Rosenbrock-Wanner Methods: Construction and Mission

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February 28, 2020

Abstract

This paper is concerned with the history of Rosenbrock-Wanner methods first initiated by Rosenbrock in 1963. His original ideas are highlighted and the main developments over 56 years are reviewed.

Keywords: linearly implicit time integrators, stiff systems, Rosenbrock-Wanner methods, W-methods, two-step Rosenbrock-Peer methods, two-step W-methods

2010 Mathematics Subject Classification: 65L04, 65L06, 65L11, 65M20

1 Introduction

Howard Harry Rosenbrock (1920-2010) suggested in his famous paper from 1963 [53] to replace the iterative process for the solution of nonlinear problems within an implicit time integrator by a finite number of solutions of linear systems. He summarized: Some general implicit processes are given for the solution of simultaneous first-order differential equations. These processes, which use successive substitution, are implicit analogues of the (explicit) Runge-Kutta processes. They require the solution in each time step of one or more sets of simultaneous linear equations, usually of a special and simple form. Processes of any required order can be devised, and they can be made to have a wide margin of stability when applied to a linear problem. Thus, Rosenbrock methods avoid the problem of convergence for the solution of systems of nonlinear equations, making them a good alternative to fully implicit Runge-Kutta methods. In this note, I will give a brief historical overview and explain main construction principles including widely used members of the whole family of linearly implicit methods such as Rosenbrock-Wanner methods, W-methods, and recently developed two-step Rosenbrock-Peer and W-methods. Rosenbrock methods
have made their way into real-life applications and become part of very sufficient adaptive multilevel PDE-solvers, see e.g. [26]. Nowadays, there still is an increasing interest in these methods, which would have delighted Rosenbrock who concluded his paper by expressing his wish: *The processes described above have been explored only cursorily, and it is hope that this note may stimulate others to investigate their possibilities. It certainly did.*

Who was Howard H. Rosenbrock? Rosenbrock was born on December 16, 1920 in Ilford, England. He graduated 1941 from University College London with a 1st class honors degree in Electrical Engineering and received his PhD from London University in 1955. During the 1960s he worked at the Cambridge University and the MIT. In 1966, he became the Chair of Control Engineering at the University of Manchester, Institute of Science and Technology. He died on 21 October 2010. Rosenbrock produced over 120 scientific papers, 7 books, and about 30 papers on the philosophical basis of science and technology. An obituary was published in [78].

2 The Original Idea of Rosenbrock

In what follows, I will first review the original ideas of Rosenbrock as described in [53]. The writing is presented in a modern style, but a few text passages are included as pictures.

As starting point in his paper, Rosenbrock took a look at the (spatial) semi-discretization of the one-dimensional linear heat equation, i.e., formulas (1) and (2) in Fig. 1. He stated: *Any explicit numerical method of solving eqn. (2) (e.g. Runge-Kutta) replaces the exponentials by their truncated Taylor’s series during one time interval of the solution. The exponentials tend to zero as \( t \) becomes large, whereas the truncated Taylor’s series tend to infinity. A severe limitation on the length of the time intervals is thus introduced.*

To illustrate these fundamental observations, let us consider the heat equation in the form

\[
\begin{align*}
\partial_t u &= \nabla \cdot (D \nabla u), \quad x \in \Omega, \quad t \in (0, T], \\
u(x, t) &= 0, \quad x \in \partial\Omega, \quad t \in (0, T], \\
u(x, 0) &= u_0(x), \quad x \in \Omega,
\end{align*}
\]  

(1)

with domain \( \Omega \subset \mathbb{R}^d \) (\( d \geq 1 \)) and a symmetric positive definite matrix \( D(x) \in \mathbb{R}^{d \times d} \).
We have the following stability results:

\[ \|u(t)\|_{L^2(\Omega)} \leq \|u_0\|_{L^2(\Omega)}, \quad t \in [0,T], \]  
\[ u(t) \to 0 \text{ for } t \to \infty. \]  

(2)

(3)

A Method of Lines approach (let’s take finite differences for simplicity) yields the system of ordinary differential equations

\[ \frac{\partial U(t)}{\partial t} = AU(t), \quad t \in (0,T], \]
\[ U(0) = U_0, \]  

(4)

where the vector \( U(t) \) collects approximations at certain spatial points. The matrix \( A \) is symmetric negative definite and therefore exhibits negative real eigenvalues - the values \(-k_i\) in the exponentials mentioned by Rosenbrock in Fig. 1. An explicit Runge-Kutta methods computes approximations \( U_n \approx U(t_n) \) with \( t_n = nh, \ n \geq 1 \) through

\[ U_{n+1} = R_{\text{ERK}}(hA)U_n, \quad n = 0,1,\ldots \]
\[ U_0 = U^0, \]  

