# A note on the Rosenbrock formulae

Emanuele Galligani and Federico Perini

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Università degli Studi di Modena e Reggio Emilia

Department of Engineering ''Enzo Ferrari''

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**Abstract.** In this report the Rosenbrock formulae are considered. These formulae are particularly suited for the integration of stiff differential systems such as the ones arising from reaction kinetics combustion modeling.
The numerical techniques for the analysis of the A-stability and of the L-stability of a third order Rosenbrock formula are reported.

**Key Words:** semi-implicit Runge-Kutta methods, stiff problems.

**MSC2010:** 65L06, 65L04.

# 1 Introduction and notations

Let us consider the initial value problem in autonomous form described by $m$ differential equations

$$\boldsymbol{u}'(t) = \boldsymbol{f}(\boldsymbol{u}(t)) \qquad t > t_0, \tag{1}$$

subject by the given conditions

$$\boldsymbol{u}(t_0) = \boldsymbol{u}_0. \tag{2}$$

The $q-$stage semi-implicit Runge-Kutta methods introduced by Rosenbrock in [26] for the computation of the approximation $\boldsymbol{u}_n$ of the solution $\boldsymbol{u}(t_n)$ at the point $t_n$ of (1)–(2), has the form (e.g., [20, p. 247])

$$\boldsymbol{u}_{n+1} = \boldsymbol{u}_n + h\sum_{j=1}^{q} c_j \boldsymbol{K}_j, \tag{3}$$

where $h$ is the step length ($t_{n+1} = t_n + h$) and

$$\begin{array}{rcl}
\boldsymbol{K}_1 & = & \boldsymbol{f}(\boldsymbol{u}_n) + \alpha_1 h J(\boldsymbol{u}_n)\boldsymbol{K}_1; \\
\boldsymbol{K}_2 & = & \boldsymbol{f}(\boldsymbol{u}_n + hb_{21}\boldsymbol{K}_1) + \alpha_2 h J(\boldsymbol{u}_n + h\beta_{21}\boldsymbol{K}_1)\boldsymbol{K}_2; \\
\boldsymbol{K}_3 & = & \boldsymbol{f}(\boldsymbol{u}_n + hb_{31}\boldsymbol{K}_1 + hb_{32}\boldsymbol{K}_2) + \alpha_3 h J(\boldsymbol{u}_n + h\beta_{31}\boldsymbol{K}_1 + \beta_{32}\boldsymbol{K}_2)\boldsymbol{K}_3; \\
\vdots & & \\
\boldsymbol{K}_q & = & \boldsymbol{f}(\boldsymbol{u}_n + h\sum_{i=1}^{q-1} b_{qi}\boldsymbol{K}_i) + \alpha_q h J(\boldsymbol{u}_n + h\sum_{i=1}^{q-1}\beta_{qi}\boldsymbol{K}_i)\boldsymbol{K}_q.
\end{array} \tag{4}$$

Here $J(\boldsymbol{u}_n)$ is the Jacobian matrix evaluated at $\boldsymbol{u}_n$. The method described by the formulae (3)–(4) is even called Rosenbrock method (procedure) or Runge-Kutta-Rosenbrock method.[1] Formulae (3)–(4) are called Rosenbrock formulae.

We remind some notations that are used in the following.
The Jacobian matrix evaluated at $\boldsymbol{u} \equiv \boldsymbol{u}(t)$ is defined as

$$J(\boldsymbol{u}) = \begin{pmatrix} \frac{\partial f_1}{\partial u_1}(\boldsymbol{u}) & \dots & \frac{\partial f_1}{\partial u_m}(\boldsymbol{u}) \\ \vdots & & \vdots \\ \frac{\partial f_m}{\partial u_1}(\boldsymbol{u}) & \dots & \frac{\partial f_m}{\partial u_m}(\boldsymbol{u}) \end{pmatrix},$$

the gradient of the function $f_i$, $i = 1, ..., m$, at $\boldsymbol{u}$ is

$$\nabla f_i(\boldsymbol{u}) = \begin{pmatrix} \frac{\partial f_i}{\partial u_1}(\boldsymbol{u}) \\ \vdots \\ \frac{\partial f_i}{\partial u_m}(\boldsymbol{u}) \end{pmatrix},$$

and the Hessian matrix of $f_i$, $i = 1, ..., m$, at $\boldsymbol{u}$ is

$$H_i(\boldsymbol{u}) = \begin{pmatrix} \frac{\partial^2 f_i}{\partial u_1^2}(\boldsymbol{u}) & \dots & \frac{\partial^2 f_i}{\partial u_1 \partial u_m}(\boldsymbol{u}) \\ \vdots & & \vdots \\ \frac{\partial^2 f_i}{\partial u_m \partial u_1}(\boldsymbol{u}) & \dots & \frac{\partial^2 f_i}{\partial u_m^2}(\boldsymbol{u}) \end{pmatrix}.$$

The Taylor expansions in several variables of the function $f_i$, $i = 1, ..., m$, at $\boldsymbol{u} + \boldsymbol{v}$ with respect to $\boldsymbol{u}$, are

$$f_i(\boldsymbol{u} + \boldsymbol{v}) = f_i(\boldsymbol{u}) + \nabla f_i(\boldsymbol{u})^T \boldsymbol{v} + \frac{1}{2}\boldsymbol{v}^T H_i(\boldsymbol{u})\boldsymbol{v} + ... \tag{5}$$

[1] Rosenbrock in [26] call these formulae *implicit processes*.

Thus by Kronecker product definition (e.g., [24, p. 236]), for all the components of the vector $\boldsymbol{f}$ we have

$$\boldsymbol{f}(\boldsymbol{u}+\boldsymbol{v}) = \boldsymbol{f}(\boldsymbol{u}) + J(\boldsymbol{u})\boldsymbol{v} + \frac{1}{2}\left(\ I \otimes \boldsymbol{v}^T\ \right) \begin{bmatrix} H_1(\boldsymbol{u}) \\ \vdots \\ H_m(\boldsymbol{u}) \end{bmatrix} \boldsymbol{v} + ...$$

Here $I$ is the identity matrix of order $m$. Thus, setting[2]

$$H(\boldsymbol{v},\boldsymbol{u}) = \left(\ I \otimes \boldsymbol{v}^T\ \right) \begin{bmatrix} H_1(\boldsymbol{u}) \\ \vdots \\ H_m(\boldsymbol{u}) \end{bmatrix}, \tag{6}$$

we obtain

$$\boldsymbol{f}(\boldsymbol{u}+\boldsymbol{v}) = \boldsymbol{f}(\boldsymbol{u}) + J(\boldsymbol{u})\boldsymbol{v} + \frac{1}{2}H(\boldsymbol{v},\boldsymbol{u})\boldsymbol{v} + ... \tag{7}$$

The Taylor expansions in several variables of the derivatives of $f_i$, $i = 1, ..., m$, at $\boldsymbol{u}+\boldsymbol{v}$ with respect to $\boldsymbol{u}$, are

$$\begin{aligned}
\frac{\partial f_i}{\partial u_1}(\boldsymbol{u}+\boldsymbol{v}) &= \frac{\partial f_i}{\partial u_1}(\boldsymbol{u}) + \frac{\partial}{\partial u_1}\left(\frac{\partial f_i}{\partial u_1}(\boldsymbol{u})\right) v_1 + \frac{\partial}{\partial u_2}\left(\frac{\partial f_i}{\partial u_1}(\boldsymbol{u})\right) v_2 + ... + \frac{\partial}{\partial u_m}\left(\frac{\partial f_i}{\partial u_1}(\boldsymbol{u})\right) v_m + ... \\
&\vdots \\
\frac{\partial f_i}{\partial u_m}(\boldsymbol{u}+\boldsymbol{v}) &= \frac{\partial f_i}{\partial u_m}(\boldsymbol{u}) + \frac{\partial}{\partial u_1}\left(\frac{\partial f_i}{\partial u_m}(\boldsymbol{u})\right) v_1 + \frac{\partial}{\partial u_2}\left(\frac{\partial f_i}{\partial u_m}(\boldsymbol{u})\right) v_2 + ... + \frac{\partial}{\partial u_m}\left(\frac{\partial f_i}{\partial u_m}(\boldsymbol{u})\right) v_m + ...
\end{aligned}$$

then,

$$\begin{aligned}
J(\boldsymbol{u}+\boldsymbol{v}) &= J(\boldsymbol{u}) + \\
&+ \begin{pmatrix} \frac{\partial}{\partial u_1}\left(\frac{\partial f_1}{\partial u_1}(\boldsymbol{u})\right) v_1 + ... + \frac{\partial}{\partial u_m}\left(\frac{\partial f_1}{\partial u_1}(\boldsymbol{u})\right) v_m & \ldots & \frac{\partial}{\partial u_1}\left(\frac{\partial f_1}{\partial u_m}(\boldsymbol{u})\right) v_1 + ... + \frac{\partial}{\partial u_m}\left(\frac{\partial f_1}{\partial u_m}(\boldsymbol{u})\right) v_m \\ \vdots & & \vdots \\ \frac{\partial}{\partial u_1}\left(\frac{\partial f_m}{\partial u_1}(\boldsymbol{u})\right) v_1 + ... + \frac{\partial}{\partial u_m}\left(\frac{\partial f_m}{\partial u_1}(\boldsymbol{u})\right) v_m & \ldots & \frac{\partial}{\partial u_1}\left(\frac{\partial f_m}{\partial u_m}(\boldsymbol{u})\right) v_1 + ... + \frac{\partial}{\partial u_m}\left(\frac{\partial f_m}{\partial u_m}(\boldsymbol{u})\right) v_m \end{pmatrix} + ... \\
&= J(\boldsymbol{u}) + \begin{pmatrix} \frac{\partial^2 f_1}{\partial u_1^2}(\boldsymbol{u})v_1 + ... + \frac{\partial^2 f_1}{\partial u_m \partial u_1}(\boldsymbol{u})v_m & \ldots & \frac{\partial^2 f_1}{\partial u_1 \partial u_m}(\boldsymbol{u})v_1 + ... + \frac{\partial^2 f_1}{\partial u_m^2}(\boldsymbol{u})v_m \\ \vdots & & \vdots \\ \frac{\partial^2 f_m}{\partial u_1^2}(\boldsymbol{u})v_1 + ... + \frac{\partial^2 f_m}{\partial u_m \partial u_1}(\boldsymbol{u})v_m & \ldots & \frac{\partial^2 f_m}{\partial u_1 \partial u_m}(\boldsymbol{u})v_1 + ... + \frac{\partial^2 f_m}{\partial u_m^2}(\boldsymbol{u})v_m \end{pmatrix} + ...
\end{aligned}$$

