk} \omega_{kl} \omega_{lm} \alpha_m^2 = b_3 \omega_{33} \alpha_3 \alpha_{32} \omega_{22}^2 \alpha_2^2 = \frac{1}{\gamma^3} b_3 \alpha_3 \alpha_{32} \alpha_2^2.$$

It follows $\frac{2}{3}\gamma^2 = 2\gamma^3$ and $\gamma = \frac{1}{3}$ but this is a contradiction to (D3b).

Let us now consider Rosenbrock methods with 4 internal stages. The order conditions in this case read as [2]

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

The following result is taken from [12].

Lemma 2. *The conditions for PDEs* (26) *can be simplified by the help of* (A1), (A2), (A3a) *and* (A3b) *to*

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

Remark. 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 [2].

The algebraic order condition reads as [2]

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

The inverse of the matrix B is given by

$$B^{-1} = (\omega_{ij})_{i,\,j=1}^{4}$$
$$= \begin{pmatrix} \frac{1}{\gamma} & 0 & 0 & 0 \\ \frac{-\beta_{21}}{\gamma^2} & \frac{1}{\gamma} & 0 & 0 \\ -\frac{-\beta_{21}\beta_{32} + \gamma\beta_{31}}{\gamma^3} & \frac{-\beta_{32}}{\gamma^2} & \frac{1}{\gamma} & 0 \\ -\frac{\beta_{21}\beta_{32}\beta_{43} - \gamma\beta_{31}\beta_{43} + \gamma^2\beta_{41}}{\gamma^4} & -\frac{-\beta_{32}\beta_{43} + \gamma\beta_{42}}{\gamma^3} & \frac{-\beta_{43}}{\gamma^2} & \frac{1}{\gamma} \end{pmatrix}.$$

Lemma 3. *A Rosenbrock method which satisfies* (A1)-(A3b) *and* (D3a)-(D3c) *fulfils* (E3) *too.*

Proof. See [12].

Lemma 4. *A Rosenbrock method which satisfies* (A1)-(A3b) *and* (D3a)-(D3c) *fulfils* (F3a) *too.*

Proof. The condition (F3a) can be written as follows:

$$2 = \sum b_i\omega_{ij}\omega_{jk}\alpha_k^2$$
$$= b_2\omega_{22}^2\alpha_2^2 + b_3(\omega_{32}\omega_{22}\alpha_2^2 + \omega_{33}\omega_{32}\alpha_2^2 + \omega_{33}^2\alpha_3^2)$$
$$+ b_4(\omega_{42}\omega_{22}\alpha_2^2 + \omega_{43}(\omega_{32}\alpha_2^2 + \omega_{33}\alpha_3^2) + \omega_{44}(\omega_{42}\alpha_2^2 + \omega_{43}\alpha_3^2 + \omega_{44}\alpha_4^2)$$
$$= \frac{1}{\gamma^2}(b_2\alpha_2^2 + b_3\alpha_3^2 + b_4\alpha_4^2) - \frac{2}{\gamma^3}(b_3\beta_{32}\alpha_2^2$$
$$+ b_4(\beta_{42}\alpha_2^2 + \beta_{43}\alpha_3^2)) + \frac{3}{\gamma^4}b_4\beta_{43}\beta_{32}\alpha_2^2.$$

Using the conditions (A3a), (D3a) and (D3b), we obtain

$$\sum b_i \omega_{ij} \omega_{jk} \alpha_k^2 = \frac{1}{3\gamma^2} - \frac{2}{3\gamma^2}(6\gamma^2 - 9\gamma + 2) + \frac{1}{\gamma^2}(6\gamma^2 - 6\gamma + 1) = 2.$$

We also observe that the conditions (F3b) and (F3c) can be written as follows:

$$\frac{2}{3} = \sum b_i \alpha_i \alpha_{ij} \omega_{jk} \omega_{kl} \alpha_l^2 = b_3 \alpha_3 \alpha_{32} \omega_{22}^2 \alpha_2^2 + b_4 \alpha_4 (\alpha_{42} \omega_{22}^2 \alpha_2^2$$

$$+ \alpha_{43}(\omega_{32}\omega_{22}\alpha_2^2 + \omega_{33}\omega_{32}\alpha_2^2 + \omega_{33}^2\alpha_2^2))$$

$$= \frac{1}{\gamma^2}(b_3\alpha_3\alpha_{32}\alpha_2^2 + b_4\alpha_4(\alpha_{42}\alpha_2^2 + \alpha_{43}\alpha_3^2)) - \frac{2}{\gamma^3} b_4\alpha_4\alpha_{43}\beta_{32}\alpha_2^2,$$

$$2 = \sum b_i \omega_{ij} \alpha_j \alpha_{jk} \omega_{kl} \omega_{lm} \alpha_m^2 = b_3 \omega_{33} \alpha_3 \alpha_{32} \omega_{22}^2 \alpha_2^2$$

$$+ b_4(\omega_{43}\alpha_3\alpha_{32}\omega_{22}^2\alpha_2^2 + \omega_{44}\alpha_4(\alpha_{42}\omega_{22}^2\alpha_2^2$$

$$+ \alpha_{43}(\omega_{32}\omega_{22}\alpha_2^2 + \omega_{33}\omega_{32}\alpha_2^2 + \omega_{33}^2\alpha_3^2)))$$

$$= \frac{1}{\gamma^3}(b_3\alpha_3\alpha_{32}\alpha_2^2 + b_4\alpha_4(\alpha_{42}\alpha_2^2 + \alpha_{43}\alpha_3^2))$$

$$- \frac{1}{\gamma^4}(b_4\beta_{43}\alpha_3\alpha_{32}\alpha_2^2 + 2b_4\alpha_4\beta_{32}\alpha_{43}\alpha_2^2) = \frac{2}{3\gamma^3} - \frac{1}{\gamma^4} b_4\beta_{43}\alpha_3\alpha_{32}\alpha_2^2.$$