(5)

where

\[ R_{\text{ERK}}(z) = 1 + z + \ldots + \frac{z^p}{p!} + \sum_{i=p+1}^{s} \alpha_i z^i = e^z + \mathcal{O}(z^{p+1}). \]  

(6)

The stability requirements for the semi-discretized solution

\[ \|U_{n+1}\|_2 \leq \|U_n\|_2, \quad U_n \to 0 \text{ for } n \to \infty, \]  

(7)
request $|R_{ERK}(z)| < 1$ for $z$ along the negative real axis. Due to the nature of the approximation \( \frac{1}{2} \), small time steps $h$ are necessary to guarantee stability. Moreover, the finer the spatial discretization, the smaller the time steps must be, showing that explicit methods, in general, are inefficient for the solution of such kind of (stiff) problems.

Crank and Nicholson (1947) pointed out that the restriction could be completely removed in linear problems by using the trapezoidal rule

\[
K_r = h_r \left( \frac{1}{2} \phi_{r-1} + \frac{1}{2} \phi_r \right) \quad (3)
\]

\[
x'_r = x'_{r-1} + k_r \quad (4)
\]

where $h_r$ is the length of the $r$th time step, and the dash distinguishes the numerical from the exact solution of eqn. 2. This process replaces the exponentials occurring in the solution of eqn. (2) by the approximation

\[
\psi_r(t) = \frac{1 - \frac{1}{2} k_r t}{1 + \frac{1}{2} k_r t} \quad (5)
\]

during each time interval.

Figure 2: © The Computer Journal, part of page 329 of [53].

An alternative is the implicit Crank-Nicolson method already proposed in 1947 [3], see also Fig. 2. It reads

\[
U_{n+1} = R_{CN}(hA) U_n, \quad n = 0, 1, \ldots \\
U_0 = U^0, \quad \quad (8)
\]

with

\[
R_{CN}(z) = \frac{1 + z/2}{1 - z/2} = e^z + O(z^3). \quad (9)
\]

The method is unconditionally stable, since $|R_{CN}(z)| \leq 1$ for all $z$ lying in the left complex half plane. However, the damping properties at infinity are unsatisfactory. This lack has been also mentioned by Rosenbrock: The procedure given in eqns. (3) and (4) has been widely used. It is perhaps not widely known, however, that instability can arise even with this process when the $\phi$ are non-linear functions of $x$. This is hardly surprising, since $\psi_r(t) \to -1$ as $t \to \infty$, so that even in a linear problem stability is only just maintained for large $t$.

However, his main observation was that when the functions $\phi$ are non-linear, implicit equations such as eqn. (3) can in general be solved only by iteration. This
is a severe drawback, as it adds to the problem of stability, that of convergence of the iterative process. As consequence, he set up a generalized implicit process with linear equations that can be solved rapidly and easily. How is it done?

\[
(k_r)_r = h_r \left\{ (\phi_r)_{r-1} + \frac{1}{2} \sum_j \left( \frac{\partial \phi_j}{\partial x_j} \right)_r (k_j)_r \right\}. \tag{9}
\]

This set of linear equations can be solved directly for \( k_r \), and if each \( \phi \) depends on only a few of the \( x \) the solution can be carried out rapidly and easily.

Let us now consider the autonomous system of nonlinear ordinary differential equations

\[
\begin{align*}
\frac{\partial t}{\partial t} U(t) &= F(U(t)), \quad t \in (0, T], \\
U(0) &= U^0.
\end{align*} \tag{10}
\]

and apply the Crank-Nicolson method to it, resulting in

\[
\begin{align*}
U_{n+1} &= U_n + \frac{h}{2} (F(U_n) + F(U_{n+1})), \quad n = 0, 1, \ldots \\
U_0 &= U^0.
\end{align*} \tag{11}
\]

With \( U_n \) as starting values, Newton’s method to approximate \( U_{n+1} \) gives the sequence of linear equations

\[
\begin{align*}
U_{n+1}^{(0)} &= U_n, \\
\left( I - \frac{h}{2} F'(U_{n+1}^{(k)}) \right) K_{n+1}^{(k+1)} &= - \left( U_{n+1}^{(k)} - U_n - \frac{h}{2} \left( F(U_{n+1}^{(k)}) + F(U_n) \right) \right), \\
U_{n+1}^{(k+1)} &= U_{n+1}^{(k)} + K_{n+1}^{(k+1)}, \quad k = 0, 1, \ldots.
\end{align*} \tag{12}
\]