Thus by Kronecker product definition, we can write

$$J(\boldsymbol{u}+\boldsymbol{v}) = J(\boldsymbol{u}) + \left(\ I \otimes \boldsymbol{v}^T\ \right) \begin{bmatrix} H_1(\boldsymbol{u}) \\ \vdots \\ H_m(\boldsymbol{u}) \end{bmatrix} + ...$$

and by the definition (6), we can write

$$J(\boldsymbol{u}+\boldsymbol{v}) = J(\boldsymbol{u}) + H(\boldsymbol{v},\boldsymbol{u}) + ... \tag{8}$$

[2] We observe that for any vectors $\boldsymbol{u}$, $\boldsymbol{v}$ and $\tilde{\boldsymbol{v}}$ of $m$ components and any real scalars $\alpha$ and $\beta$ we have

$$\begin{aligned}
H(\alpha\boldsymbol{v} + \beta\tilde{\boldsymbol{v}}, \boldsymbol{u}) &= \alpha H(\boldsymbol{v},\boldsymbol{u}) + \beta H(\tilde{\boldsymbol{v}},\boldsymbol{u}); \\
H_{\boldsymbol{u}}(\alpha\boldsymbol{v} + \beta\tilde{\boldsymbol{v}}, \boldsymbol{u}) &= \alpha H_{\boldsymbol{u}}(\boldsymbol{v},\boldsymbol{u}) + \beta H_{\boldsymbol{u}}(\tilde{\boldsymbol{v}},\boldsymbol{u}).
\end{aligned}$$

By omitting the point of evaluation of the functions, we have the following notations for higher order derivatives of $\boldsymbol{u}$.
For the second derivatives of $\boldsymbol{u}$ we have

$$\boldsymbol{u}'' = \begin{pmatrix} u_1'' \\ \vdots \\ u_m'' \end{pmatrix} = \begin{pmatrix} \frac{d}{dt} f_1 \\ \vdots \\ \frac{d}{dt} f_m \end{pmatrix} = \begin{pmatrix} \frac{\partial f_1}{\partial u_1} u_1' + \dots + \frac{\partial f_1}{\partial u_m} u_m' \\ \vdots \\ \frac{\partial f_m}{\partial u_1} u_1' + \dots + \frac{\partial f_m}{\partial u_m} u_m' \end{pmatrix} = \begin{pmatrix} \frac{\partial f_1}{\partial u_1} f_1 + \dots + \frac{\partial f_1}{\partial u_m} f_m \\ \vdots \\ \frac{\partial f_m}{\partial u_1} f_1 + \dots + \frac{\partial f_m}{\partial u_m} f_m \end{pmatrix} = J\boldsymbol{f}. \quad (9)$$

Here, we can denote $\boldsymbol{f}' = (\frac{d}{dt} f_1, \dots, \frac{d}{dt} f_m)^T$.
For the third order derivatives we have,

$$\boldsymbol{u}''' = \begin{pmatrix} u_1''' \\ \vdots \\ u_m''' \end{pmatrix} \quad \Longrightarrow \quad \begin{cases} u_1''' = \frac{d}{dt}\left(\frac{\partial f_1}{\partial u_1} f_1\right) + \dots + \frac{d}{dt}\left(\frac{\partial f_1}{\partial u_m} f_m\right) = \\ \vdots \\ u_m''' = \frac{d}{dt}\left(\frac{\partial f_m}{\partial u_1} f_1\right) + \dots + \frac{d}{dt}\left(\frac{\partial f_m}{\partial u_m} f_m\right) = \end{cases}$$

$$\begin{aligned} &= \frac{\partial}{\partial u_1}\left(\frac{\partial f_1}{\partial u_1} f_1\right) u_1' + \dots + \frac{\partial}{\partial u_m}\left(\frac{\partial f_1}{\partial u_1} f_1\right) u_m' + \dots + \frac{\partial}{\partial u_1}\left(\frac{\partial f_1}{\partial u_m} f_m\right) u_1' + \dots + \frac{\partial}{\partial u_m}\left(\frac{\partial f_1}{\partial u_m} f_m\right) u_m' = \\ &\vdots \\ &= \frac{\partial}{\partial u_1}\left(\frac{\partial f_m}{\partial u_1} f_1\right) u_1' + \dots + \frac{\partial}{\partial u_m}\left(\frac{\partial f_m}{\partial u_1} f_1\right) u_m' + \dots + \frac{\partial}{\partial u_1}\left(\frac{\partial f_m}{\partial u_m} f_m\right) u_1' + \dots + \frac{\partial}{\partial u_m}\left(\frac{\partial f_m}{\partial u_m} f_m\right) u_m' = \end{aligned}$$

$$\begin{aligned} &= \left(\frac{\partial^2 f_1}{\partial u_1^2} f_1 + (\frac{\partial f_1}{\partial u_1})^2\right) f_1 + \dots + \left(\frac{\partial^2 f_1}{\partial u_m \partial u_1} f_1 + \frac{\partial f_1}{\partial u_1}\frac{\partial f_1}{\partial u_m}\right) f_m + \dots + \left(\frac{\partial^2 f_1}{\partial u_1 \partial u_m} f_m + \frac{\partial f_1}{\partial u_1}\frac{\partial f_m}{\partial u_1}\right) f_1 + \dots + \left(\frac{\partial^2 f_1}{\partial u_m^2} f_m + \frac{\partial f_1}{\partial u_m}\frac{\partial f_m}{\partial u_m}\right) f_m \\ &\vdots \\ &= \left(\frac{\partial^2 f_m}{\partial u_1^2} f_1 + \frac{\partial f_m}{\partial u_1}\frac{\partial f_1}{\partial u_1}\right) f_1 + \dots + \left(\frac{\partial^2 f_m}{\partial u_m \partial u_1} f_1 + \frac{\partial f_m}{\partial u_m}\frac{\partial f_1}{\partial u_m}\right) f_m + \dots. + \left(\frac{\partial^2 f_m}{\partial u_1 \partial u_m} f_m + \frac{\partial f_m}{\partial u_m}\frac{\partial f_m}{\partial u_1}\right) f_1 + \dots + \left(\frac{\partial^2 f_m}{\partial u_m^2} f_m + (\frac{\partial f_m}{\partial u_m})^2\right) f_m \end{aligned}$$

Then, we have

$$\begin{aligned} u_1''' &= \begin{pmatrix} f_1 & \dots & f_m \end{pmatrix} \begin{pmatrix} \frac{\partial^2 f_1}{\partial u_1^2} & \dots & \frac{\partial^2 f_1}{\partial u_1 \partial u_m} \\ \vdots & & \vdots \\ \frac{\partial^2 f_1}{\partial u_m \partial u_1} & \dots & \frac{\partial^2 f_1}{\partial u_m^2} \end{pmatrix} \begin{pmatrix} f_1 \\ \vdots \\ f_m \end{pmatrix} + \\ &\quad + \begin{pmatrix} \frac{\partial f_1}{\partial u_1} & \dots & \frac{\partial f_1}{\partial u_m} \end{pmatrix} \begin{pmatrix} \frac{\partial f_1}{\partial u_1} & \dots & \frac{\partial f_1}{\partial u_m} \\ \vdots & & \vdots \\ \frac{\partial f_m}{\partial u_1} & \dots & \frac{\partial f_m}{\partial u_m} \end{pmatrix} \begin{pmatrix} f_1 \\ \vdots \\ f_m \end{pmatrix} \\ &\vdots \\ u_m''' &= \begin{pmatrix} f_1 & \dots & f_m \end{pmatrix} \begin{pmatrix} \frac{\partial^2 f_m}{\partial u_1^2} & \dots & \frac{\partial^2 f_m}{\partial u_1 \partial u_m} \\ \vdots & & \vdots \\ \frac{\partial^2 f_m}{\partial u_m \partial u_1} & \dots & \frac{\partial^2 f_m}{\partial u_m^2} \end{pmatrix} \begin{pmatrix} f_1 \\ \vdots \\ f_m \end{pmatrix} + \\ &\quad + \begin{pmatrix} \frac{\partial f_m}{\partial u_1} & \dots & \frac{\partial f_m}{\partial u_m} \end{pmatrix} \begin{pmatrix} \frac{\partial f_1}{\partial u_1} & \dots & \frac{\partial f_1}{\partial u_m} \\ \vdots & & \vdots \\ \frac{\partial f_m}{\partial u_1} & \dots & \frac{\partial f_m}{\partial u_m} \end{pmatrix} \begin{pmatrix} f_1 \\ \vdots \\ f_m \end{pmatrix} \end{aligned}$$

that is, by omitting the dependency of the evaluation point $\boldsymbol{u}$ of $H_i$, for $i = 1, \dots, m$, we can write

$$u_i''' = \boldsymbol{f}^T H_i \boldsymbol{f} + \nabla f_i^T J \boldsymbol{f}. \quad (10)$$

Thus by Kronecker product definition and by (6) we can write

$$\boldsymbol{u}''' = \left( \; I \otimes \boldsymbol{f}^T \; \right) \begin{bmatrix} H_1 \\ \vdots \\ H_m \end{bmatrix} \boldsymbol{f} + J^2 \boldsymbol{f} = H(\boldsymbol{f})\boldsymbol{f} + J^2 \boldsymbol{f}, \tag{11}$$

where we used the definition in (6).[3]

Finally, we keep in mind the Taylor expansion of $\boldsymbol{u}(t)$ at $t = t_{n+1}$ with respect to $t = t_n$; for sake of simplicity of notation, we denote $\boldsymbol{u} \equiv \boldsymbol{u}(t_n)$, $\boldsymbol{f} \equiv \boldsymbol{f}(\boldsymbol{u}(t_n))$, $J \equiv J(\boldsymbol{u}(t_n))$, $H_i \equiv H_i(\boldsymbol{u}(t_n))$ and $H(\boldsymbol{f}) \equiv H(\boldsymbol{f}(\boldsymbol{u}(t_n)), \boldsymbol{u}(t_n))$. Then, from (1), (9) and (11), we have

$$\boldsymbol{u}(t_{n+1}) = \boldsymbol{u} + h\boldsymbol{f} + \frac{h^2}{2} J\boldsymbol{f} + \frac{h^3}{6}(H(\boldsymbol{f})\boldsymbol{f} + J^2 \boldsymbol{f}) + O(h^4). \tag{12}$$

