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ROS3P—AN ACCURATE THIRD-ORDER ROSENBROCK SOLVER DESIGNED FOR PARABOLIC PROBLEMS *

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Abstract.

In this note we present a new Rosenbrock solver which is third-order accurate for nonlinear parabolic problems. Since Rosenbrock methods suffer from order reduction when they are applied to partial differential equations, additional order conditions have to be satisfied. Although these conditions have been known for a longer time, from the practical point of view only little has been done to construct new methods. Steinebach modified the well-known solver RODAS of Hairer and Wanner to preserve its classical order four for special problem classes including linear parabolic equations. His solver RODASP, however, drops down to order three for nonlinear parabolic problems. Our motivation here was to derive an efficient third-order Rosenbrock solver for the nonlinear situation. Such a method exists with three stages and two function evaluations only. A comparison with other third-order methods shows the substantial potential of our new method.

AMS subject classification: 65M12, 65L06.

Key words: Nonlinear parabolic equations, Rosenbrock methods, order reduction.

1 Introduction.

Diverse physical phenomena occurring in a wide range of industrial applications are modelled by systems of time-dependent partial differential equations (PDEs). Due to the great complexity of the established models, the numerical analysis of PDEs is often the central tool to assess the models and to gain profound knowledge about the underlying physical processes. Much progress has been achieved in the development and design of efficient and robust simulation programs for solving time-dependent PDEs. One of those programs is the Kardos package which was developed at the Konrad–Zuse–Zentrum in Berlin to solve a general class of nonlinear evolution problems. The most important feature of Kardos is that the quality of the numerical approximations is judged during the computation and an adaptive strategy is automatically determined to improve the accuracy where needed [3]. Kardos uses linearly implicit one-step methods of Rosenbrock type and multilevel finite elements to discretize in time and space, respectively. In the

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solution of PDEs using an adaptive mesh, one-step methods have an inherent advantage over multistep methods such as BDF. Since each interpolation of variables onto a new mesh generates a discontinuity in time, a multistep method usually must be restarted at lower order, whereas one-step methods can continue at higher order. In addition, Rosenbrock methods avoid the solution of nonlinear equations, working the exact Jacobian directly into the integration formula (Rosenbrock [9], Hairer and Wanner [2]). Nowadays they are widely accepted to work satisfactorily for moderate accuracy requirements which are typical for the solution of PDEs.

It is a known fact that one-step methods such as Rosenbrock, Runge–Kutta, and extrapolation methods suffer from order reduction when they are applied to stiff ODEs and semi-discrete PDEs (see e.g. Sanz-Serna et al. [11], Verwer [15]). For nonlinear parabolic PDEs, this phenomenon was theoretically investigated in a sequence of papers by Lubich, Ostermann, and Roche [6, 7, 4, 5]. Their results show that the temporal order of convergence is mainly influenced by the spatial regularity of the solution, which usually depends on the boundary conditions. Consequently, one-step methods having a high order of accuracy will loose this advantage for real-life PDEs supplemented with complex boundary conditions. To avoid this disturbing feature, Runge–Kutta methods with high stage order (see e.g. Bendtsen [1]) have to be used [5]. Since Rosenbrock methods have stage order one, their coefficients have to satisfy additional conditions to obtain a higher order of convergence [7, 4] as well. Analogous conditions for the stiff ODE case related to B-convergence properties were announced previously in [14, 12]. Improved Rosenbrock methods which preserve the classical order of convergence for linear parabolic PDEs were given by Scholz [12] and Steinebach [13] up to order four. As a direct consequence of the results given in [4], the family of 3-stage Rosenbrock methods proposed by Scholz ([12, Prep. 5]) could be used to construct a third-order accurate method for nonlinear parabolic PDEs, but there one of the intermediate time points lies outside the time step—a property which one should try to avoid.

Here we want to construct a third-order method which evaluates the functions at the beginning and at the end of each time step. Such methods are particularly valuable when time-dependent terms are present in the PDE operator. More precisely, since a Rosenbrock method evaluates the functions at $t_n + \alpha_i \tau$, $i = 1, 2, \ldots$, to integrate from t_n to t_{n+1} with a step of length τ, rapid solution changes, e.g. due to time-dependent boundary conditions or forcing functions, can only be detected properly within the interval $[t_n, t_n + \alpha_m \tau]$ where $\alpha_m = \max_i \alpha_i$. Serious errors in the numerical solution are possible with formulas the evaluations of which do not span the whole interval $[t_n, t_{n+1}]$. It turns out that a third-order method with $\alpha_m = 1$ exists for three stages employing only two function evaluations. This method is A-stable with $R(\infty) \approx 0.73$, fulfills the additional conditions from [7, 4] for avoiding order reduction, and fulfills also the third-order conditions for differential-algebraic equations (DAEs) of index one. We call this method ROS3P where P stands for parabolic PDEs. A second-order embedding with the same stability properties can be derived easily for error estimation.