Summarizing our results, we have

$$\begin{cases} \text{(F3b)} \quad \gamma(b_3\alpha_3\alpha_{32}\alpha_2^2 + b_4\alpha_4(\alpha_{42}\alpha_2^2 + \alpha_{43}\alpha_3^2)) - 2b_4\alpha_4\alpha_{43}\beta_{32}\alpha_2^2 = \frac{2}{3}\gamma^3 \\ \text{(F3c)} \quad b_4\beta_{43}\alpha_3\alpha_{32}\alpha_2^2 = \frac{2}{3}\gamma^3 - 2\gamma^4. \end{cases}$$

The embedded methods should be L-stable, too. Therefore, we need the following result from [12].

Lemma 5. *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*

$$\hat{b}_4 = \frac{1}{\beta_3\beta_{43}}\left[\gamma^3 - 2\gamma^2 + \frac{1}{2}\gamma\right]. \tag{3.11}$$

Proof. See [12].

3.1. An *L*-stable Rosenbrock W-method

Our first method is *L*-stable and satisfies the conditions (A1)-(A3b), (B2), (C3a)-(C3c), (D3a)-(D3c), (F3b) and (F3c). We call the method ROSI2P1, where ROS stands for Rosenbrock, I2 for index 2 problems, P for semidiscretized PDE problems and 1 is an internal number. To find a solution of the equations given above, we have used the computer algebra system MAPLE. We choose the free variables as follows: $\alpha_2 = 1/2$, $\alpha_3 = 3/4$, and $\alpha_4 = 1$. The coefficients of ROSI2P1 are given in Table 1. The embedded method satisfies the conditions (A1), (A2) and (3.11). Moreover, we set $\hat{b}_3 = 0$. The resulting system of equations can be solved easily.

Table 1. Set of coefficients for ROSI2P1

$\gamma = 4.3586652150845900e-01$	
$\alpha_{21} = 5.0000000000000000e-01$	$\gamma_{21} = -5.0000000000000000e-01$
$\alpha_{31} = 5.5729261836499822e-01$	$\gamma_{31} = -6.4492162993321323e-01$
$\alpha_{32} = 1.9270738163500176e-01$	$\gamma_{32} = 6.3491801247597734e-02$
$\alpha_{41} = -3.0084516445435860e-01$	$\gamma_{41} = 9.3606009252719842e-03$
$\alpha_{42} = 1.8995581939026787e+00$	$\gamma_{42} = -2.5462058718013519e-01$
$\alpha_{43} = -5.9871302944832006e-01$	$\gamma_{43} = -3.2645441930944352e-01$
$b_1 = 5.2900072579103834e-02$	$\hat{b}_1 = 1.4974465479289098e-01$
$b_2 = 1.3492662311920438e+00$	$\hat{b}_2 = 7.0051069041421810e-01$
$b_3 = -9.1013275270050265e-01$	$\hat{b}_3 = 0.0000000000000000e+00$
$b_4 = 5.0796644892935516e-01$	$\hat{b}_4 = 1.4974465479289098e-01$

3.2. A stiffly accurate Rosenbrock method

Definition 2. A Rosenbrock method satisfying

$$\beta_{si} = b_i,\ i = 1, \dots, s, \text{ and } \alpha_s = 1 \qquad (3.12)$$

is called *stiffly accurate*.

Methods which satisfy (3.12) yield asymptotically exact results for the problem $\dot{u} = \lambda(u - \varphi(t)) + \dot{\varphi}(t)$. A stiffly accurate Rosenbrock method is L-stable, i.e., $\gamma \approx 0.4358665$ [2] or [12].

Our conditions simplify by the help of (3.12) to [9] and [12]