[3]From (6), we have

$$H(\boldsymbol{f}) \equiv H(\boldsymbol{f}, \boldsymbol{u}) = \left( \; I \otimes \boldsymbol{f}^T \; \right) \begin{bmatrix} H_1(\boldsymbol{u}) \\ \vdots \\ H_m(\boldsymbol{u}) \end{bmatrix}.$$

## 2 Two- and three-stage semi-implicit Runge-Kutta methods of order three

Let us consider the Rosenbrock procedure (3)–(4) with $q = 2$ and $q = 3$. From (4) we can write[4]

$$\begin{aligned}
\boldsymbol{K}_1 &= (I - \alpha_1 h J(\boldsymbol{u}_n))^{-1} \boldsymbol{f}(\boldsymbol{u}_n);\\
\boldsymbol{K}_2 &= (I - \alpha_2 h J(\boldsymbol{u}_n + h\beta_{21}\boldsymbol{K}_1))^{-1} \boldsymbol{f}(\boldsymbol{u}_n + h b_{21}\boldsymbol{K}_1);\\
\boldsymbol{K}_3 &= (I - \alpha_3 h J(\boldsymbol{u}_n + h\beta_{31}\boldsymbol{K}_1 + \beta_{32}\boldsymbol{K}_2))^{-1} \boldsymbol{f}(\boldsymbol{u}_n + h b_{31}\boldsymbol{K}_1 + h b_{32}\boldsymbol{K}_2).
\end{aligned}$$

For $h$ sufficiently small, we can apply Neumann Lemma (e.g., [23, p. 26]) and we have

$$(I - \alpha h J(\boldsymbol{v}))^{-1} = I + \sum_{i=1}^{\infty} (\alpha h J(\boldsymbol{v}))^i. \tag{13}$$

Thus,

$$\begin{aligned}
\boldsymbol{K}_1 &= (I - \alpha_1 h J(\boldsymbol{u}_n))^{-1} \boldsymbol{f}(\boldsymbol{u}_n)\\
&= (I + \alpha_1 h J(\boldsymbol{u}_n) + \alpha_1^2 h^2 J(\boldsymbol{u}_n)^2 + O(h^3)) \boldsymbol{f}(\boldsymbol{u}_n)\\
&= \boldsymbol{f}(\boldsymbol{u}_n) + \alpha_1 h J(\boldsymbol{u}_n)\boldsymbol{f}(\boldsymbol{u}_n) + \alpha_1^2 h^2 J(\boldsymbol{u}_n)^2 \boldsymbol{f}(\boldsymbol{u}_n) + O(h^3).
\end{aligned} \tag{14}$$

From (7) for $\boldsymbol{f}(\boldsymbol{u}_n + h b_{21}\boldsymbol{K}_1)$ and from the expression of $\boldsymbol{K}_1$ in (14), we have

$$\begin{aligned}
\boldsymbol{K}_2 &= (I - \alpha_2 h J(\boldsymbol{u}_n + h\beta_{21}\boldsymbol{K}_1))^{-1} \boldsymbol{f}(\boldsymbol{u}_n + h b_{21}\boldsymbol{K}_1)\\
&= (I - \alpha_2 h J(\boldsymbol{u}_n + h\beta_{21}\boldsymbol{K}_1))^{-1} \left( \boldsymbol{f}(\boldsymbol{u}_n) + h b_{21} J(\boldsymbol{u}_n)\boldsymbol{K}_1 + \frac{b_{21}^2 h^2}{2} H(\boldsymbol{K}_1, \boldsymbol{u}_n)\boldsymbol{K}_1 + O(h^3) \right)\\
&= (I - \alpha_2 h J(\boldsymbol{u}_n + h\beta_{21}\boldsymbol{K}_1))^{-1} (\boldsymbol{f}(\boldsymbol{u}_n) + h b_{21} J(\boldsymbol{u}_n)\boldsymbol{f}(\boldsymbol{u}_n) +\\
&\quad + h^2 \left[ b_{21}\alpha_1 J(\boldsymbol{u}_n)^2 \boldsymbol{f}(\boldsymbol{u}_n) + \frac{b_{21}^2}{2} H(\boldsymbol{f}(\boldsymbol{u}_n), \boldsymbol{u}_n)\boldsymbol{f}(\boldsymbol{u}_n) \right] + O(h^3)).
\end{aligned}$$

From (8) and the expression of $\boldsymbol{K}_1$ in (14), we write

$$\begin{aligned}
J(\boldsymbol{u}_n + h\beta_{21}\boldsymbol{K}_1) &= J(\boldsymbol{u}_n) + h\beta_{21} H(\boldsymbol{K}_1, \boldsymbol{u}_n) + O(h^2)\\
&= J(\boldsymbol{u}_n) + h\beta_{21} H(\boldsymbol{f}(\boldsymbol{u}_n), \boldsymbol{u}_n) + O(h^2),
\end{aligned}$$

and the equality in (13) yields

$$\begin{aligned}
(I - \alpha_2 h J(\boldsymbol{u}_n + h\beta_{21}\boldsymbol{K}_1))^{-1} &= I + \alpha_2 h J(\boldsymbol{u}_n + h\beta_{21}\boldsymbol{K}_1) + \alpha_2^2 h^2 J(\boldsymbol{u}_n + h\beta_{21}\boldsymbol{K}_1)^2 + O(h^3)\\
&= I + \alpha_2 h J(\boldsymbol{u}_n) + \alpha_2 h^2 \beta_{21} H(\boldsymbol{f}(\boldsymbol{u}_n), \boldsymbol{u}_n) + \alpha_2^2 h^2 J(\boldsymbol{u}_n)^2 + O(h^3).
\end{aligned}$$

Then, we have

$$\begin{aligned}
\boldsymbol{K}_2 &= \left(I + \alpha_2 h J(\boldsymbol{u}_n) + \alpha_2 h^2 \beta_{21} H(\boldsymbol{f}(\boldsymbol{u}_n), \boldsymbol{u}_n) + \alpha_2^2 h^2 J(\boldsymbol{u}_n)^2 + O(h^3)\right) \times\\
&\quad \times \left( \boldsymbol{f}(\boldsymbol{u}_n) + h b_{21} J(\boldsymbol{u}_n)\boldsymbol{f}(\boldsymbol{u}_n) + h^2 \left[ b_{21}\alpha_1 J(\boldsymbol{u}_n)^2 \boldsymbol{f}(\boldsymbol{u}_n) + \frac{b_{21}^2}{2} H(\boldsymbol{f}(\boldsymbol{u}_n), \boldsymbol{u}_n)\boldsymbol{f}(\boldsymbol{u}_n) \right] + O(h^3) \right)\\
&= \boldsymbol{f}(\boldsymbol{u}_n) + h\left[b_{21} + \alpha_2\right] J(\boldsymbol{u}_n)\boldsymbol{f}(\boldsymbol{u}_n) +\\
&\quad + h^2 \left[ (b_{21}(\alpha_1 + \alpha_2) + \alpha_2^2) J(\boldsymbol{u}_n)^2 f(\boldsymbol{u}_n) + (\frac{b_{21}^2}{2} + \alpha_2\beta_{21}) H(\boldsymbol{f}(\boldsymbol{u}_n), \boldsymbol{u}_n)\boldsymbol{f}(\boldsymbol{u}_n) \right] + O(h^3).
\end{aligned} \tag{15}$$

Analogously, from (7) for $\boldsymbol{f}(\boldsymbol{u}_n + h b_{31}\boldsymbol{K}_1 + h b_{32}\boldsymbol{K}_2)$ and by using the expressions of $\boldsymbol{K}_1$ and $\boldsymbol{K}_2$ in (14) and (15) respectively, and, in addition, from the Neumann Lemma (13) with the expressions (14) and (15) again, we can write

$$\begin{aligned}
\boldsymbol{K}_3 &= \boldsymbol{f}(\boldsymbol{u}_n) + h\left[b_{31} + b_{32} + \alpha_3\right] J(\boldsymbol{u}_n)\boldsymbol{f}(\boldsymbol{u}_n) +\\
&\quad + h^2 \left[b_{31}\alpha_1 + b_{32}(b_{21} + \alpha_2) + \alpha_3^2 + \alpha_3(b_{21} + \alpha_2)\right] J(\boldsymbol{u}_n)^2 \boldsymbol{f}(\boldsymbol{u}_n) +\\
&\quad + h^2 \left[ \frac{1}{2}(b_{31} + b_{32})^2 + \alpha_3(\beta_{31} + \beta_{32}) \right] H(\boldsymbol{f}(\boldsymbol{u}_n), \boldsymbol{u}_n)\boldsymbol{f}(\boldsymbol{u}_n) + O(h^3).
\end{aligned} \tag{16}$$

[4]By inversion of a matrix we do not mean the actual matrix inversion. What is required is the solution of a system of algebraic linear equations that can be realized by factorization methods or by iterative methods.