The fundamental idea of Rosenbrock was to use only one step of Newton’s method, which reads for \( k = 0 \)

\[
\left( I - \frac{h}{2} F'(U_n) \right) K_{n+1} = h F(U_n), \tag{13}
\]

or equivalently

\[
K_{n+1} = h \left( F(U_n) + \frac{1}{2} F'(U_n) K_{n+1} \right). \tag{14}
\]
In his paper, Rosenbrock did not mention how he derived his formula (9), see Fig. 3 and left it to the reader as an exercise.

In a next step, he proposed to use Kopal’s treatment of the Runge-Kutta processes [24] to design a generalized implicit process shown in Fig. 4. Note that the

![A generalized implicit process may be obtained from eqn. (9) by analogy with Kopal’s treatment of the Runge-Kutta processes (Kopal, 1955).](image)

A generalized implicit process may be obtained from eqn. (9) by analogy with Kopal’s treatment of the Runge-Kutta processes (Kopal, 1955). Let

\[ A(x) = (A_g(x)) = \left( \frac{\partial \phi_i(x)}{\partial x_j} \right) \]  

(10)

and write

\[ k_r = h_r \{ \phi(x_r' - 1) + a_1 A(x_r' - 1)k \} \]  

(11)

\[ l_r = h_r \{ \phi(x_r' - 1 + b_2 k_r) + a_2 A(x_r' - 1 + c_1 l_r) \} \]  

(12)

\[ m_r = h_r \{ \phi(x_r' - 1 + b_2 k_r + d_1 l_r) + a_3 A(x_r' - 1 + c_2 k_r + c_1 l_r)m_r \} \]  

(13)

\[ \cdots \]

\[ \dot{x}' = x_r' - 1 + R_1 k_r + R_2 l_r + R_3 m_r + \ldots \]  

(14)

Figure 4: © The Computer Journal, part of page 329 of [53].

Jacobian is evaluated at different solutions. Rosenbrock did a consistency analysis: By a straightforward but tedious calculation it is possible to expand \( x_r' - x_r' - 1 \) in eqn. (14) as a power series in \( h_r \), and to compare this with the Taylor’s series. He derived order conditions for two stages up to order four. Finally, I summarize his findings:

- There is no 2-stage third-order method with \( R(\infty) = 0 \).

- He constructed a 2-stage third-order method with \( R(\infty) = -0.8 \).

- He constructed a 2-stage second-order method with \( R(\infty) = 0 \).

Compared to the second-order Crank-Nicolson method, Rosenbrock found a 2-stage second-order method with optimal damping property at infinity and only two linear equations that have to be solved in each time step. General \( s \)-stage Rosenbrock or Rosenbrock-Runge-Kutta methods can be written in the (modern) form

\[
(1 - h t_{ii} F'(U_n + \sum_{j=1}^{i-1} \delta_{ij} K_j)) K_i = h F(U_n + \sum_{j=1}^{i-1} \alpha_{ij} K_j), \quad i = 1, \ldots, s, \quad (15)
\]

\[
U_{n+1} = U_n + \sum_{i=1}^{s} b_i K_i.
\]

This formulation is the starting point for further improvements.
3 The Improvement by Wanner

Around 1973, Gerhard Wanner became interested in Rosenbrock schemes and added his famous sum, \( hF'(U_n) \sum_{j=1}^{i-1} \gamma_{ij} K_j \), on the right hand side in (15), keeping at the same time the Jacobian fixed, i.e., using \( F'(U_n) \) for all stages [75, 1977]. Rosenbrock-Wanner methods (short ROW methods) with \( s \) stages have the general form

\[
(I - h \gamma_{ii} F'(U_n)) K_i = hF(U_n + \sum_{j=1}^{i-1} \alpha_{ij} K_j) + hF'(U_n) \sum_{j=1}^{i-1} \gamma_{ij} K_j, \quad i = 1, \ldots, s, \tag{16}
\]

\[
U_{n+1} = U_n + \sum_{i=1}^s b_i K_i.
\]

In the spirit of Rosenbrock, they can be derived from diagonally implicit Runge-Kutta methods (short DIRK methods), applying only one simplified Newton step with the Jacobian \( F'(U_n) \) and using already calculated stage values as starting values in the calculation of subsequent stages. Applied to (10), the nonlinear system for the stage values \( K_i \) of a DIRK method with lower triangular coefficient matrix \( D = (d_{ij}) \) reads

\[
K_i = hF(U_n + \sum_{j=1}^i d_{ij} K_j), \quad i = 1, \ldots, s. \tag{17}
\]