We shall present comparative convergence and efficiency results for two different nonlinear parabolic problems, illustrating that ROS3P behaves indeed like a third-order method for nonlinear parabolic equations. It is worthwhile to mention

that ROS3P which was added to the Kardos package performed better in various problem classes where complex boundary conditions are present.

2 Rosenbrock methods.

Applied to the initial-value problem

$$\partial_t u = F(t,u), \quad u(0) = u_0, \quad 0 < t \le T, \tag{2.1}$$

with the step size $\tau > 0$ a linearly implicit one-step method of Rosenbrock type has the form

$$\begin{cases} (I - \tau\gamma_{ii}\,\partial_u F(t_n,u_n))\,K_{ni} = F\Big(t_n + \alpha_i\tau, u_n + \tau\sum\limits_{j=1}^{i-1}\alpha_{ij}K_{nj}\Big) \\ \qquad + \tau\,\partial_u F(t_n,u_n)\sum\limits_{j=1}^{i-1}\gamma_{ij}K_{nj} + \tau\gamma_i\,\partial_t F(t_n,u_n), \quad i = 1,\dots,s, \\ u_{n+1} = u_n + \tau\sum\limits_{i=1}^{s} b_i K_{ni}, \end{cases} \tag{2.2}$$

with

$$\alpha_i = \sum_{j=1}^{i-1}\alpha_{ij}, \quad \text{and} \quad \gamma_i = \sum_{j=1}^{i}\gamma_{ij}\,.$$

The operator $F(t,u)$ in (2.1) stands either for a PDE operator supplemented with appropriate boundary conditions or for a semi-discrete PDE operator which typically arises in the method of lines approach. The notations ∂_t and ∂_u denote partial derivatives with respect to t and u.

For convenience, we set $\alpha_{ij} = 0$ for $j \ge i$, $\gamma_{ij} = 0$ for $j > i$, and use the notation

$$\beta_{ij} = \alpha_{ij} + \gamma_{ij}, \quad \beta_i = \sum_{j=1}^{i-1}\beta_{ij}, \quad B = (\beta_{ij})_{i,j=1}^{s},$$
$$b = (b_1,\dots,b_s)^T, \quad \alpha^k = (\alpha_1^k,\dots,\alpha_s^k)^T, \quad \mathbf{1} = (1,\dots,1)^T \in \mathbb{R}^s\,.$$

We assume $\gamma_{ii} = \gamma > 0$ for all i, which is the standard simplification to derive Rosenbrock methods with one and the same matrix on the left-hand side of (2.2).

3 Order conditions for a third-order method with $s = 3$.

The consistency conditions for order three are (see e.g. Hairer and Wanner [2])

$$\begin{cases} \text{(A1)} & b_1 + b_2 + b_3 = 1, \\ \text{(A2)} & b_2\beta_2 + b_3\beta_3 = \frac{1}{2} - \gamma, \\ \text{(A3a)} & b_2\alpha_2^2 + b_3\alpha_3^2 = \frac{1}{3}, \\ \text{(A3b)} & b_3\beta_2\beta_{32} = \frac{1}{6} - \gamma + \gamma^2\,. \end{cases} \tag{3.1}$$

Additional conditions have to be satisfied to avoid order reduction for one-step methods of Rosenbrock type (see Lubich and Ostermann [4]). To obtain full order three we have to fulfill

$$b^T B^j (2B^2 \mathbf{1} - \alpha^2) = 0 \quad \text{for } 1 \le j \le 2,$$

which can be simplified taking into account (3.1) to

$$\begin{cases} \text{(B1)} & b_3\beta_{32}\alpha_2^2 = \frac{1}{6} - \frac{2}{3}\gamma, \\ \text{(B2)} & \gamma = \frac{1}{2} \pm \frac{1}{6}\sqrt{3} \quad (\gamma^2 - \gamma + \frac{1}{6} = 0)\,. \end{cases} \tag{3.2}$$