By substituting the expression (14) of $\boldsymbol{K}_1$ and (15) of $\boldsymbol{K}_2$ in the method (3) we obtain for $q = 2$

$$\boldsymbol{u}_{n+1} = \boldsymbol{u}_n + h\tilde{e}_1 \boldsymbol{f}(\boldsymbol{u}_n) + h^2 \tilde{e}_2 J(\boldsymbol{u}_n)\boldsymbol{f}(\boldsymbol{u}_n) + h^3 \left[\tilde{e}_3 J(\boldsymbol{u}_n)^2 f(\boldsymbol{u}_n) + \tilde{e}_4 H(\boldsymbol{f}(\boldsymbol{u}_n), \boldsymbol{u}_n)\boldsymbol{f}(\boldsymbol{u}_n)\right] + O(h^4), \qquad (17)$$

where the coefficients $\tilde{e}_1$, $\tilde{e}_2$, $\tilde{e}_3$ and $\tilde{e}_4$ have the expressions

$$\begin{aligned} \tilde{e}_1 &= c_1 + c_2; \\ \tilde{e}_2 &= c_1\alpha_1 + c_2(b_{21} + \alpha_2); \\ \tilde{e}_3 &= c_1\alpha_1^2 + c_2 b_{21}(\alpha_1 + \alpha_2) + c_2\alpha_2^2; \\ \tilde{e}_4 &= \frac{c_2 b_{21}^2}{2} + c_2\alpha_2\beta_{21}; \end{aligned} \qquad (18)$$

and, for $q = 3$

$$\boldsymbol{u}_{n+1} = \boldsymbol{u}_n + h e_1 \boldsymbol{f}(\boldsymbol{u}_n) + h^2 e_2 J(\boldsymbol{u}_n)\boldsymbol{f}(\boldsymbol{u}_n) + h^3 \left[e_3 J(\boldsymbol{u}_n)^2 f(\boldsymbol{u}_n) + e_4 H(\boldsymbol{f}(\boldsymbol{u}_n), \boldsymbol{u}_n)\boldsymbol{f}(\boldsymbol{u}_n)\right] + O(h^4), \qquad (19)$$

where the coefficients $e_1$, $e_2$, $e_3$ and $e_4$ have the expressions

$$\begin{aligned} e_1 &= c_1 + c_2 + c_3; \\ e_2 &= c_1\alpha_1 + c_2(b_{21} + \alpha_2) + c_3(b_{31} + b_{32} + \alpha_3); \\ e_3 &= c_1\alpha_1^2 + c_2 b_{21}(\alpha_1 + \alpha_2) + c_2\alpha_2^2 + c_3 b_{31}\alpha_1 + c_3 b_{32}(b_{21} + \alpha_2) + c_3\alpha_3^2 + c_3\alpha_3(b_{21} + \alpha_2); \\ e_4 &= \frac{c_2 b_{21}^2}{2} + c_2\alpha_2\beta_{21} + \frac{c_3}{2}(b_{31} + b_{32})^2 + c_3\alpha_3(\beta_{31} + \beta_{32}). \end{aligned} \qquad (20)$$

In order that the two-stage Runge-Kutta method (3)–(4) (with $q = 2$) has order three, we have to compare (17) with (12); then the coefficients in (18) should satisfy the conditions

$$\tilde{e}_1 = 1; \quad \tilde{e}_2 = \frac{1}{2}; \quad \tilde{e}_3 = \frac{1}{6}; \quad \tilde{e}_4 = \frac{1}{6}. \qquad (21)$$

Two-stage, third order semi-implicit Runge-Kutta schemes that have enjoyed great popularity are Rosenbrock's formula ([26]) where the coefficients are

$$\alpha_1 = 1 + \frac{\sqrt{6}}{6}; \qquad \alpha_2 = 1 - \frac{\sqrt{6}}{6}; \qquad b_{21} = \beta_{21} = \frac{-6 - \sqrt{6} + \sqrt{58 + 20\sqrt{6}}}{6 + 2\sqrt{6}} \simeq 0.17378667;$$

$$c_2 = \frac{\frac{\sqrt{6}}{6} + \frac{1}{2}}{2\frac{\sqrt{6}}{6} - b_{21}}; \qquad c_1 = 1 - c_2,$$

and Calahan's formula ([14]) where the coefficients are

$$\alpha_1 = \alpha_2 = \frac{3 + \sqrt{3}}{6}; \qquad b_{21} = -\frac{2}{\sqrt{3}}; \qquad \beta_{21} = 0; \quad c_1 = \frac{3}{4}; \qquad c_2 = \frac{1}{4}.$$

Analogously, by comparing (19) with (12), the three-stage Runge-Kutta method (3)–(4) (with $q = 3$) has order three if we choose

$$e_1 = 1; \quad e_2 = \frac{1}{2}; \quad e_3 = \frac{1}{6}; \quad e_4 = \frac{1}{6}. \qquad (22)$$

In the next three sections the stability of two- and three-stage semi-implicit Runge-Kutta methods of order three is analysed.

# 3 A-stability for two-stage semi-implicit Runge-Kutta methods of order three

Now we wish to study the stability of the Rosenbrock procedure (3)–(4) when $q = 2$.
We recall that a method is called A-stable if and only if $|u_{n+1}/u_n| = |R(z)| \leq 1$, $z = h\lambda$, when the method is applied with any positive step size $h$ to the scalar equation $u'(t) = \lambda u(t)$, where $\lambda$ is a complex constant with non positive real part, i.e., $\Re(z) \leq 0$ (e.g., [18, p. 74]).
The term $R(z)$ is called the stability function.
Furthermore, a method is called L-stable if it is A-stable and $|R(z)| \to 0$ as $z \to -\infty$ (e.g., [20, p. 237]).
Let us consider the two-stage semi-implicit Runge-Kutta method (3)–(4) applied to the scalar equation

$$u'(t) = \lambda u(t). \tag{23}$$

Here, $m = 1$. We have,

$$u_{n+1} = u_n + hc_1K_1 + hc_2K_2,$$

with

$$K_1 = \frac{\lambda u_n}{1 - \alpha_1 h\lambda}; \qquad K_2 = \frac{\lambda(u_n + hb_{21}K_1)}{1 - \alpha_2 h\lambda} = \left(\lambda u_n + b_{21}\frac{h\lambda^2}{1 - \alpha_1 h\lambda}u_n\right)/(1 - \alpha_2 h\lambda),$$

differently written,

$$K_1 = \frac{\lambda}{1 - \alpha_1 z}u_n; \qquad K_2 = \frac{\lambda}{(1 - \alpha_1 z)(1 - \alpha_2 z)}(1 + (b_{21} - \alpha_1)z)u_n,$$

and then,

$$\begin{aligned} \frac{u_{n+1}}{u_n} &= 1 + c_1\frac{z}{1 - \alpha_1 z} + c_2\frac{z(1 + (b_{21} - \alpha_1)z)}{(1 - \alpha_1 z)(1 - \alpha_2 z)} \\ &= \frac{1 + (c_1 + c_2 - (\alpha_1 + \alpha_2))z + (\alpha_1\alpha_2 - c_1\alpha_2 - c_2\alpha_1 + c_2b_{21})z^2}{1 - (\alpha_1 + \alpha_2)z + \alpha_1\alpha_2 z^2}. \end{aligned} \tag{24}$$

In order that the two-stage semi-implicit Runge-Kutta method has order three, conditions (21) should be satisfied. For the problem (23), the formula (17) becomes

$$u_{n+1} = u_n + h\lambda\tilde{e}_1 u_n + h^2\lambda^2\tilde{e}_2 u_n + h^3\left[\lambda^3\tilde{e}_3 u_n + 0 \cdot \tilde{e}_4\right] + O(h^4),$$

and conditions (18) and (21) are

$$c_1 + c_2 = 1; \tag{25}$$

$$c_2 b_{21} = \frac{1}{2} - c_1\alpha_1 - c_2\alpha_2; \tag{26}$$

$$c_1\alpha_1^2 + c_2b_{21}(\alpha_1 + \alpha_2) + c_2\alpha_2^2 = \frac{1}{6} \qquad \Longrightarrow \qquad \left(\frac{1}{2} - c_2\alpha_2\right)\alpha_1 + \left(\frac{1}{2} - c_1\alpha_1\right)\alpha_2 = \frac{1}{6}.$$

The last (third) equation can be written

$$\frac{1}{2}(\alpha_1 + \alpha_2) - \alpha_1\alpha_2 = \frac{1}{6}. \tag{27}$$

By using (25) and (26), the coefficient of $z^2$ of the numerator in the last expression of (24) can be written

$$\begin{aligned} \alpha_1\alpha_2 - c_1\alpha_2 - c_2\alpha_1 + c_2b_{21} &= \alpha_1\alpha_2 - c_1\alpha_2 - c_2\alpha_1 + \frac{1}{2} - c_1\alpha_1 - c_2\alpha_2 = \\ &= \alpha_1\alpha_2 - c_1(\alpha_1 + \alpha_2) - c_2(\alpha_1 + \alpha_2) + \frac{1}{2} = \alpha_1\alpha_2 - (\alpha_1 + \alpha_2) + \frac{1}{2}. \end{aligned}$$

Then,

$$\frac{u_{n+1}}{u_n} = R(z) \equiv \frac{P(z)}{Q(z)} = \frac{1+(1-(\alpha_1+\alpha_2))z+(\alpha_1\alpha_2-(\alpha_1+\alpha_2)+\frac{1}{2})z^2}{1-(\alpha_1+\alpha_2)z+\alpha_1\alpha_2 z^2}.$$

For sufficiently small values of $z$, from the infinite geometric series, we have

$$\begin{aligned}
\frac{u_{n+1}}{u_n} &= \left[1+(1-(\alpha_1+\alpha_2))z+(\alpha_1\alpha_2-(\alpha_1+\alpha_2)+\frac{1}{2})z^2\right][1+((\alpha_1+\alpha_2)z-\alpha_1\alpha_2 z^2)+ \\
&\quad +((\alpha_1+\alpha_2)z+\alpha_1\alpha_2 z^2)^2+((\alpha_1+\alpha_2)z+\alpha_1\alpha_2 z^2)^3+...] \\
&= \left[1+(1-(\alpha_1+\alpha_2))z+(\alpha_1\alpha_2-(\alpha_1+\alpha_2)+\frac{1}{2})z^2\right][1+(\alpha_1+\alpha_2)z+((\alpha_1+\alpha_2)^2-\alpha_1\alpha_2)z^2+ \\
&\quad +((\alpha_1+\alpha_2)^3-2\alpha_1\alpha_2(\alpha_1+\alpha_2))z^3+O(z^4)] \\
&= 1+(\alpha_1+\alpha_2)z+((\alpha_1+\alpha_2)^2-\alpha_1\alpha_2)z^2+((\alpha_1+\alpha_2)^3-2\alpha_1\alpha_2(\alpha_1+\alpha_2))z^3+ \\
&\quad +(1-(\alpha_1+\alpha_2))z+(1-(\alpha_1+\alpha_2))(\alpha_1+\alpha_2)z^2+(1-(\alpha_1+\alpha_2))((\alpha_1+\alpha_2)^2-\alpha_1\alpha_2)z^3+ \\
&\quad +(\alpha_1\alpha_2-(\alpha_1+\alpha_2)+\frac{1}{2})z^2+(\alpha_1\alpha_2-(\alpha_1+\alpha_2)+\frac{1}{2})(\alpha_1+\alpha_2)z^3+O(z^4) \\
&= 1+z+\frac{1}{2}z^2+(\frac{1}{2}(\alpha_1+\alpha_2)-\alpha_1\alpha_2)z^3+O(z^4).
\end{aligned}$$