One-step of a Newton-like iteration

\[
(I - hd_{ii} F'(U_n)) \left( K_i - K_i^{(0)} \right) = hF \left( U_n + \sum_{j=1}^{i-1} d_{ij} K_j + d_{ii} K_j^{(0)} \right) - K_i^{(0)} \tag{18}
\]

with starting values

\[
K_1^{(0)} = 0, \quad K_i^{(0)} = -\sum_{j=1}^{i-1} \frac{\gamma_{ij}}{d_{ii}} K_j, \quad i = 2, \ldots, s, \tag{19}
\]

yields the ROW method (16) with \( \alpha_{ij} = d_{ij} - \gamma_{ij} \) and \( \gamma_{ii} = d_{ii} \). Compared to Rosenbrock’s original form (15), the coefficients \( \delta_{ij} \) were removed to avoid recalculation of Jacobians and new coefficients \( \gamma_{ij} \) were added to have enough parameters for consistency and good stability properties.

A usual simplification is to set \( \gamma_{ij} = \gamma \) for all \( i = 1, \ldots, s \). In case of direct solvers, it allows to reuse an LU-decomposition of the linear system matrix \( I - h \gamma F'(U_n) \). It also simplifies iterative solvers, when matrix decompositions as preconditioners are used. To avoid the matrix-vector multiplication, one introduces \( S_i = \sum_{j=1}^{i-1} \gamma_{ij} K_j \) and solves

\[
\left( \frac{I}{h \gamma} - F'(U_n) \right) S_i = F(U_n + \sum_{j=1}^{i-1} a_{ij} S_j) + \sum_{j=1}^{i-1} \frac{c_{ij}}{h} S_j, \quad i = 1, \ldots, s, \tag{20}
\]

\[
U_{n+1} = U_n + \sum_{i=1}^s m_i S_i.
\]
Defining the matrix \( \Gamma = (\gamma_{ij})_{i,j=1}^{s} \) with \( \gamma_{ii} \neq 0 \) for all \( i \), the new parameters are derived from

\[
(a_{ij})_{i,j=1}^{s} = (\alpha_{ij})_{i,j=1}^{s} = \Gamma^{-1}, \quad (c_{ij})_{i,j=1}^{s} = \text{diag}(\gamma_{11}^{-1}, \ldots, \gamma_{ss}^{-1}) - \Gamma^{-1},
\]

\[
(m_{1}, \ldots, m_{s}) = (b_{1}, \ldots, b_{s})\Gamma^{-1}.
\]

Further generalizations to non-autonomous systems and systems of the special multiplicative form

\[ M(t,U)\partial_{t}U = F(t,U), \]

where \( M \) might be singular, are also possible

\[ [14, 35]. \]

So far, the Jacobian has to be computed at every time step, which can be quite costly. Steihaug and Wolfbrandt [64, 1979] developed so-called W-methods that avoid exact Jacobians, i.e., \( F'(U_{n}) \approx T_{n} \) with arbitrary matrix \( T_{n} \). The idea is to keep the Jacobian unchanged over several time steps while still ensuring stability. Less restrictive time lagged approximations of the form \( T_{n} \approx F'(U_{n}) + \mathcal{O}(h) \) were proposed by Scholz and Verwer [60, 1983], see also Scholz [57, 58, 1978/79], and Kaps and Ostermann [25, 80, 1988/89]. Rahumanthan and Stanescu recently discussed high-order W-methods [46, 2010]. They have been also applied to optimal control problems in Lang and Verwer [30, 2013].

The linear equations in (20) can be successively solved. Order conditions were derived by applying the theory of Butcher series. They can be found in Wolfbrandt [80, 1977], Kaps [19, 1977], Nørsett and Wolfbrandt [54, 1979], and Kaps and Wanner [23, 1981]. Further details and many more information are given in the books of Van der Houven [5, 1976] and Hairer and Wanner [14, 1991].

For later use, I briefly recall the definition of a few fundamental stability concepts.