$$\begin{cases} \text{(A1')} & b_1 + b_2 + b_3 = 1 - \gamma \\ \text{(A2')} & b_2\beta_2 + b_3\beta_3 = \frac{1}{2} - 2\gamma + \gamma^2 \\ \text{(A3a')} & b_2\alpha_2^2 + b_3\alpha_3^2 = \frac{1}{3} - \gamma \\ \text{(A3b')} & b_3\beta_{32}\beta_2 = \frac{1}{6} - \frac{3}{2}\gamma + 3\gamma^2 - \gamma^3 \\ \text{(B2')} & b_2\alpha_2 + b_3\alpha_3 = \frac{1}{2} - \gamma \\ \text{(C3a')} & b_3\alpha_{32}\alpha_2 + \gamma(\alpha_{42}\alpha_2 + \alpha_{43}\alpha_3) = \frac{1}{6} \\ \text{(C3b')} & b_3\alpha_{32}\beta_2 + \gamma(\alpha_{42}\beta_2 + \alpha_{43}\beta_3) = \frac{1}{6} - \frac{\gamma}{2} \\ \text{(C3c')} & b_3\beta_{32}\alpha_2 = \frac{1}{6} - \gamma + \gamma^2 \\ \text{(D3a')} & b_3\beta_{32}\alpha_2^2 = 2\gamma^3 - 2\gamma^2 + \frac{1}{3}\gamma \\ \text{(D3c')} & b_3\beta_{32}\beta_2 = 0 \\ \text{(F3b')} & \gamma(\alpha_{42}\alpha_2^2 + \alpha_{43}\alpha_3^2) - 2\alpha_{43}\beta_{32}\alpha_2^2 = 2\gamma^3 \\ \text{(F3c')} & b_3\alpha_3\alpha_{32}\alpha_2^2 = \frac{2}{3}\gamma^2 - 2\gamma^3. \end{cases}$$

The new method should satisfy the conditions (A1')-(A3b'), (D3a'), (D3c'), (F3b') and (F3c'). Moreover, we set $\alpha_2 = 1/2$, $\alpha_{41} = \alpha_{31}$, $\alpha_{42} = \alpha_{32}$ and $\alpha_{43} = 0$, i.e., the method needs only three function evaluations. First, we note that $\beta_2 = 0$. This follows from (D3a') and (D3c'). With (F3b'), we get $\alpha_{42} = 8\gamma^2$. Inserting this result into (F3c') yields $b_3 = 1/3 - \gamma$. Using (D3a'), we obtain

$$\beta_{32} = 4\,\frac{2\gamma^3 - 2\gamma^2 + 1/3\,\gamma}{1/3 - \gamma}.$$

The remaining coefficients can be computed by the help of (A1'), (A2') and (A3a'). The new method is called ROSI2P2 and its coefficients are given in Table 2. The embedded method satisfies the conditions (A1), (A2) and (3.11). Moreover, we set $\hat{b}_3 = 1/2$. This system of equations can be solved easily.

Table 2. Set of coefficients for ROSI2P2

$\gamma = 4.3586652150845900e-01$	
$\alpha_{21} = 5.0000000000000000e-01$	$\gamma_{21} = -5.0000000000000000e-01$
$\alpha_{31} = -5.1983699657507165e-01$	$\gamma_{31} = -4.0164172503011392e-01$
$\alpha_{32} = 1.5198369965750715e+00$	$\gamma_{32} = 1.1742718526976650e+00$
$\alpha_{41} = -5.1983699657507165e-01$	$\gamma_{41} = 1.1865036632417383e+00$
$\alpha_{42} = 1.5198369965750715e+00$	$\gamma_{42} = -1.5198369965750715e+00$
$\alpha_{43} = 0.0000000000000000e+00$	$\gamma_{43} = -1.0253318817512568e-01$
$b_1 = 6.6666666666666663e-01$	$\hat{b}_1 = -9.5742384859111473e-01$
$b_2 = 0.0000000000000000e-00$	$\hat{b}_2 = 2.9148476971822297e+00$
$b_3 = -1.0253318817512568e-01$	$\hat{b}_3 = 5.0000000000000000e-01$
$b_4 = 4.3586652150845900e-01$	$\hat{b}_4 = -1.4574238485911146e+00$

3.3. A stiffly accurate Rosenbrock method with $J = f_u + \mathcal{O}(h)$ and $T = 0$

The new method should satisfy the conditions (A1')-(A3b'), (B2'), (C3c'), (D3a'), (D3c'), (F3b'), (F3c') and (G3). The condition (G3) can be simplified to

$$b_4\alpha_{43}\alpha_3^2\alpha_{32}\alpha_2^2 = \frac{4}{3}\gamma^4.$$

In the case of stiffly accurate Rosenbrock method, we obtain

$$\alpha_{43}\alpha_3^2\alpha_{32}\alpha_2^2 = \frac{4}{3}\gamma^3.$$

As the free variable, we choose $\alpha_3 = 3/4$. As in the previous section, we have $\beta_2 = 0$. The variable $\alpha_2 = 2\gamma$ can be determined by (D3a') and (C3c'). The equations (A3a) and (B2) form a linear system of equations in the variables b_2 and b_3. Then the remaining coefficients can be determined easily. The method is called ROSI2Pw and the coefficients are given in Table 3. The embedded method satisfies the conditions (A1), (A2) and (3.11). Moreover, we set $\hat{b}_3 = 0$. This system of equations can be solved easily.