Using (B2) we find $b_3\beta_{32}\alpha_2^2 \neq 0$ in (B1). Consequently, $\beta_2 = 0$ in (A3b) due to (B2). Now we fix β_3, α_2, and α_3 to compute $b^T = (b_1, b_2, b_3)$ from (A1)–(A3a). This leads to

$$\begin{cases} b_2 = \dfrac{\frac{1}{3}\beta_3 - (\frac{1}{2} - \gamma)\alpha_3^2}{\alpha_2^2\beta_3}, \\ b_3 = \dfrac{\frac{1}{2} - \gamma}{\beta_3}, \\ b_1 = 1 - b_2 - b_3. \end{cases} \tag{3.3}$$

Replacing b_3 in (B1), we derive

$$\beta_{32} = \frac{1 - 4\gamma}{(3 - 6\gamma)\alpha_2^2}\,\beta_3, \tag{3.4}$$

and conclude remembering that $\beta_{31} = \beta_3 - \beta_{32}$. The free parameters are β_3, α_2, and α_3.

4 Algebraic order conditions for a third-order method with $s = 3$.

To reach order three for DAEs too, the following algebraic order condition has to be satisfied (see Roche [8])

$$(C1) \quad b_2 w_{22}\alpha_2^2 + b_3(w_{32}\alpha_2^2 + w_{33}\alpha_3^2) = 1, \tag{4.1}$$

where $(w_{ij})_{i,j=1}^s = B^{-1}$. A simple calculation shows

LEMMA 4.1. *A Rosenbrock method which satisfies* (A1)–(A3b) *and* (B1)–(B2) *fulfills also* (C1).

PROOF. Invert B and use (A3a), (B1), and (B2) to get (C1). □

5 ROS3P—An A-stable method.

We choose $\gamma = \gamma_+ = 1/2 + \sqrt{3}/6$ to get A-stability with $|R(\infty)| \approx 0.73$, where $R(z) = 1 + zb^T(I - zB)^{-1}\mathbf{1}$ is the stability function. The second value $\gamma_- = 1/2 - \sqrt{3}/6$ does not give an A-stable method; see Table 6.3 in [2]. In order to include only two function evaluations, one at the beginning of the time step and one at the end, we set $\alpha_{21} = \alpha_{31} = 1$, and $\alpha_{32} = 0$. From $\beta_{21} = 0$, we derive $\gamma_{21} = -1$.

Positive values for the vector b can be achieved by setting $\beta_3 = 3/2 - 3\gamma$, which yields $b_1 = 2/3$, $b_2 = 0$, and $b_3 = 1/3$. Simple calculations give $\beta_{32} = 1/2 - 2\gamma$ and $\beta_{31} = 1 - \gamma$ leading to $\gamma_{32} = 1/2 - 2\gamma$ and $\gamma_{31} = -\gamma$. Finally, we construct an embedded method of second order replacing the coefficients b_i in (2.2) by different coefficients $\hat{b}_i$. Since $\beta_2 = 0$, we have to include all $\hat{b}_i$, $i = 1, 2, 3$. The order conditions are

$$\text{(5.1)} \qquad \begin{cases} (\hat{\text{A}}1) & \hat{b}_1 + \hat{b}_2 + \hat{b}_3 = 1, \\ (\hat{\text{A}}2) & \hat{b}_3\beta_3 = \frac{1}{2} - \gamma\,. \end{cases}$$

From (Â2) we find $\hat{b}_3 = 1/3$. We set $\hat{b}_1 = 1/3$ and $\hat{b}_2 = 1/3$ in order to fulfill (Â1), which is only one possibility.

Table 5.1: Set of coefficients for the 3-stage ROS3P method.

$\gamma = 7.886751345948129e{-}01$	
$a_{21} = 1.267949192431123e+00$	$c_{21} = -1.607695154586736e+00$
$a_{31} = 1.267949192431123e{+}00$	$c_{31} = -3.464101615137755e{+}00$
$a_{32} = 0.000000000000000e{+}00$	$c_{32} = -1.732050807568877e{+}00$
$\alpha_1 = 0.000000000000000e{+}00$	$\gamma_1 = 7.886751345948129e{-}01$
$\alpha_2 = 1.000000000000000e{+}00$	$\gamma_2 = -2.113248654051871e{-}01$
$\alpha_3 = 1.000000000000000e{+}00$	$\gamma_3 = -1.077350269189626e{+}00$
$m_1 = 2.000000000000000e{+}00$	$\hat{m}_1 = 2.113248654051871e{+}00$
$m_2 = 5.773502691896258e{-}01$	$\hat{m}_2 = 1.000000000000000e{+}00$
$m_3 = 4.226497308103742e{-}01$	$\hat{m}_3 = 4.226497308103742e{-}01$