From (27), we have

$$\frac{u_{n+1}}{u_n} = 1+z+\frac{1}{2}z^2+\frac{1}{6}z^3+O(z^4).$$

that is the stability function $R(z)$ of the method approximates the exponential function $e^z$.
Since the two-stage semi-implicit Runge-Kutta method (3) of order three

$$u_{n+1} = \frac{P(z)}{Q(z)}u_n,$$

has the polynomials $P(z)$ and $Q(z)$ of the same degree, then by the well known result of Birkhoff and Varga (1965, e.g., [20, p. 237]), the method is A-stable.
Furthermore we see that a two-stage semi-implicit Runge-Kutta method of order three can not be L-stable.[5]
Indeed, by the well known result of Ehle (1969, e.g., [20, p. 237]), the polynomial $P(z)$ must have degree equal to one. That is, condition

$$\alpha_1\alpha_2-(\alpha_1+\alpha_2)+\frac{1}{2}=0, \tag{28}$$

or taking into account of formula (24), the condition

$$\alpha_1\alpha_2-c_1\alpha_2-c_2\alpha_1+c_2b_{21}=0,$$

holds. By adding this last condition to (18) and (21), we have the nonlinear system

$$\begin{cases} c_1+c_2=1 \\ c_1\alpha_1+c_2(b_{21}+\alpha_2)=\frac{1}{2} \\ c_1\alpha_1^2+c_2b_{21}(\alpha_1+\alpha_2)+c_2\alpha_2^2=\frac{1}{6} \\ \frac{c_2b_{21}^2}{2}+c_2\alpha_2\beta_{21}=\frac{1}{6} \\ \alpha_1\alpha_2-c_1\alpha_2-c_2\alpha_1+c_2b_{21}=0 \end{cases} \tag{29}$$

This nonlinear system does not admit a solution.[6]

[5] In [5, Theor. 2] is proved that the order of an L-stable, $q$-stage semi-implicit Runge-Kutta method is at most $q$.
[6] Indeed, setting $x=\alpha_1\alpha_2$ and $y=\alpha_1+\alpha_2$, the third equation of (29) can be written as (27)

$$\frac{1}{2}y-x=\frac{1}{6},$$

# 4 A-stability and L-stability for three-stage semi-implicit Runge-Kutta methods of order three

Let us consider the Rosenbrock procedure (3)–(4) when $q = 3$, applied to the scalar equation (23)

$$u'(t) = \lambda u(t).$$

Here, $m = 1$. We have,

$$u_{n+1} = u_n + hc_1K_1 + hc_2K_2 + hc_3K_3,$$

with

$$K_1 = \frac{\lambda u_n}{1-\alpha_1 h\lambda}; \qquad K_2 = \frac{\lambda(u_n + hb_{21}K_1)}{1-\alpha_2 h\lambda} = \left(\lambda + b_{21}\frac{h\lambda^2}{1-\alpha_1 h\lambda}\right) u_n/(1-\alpha_2 h\lambda);$$

$$K_3 = \frac{\lambda(u_n + hb_{31}K_1 + hb_{32}K_2)}{1-\alpha_3 h\lambda} = \frac{\lambda}{1-\alpha_3 h\lambda}\left[1 + b_{31}\frac{\lambda h}{1-\alpha_1 h\lambda} + b_{32}\frac{\lambda h}{1-\alpha_2 h\lambda}\left(1 + b_{21}\frac{\lambda h}{1-\alpha_1 h\lambda}\right)\right] u_n.$$

Set $z = h\lambda$ we have

$$K_1 = \frac{\lambda}{1-\alpha_1 z}u_n; \qquad K_2 = \frac{\lambda}{(1-\alpha_1 z)(1-\alpha_2 z)}(1 + (b_{21}-\alpha_1)z)u_n;$$

$$K_3 = \frac{\lambda}{1-\alpha_3 z}\left[1 + \frac{b_{31}z}{1-\alpha_1 z} + \frac{b_{32}z}{1-\alpha_2 z}\left(1 + b_{21}\frac{z}{1-\alpha_1 z}\right)\right] u_n.$$

By easy calculations we obtain the following expression for $K_3$

$$K_3 = \frac{\lambda\left[1 + (b_{31}+b_{32}-\alpha_1-\alpha_2)z + (b_{32}(b_{21}-\alpha_1) - \alpha_2(b_{31}-\alpha_1))z^2\right]}{(1-\alpha_1 z)(1-\alpha_2 z)(1-\alpha_3 z)}u_n,$$

and then,

$$\begin{aligned}\frac{u_{n+1}}{u_n} &= 1 + c_1\frac{z}{1-\alpha_1 z} + c_2\frac{z(1+(b_{21}-\alpha_1)z)}{(1-\alpha_1 z)(1-\alpha_2 z)} + \\ &+ c_3\frac{z\left[1 + (b_{31}+b_{32}-\alpha_1-\alpha_2)z + (b_{32}(b_{21}-\alpha_1) - \alpha_2(b_{31}-\alpha_1))z^2\right]}{(1-\alpha_1 z)(1-\alpha_2 z)(1-\alpha_3 z)}.\end{aligned}$$

The method can be written as

$$\frac{u_{n+1}}{u_n} = R(z),$$

where $R(z) = P(z)/Q(z)$ with

$$\begin{aligned}Q(z) &= (1-\alpha_1 z)(1-\alpha_2 z)(1-\alpha_3 z) \\ &= 1 - (\alpha_1+\alpha_2+\alpha_3)z + (\alpha_1\alpha_2 + \alpha_1\alpha_3 + \alpha_2\alpha_3)z^2 - \alpha_1\alpha_2\alpha_3 z^3,\end{aligned} \tag{30}$$

and by easy calculations

$$\begin{aligned}P(z) &= 1 + (c_1+c_2+c_3-\alpha_1-\alpha_2-\alpha_3)z + [\alpha_1\alpha_2 + \alpha_1\alpha_3 + \alpha_2\alpha_3 - c_1(\alpha_2+\alpha_3) - \\ &\quad - c_2(\alpha_1+\alpha_3-b_{21}) - c_3(\alpha_1+\alpha_2-b_{31}-b_{32})]\,z^2 + \\ &\quad + [-\alpha_1\alpha_2\alpha_3 + c_1\alpha_2\alpha_3 + c_2\alpha_1\alpha_3 + c_3\alpha_1\alpha_2 - c_2\alpha_3 b_{21} - c_3 b_{31}\alpha_2 - c_3 b_{32}\alpha_1 + c_3 b_{32} b_{21}]\,z^3.\end{aligned} \tag{31}$$

---

and the fifth equation of (29), written as (28), yields

$$x - y = -\frac{1}{2}.$$

This two last equations in $x$ and $y$ produce the solution $x = 1/6$ and $y = 2/3$. Then we have the simple algebraic equation in $\alpha_1$

$$\alpha_1(\frac{2}{3} - \alpha_1) = \frac{1}{6}, \qquad \Longrightarrow \qquad -\alpha_1^2 + \frac{2}{3}\alpha_1 - \frac{1}{6} = 0,$$

that does not admit real solutions.

We observe that the polynomials $P(z)$ and $Q(z)$ has the same degree. Then, in order to have the A-stability of the three-stage semi-implicit Runge-Kutta method of third order, we should have that the stability function $R(z)$ of the method approximates the exponential functions $e^z$ with an error of $O(z^4)$. We must have that the following equality holds

$$P(z) = (1 + z + \frac{z^2}{2} + \frac{z^3}{6})Q(z). \tag{32}$$

The right hand side of (32) becomes

$$\begin{aligned}
&(1 + z + \frac{z^2}{2} + \frac{z^3}{6})(1 - (\alpha_1 + \alpha_2 + \alpha_3)z + (\alpha_1\alpha_2 + \alpha_1\alpha_3 + \alpha_2\alpha_3)z^2 - \alpha_1\alpha_2\alpha_3 z^3) = \\
&= 1 + (1 - \alpha_1 - \alpha_2 - \alpha_3)z + (\frac{1}{2} + \alpha_1\alpha_2 + \alpha_1\alpha_3 + \alpha_2\alpha_3 - \alpha_1 - \alpha_2 - \alpha_3)z^2 + \\
&+(\frac{1}{6} - \alpha_1\alpha_2\alpha_3 + \alpha_1\alpha_2 + \alpha_1\alpha_3 + \alpha_2\alpha_3 - \frac{1}{2}(\alpha_1 + \alpha_2 + \alpha_3))z^3.
\end{aligned} \tag{33}$$

In order that expression in (33) is equal to the one of $P(z)$ in (31) we must have the following conditions given by the coefficients of $z$ and $z^2$:

$$c_1 + c_2 + c_3 = 1, \tag{34}$$

and

$$-c_1(\alpha_2 + \alpha_3) - c_2(\alpha_1 + \alpha_3 - b_{21}) - c_3(\alpha_1 + \alpha_2 - b_{31} - b_{32}) = \frac{1}{2} - \alpha_1 - \alpha_2 - \alpha_3,$$

that, by adding $-c_1\alpha_1 - c_2\alpha_2 - c_3\alpha_3$ and keeping into account of (34), becomes

$$c_1\alpha_1 + c_2(\alpha_2 + b_{21}) + c_3(\alpha_3 + b_{31} + b_{32}) = \frac{1}{2}. \tag{35}$$

The formulae (34) and (35) are the first and the second formula of (20) and (22), that are two conditions in order that the method has order three.
In order to equal the coefficients of $z^3$ of (33) and (31) we must have

$$\begin{aligned}
c_1\alpha_2\alpha_3 + c_2\alpha_1\alpha_3 + c_3\alpha_1\alpha_2 - c_2\alpha_3 b_{21} - c_3 b_{31}\alpha_2 - c_3 b_{32}\alpha_1 + c_3 b_{32} b_{21} \quad = \quad & \frac{1}{6} - \frac{1}{2}(\alpha_1 + \alpha_2 + \alpha_3) + \\
& +\alpha_1\alpha_2 + \alpha_1\alpha_3 + \alpha_2\alpha_3,
\end{aligned}$$

that is

$$\begin{aligned}
-c_2\alpha_3 b_{21} - c_3 b_{31}\alpha_2 - c_3 b_{32}\alpha_1 + c_3 b_{32} b_{21} \quad = \quad & \frac{1}{6} - \frac{1}{2}(\alpha_1 + \alpha_2 + \alpha_3) + \\
& +\alpha_1\alpha_2 + \alpha_1\alpha_3 + \alpha_2\alpha_3 - \\
& -c_1\alpha_2\alpha_3 - c_2\alpha_1\alpha_3 - c_3\alpha_1\alpha_2.
\end{aligned}$$