Table 3. Set of coefficients for ROSI2Pw

$\gamma = 4.3586652150845900e - 01$	
$\alpha_{21} = 8.7173304301691801e - 01$	$\gamma_{21} = -8.7173304301691801e - 01$
$\alpha_{31} = 7.8938917169345013e - 01$	$\gamma_{31} = -8.4175599602920992e - 01$
$\alpha_{32} = -3.9389171693450180e - 02$	$\gamma_{32} = -1.2977652642309580e - 02$
$\alpha_{41} = 6.2787416864263046e - 01$	$\gamma_{41} = -3.7964867148089526e - 01$
$\alpha_{42} = 6.9295440480994763e + 00$	$\gamma_{42} = -8.3490231248017537e + 00$
$\alpha_{43} = -6.5574182167421071e + 00$	$\gamma_{43} = 8.2928052747741905e + 00$
$b_1 = 2.4822549716173517e - 01$	$\hat{b}_1 = 4.4315753191688778e - 01$
$b_2 = -1.4194790767022774e + 00$	$\hat{b}_2 = 4.4315753191688778e - 01$
$b_3 = 1.7353870580320832e + 00$	$\hat{b}_3 = 0.0000000000000000e + 00$
$b_4 = 4.3586652150845900e - 01$	$\hat{b}_4 = 1.1368493616622447e - 01$

3.4. A stiffly accurate Rosenbrock W-method

In the following, a Rosenbrock method is constructed which satisfies the conditions (A1')-(A3b'), (B2'), (C3a')-(C3c'), (D3a'), (D3c'), (F3b') and (F3c'). We have 12 equations and 12 unknowns. Note that 5 unknowns are determined by (3.12). There are no free variables. The coefficients $\alpha_2 = 2\gamma$ and $\beta_2 = 0$ can be computed as in the previous section. Let us assume that we know the coefficient α_3. Then (A3a') and (B2') form a linear system of equations in the unknowns b_2 and b_3. The solution depends on α_3 and is given by

$$b_2 = \frac{1}{12}\frac{6\alpha_3\gamma + 2 - 6\gamma - 3\alpha_3}{\gamma(2\gamma - \alpha_3)}, \; b_3 = -\frac{1}{3}\frac{6\gamma^2 - 6\gamma + 1}{\alpha_3(2\gamma - \alpha_3)}.$$

It follows

$$(\mathrm{A2'}) \Rightarrow \beta_3 = -\frac{3}{2}\frac{(1-4\gamma+2\gamma^2)\alpha_3(2\gamma-\alpha_3)}{6\gamma^2-6\gamma+1},$$

$$(\mathrm{C3b'}) \Rightarrow \alpha_{43} = \frac{1}{9}\frac{(-1+3\gamma)(6\gamma^2-6\gamma+1)}{\gamma(1-4\gamma+2\gamma^2)\alpha_3(2\gamma-\alpha_3)},$$

$$(\mathrm{C3c'}) \Rightarrow \beta_{32} = -\frac{1}{4}\frac{\alpha_3(2\gamma-\alpha_3)}{\gamma},$$

$$(\mathrm{F3c'}) \Rightarrow \alpha_{32} = \frac{1}{2}\frac{(2\gamma-\alpha_3)(-1+3\gamma)}{6\gamma^2-6\gamma+1}$$

$$\begin{aligned}(\mathrm{F3b'}) \Rightarrow \alpha_{42} = {} & \frac{1}{36\gamma^3(2\gamma-\alpha_3)(1-4\gamma+2\gamma^2)}(-36\gamma^4-144\gamma^5 \\ & +72\gamma^4\alpha_3+72\gamma^6-36\gamma^5\alpha_3+96\gamma^3 \\ & -24\alpha_3\gamma^2-36\gamma^2+9\alpha_3\gamma+4\gamma-\alpha_3),\end{aligned}$$

$$\begin{aligned}(\mathrm{C3a'}) \Rightarrow \alpha_3 = {} & -\frac{1}{2\gamma}(-48\alpha_3\gamma^2+162\gamma^3\alpha_3-132\gamma^4\alpha_3+12\alpha_3^2\gamma \\ & -36\alpha_3^2\gamma^2+6\alpha_3^2\gamma^3+12\gamma^3-84\gamma^4+168\gamma^5 \\ & -72\gamma^6-108\gamma^5\alpha_3+72\gamma^4\alpha_3^2+72\alpha_3\gamma^6-36\gamma^5\alpha_3^2 \\ & +4\alpha_3\gamma-\alpha_3^2)/(3\gamma-1)(6\gamma^2-6\gamma+1).\end{aligned}$$

The solution of the last equation can be computed by the help of MAPLE. One solution is $\alpha_3 = 2\gamma$, but this is a contradiction to b_2 and b_3. A second solution is given by

$$\alpha_3 = 6\frac{\gamma^2(-14\gamma^2+6\gamma^3-1+7\gamma)}{-12\gamma+36\gamma^2-6\gamma^3-72\gamma^4+36\gamma^5+1} \approx -1.55.$$

Unfortunately, $\alpha_3 < 0$. The method is called ROSI2PW and the coefficients are given by Table 4. The embedded method satisfies the conditions (A1), (A2) and (3.11). Moreover, we set $\hat{b}_3 = 0$. This system of equations can be solved easily.

