



$L(\theta)$ -stable peer methods with reused stages for advection–diffusion–reaction problems

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Received: 1 August 2025 / Accepted: 12 May 2026
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Abstract

This paper addresses the efficient numerical solution of large and stiff initial value problems (IVPs) arising from the space discretization of systems of nonlinear advection–diffusion–reaction partial differential equations (PDEs). To this end, we introduce a new family of linearly implicit two-step peer methods that leverage specialized preconditioners and exploit the reuse of previously computed stages. The proposed methods are constructed to ensure strong stability properties, specifically, L -stability or $L(\theta)$ -stability with θ approaching 90° , while maintaining low error constants. Compared to recently developed linearly implicit peer schemes, the new methods significantly reduce both the number of required function evaluations and linear systems to solve at each time step, also resulting in notably diminished error constants. Numerical experiments on nonlinear advection–diffusion–reaction problems testify to the efficiency of the new methods and confirm their accuracy and stability properties.

Keywords Two-step peer methods · Reused stages · TASE operators · Stiff initial value problems · PDEs

Mathematics Subject Classification (2010) 65L04 · 65L05 · 65L06 · 65L20 · 65M12 · 65M20 · 65M22

Communicated by: Gianluigi Rozza

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1 Introduction

The numerical solution of initial value problems (IVPs) arising from the discretization in space of partial differential equations (PDEs) represents a topic on which research activity is very intense. In fact, PDEs are a rather widely used model for the description of real-world phenomena, and of biological, chemical, and physical processes. Just to mention a few, interesting applications that can be modeled with PDEs are the evolution of vegetation in arid and semi-arid environments [12], corrosion of materials [15], and charge/discharge processes in electric batteries [16]. The aim of this paper is therefore to propose new numerical methods for IVPs

$$\begin{cases} \frac{d}{dt}y(t) = f(t, y(t)), \\ y(t_0) = y_0, \end{cases} \quad t \in [t_0, t_{\text{end}}], \quad f : \mathbb{R} \times \mathbb{R}^m \rightarrow \mathbb{R}^m, \quad (1.1)$$

arising mainly from the space discretization of nonlinear advection–diffusion–reaction PDEs. Since such problems are often large and have severe stiffness, our goal is to develop stable numerical methods characterized by low computational cost.

Well-known numerical methods for the solution of IVPs are the Runge–Kutta (RK) ones, which depending on the choice of the coefficients can be explicit or implicit. Explicit methods require in principle low computational effort, but are not suitable for stiff problems since they do not have good stability, leading to the use of excessively small time step sizes to provide an appropriate solution (see, e.g., [20]). Implicit methods can have good stability, but in general require at each time step the solution of a system of nonlinear equations of size proportional to m , being m the size of the problem (1.1), and are therefore infeasible for space discretized PDEs. By suitably modifying the diagonally implicit RK methods, that are particular implicit RK methods, linearly implicit methods have been proposed, which can have good stability properties and are characterized by computational cost mainly given by the solution of a fixed number of linear systems at each step. Well-known linearly implicit schemes are the Rosenbrock and W-methods [19].

Starting from the two-step W-methods, in the 2000s Weiner and co-workers proposed another class of numerical schemes for IVPs, called peer methods [27–30]. They are constructed by requiring all related stages to have the same order of consistency, and this can avoid order reduction on highly stiff problems or can facilitate the derivation of a continuous approximant of the discrete solution. Additionally, for certain choices of the coefficients, peer methods can be parallelized. These characteristics make peer methods promising, and indeed, several researchers have become interested in them. In recent years, some classes of explicit and implicit peer methods have been proposed (see, e.g., [1, 6, 23, 25]) that are competitive with other numerical schemes for IVPs. Furthermore, as described below, by using appropriate techniques, linearly implicit peer methods for the solution of stiff IVPs have been derived [13, 26].

Among the classes of explicit peer methods, interesting numerical schemes are the ones with shifted or reused stages, which have been proposed by Horváth and co-workers [21], Klinge and co-workers [24], and Calvo and co-workers [6]. Indeed, exploiting a particular structure of the methods, these authors showed that it is possible

to reduce the number of function evaluations required at the current time step by using stages already computed in the previous steps. Specifically, Horváth et al. and Klinge et al. [21, 24] proposed two-step s -stage peer methods, where s_e stages are the effective ones, i.e., the ones actually computed at the current time step, while the remaining $s_r = s - s_e$ stages can be recovered from the previous s_r time steps. To recover stages only from the previous time step, and not from all previous s_r time steps, Calvo et al. [6] subsequently further modified these methods. They derived explicit two-step peer schemes with just two effective stages up to order five. Thus, the mentioned peer methods allow to reach high order of consistency by considering a low number of effective stages. However, they are explicit and therefore unsuitable for the numerical solution of large stiff IVPs. In this work, we introduce new linearly implicit peer methods with good stability properties and exploit the idea of reused stages for them. We prove that this allows to reduce not only the number of required function evaluations, but also the number of linear systems to be solved at each time step.