Since (34), we have

$$\begin{aligned}
-c_2\alpha_3 b_{21} - c_3 b_{31}\alpha_2 - c_3 b_{32}\alpha_1 + c_3 b_{32} b_{21} \quad = \quad & \frac{1}{6} - \frac{1}{2}(\alpha_1 + \alpha_2 + \alpha_3) + \\
& +(\alpha_1\alpha_2 + \alpha_1\alpha_3 + \alpha_2\alpha_3)(c_1 + c_2 + c_3) - \\
& -c_1\alpha_2\alpha_3 - c_2\alpha_1\alpha_3 - c_3\alpha_1\alpha_2,
\end{aligned}$$

and then,

$$\begin{aligned}
-c_2\alpha_3 b_{21} - c_3 b_{31}\alpha_2 - c_3 b_{32}\alpha_1 + c_3 b_{32} b_{21} \quad = \quad & \frac{1}{6} - \frac{1}{2}(\alpha_1 + \alpha_2 + \alpha_3) + \\
& +c_1\alpha_1(\alpha_2 + \alpha_3) + c_2\alpha_2(\alpha_1 + \alpha_3) + c_3\alpha_3(\alpha_1 + \alpha_2).
\end{aligned} \tag{36}$$

Let us consider the second equation of (20) and (22) or equation (35) that can be written

$$c_2 b_{21} + c_3(b_{31} + b_{32}) = \frac{1}{2} - c_1\alpha_1 - c_2\alpha_2 - c_3\alpha_3,$$

and multiplying each term for $\alpha_1 + \alpha_2 + \alpha_3$, we have

$$\begin{aligned} c_2 b_{21}(\alpha_1+\alpha_2+\alpha_3) + c_3 b_{31}(\alpha_1+\alpha_2+\alpha_3) + c_3 b_{32}(\alpha_1+\alpha_2+\alpha_3) &= \frac{1}{2}(\alpha_1+\alpha_2+\alpha_3) - \\ &-c_1\alpha_1(\alpha_1+\alpha_2+\alpha_3) - \\ &-c_2\alpha_2(\alpha_1+\alpha_2+\alpha_3) - \\ &-c_3\alpha_3(\alpha_1+\alpha_2+\alpha_3). \end{aligned} \tag{37}$$

Now, let us consider the third equation of (20) and (22)

$$c_3 b_{32} b_{21} = \frac{1}{6} - c_3\alpha_1 b_{31} - c_3\alpha_2 b_{32} - c_3\alpha_3 b_{21} - c_3\alpha_3\alpha_2 - c_2 b_{21}(\alpha_1+\alpha_2) - c_1\alpha_1^2 - c_2\alpha_2^2 - c_3\alpha_3^2.$$

By adding the term $-c_2\alpha_3 b_{21} - c_3\alpha_2 b_{31} - c_3\alpha_1 b_{32}$ to both the members of the last equation, it becomes

$$\begin{aligned} -c_2\alpha_3 b_{21} - c_3\alpha_2 b_{31} - c_3\alpha_1 b_{32} + c_3 b_{32} b_{21} &= \frac{1}{6} - c_2 b_{21}(\alpha_1+\alpha_2+\alpha_3) - \\ &-c_3 b_{32}(\alpha_1+\alpha_2) - c_3 b_{31}(\alpha_1+\alpha_2) - \\ &-c_3 b_{21}\alpha_3 - c_3\alpha_2\alpha_3 - c_1\alpha_1^2 - c_2\alpha_2^2 - c_3\alpha_3^2. \end{aligned} \tag{38}$$

The right hand side of (38) can be written

$$\begin{aligned} &\frac{1}{6} - c_2 b_{21}(\alpha_1+\alpha_2+\alpha_3) - c_3 b_{32}(\alpha_1+\alpha_2+\alpha_3) + c_3 b_{32}\alpha_3 - c_3 b_{31}(\alpha_1+\alpha_2+\alpha_3) + c_3 b_{31}\alpha_3 - \\ &\quad -c_3 b_{21}\alpha_3 - c_3\alpha_2\alpha_3 - c_1\alpha_1^2 - c_2\alpha_2^2 - c_3\alpha_3^2, \end{aligned}$$

and by (37), this last expression can be written as

$$\begin{aligned} &\frac{1}{6} - \frac{1}{2}(\alpha_1+\alpha_2+\alpha_3) + c_1\alpha_1(\alpha_1+\alpha_2+\alpha_3) + c_2\alpha_2(\alpha_1+\alpha_2+\alpha_3) + c_3\alpha_3(\alpha_1+\alpha_2+\alpha_3) + \\ &\quad +c_3 b_{32}\alpha_3 + c_3 b_{31}\alpha_3 - c_3 b_{21}\alpha_3 - c_3\alpha_2\alpha_3 - c_1\alpha_1^2 - c_2\alpha_2^2 - c_3\alpha_3^2, \end{aligned}$$

that is equal to

$$\begin{aligned} &\frac{1}{6} - \frac{1}{2}(\alpha_1+\alpha_2+\alpha_3) + c_1\alpha_1(\alpha_1+\alpha_2) + c_2\alpha_2(\alpha_1+\alpha_3) + c_3\alpha_3(\alpha_1+\alpha_2) + \\ &\quad +c_3\alpha_3(b_{32} + b_{31} - b_{21} - \alpha_2). \end{aligned} \tag{39}$$

Then, from (39), we have that (38), i.e., the third equation of (20) and (22), $e_3 = 1/6$, is

$$\begin{aligned} -c_2\alpha_3 b_{21} - c_3\alpha_2 b_{31} - c_3\alpha_1 b_{32} + c_3 b_{32} b_{21} &= \frac{1}{6} - \frac{1}{2}(\alpha_1+\alpha_2+\alpha_3) + \\ &+c_1\alpha_1(\alpha_1+\alpha_2) + c_2\alpha_2(\alpha_1+\alpha_3) + \\ &+c_3\alpha_3(\alpha_1+\alpha_2) + c_3\alpha_3(b_{32} + b_{31} - b_{21} - \alpha_2), \end{aligned}$$

and this is equivalent to equation (36), if and only if the condition

$$c_3\alpha_3(b_{32} + b_{31} - b_{21} - \alpha_2) = 0, \tag{40}$$

holds.

Thus, in order that the three-stage semi-implicit Runge-Kutta method has order three and be A-stable, the conditions (20) and (22) and (40) must be satisfied, i.e.,

$$\left\{ \begin{array}{rcl} c_1 + c_2 + c_3 &=& 1; \\ c_1\alpha_1 + c_2(b_{21}+\alpha_2) + c_3(b_{31} + b_{32} + \alpha_3) &=& 1/2; \\ c_1\alpha_1^2 + c_2 b_{21}(\alpha_1+\alpha_2) + c_2\alpha_2^2 + c_3 b_{31}\alpha_1 + c_3 b_{32}(b_{21}+\alpha_2) + c_3\alpha_3^2 + c_3\alpha_3(b_{21}+\alpha_2) &=& 1/6; \\ \frac{c_2 b_{21}^2}{2} + c_2\alpha_2\beta_{21} + \frac{c_3}{2}(b_{31}+b_{32})^2 + c_3\alpha_3(\beta_{31}+\beta_{32}) &=& 1/6; \\ c_3\alpha_3(b_{32} + b_{31} - b_{21} - \alpha_2) &=& 0. \end{array} \right.$$

# 5 A three-stage semi-implicit Runge-Kutta method

## 5.1 Conditions for order three and for A-stability

When we consider the Rosenbrock procedure (3)–(4) with $q = 3$, because of the expression of $\boldsymbol{K}_1$, $\boldsymbol{K}_2$ and $\boldsymbol{K}_3$

$$\begin{aligned}
\boldsymbol{K}_1 &= (I - \alpha_1 hJ(\boldsymbol{u}_n))^{-1}\boldsymbol{f}(\boldsymbol{u}_n);\\
\boldsymbol{K}_2 &= (I - \alpha_2 hJ(\boldsymbol{u}_n + h\beta_{21}\boldsymbol{K}_1))^{-1}\boldsymbol{f}(\boldsymbol{u}_n + hb_{21}\boldsymbol{K}_1);\\
\boldsymbol{K}_3 &= (I - \alpha_3 hJ(\boldsymbol{u}_n + h\beta_{31}\boldsymbol{K}_1 + \beta_{32}\boldsymbol{K}_2))^{-1}\boldsymbol{f}(\boldsymbol{u}_n + hb_{31}\boldsymbol{K}_1 + hb_{32}\boldsymbol{K}_2);
\end{aligned}$$

at each time step $t_n$, we have to solve three linear systems where the coefficient matrix is the Jacobian evaluated at three different points.
Hence, we may measure the computational efficiency of a method in terms of:

(i) number of Jacobian evaluations;

(ii) number of matrix factorizations;[7]

(iii) number of functional evaluations.

Then, it is desirable to develop methods which are computationally efficient and yet maintain maximum accuracy.
We see a three-stage semi-implicit Runge-Kutta method of order three that requires only one Jacobian evaluation and then, only one factorization matrix, and three functional evaluation at each time step $t_n$.
As the Calahan's formulae for two-stage semi-implicit Runge-Kutta methods, we consider a method ([4]) where

$$\alpha \equiv \alpha_1 = \alpha_2 = \alpha_3, \qquad \beta_{21} = \beta_{31} = \beta_{32} = 0.$$

In this case, the formulae (20) and (22) to have a method of order three, become

$$\begin{aligned}
c_1 + c_2 + c_3 &= 1;\\
c_2 b_{21} + c_3(b_{31} + b_{32}) &= \frac{1}{2} - \alpha;\\
c_3 b_{21} b_{32} &= \frac{1}{6} - \alpha^2 - c_3\alpha^2 - (c_2 b_{21} + c_3(b_{31} + b_{32}))\alpha - b_{21}(c_2 + c_3)\alpha \qquad (41)\\
&= \frac{1}{6} - (\frac{1}{2} + b_{21}(c_2 + c_3))\alpha - c_3\alpha^2;\\
c_2\frac{b_{21}^2}{2} + c_3\frac{1}{2}(b_{31} + b_{32})^2 &= \frac{1}{6}.
\end{aligned}$$

Furthermore, from the expression of $P(z)$ in (31), we can write

$$\begin{aligned}
P(z) &= 1 + (1 - 3\alpha)z + \left[3\alpha^2 - c_1 2\alpha - c_2(2\alpha - b_{21}) - c_3(2\alpha - b_{31} - b_{32})\right] z^2 + \\
&\quad + \left[-\alpha^3 + \alpha^2 - c_2\alpha b_{21} + c_3 b_{21} b_{32} - c_3\alpha(b_{31} + b_{32})\right] z^3. \qquad (42)
\end{aligned}$$

Keeping into account the first and the second equation of (41), the coefficient of $z^2$ in (42) becomes

$$3\alpha^2 - 3\alpha + \frac{1}{2}. \qquad (43)$$

Keeping into account the second and the third equation of (41), the coefficient of $z^3$ in (42) becomes

$$-\alpha^3 + (2 - c_3)\alpha^2 - (1 + b_{21}(c_2 + c_3))\alpha + \frac{1}{6}. \qquad (44)$$

[7] We consider to solve the linear algebraic system, whose coefficient matrix is the Jacobian, by factorization methods as Gaussian elimination method.