Table 4. Set of coefficients for ROSI2PW

$\gamma = 4.3586652150845900e-01$	
$\alpha_{21} = 8.7173304301691801e-01$	$\gamma_{21} = -8.7173304301691801e-01$
$\alpha_{31} = -7.9937335839852708e-01$	$\gamma_{31} = 3.0647867418622479e+00$
$\alpha_{32} = -7.9937335839852708e-01$	$\gamma_{32} = 3.0647867418622479e+00$
$\alpha_{41} = 7.0849664917601007e-01$	$\gamma_{41} = -1.0424832458800504e-01$
$\alpha_{42} = 3.1746327955312481e-01$	$\gamma_{42} = -3.1746327955312481e-01$
$\alpha_{43} = -2.5959928729134892e-02$	$\gamma_{43} = -1.4154917367329144e-02$
$b_1 = 6.0424832458800504e-01$	$\hat{b}_1 = 4.4315753191688778e-01$
$b_2 = 0.0000000000000000e-00$	$\hat{b}_2 = 4.4315753191688778e-01$
$b_3 = -4.0114846096464034e-02$	$\hat{b}_3 = 0.0000000000000000e+00$
$b_4 = 4.3586652150845900e-01$	$\hat{b}_4 = 1.1368493616622447e-01$

4. Comparison of Rosenbrock Methods and Numerical Results

All examples were solved numerically by the help of the FEM-package MooNMD3.0 [4]. We have compared the new methods with other well-known Rosenbrock methods such as ROS3P, ROS3Pw and ROS34PW2. An overview of the selected Rosenbrock methods is given in Table 5.

We applied these schemes to a PDAE of index 2 and to the Navier-Stokes equations with different right-hand sides. For the definition of the index of linear PDAEs, we refer to the paper [11].

The global error $\underline{\epsilon}$ is measured in the discrete L_2-norm

$$\| \underline{\epsilon} \|_{l_2(J,V)} := \left(\tau_N \sum_{n=0}^{N} \| \mathbf{u}_n - \mathbf{u}(t_n) \|_V^2 \right)^{1/2},$$

where J denotes the time-interval, $V = L_2(\Omega)$ or $H^1(\Omega)$, and τ_N is a time-step depending on $N \in \mathbb{N}$. Some examples were computed with variable time-step lengths by the help of the PI-controller [2].

Table 5. 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	4	3	yes	yes	no	0	yes	[LR90]
ROS3Pw	3	3	yes	no	yes	0.73	no	[RA05b]
ROS34PW2	4	3	yes	no	yes	0	yes	[RA05b]
ROSI2P1	4	3	yes	yes	yes	0	no	see Section 3.1
ROSI2P2	4	3	yes	yes	yes	0	yes	see Section 3.2
ROSI2Pw	4	3	yes	yes	yes	0	yes	see Section 3.3
ROSI2PW	4	3	yes	yes	yes	0	yes	see Section 3.4

Example 1. Let $d := 2$, $J := (0, 1)$ and $\Omega := (0, 1)^2$. We consider the following nonlinear PDAE

$$\begin{aligned}
&\dot{u}_1 - \Delta u_1 - u_3 \dot{u}_2 + \dot{u}_3 u_2 = -2t^\alpha && \text{in } J \times \Omega,\\
&\Delta u_2 = 0 && \text{in } J \times \Omega,\\
&\Delta u_3 = 0 && \text{in } J \times \Omega,\\
&\dot{u}_4 - \Delta u_4 - \Delta u_1 = -e^{-t}(x^2 + 2) - 2t^\alpha && \text{in } J \times \Omega,
\end{aligned} \tag{4.13}$$

where $\alpha \geq 1$ is a parameter. The initial conditions and the non-homogeneous Dirichlet boundary conditions are chosen such that

$$u_1(t, x, y) = x^2 t^\alpha,$$

$$u_2(t, x, y) = x \sin t^\alpha,$$

$$u_3(t, x, y) = x \cos t^\alpha,$$

$$u_4(t, x, y) = 1 + e^{-t}x^2$$

is the solution of (4.14). In the numerical experiments, we set $\alpha = 50$. For the semidiscretization in space, we used central finite differences on a square grid with step length $h = 1/100$. The computations were carried out with time-steps $\tau_N = 1/10N$ with $N = 1, 2, 4, 8, 16, 32, 64, 128$. The Jacobian is computed exactly. Note that all occurring discretization errors result from the temporal discretization. Figure 1 illustrates the results of the calculation, where the error is measured in the $l_2(J, L_2(\Omega))$-norm. In the lower part of the figure, the graphs of the following methods show a close overlay (from bottom to top): RODASP (a fourth-order method!), ROSI2P2, ROSI2PW, ROSI2P1, ROSI2Pw. For these methods, the experimental order of convergence is about 3.4 (see Table 6).

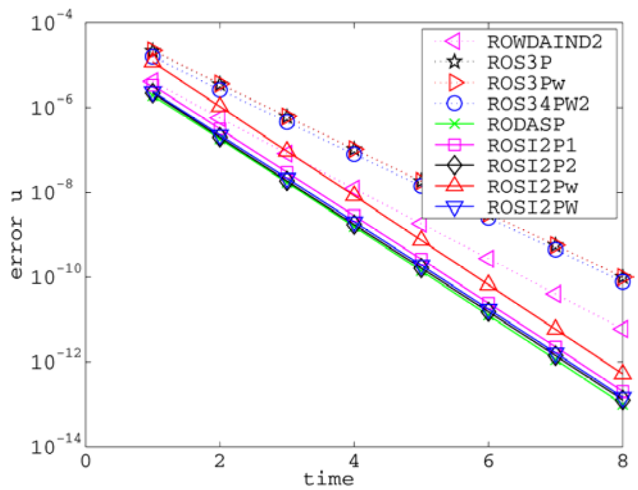


Figure 1. Example 1, results.