In the following, we give the defining formula coefficients for the transformed form of a Rosenbrock scheme, which is usually employed in practice to avoid matrix-vector operations.

$$\text{(5.2)} \qquad \begin{cases} \left(\dfrac{I}{\tau\gamma} - \partial_u F(t_n, u_n)\right) U_{ni} = F\left(t_n + \alpha_i\tau, u_n + \displaystyle\sum_{j=1}^{i-1} a_{ij}U_{nj}\right) \\ \qquad\qquad + \displaystyle\sum_{j=1}^{i-1} \frac{c_{ij}}{\tau} U_{nj} + \tau\gamma_i\, \partial_t F(t_n, u_n)\,, \quad i = 1, \ldots, s, \\ u_{n+1} = u_n + \displaystyle\sum_{i=1}^{s} m_i U_{ni}\,, \\ \hat{u}_{n+1} = u_n + \displaystyle\sum_{i=1}^{s} \hat{m}_i U_{ni}. \end{cases}$$

The difference $u_{n+1} - \hat{u}_{n+1}$ can be used as a local error estimator. The coefficients of the whole method called ROS3P are presented in Table 5.1.

6 Convergence test.

To test our scheme we consider the equation

$$\partial_t u - \nu\nabla^2 u + u\partial_x u + u\partial_y u = 0\,, \quad 0 < t \le T = 0.1\,, \tag{6.1}$$

defined on the domain $\Omega = (0, 1/2) \times (0, 1/2)$. The initial and Dirichlet boundary conditions are chosen from the exact solution

$$u(x, y, t) = 1/(1 + exp((x + y - t)/(2\nu)).$$

Table 6.1: Problem (6.1) with time-dependent Dirichlet boundary conditions. The observed temporal orders of convergence measured in the global L^2-norm reveal $p = 2.25$ for RODAS3 and ROWDA3, and $p = 3$ for ROS3P.

	RODAS3		ROWDA3		ROS3P	
τ	$\|\underline{\epsilon}\|_{l^2(L^2)}$	q_{num}	$\|\underline{\epsilon}\|_{l^2(L^2)}$	q_{num}	$\|\underline{\epsilon}\|_{l^2(L^2)}$	q_{num}
$\frac{1}{100}$	6.59^{-7}_{10}		9.03^{-7}_{10}		3.02^{-7}_{10}	
$\frac{1}{200}$	1.37^{-7}_{10}	2.26	1.88^{-7}_{10}	2.26	4.23^{-8}_{10}	2.84
$\frac{1}{400}$	2.86^{-8}_{10}	2.26	3.93^{-8}_{10}	2.26	5.69^{-9}_{10}	2.89
$\frac{1}{800}$	5.99^{-9}_{10}	2.25	8.22^{-9}_{10}	2.26	7.39^{-10}_{10}	2.95

Table 6.2: Problem (6.1) with time-dependent Dirichlet boundary conditions. The observed temporal orders of convergence measured in the global H^1-norm reveal $p = 1.75$ for RODAS3 and ROWDA3, and $p = 3$ for ROS3P.

	RODAS3		ROWDA3		ROS3P	
τ	$\|\underline{\epsilon}\|_{l^2(H^1)}$	q_{num}	$\|\underline{\epsilon}\|_{l^2(H^1)}$	q_{num}	$\|\underline{\epsilon}\|_{l^2(H^1)}$	q_{num}
$\frac{1}{100}$	4.02^{-5}_{10}		5.18^{-5}_{10}		4.91^{-6}_{10}	
$\frac{1}{200}$	1.19^{-5}_{10}	1.76	1.53^{-5}_{10}	1.76	7.50^{-7}_{10}	2.71
$\frac{1}{400}$	3.54^{-6}_{10}	1.75	4.56^{-6}_{10}	1.75	1.05^{-7}_{10}	2.83
$\frac{1}{800}$	1.05^{-6}_{10}	1.75	1.35^{-6}_{10}	1.76	1.38^{-8}_{10}	2.93

We set $\nu = 0.1$ and solve the equation with the finite element code Kardos for a sequence of time steps $\tau_N = T/N$ with $N = 10, 20, 40, 80$. Standard 4th-order Lagrange finite elements and a uniform grid consisting of 16384 triangles are used to keep the spatial discretization to a nearly insignificant level.