Applied to the famous scalar Dahlquist’s test equation \( y' = \lambda y, \ y_{0} = 1 \) with \( \lambda \in \mathbb{C} \), a ROW method (as any other Runge-Kutta method) gives \( U_{n+1} = R(z)U_{n} \), where \( z = \lambda h \). The function \( R(z) \) is called the stability function of the method and the set \( S = \{ z \in \mathbb{C} : |R(z)| \leq 1 \} \) defines its stability domain. The exact solution of the test equation is stable in the entire negative complex half plane \( C^{-} = \{ z : \text{Re}(z) \leq 0 \} \), and it seems likely that a numerical method should preserve this stability property. Dahlquist (1963) called a method \textit{A-stable} if \( C^{-} \subseteq S \). If in addition \( \lim_{z \to -\infty} R(z) = 0 \), the method is called \textit{L-stable} - a property that was introduced by Ehle (1969) and guarantees a fast damping for those \( z \) having very large negative real parts. A convenient way to ensure \( L \)-stability for ROW methods is to require \( \alpha_{si} + \gamma_{si} = b_{i} \) for \( i = 1, \ldots, s \), and \( \sum_{j} \alpha_{sj} = 1 \). Such methods are called \textit{stiffly accurate}. A weaker concept was established by Widlund (1967) who called a method \textit{A(\( \alpha \))-stable} if the sector \( S_{\alpha} = \{ z : |\text{arg}(-z)| \leq \alpha, \ z \neq 0 \} \) is contained in its stability region.

There are \textit{A-stable} and \textit{L-stable} ROW methods available. ROW methods share their linear stability properties with (singly) diagonally implicit Runge-Kutta methods introduced by Alexander [11, 1977]. The role of the stability parameter \( \gamma \) was studied in Wanner [76, 1980]. Continuous extensions of Rosenbrock-type methods for a frequent graphical output were introduced by Ostermann [39, 1990].
4 Development of Rosenbrock-Wanner Methods

First Solvers. The theoretical investigation of Rosenbrock-Wanner methods at the end of the 70s laid the starting point for a broad and fast development of efficient solvers. The fourth-order codes GRK4A and GRK4T proposed by Kaps and Rentrop [22, 1979] were equipped with a step size control based on embedded formulas of order three. The first one is A-stable whereas the second is only A(89.3°)-stable, but comes with smaller truncation errors. They were successfully tested on the 25 stiff test problems of Enright, Hull and Lindberg [7, 1975]. Gottwald and Wanner presented their back-stepping algorithm to improve the reliability of Rosenbrock methods [11, 1981]. Time-lagged Jacobian matrices and a modified Richardson extrapolation for variable steps size control within a fourth-order A-stable Rosenbrock-Wanner scheme (named RKRMC) were tested by Verwer, Scholz, Blom, and Louter-Nool [74, 1983]. Further analysis and experiments have been made by Verwer [72, 73, 1982]. Implementation issues were discussed by Shampine [62, 1982]. Veldhuizen investigated the D-stability of the Kaps-Rentrop methods [71, 1984]. There are two options to estimate local errors: embedding and Richardson extrapolation. Kaps, Poon, and Bui did a careful comparison of these two strategies in [21, 1985]. The performance of Rosenbrock methods for large scale combustion problems discretized by the Method of Lines was investigated by Ostermann, Kaps, and Bui [40, 1986].

Partitioned Methods. It is often useful to split the solution vector $U(t)$ into stiff and non-stiff components, say $U_s(t)$ and $U_n(t)$. After an appropriate reordering of the original equations, this gives a partitioned system

$$
\begin{align*}
U'_s(t) &= F_s(U_s(t), U_n(t)), & U_s(0) = U_s^0, \\
U'_n(t) &= F_n(U_s(t), U_n(t)), & U_n(0) = U_n^0.
\end{align*}
$$

(22)

Now it is quite natural to apply a Rosenbrock-type scheme to the stiff part and an explicit Runge-Kutta method to the non-stiff part. Rentrop combined an A-stable Rosenbrock (3)4-pair with a common (4)5-Runge-Kutta-pair and studied strategies for stiffness detection in [50, 1985]. A drawback of such an approach is the occurrence of additional coupling conditions which usually does not allow the simple combination of two favourite schemes. An alternative is to use the setting of W-methods to directly incorporate the partitioning on the level of the Jacobian calculation, e.g., only take into account derivatives of $F_s$ and drop the other ones. Such methods were analysed by Strehmel, Weiner, and Dannehl [69, 1990] under the heading partitioned linearly implicit Runge-Kutta methods including ROW- and W-methods. Later on, Wensch designed an eight-stage fourth-order partitioned Rosenbrock method for multibody systems in index-3 formulation [70, 1998].