The most inaccurate results were obtained by the use of the methods for PDAEs of index 1, namely ROS3P, ROS3Pw and ROS34PW2. This is due to the fact that these methods do not satisfy the conditions (F3b) and (F3c). The method ROWDAIND2 satisfies these conditions but it has an order reduction because a semidiscretized PDAE is solved. The best results were obtained by means of the solvers ROSI2P2, ROSI2PW, ROSI2P1 and ROSI2Pw.

Table 6. Example 1, experimental order of convergence

Scheme	p	$N = 1, \ldots, 32$	$N = 1, \ldots, 64$	$N = 1, \ldots, 128$
ROS3P	3	2.51	2.50	2.50
ROWDAIND2	3	2.75	2.75	2.76
ROS3Pw	3	2.51	2.51	2.50
RODASP	4	3.48	3.49	3.49
ROSI2P1	3	3.43	3.45	3.46
ROSI2P2	3	3.43	3.44	3.45
ROSI2Pw	3	3.49	3.49	3.50
ROSI2PW	3	3.43	3.45	3.46

In the next examples, we consider the Navier-Stokes equations

$$\begin{aligned}
&\dot{u} - Re^{-1}\Delta u + (u \cdot \nabla)u + \nabla p = f && \text{in } J \times \Omega,\\
&\nabla \cdot u = 0 && \text{in } J \times \Omega,\\
&u = g && \text{on } J \times \partial\Omega,\\
&u(0, x) = u_0 && x \in \Omega,
\end{aligned} \tag{4.14}$$

where Re denotes the positive Reynolds number, J is a real (time-) interval, $\Omega \subset \mathbb{R}^d$ is a spatial domain.

Example 2. Let $d := 2$, $J := (0, 1)$ and $\Omega := (0, 1)^2$. In (4.14), 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 (4.14). Moreover, we set $Re = 1$. We used the Q_2/P_1^{disc} discretization on a square mesh with an edge length $h = 1/64$ and solved the problem with variable time-step sizes. The Jacobian was computed exactly. Note that for any t the solution can be represented exactly by the discrete functions. Hence, all occurring discretization errors 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. Figure 2 shows the results of the calculation.

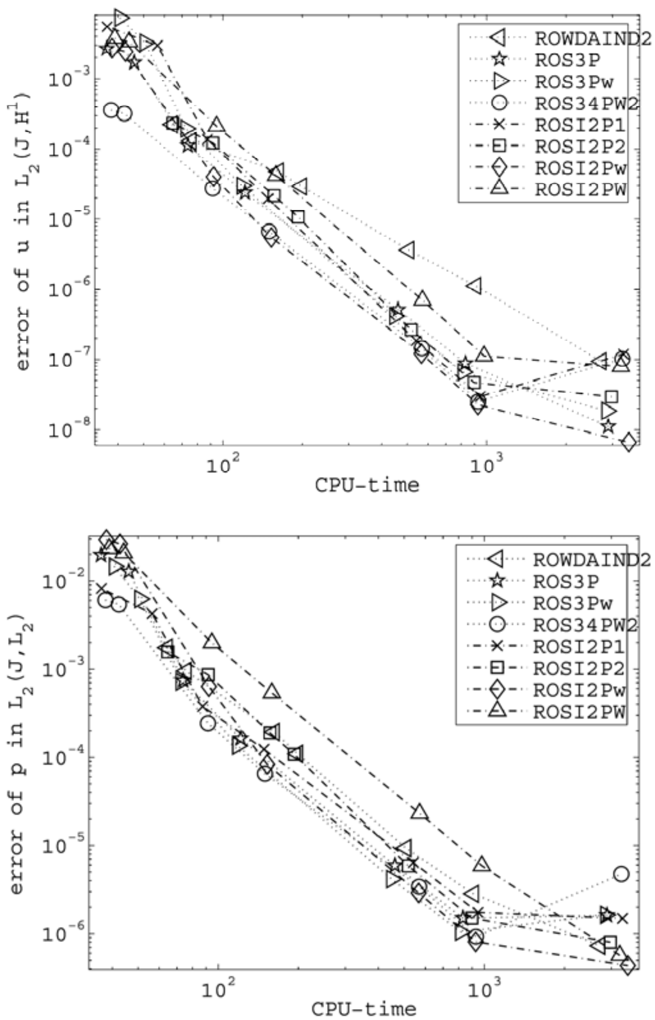


Figure 2. Example 2, results.

Considering the velocity error the scheme, ROWDAIND2 gave the most inaccurate results. The method ROSI2PW showed bad results for pressure error. The best results were obtained by the help of ROSI2Pw. Nevertheless, the remaining schemes gave acceptable results, too.