The global error is measured in the discrete norms

$$\|\underline{\epsilon}\|_{l^2_{N+1}(V)} = \left(\tau_N \sum_{n=0}^{N} \|u_n - u(t_n)\|_V^2\right)^{1/2}$$

where $V = L^2(\Omega)$ and $V = H^1(\Omega)$ equipped with the norms

$$\|v\|^2_{L^2(\Omega)} = \int_\Omega v^2\,dxdy\,, \quad \|v\|^2_{H^1(\Omega)} = \int_\Omega \left(v^2 + (\partial_x v)^2 + (\partial_y v)^2\right)\,dxdy.$$

The numerically observed temporal order of convergence is computed by

$$q_{num} = \log_2 \|\underline{\epsilon}\|_{l^2_{N+1}(V)} - \log_2 \|\underline{\epsilon}\|_{l^2_{2N+1}(V)}.$$

We have compared ROS3P with RODAS3 [10] and ROWDA3 [8], which are also third-order accurate for differential-algebraic equations, but do not satisfy conditions (3.2) which avoid order reduction. The test case chosen is critical with respect to the attainable order due to the time-dependent Dirichlet boundary conditions. The results given in Table 6.1 and Table 6.2 reveal that RODAS3 and ROWDA3 suffer from severe order reductions whereas the full order three of ROS3P clearly shows up. The fractional order $p = 2.25$ for the $l^2(L^2)$-norm was explained theoretically by Lubich and Ostermann ([4, Theorem 5.2]). A discussion about the order $p = 1.75$ for the $l^2(H^1)$-norm can be found in Lang ([3, VI.§1, Example 1]).

7 Efficiency test.

Now we use the Kardos software to check the efficiency of ROS3P, involving an automatic stepsize control and adaptively generated grids which evolves with the solution. First we choose once again equation (6.1) and perform a sequence of different computations in order to find well-balanced temporal and spatial tolerances. The left picture of Figure 7.1 shows the corresponding computing times necessary to obtain a certain accuracy measured in the $l^2(H^1)$-norm with variable time steps.

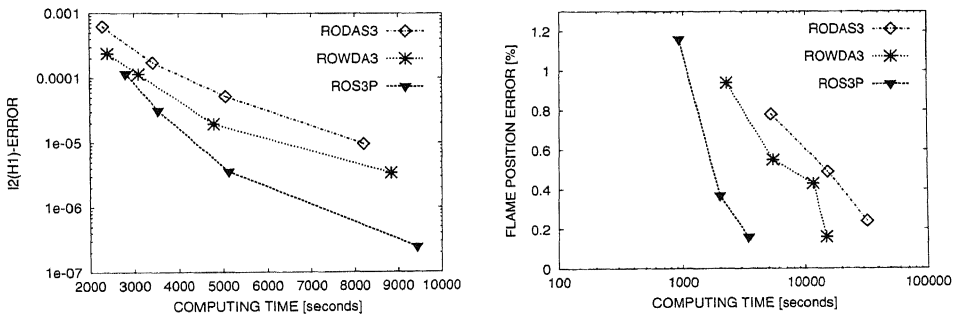

Figure 7.1: Comparison of errors and computing times for problem (6.1) (left) and combustion problem (right) solved with variable stepsizes and adaptive spatial grids. The results clearly show that ROS3P performs best with respect to achieved accuracies.

In a second test, we consider a more practically relevant combustion problem fully described in Lang ([3, VII.§2.1]). The underlying equations are of reaction-diffusion type with a highly nonlinear reaction term arising from an Arrhenius

law. A freely propagating laminar flame is disturbed by a heat absorbing obstacle modeled by an inhomogeneous solution-dependent boundary condition. Since this heat flux condition mainly influences the flame speed, the accuracy and efficiency of a method can be judged by the reached deviation from the exact flame position after leaving the obstacle. The right picture of Figure 7.1 shows the deviation expressed in percentages versus computing time for the methods compared here.

In both cases ROS3P outperforms the other third-order methods, where its potential is more evident for the flame problem. We mention that RODASP, the method of Steinebach [13], gives comparable good results for problem (6.1), but becomes too expensive and therefore inefficient for the combustion problem.

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