The partitioning can be also used to set up multirate schemes, where different step sizes for active and latent components are explicitly introduced in the discretization. In Günther and Rentrop [13, 1993], multirate Rosenbrock-Wanner methods
were used for the simulation of electrical networks. One general shortcoming of multirate methods is the coupling between the components by interpolating and extrapolating state variables. Stability of multirate Rosenbrock methods were studied in Savcenco \cite{55, 56, 2008/09} and Kuhn and Lang \cite{25, 2014}.

**Differential-Algebraic Equations.** In the late 80s, Rosenbrock methods were also applied to differential-algebraic equations (DAEs) of index one:

\[
U'(t) = F(U(t), Z(t)), \quad U(0) = U^0, \\
0 = G(U(t), Z(t)), \quad Z(0) = Z^0, 
\]

where it is assumed that \((\partial Z G)^{-1}\) exists and is bounded in a neighbourhood of the solution. The main idea used by Roche \cite{52, 1988} is to add \(\varepsilon Z'(t)\) on the left hand side of the second equation and consider the DAE \((23)\) as a limit case of the stiff singular perturbation problem for \(\varepsilon \to 0\). This limit typically destroys the classical order of the Rosenbrock methods and gives rise to a new consistency theory derived by means of a modified Butcher-like tree model for the \(U\)- and \(Z\)-components. Note that the Kaps-Rentrop methods from \cite{22} drop down to order two when applied to \((23)\). Similar observations have been made earlier by Verwer \cite{73, 1982}. Two new ROW-methods (named DAE34 and RKF4DA) with stepsize control and an index-1 monitor were proposed and tested by Rentrop, Roche and Steinebach \cite{51, 1989}.

A desirable property when solving stiff or differential-algebraic equations is to have an L-stable method, i.e., a method with \(R(\infty) = 0\). This is always the case for stiffly accurate Rosenbrock methods which approximate the algebraic component \(Z\) of the extreme DAEs, \(U' = 1\) and \(0 = G(U, Z)\), through one simplified Newton iteration. This nicely meets the original idea of Rosenbrock. In their book, Hairer and Wanner \cite{14, 1991} constructed the famous stiffly accurate six-stage fourth-order Rosenbrock solver RODAS with an embedded method of order three. Special index-2 DAEs were treated in Lubich and Roche \cite{35, 1990} and results for index-3 multi-body systems can be found in Wensch \cite{79, 1998}. Günther, Hoschek, and Rentrop constructed special index-2 Rosenbrock methods for electric circuit simulations \cite{12, 2000}. Recently, Jax and Steinebach \cite{17, 2017} introduced a new type of ROW methods for solving DAEs of the form \((23)\). Taking ideas from W-methods, they allow arbitrary approximations to Jacobian entries resulting from the differential part.

**Extrapolation.** An interesting, general approach to construct higher order methods for differential as well as differential-algebraic equations is to use extrapolation. Deuflhard and Nowak \cite{6, 1987} proposed to extrapolate the linearly implicit Euler discretization (as the simplest Rosenbrock method) to solve chemical reaction kinetics and electric circuits and implemented the well-known variable-order \textsc{Limex} code with step size control. They also provided the impetus for Lubich to explain the error behaviour of such methods by perturbed asymptotic analysis \cite{33, 1989}.
**B-Convergence and Order Reduction.** One-step methods and so Rosenbrock schemes suffer from order reduction, especially when they are applied to nonlinear parabolic partial differential equations. Sharp error estimates showing fractional orders of convergence for Rosenbrock and W-methods were first established by Lubich, Ostermann, and Roche [41, 34, 1993/95]. This phenomenon is related to the B-convergence of linearly implicit methods studied by Strehmel and Weiner [67, 1987]. Barriers for the order of B-convergence were given by Scholz [59, 1989]. In their book, Strehmel and Weiner [68, 1992] gave convergence results for spatial discretizations of semilinear parabolic equations with constant operator and a Lipschitz continuous non-linearity. However, the B-convergence technique does not give the sharp fractional temporal convergence rates. It is now much better understood than before why (lower) fractional orders occur. This reduction is not induced by lack of smoothness of the solution but rather by the presence of powers of the spatial differential operators in the local truncation error. Concerning W-methods, the order reduction is more severe compared with Rosenbrock methods. Loss of accuracy happens long before stability is affected. Fortunately, there are additional consistency conditions that imply also higher order of convergence as shown in Lubich and Ostermann [34, 1995].