Example 3. As in the previous example, we consider the Navier-Stokes equations (4.14) but with Dirichlet boundary conditions on the whole boundary and with the solution

$$u_1(t, x, y) = t^3 y^2,$$

$$u_2(t, x, y) = \exp(-50t)x,$$

$$p(t, x, y) = (10 + t)\exp(-t)(x + y - 1).$$

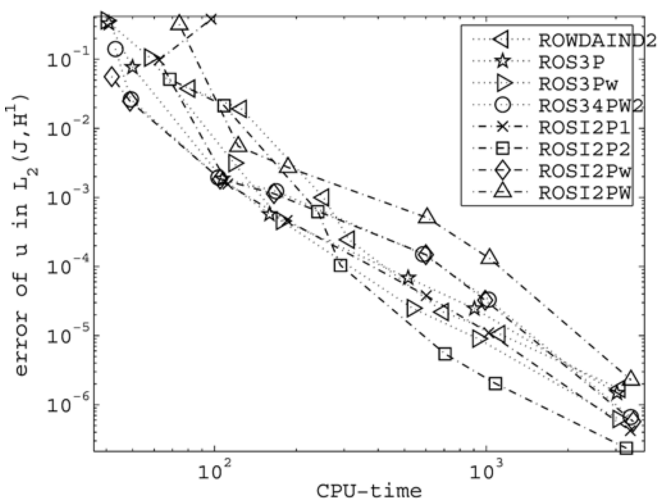
The computations were carried out with $Re = 1000$, a spatial grid consisting of squares of edge length $h = 1/32$, and variable time-step sizes. This setting gives 8 450 velocity d.o.f. and 3 072 pressure d.o.f. for the Q_2/P_1^{disc} finite element discretization.

The method ROSI2PW gave bad results for both errors. The best results were obtained by the use of ROSI2P2 for both components. Considering the pressure error, the method ROWDAIND2 gave very good results, too. Nevertheless, the remaining schemes gave acceptable results, too.

Example 4. Here, we consider the flow around a cylinder. This example was defined as a *benchmark problem* in [14] and studied numerically in detail in [3]. Figure 4 presents the flow domain Ω. The right hand side of the Navier-Stokes equations (4.14) is $f := 0$, the time interval is $J := (0, 8)$ and the inflow and outflow boundary conditions are given by

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

On all remaining boundary parts, 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 $\nu = 10^{-3}\mathrm{m}^2\mathrm{s}^{-1}$ is $0 \leq Re(t) \leq 100$.



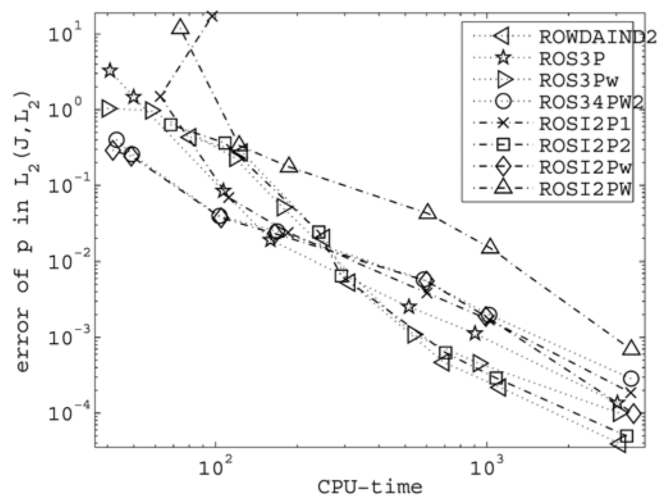


Figure 3. Example 3, results.

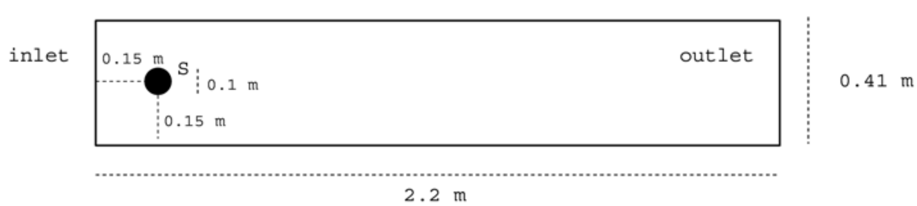


Figure 4. Example 4, the channel with the cylinder.

The coarsest grid (level 0) is presented in Figure 5. All computations were 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 as $\tau = 0.01$.

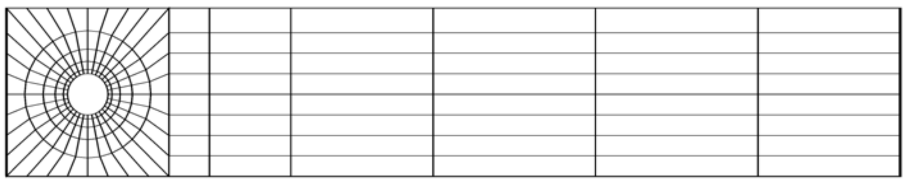


Figure 5. Example 4, the coarsest grid (level 0).

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

$$c_d(t) = -20[(u_t, v_d) + (\nu\nabla u, \nabla v_d) + ((u \cdot \nabla)u, v_d) - (p, \cdot \nabla v_d)],$$

$$c_l(t) = -20[(u_t, v_l) + (\nu\nabla u, \nabla v_l) + ((u \cdot \nabla)u, v_l) - (p, \cdot \nabla v_l)],$$

for all functions $v_d \in (H^1(\Omega))^2$ with $v_d|_S = (0, 1)^\top$ 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 from [14] 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 [3].

Figure 6 shows the lift and drag coefficients and the pressure difference as functions of time. In all graphs, also the reference curve from [3] is given. We see that the backward Euler scheme (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 the lift coefficient curves (Figure 6), it becomes obvious that all methods are relatively close the reference curve. The best results were obtained by the Rosenbrock methods.