From the second equation of (41), we can write

$$-\alpha c_2 b_{21} = -\frac{\alpha}{2} + \alpha^2 + \alpha c_3(b_{31} + b_{32}),$$

then, the expression (44) becomes

$$-\alpha^3 + 3\alpha^2 - \frac{3}{2}\alpha + \frac{1}{6} + c_3\alpha(b_{31} + b_{32} - b_{21} - \alpha).$$

If we require that the condition for the A-stability (40) holds, i.e.,

$$c_3\alpha(b_{32} + b_{31} - b_{21} - \alpha) = 0,$$

then, the coefficient of $z^3$ becomes

$$-\alpha^3 + 3\alpha^2 - \frac{3}{2}\alpha + \frac{1}{6}. \tag{45}$$

This value for the coefficient of $z^3$ can be also obtained if, in the expression (44), we require

$$\begin{cases} 2 - c_3 &= 3; \\ 1 + b_{21}(c_2 + c_3) &= 3/2. \end{cases} \tag{46}$$

### 5.2 Computation of the coefficients

We compute the coefficients of the method in terms of the parameter $\alpha$.
Let us consider the conditions (41) and (46):

$$\begin{aligned} c_1 + c_2 + c_3 &= 1; \\ c_2 b_{21} + c_3(b_{31} + b_{32}) &= \frac{1}{2} - \alpha; \\ c_3 b_{21} b_{32} &= \frac{1}{6} - (\frac{1}{2} + b_{21}(c_2 + c_3))\alpha - c_3\alpha^2; \\ c_2\frac{b_{21}^2}{2} + c_3\frac{1}{2}(b_{31} + b_{32})^2 &= \frac{1}{6}; \\ 2 - c_3 &= 3; \\ 1 + b_{21}(c_2 + c_3) &= 3/2. \end{aligned} \tag{47}$$

From the fifth equation of (47), we obtain

$$c_3 = -1. \tag{48}$$

From the sixth equation of (47) and keeping into account of (48), we have

$$c_2 b_{21} = \frac{1}{2} + b_{21}. \tag{49}$$

From the first equation of (47) and keeping into account of (48), we have

$$c_1 + c_2 = 2. \tag{50}$$

From the second equation of (47) and keeping into account of (48) and (49), we have

$$b_{31} + b_{32} = b_{21} + \alpha. \tag{51}$$

From the third equation of (47) and keeping into account of (48) and (49), we have

$$-b_{32} b_{21} = \frac{1}{6} - \alpha + \alpha^2. \tag{52}$$

Multiplying by 2 the fourth equation of (47) and keeping into account of (48) and (51), we have

$$b_{21}\left[c_2 b_{21} - b_{21} - 2\alpha\right] = \frac{1}{3} + \alpha^2. \tag{53}$$

From (53) and keeping into account of (49), we have

$$b_{21} = (\frac{1}{3} + \alpha^2)/(\frac{1}{2} - 2\alpha). \tag{54}$$

Then, from (49) and keeping into account of (54), we have

$$c_2 = 1 + \frac{1}{2b_{21}} = 1 + \frac{\frac{1}{2} - 2\alpha}{2(\frac{1}{3} + \alpha^2)}. \tag{55}$$

Then, from (50) and keeping into account of (55), we have

$$c_1 = 2 - c_2 = 1 - \frac{\frac{1}{2} - 2\alpha}{2(\frac{1}{3} + \alpha^2)}. \tag{56}$$

Then, from (52) and keeping into account of (54), we have

$$b_{32} = \frac{1}{b_{21}}(-\frac{1}{6} + \alpha - \alpha^2) = \frac{\frac{1}{2} - 2\alpha}{\frac{1}{3} + \alpha^2}(-\frac{1}{6} + \alpha - \alpha^2). \tag{57}$$

and then, the value of $b_{31}$ is obtained from (51) keeping into account of (54) and (57), i.e.,

$$b_{31} = b_{21} + \alpha - b_{32} = \frac{-\alpha^2 + \frac{1}{2}\alpha + \frac{1}{3}}{\frac{1}{2} - 2\alpha} - \left(\frac{\frac{1}{2} - 2\alpha}{\frac{1}{3} + \alpha^2}(-\frac{1}{6} + \alpha - \alpha^2)\right). \tag{58}$$

### 5.3 Values of $\alpha$ for stability

In this subsection we determine the value of $\alpha$ to have an A-stable method of order three. Let us consider the scalar problem (23), we write the semi-implicit Runge-Kutta method, with the coefficients determined as in the previous subsection, as

$$u_{n+1} = R(z)u_n,$$

and we want that the function $R(z)$ is an A-acceptable (A-stable) approximation of the third order of $e^z$, i.e.,

$$e^z = R(z) + O(z^4),$$

and $|R(z)| \leq 1$ for $\Re(z) \leq 0$.
We have (see (42) with (43), (45) and see (30))

$$R(z) \equiv \frac{P(z)}{Q(z)} = \frac{1 + (1 - 3\alpha)z + (3\alpha^2 - 3\alpha + \frac{1}{2})z^2 + (-\alpha^3 + 3\alpha^2 - \frac{3}{2}\alpha + \frac{1}{6})z^3}{(1 - \alpha z)^3}.$$

It is straightforward to show that $|R(z)| \leq 1$ for $\Re(z) = 0$ and since $|R(z)|$ is analytic in $\Re(z) \leq 0$, it is concluded that $|R(z)| \leq 1$ for $\Re(z) \leq 0$ due to the maximum modulus theorem (e.g., [3, §16.17]).
Set $z = \xi + i\eta$, we choose the values of $\alpha$ in order to have $R(i\eta)$ strictly bounded in modulus by 1, i.e.,

$$|R(i\eta)| < 1.$$

Then,

$$\begin{aligned} R(i\eta) &= \frac{1 + i(1 - 3\alpha)\eta - (3\alpha^2 - 3\alpha + \frac{1}{2})\eta^2 + i(\alpha^3 - 3\alpha^2 + \frac{3}{2}\alpha - \frac{1}{6})\eta^3}{1 - i3\alpha\eta - 3\alpha^2\eta^2 + i\alpha^3\eta^3} \\ &= \frac{[1 - (3\alpha^2 - 3\alpha + \frac{1}{2})\eta^2] + i[(1 - 3\alpha)\eta + (\alpha^3 - 3\alpha^2 + \frac{3}{2}\alpha - \frac{1}{6})\eta^3]}{(1 - 3\alpha^2\eta^2) - i(3\alpha\eta - \alpha^3\eta^3)}. \end{aligned}$$

Thus, we can obtain

$$
\begin{aligned}
|R(i\eta)|^2 &= \frac{[1-(3\alpha^2-3\alpha+\frac{1}{2})\eta^2]^2+[(1-3\alpha)\eta+(\alpha^3-3\alpha^2+\frac{3}{2}\alpha-\frac{1}{6})\eta^3]^2}{(1-3\alpha^2\eta^2)^2+(3\alpha\eta-\alpha^3\eta^3)^2} \\
&= \frac{1}{1+3\alpha^2\eta^2+3\alpha^4\eta^4+\alpha^6\eta^6}\Bigg[1+3\alpha^2\eta^2+(3\alpha^4+2\alpha^3-3\alpha^2+\alpha-\frac{1}{12})\eta^4+ \\
&\quad +(\alpha^3-3\alpha^2+\frac{3}{2}\alpha-\frac{1}{6})^2\eta^6\Bigg].
\end{aligned} \tag{59}
$$

For $\alpha = 1$ we have $|R(i\eta)| < 1$ then, $R(z)$ is an A-acceptable approximation of $e^z$.
Thus, from (48) and (54)–(58), a three-stage semi-implicit Runge-Kutta method of order three and A-stable is given by the coefficients

$$
\begin{aligned}
&\alpha = 1; \quad b_{21} = -8/9; \quad b_{31} = -11/144; \quad b_{32} = 3/16; \\
&c_1 = 7/16; \quad c_2 = 25/16; \quad c_3 = -1.
\end{aligned}
$$

Now, we require that $R(z)$ is a third order, L-acceptable (L-stable) approximation of $e^z$. Then, we have to choose the parameter $\alpha$ in such a way that the coefficient of $z^3$ of $P(z)$ is equal to zero.
From (45) we should have for positive values of $\alpha$

$$
-(\alpha^3-3\alpha^2+\frac{3}{2}\alpha-\frac{1}{6}) = 0. \tag{60}
$$

Formula (60) is the condition for the L-stability of the method.
This last equation can be written in the form

$$
-\alpha^3\left(1-3\frac{1}{\alpha}+\frac{3}{2}\left(\frac{1}{\alpha}\right)^2-\frac{1}{6}\left(\frac{1}{\alpha}\right)^3\right) = 0.
$$

Since $L_3(x) = 1-3x+3/2x^2-1/6x^3$ is the Laguerre orthogonal polynomial of third degree (e.g., see [17, p. 39]), we have to choose the parameter $\alpha$ equal to the reciprocal of a zero of this polynomial.
Among the three zeros of the Laguerre polynomial $L_3(x)$ we choose the one such that the condition $|R(i\eta)| < 1$ is satisfied.
From formula (59) we have

$$
|R(i\eta)|^2 = \frac{1+3\alpha^2\eta^2+(3\alpha^4+2\alpha^3-3\alpha^2+\alpha-\frac{1}{12})\eta^4+(\alpha^3-3\alpha^2+\frac{3}{2}\alpha-\frac{1}{6})^2\eta^6}{1+3\alpha^2\eta^2+3\alpha^4\eta^4+\alpha^6\eta^6}.
$$