Using this theoretical framework, new methods were constructed. Steinebach improved the RODAS code and designed his stiffly accurate RODASP scheme, which satisfies the new conditions for linear parabolic problems to reach order four. It was successfully applied to forecast transport in rivers, see Steinebach and Rennsteig [45, 2001]. New order-three methods with three, Ros3p, and four stages, Ros3pl, were constructed in Lang and Verwer [28, 2001] and Lang and Teleaga [27, 2008], respectively. The latter one is stiffly accurate and therefore suitable for differential-algebraic equations. It also satisfies the condition of a W-method with $O(h)$-disturbance of the Jacobian, which makes numerical differentiation for its entries less sensitive with respect to roundoff errors. A bunch of newly designed third-order Rosenbrock W-methods for partial differential-algebraic equations was published in Rang and Angermann [49, 2005]. Further improved ROW methods can be found in Rang [47, 48, 2014/15].

**Exponential Rosenbrock-type Methods.** Exponential integrators are based on a continuous linearization of the nonlinearity $F(U(t))$ along the numerical solution. This gives the linearized system

$$U'(t) = F'(U_n)U(t) + G_n(U(t)), \quad G_n(U(t)) = F(U(t)) - F'(U_n)U(t). \quad (24)$$

Exponential Rosenbrock methods make direct use of $J_n := F'(U_n)$ and $G_n(U(t))$. Hochbruck, Ostermann, and Schweitzer [15, 2009] considered the following class of
methods (here for variable time steps $h_n$):

\[
U_{ni} = e^{c_i h_n J_n} U_n + h_n \sum_{j=1}^{i-1} a_{ij}(h_n J_n) g_n(U_{nj}), \quad i = 1, \ldots, s,
\]

\[
U_{n+1} = e^{c_i h_n J_n} U_n + h_n \sum_{i=1}^{s} b_i(h_n J_n) g_n(U_{ni}).
\]

A key point is the efficient approximation of the matrix exponential times a vector by Krylov subspace methods or methods based on direct polynomial interpolation. An interpolation method with real Leja points was tested by Caliari and Ostermann [2, 2009] and showed a great potential for problems with large advection in combination with moderate diffusion and mildly stiff reactions. Higher order and parallel exponential Rosenbrock methods were proposed by Luan and Ostermann [31, 32, 2014/16].

**Miscellaneous.** Rosenbrock methods offer a simple usage due to their linear structure. Methods up to order four perform well for low and medium tolerances and work competitive in many applications. The code ode23s in the MATLAB ODE SUITE is a typical Rosenbrock scheme, see Shampine and Reichelt [63, 1997]. The Krylov-W-code ROWMAP based on the Rosenbrock method ROS4 of Hairer and Wanner has demonstrated its efficiency for large stiff systems. Numerical tests were performed in Weiner, Schmitt, and Podhaisky [77, 1997]. Rosenbrock methods are the numerical kernel in the adaptive multilevel PDAE-solver KARDOS, which is a well running working horse for a broad range of real-life applications, see Lang [26, 2000]. Combined with a linearized error transport equation based on first variational principles, they can be accompanied with a cheap global error estimation and control through tolerance proportionality. Such strategies were investigated in Lang and Verwer [29, 2007] for initial value problems and in Debrabant and Lang [4, 2015] for semilinear parabolic equations. Last but not least, a Rosenbrock code is listed in the second edition of *Numerical Recipes* by Press, Teukolsky, Vetterling, and Flannery [45, 1996].

A lot of basic information about Rosenbrock methods can be found in the books by Hairer and Wanner [14, 1991] and Strehmel and Weiner [68, 1992]. Newer developments are highlighted in Strehmel, Weiner, and Podhaisky [70, 2012]. A tremendous source of further interesting material are the proceedings of the numerous NUMDIFF-conferences held at the Martin Luther University Halle-Wittenberg since the early 1980s.

## 5 Two-Step Rosenbrock-Peer and W-Methods

As explained above, Rosenbrock methods may suffer from order reduction for very stiff problems. A closer inspection reveals that the low stage order (the first stage value is computed by the linearly implicit Euler scheme) is one of the reasons. To
raise the stage order substantially, Podhaisky, Schmitt, and Weiner \[43, 42, 2002\] studied a new class of linearly implicit two-step methods, where the previously computed stage values are taken into account. Such $s$-stage two-step W-methods have the form

$$
Y_{ni} = U_n + h_n \sum_{j=1}^{s} a_{ij} U_{n-1,j} + h_n \sum_{j=1}^{i-1} \tilde{a}_{ij} U_{nj},
$$

$$(I - \gamma h_n T_n)U_{ni} = F(Y_{ni}) + h_n T_n \sum_{j=1}^{s} \gamma_{ij} U_{n-1,j} + h_n T_n \sum_{j=1}^{i-1} \tilde{\gamma}_{ij} U_{nj},
$$

$$
i = 1, \ldots, s,
$$

$$
U_{n+1} = U_n + h_n \sum_{i=1}^{s} (b_i U_{ni} + v_i U_{n-1,i}).
$$

(26)