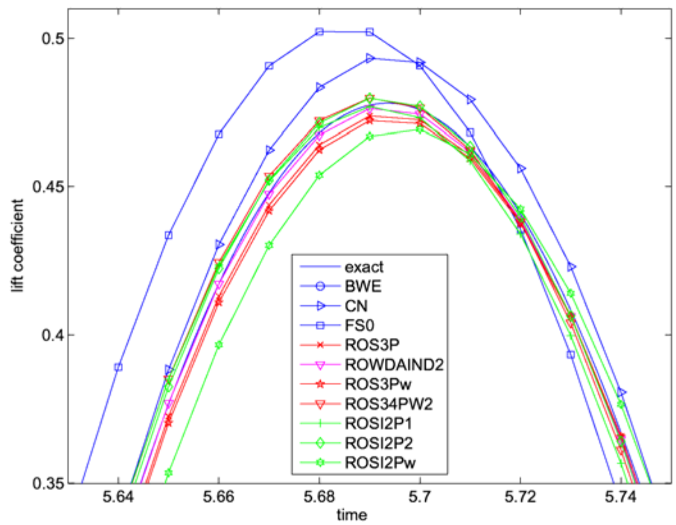


Figure 6. Example 4, lift coefficient.

In Table 7, the pressure difference at the final time $t = 8$ is given. We present the value itself, its deviation from the reference value given in [3] and the relative error. The best results were obtained by means of ROS3PW2 and ROSI2P2. All Rosenbrock methods produce quite accurate results which are much better than the results obtained by the use of the Crank-Nicolson scheme (CN) and the fractional-step θ-scheme (FS). Also, for this value, the results from BWE were the most inaccurate ones.

Example 5. We consider the Navier-Stokes equations (4.14) in three space dimensions (i.e., $d = 3$) with Dirichlet boundary conditions on the whole boundary and with the solution

$$u_1(t, x, y, z) = e^{-t}(y^2 + z),$$

$$u_2(t, x, y, z) = t^4(x - 2z^2),$$

$$u_3(t, x, y, z) = e^{-50t}(2xy + y),$$

$$p(t, x, y, z) = t^3(x + 2y + 3z - 3).$$

The computations were carried out with $Re = 1$, a spatial grid consisting of cubes of edge length $h = 1/16$, and variable time-step sizes.

Considering the velocity error, ROS3Pw and ROSI2P1 gave the best results. The most inaccurate results were obtained by the use of ROWDAIND2 and ROSI2P2. Considering the pressure error, we have a different situation. Here, ROWDAIND2 and ROSI2P2 gave the very good results. The schemes ROS3Pw yielded accurate results, too. Bad solvers for this example were ROSI2P1 and ROSI2PW.

Table 7. Pressure difference at $t = 8$, $\Delta p_{ref} = -0.1116$ from [3]

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	$-1.11570e-01$	$3.0263e-05$	$2.71e-02$
ROSI2P1	$-1.11793e-01$	$-1.9335e-04$	$1.73e-01$
ROSI2P2	$-1.11641e-01$	$-4.0951e-05$	$3.67e-02$
ROSI2Pw	$-1.11809e-01$	$-2.0880e-04$	$1.87e-01$

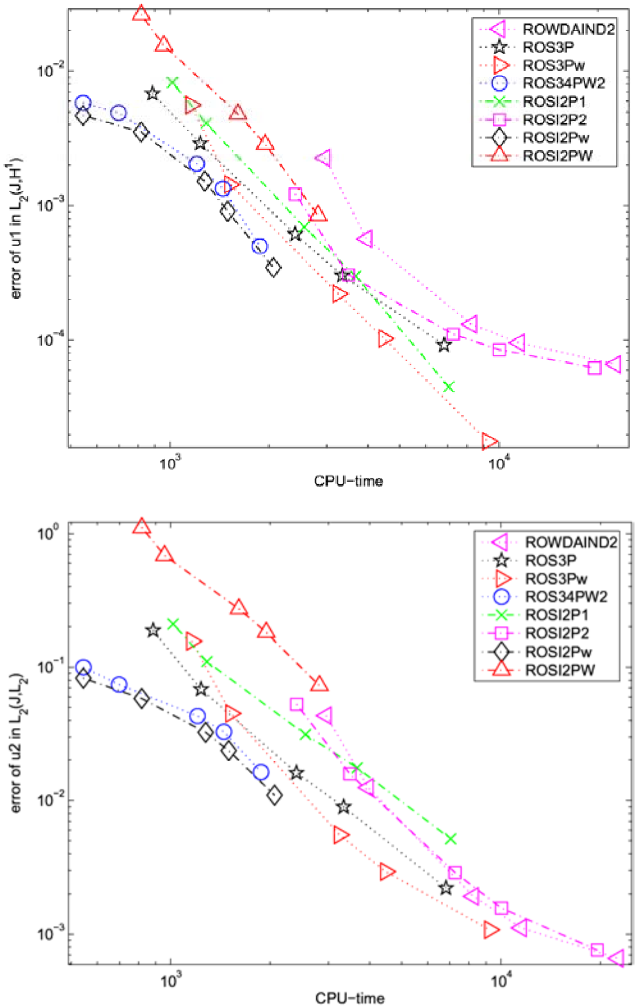


Figure 7. Example 5, results.

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