If $1/\alpha$ is a zero of Laguerre polynomial, then the coefficient of $\eta^6$ of the numerator is equal to zero.
In order that $|R(i\eta)|^2 < 1$, the coefficient of $\eta^4$ of the numerator should be less than the one of the denominator; that is

$$
3\alpha^4+2\alpha^3-3\alpha^2+\alpha-\frac{1}{12} < 3\alpha^4,
$$

or,

$$
2\alpha^3-3\alpha^2+\alpha-\frac{1}{12} < 0. \tag{61}
$$

Since the L-stability condition (60) holds, we have

$$
\alpha^3 = 3\alpha^2-\frac{3}{2}\alpha+\frac{1}{6}.
$$

By replacing the value of $\alpha^3$ of the last formula in (61), we have

$$
2(3\alpha^2-\frac{3}{2}\alpha+\frac{1}{6})-3\alpha^2+\alpha-\frac{1}{12} < 0,
$$

that is

$$3\alpha^2 - 2\alpha + \frac{1}{4} < 0.$$

This last inequality is satisfied for values of $\alpha$ in the interval $(1/6, 1/2)$.
The roots of Laguerre polynomial of third degree $L_3(x)$ are

$$x_1 = 0.415774... \qquad x_2 = 2.294280... \qquad x_3 = 6.289945$$

Then, the value for $\alpha$ is

$$\alpha = \frac{1}{x_2} = 0.4358665216...$$

Thus, from (48) and (54)–(58), a three-stage semi-implicit Runge-Kutta method of order three and L-stable is given by the coefficients:

$$\alpha = 0.4358665216; \qquad b_{21} = (\frac{1}{3} + \alpha^2)/(\frac{1}{2} - 2\alpha);$$
$$c_3 = -1; \qquad c_2 = 1 + \frac{1}{2b_{21}}; \qquad c_1 = 2 - c_2;$$
$$b_{32} = \frac{1}{b_{21}}(-\frac{1}{6} + \alpha - \alpha^2); \qquad b_{31} = b_{21} + \alpha - b_{32}.$$

## 5.4 A fourth order semi-implicit method of Bui

We include, here, a subsection where we recall a forth order, four-stage semi-implicit Runge-Kutta method presented in the papers [4] and [6] (see also [5]), where the coefficients are deduced as in the previous subsections for the three-stage semi-implicit Runge-Kutta method.
The method is defined by the following set of parameters:

$$\alpha = 0.5728160625; \qquad b_{21} = -0.5;$$
$$b_{31} = -0.1012236115; \qquad b_{32} = 0.9762236115;$$
$$b_{41} = -0.3922096763; \qquad b_{42} = 0.7151140251; \qquad b_{43} = 0.1430371625;$$
$$c_1 = 0.9451564786; \qquad c_2 = 0.341323172; \qquad c_3 = 0.5655139575; \qquad c_4 = -0.8519936081.$$

# 6 Some other semi-implicit Runge-Kutta method

The $q-$stage semi-implicit Runge-Kutta formulae (3)–(4) compute the solution towards the solution of $q$ linear systems (each of order $m$) while the (fully) implicit Runge-Kutta methods[8] need the solution of $q$ nonlinear systems (each of order $m$). Thus the semi-implicit Runge-Kutta methods are linearly implicit. The methods that avoid the solution of nonlinear systems and replace a sequence of linear systems are referred as *linearly implicit Runge-Kutta methods*:[9] the diagonally implicit Runge-Kutta (DIRK) methods (e.g., [11, p. 261]),[10] the singly-implicit Runge-Kutta (SIRK) methods ([7], [9], see e.g., [11, p. 266]) implemented in the software STRIDE ([8]), and the DESIRE methods ([12]) belong to this category of methods. These methods are referred in [11] as *implementable implicit Runge-Kutta methods*.
Furthermore, the Rosenbrock formulae can be considered as a multiderivative method (e.g., [11, p. 90]) or as a replacing of Newton iteration for the solution of the nonlinear systems arising when we apply an implicit Runge-Kutta method (e.g., [11, p. 120]).
We see also report that in [18, Chapt. 9] and in [19, Chapt IV.7], the Rosenbrock formulae are defined as follows:

$$\boldsymbol{u}_{n+1} = \boldsymbol{u}_n + h\sum_{j=1}^{q} c_j \boldsymbol{K}_j, \tag{62}$$

and $\boldsymbol{K}_j$ has the expression

$$\boldsymbol{K}_j = \boldsymbol{f}(\boldsymbol{u}_n + h\sum_{i=1}^{j-1} b_{ji}\boldsymbol{K}_i) + hJ(\boldsymbol{u}_n)\sum_{i=1}^{j}\gamma_{ji}\boldsymbol{K}_i; \qquad j = 1, ..., q. \tag{63}$$

These formulae are equal to (3)–(4) when $\gamma_{ij} = 0$, $i = 1, ..., j-1$ and $j = 1, ...q$ ($\gamma_{jj} = \alpha_j$) and $\beta_{ij} = 0$, $i = 1, ..., j-1$ and $j = 1, ...q$.
It is worthwhile to mention that codes implementing Rosenbrock formulae (62)–(63) are RODAS, RODAS5 and ROS4 (see [19, p. 143]) and RODAS3 and ROS3 ([29]).
In the following, we recall the formulae of two semi-implicit Runge-Kutta methods of order three which are A-stable and L-stable.

## 6.1 Method of Caillaud and Padmanabhan

In [13], the authors consider the three-stage Runge-Kutta method

$$\boldsymbol{u}_{n+1} = \boldsymbol{u}_n + h\sum_{j=1}^{3} c_j \boldsymbol{K}_j,$$

where the terms $K_i$, $i = 1, ..., 3$, are formulated as follows

$$\boldsymbol{K}_1 \;\; = \;\; (I - \alpha hJ(\boldsymbol{u}_n))^{-1}\boldsymbol{f}(\boldsymbol{u}_n);$$

[8]The implicit Runge-Kutta methods are defined by formula (3) where the terms $\boldsymbol{K}_j$, $j = 1, ..., q$, have the form (e.g. [10, §34])

$$\boldsymbol{K}_j = \boldsymbol{f}(\boldsymbol{u}_n + h\sum_{i=1}^{q} b_{ji}\boldsymbol{K}_i),$$

[9]Earlier names for methods in this general class are the semi-explicit methods ([22]) or semi-implicit Runge-Kutta methods ([15]). There is a wide literature on these methods (see, e.g. [10]), even engineering literature and especially chemical engineering since the Sixties (e.g., [2], [13], [16], [25], [27]). A recent paper on semi-implicit Runge-Kutta methods for chemical kinetics differential systems is, e.g., [28].

[10]The DIRK methods are defined by formula (3) where the terms $\boldsymbol{K}_j$, $j = 1, ..., q$, have the form

$$\boldsymbol{K}_j = \boldsymbol{f}(\boldsymbol{u}_n + h\sum_{i=1}^{j} b_{ji}\boldsymbol{K}_i),$$

We can easily observe that the Rosenbrock method (3)–(4) can be considered as a linearization of the diagonally implicit procedure. The DIRK methods do not require equal coefficient $b_{jj}$; the methods where the coefficients $b_{jj}$ are equal are called singly diagonally implicit Runge-Kutta (SDIRK) methods.

$$
\begin{aligned}
\boldsymbol{K}_2 &= (I-\alpha h J(\boldsymbol{u}_n))^{-1}\boldsymbol{f}(\boldsymbol{u}_n + h b_{21}\boldsymbol{K}_1);\\
\boldsymbol{K}_3 &= (I-\alpha h J(\boldsymbol{u}_n))^{-1}J(\boldsymbol{u}_n)(h b_{31}\boldsymbol{K}_1 + h b_{32}\boldsymbol{K}_2).
\end{aligned}
$$

By proceeding as in Section 2 or as in [13], this method has order 3 if the following conditions are satisfied

$$
\begin{aligned}
c_1 + c_2 &= 1;\\
c_1\alpha + c_2(b_{21}+\alpha) + c_3(b_{31}+b_{32}) &= \frac{1}{2};\\
c_1\alpha^2 + c_2(2\alpha b_{21}+\alpha^2) + c_3(2\alpha(b_{31}+b_{32}) + b_{32}b_{21}) &= \frac{1}{6};\\
c_2\frac{b_{21}^2}{2} &= \frac{1}{6}.
\end{aligned}
$$

This method is referred in [13] as ISI3.
If we choose the parameter $\alpha$ as the inverse of the root of the Laguerre orthogonal polynomial of third degree $x_2 = 2.2942803597$, i.e.,

$$\alpha = 0.4358665216$$

and the coefficients[11]

$$
\begin{aligned}
&b_{21} = \frac{3}{4}; \qquad b_{32} = \frac{4}{3}(\frac{1}{6} + \alpha^2 - \alpha); \qquad b_{31} = \frac{1}{18} - \alpha - b_{32};\\
&c_1 = \frac{11}{27}; \qquad c_2 = \frac{16}{27}; \qquad c_3 = 1.
\end{aligned}
$$

it can be shown following the previous sections that the method (referred in [13] as ISI3($-\infty$)) is A-stable and L-stable (see also [21] for L-stability).

## 6.2 A third order semi-implicit method of Bui

An A-stable and L-stable, third order, three-stage semi-implicit Runge-Kutta method has been introduced by Bui in [5], where the coefficients have the following expression:

$$
\begin{aligned}
&\alpha = 0.4358665216; \qquad b_{21} = -0.5096436824;\\
&b_{31} = 0.3270258661; \qquad b_{32} = 0.3108847731;\\
&c_1 = 0; \qquad c_2 = 0.5; \qquad c_3 = 0.5.
\end{aligned}
$$

This method has been investigated by Alexander ([1]) as a DIRK method.

[11] The authors considered $c_3 = 1$ and added the equation $c_2 b_{21}^3 = 1/4$ obtained in such a way that the term of $h^4\boldsymbol{f}(\boldsymbol{u}_n)$ vanishes.

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