Observe that $a_{ij} = \gamma_{ij} = v_i = 0$ recovers classical one-step ROW and W-methods. The special setting $\tilde{a}_{ij} = \tilde{\gamma}_{ij} = 0$ treated in \[42\] allows to compute the stage values $U_{ni}$ in parallel. Higher order parallel methods were studied by Jackiewicz, Podhaisky, and Weiner \[16, 2004\]. Computer architectures of workgroup servers having shared memory for quite a few processors are particularly suitable for these methods which have been designed for the solution of large stiff systems in combination with Krylov techniques. Methods with favorable stability properties have been constructed with stage order $q = s$ and order $p = s$ for $s \leq 4$. All methods are competitive with state-of-the-art codes for stiff ODEs.

Within the class of two-step methods, Podhaisky, Weiner, and Schmitt \[44, 2005\] also constructed $s$-stage methods where all stage values have the stage order $q = s-1$. They considered the following methods:

$$(I - \gamma h_n T_n)U_{ni} = \sum_{j=1}^{s} b_{ij} U_{n-1,j} + h_n \sum_{j=1}^{s} a_{ij} (F(U_{n-1,j}) - T_n U_{n-1,j})$$

$$+ h_n T_n \sum_{j=1}^{i-1} g_{ij} U_{nj}, \quad i = 1, \ldots, s.
$$

(27)

Here, $U_{ns} \approx U(t_{n+1})$ and the matrix $T_n$ is supposed to be an approximation to the Jacobian $F'(U(t_n))$ for stability reasons. The method is treated as a W-method, i.e., the order conditions are derived for arbitrary $T_n$. Due to their two-step and linear structure, the methods are called two-step Rosenbrock-Peer methods, where peer refers to the fact that all stage values have now one and same order. The methods constructed in \[44\] for $s = 4, \ldots, 8$ are zero-stable for arbitrary step size sequences and $L(\alpha)$-stable with large $\alpha$. For constant time steps, these methods have order $s$. Numerical experiments showed no order reduction and an efficiency superior to the fourth-order RODAS for more stringent tolerances.

With this property, peer methods commend themselves as time-stepping schemes for the solution of time-dependent partial differential equations. So they have been implemented in the already mentioned finite element software package KARDOS, see Gerisch, Lang, Podhaisky, and Weiner \[8, 2009\] and Schröder, Gerisch, and Lang \[61, 2017\]. They also performed well for compressible Euler equations, demonstrated in Jebens, Knoth, and Weiner \[18, 2012\], for shallow-water equations, reported in
Steinebach and Weiner [66, 2012], and for more complex fluid dynamics problems, see Gottermeier and Lang [9, 10, 2009/10]. More recently, linearly implicit two-step Peer methods of Rosenbrock-type have shown their reliability, robustness, and accuracy for large eddy and direct numerical simulations for turbulent unsteady flows in Massa, Noventa, Lorini, Bassi, and Ghidoni [36, 2018].

6 Summary

The idea of Rosenbrock is still alive. Avoiding the (often cumbersome) solution of nonlinear equations has not lost its attractiveness and significance over the years. The successive solution of linear equations is still a valuable option to efficiently solve systems of differential, differential-algebraic or partial differential equations. Classical one-step Rosenbrock-Wanner methods up to order four have demonstrated their good performance for low and medium tolerances. The new class of two-step Rosenbrock-Peer methods allows the construction of even higher order methods that overcome the disadvantage of order reduction and still exhibit good stability properties. Recent numerical experiments with higher tolerances are very promising.

There is still an ongoing research activity in the field of Rosenbrock methods. A recent search in the Scopus data base gave 753 documents. One of the last entries is about Strong Convergence Analysis of the Stochastic Exponential Rosenbrock Scheme for the Finite Element Discretization of Semilinear SPDEs Driven by Multiplicative and Additive Noise by Mukam and Tambue [37, 2018]. This brings me to my final remark. In view of the numerous contributions to Rosenbrock schemes, I would like to apologize in advance to those who have made significant further contributions to the topic but were not mentioned in my overview. I am prepared to receive your emails.

7 Acknowledgement

I would like to thank Rüdiger Weiner for careful reading of a first version of the manuscript. His suggestions very much helped to improve the article. I also thank the reviewers for their useful remarks.

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