To derive the new linearly implicit peer methods, we employ appropriate preconditioners belonging to the family of the so-called Time-Accurate and highly Stable-Explicit (TASE) operators. The original TASE operators were introduced in 2021 by Bassenne and co-workers [4], being generalized the same year by Calvo and co-workers [8], to improve the stability of explicit RK methods. Indeed, the use of TASE preconditioners on explicit numerical methods makes them linearly implicit and therefore potentially able to achieve good stability properties, such as A-stability or A(θ)-stability (definitions of stability will be recalled in the next sections). In recent years, several researchers have proposed new TASE operators [2, 5, 13] or analyzed the connections between RK-TASE methods (by RK-TASE methods, we mean explicit RK methods stabilized with TASE operators) and Rosenbrock and W-methods [3, 9–11, 18]. TASE operators have also been considered to improve the stability properties of numerical methods other than RK schemes. That is, Conte and co-workers [13] and Pagano [26] used the first TASE operators in [4, 8] on explicit peer methods. In particular, they derived strongly A-stable or A(θ)-stable linearly implicit peer methods with θ sometimes close to 90° , whose main computational cost is given by the solution of $s \cdot p$ linear systems per step involving p different coefficient matrices, where s is the number of stages and p is the order of consistency.

In this paper, by suitably employing the so-called singly TASE operators, which have been introduced by Calvo and co-workers in 2023 [5] to reduce the computational effort of the first RK-TASE methods in [4, 8], we derive new linearly implicit peer methods that improve the above-mentioned existing ones proposed in [13, 26] in several aspects. First of all, the new methods are L-stable or L(θ)-stable with θ close to 90° . Furthermore, they have smaller error constants and require drastically lower computational effort than the schemes in [13, 26] to achieve a given order of consistency p . Indeed, by exploiting the singly TASE operators and the idea of reused stages, for the new methods, the number of linear systems to solve at each step can be less than $s \cdot p$, and moreover, the related coefficient matrix is always the same, and this can be exploited to perform an efficient implementation. The listed properties make the new peer methods able to handle the presence of highly stiff components of the

solution and to efficiently address large problems arising from the space discretization of advection–diffusion–reaction PDEs.

The paper is structured as described below. In Sect. 2, we recall the existing two-step peer methods stabilized by TASE operators. In Sect. 3, we propose a new family of linearly implicit two-step peer methods with reused stages, analyzing their consistency and stability properties. In Sects. 4, 5, and 6, we focus on deriving peer methods of the new family of order two, three, and four, respectively, with only two effective stages. In particular, we will prove that for certain choices of coefficients, it is possible to obtain L -stable or $L(\theta)$ -stable peer methods with low error constants and computational cost. Section 7 is devoted to numerical experiments on advection–diffusion–reaction PDEs, where we will show the good performance of the new peer methods compared to other linearly implicit schemes recently introduced in the scientific literature. Finally, in Sect. 8, we discuss the obtained results and possible future directions of the research activity.

2 Explicit two-step peer methods and TASE operators

In this section, we recall existing explicit peer methods stabilized by TASE operators, highlighting their properties and anticipating the improvements we will get in the paper. Let us consider the discrete time grid $\{t_n = t_0 + nh; n = 0, \dots, N; t_N = t_{\text{end}}\}$. Classical two-step s -stage explicit peer methods for IVPs (1.1) are formulated as follows [29]:

$$Y_{n,i} = \sum_{j=1}^s a_{ij} Y_{n-1,j} + h \sum_{j=1}^s b_{ij} f(t_{n-1,j}, Y_{n-1,j}) + h \sum_{j=1}^{i-1} r_{ij} f(t_{n,j}, Y_{n,j}), \quad i = 1, \dots, s, \quad n \geq 1. \quad (2.2)$$

Here, $Y_{n,i} \approx y(t_{n,i})$, with $t_{n,i} = t_n + hc_i$, $i = 1, \dots, s$, are the stages at step n , which are also functions of those at step $n - 1$. The initial stages $Y_{0,j}$, $j = 1, \dots, s$, have to be computed using a suitable procedure, e.g., using a one-step method of appropriate order. Note that the expression of the advancing solution at the grid point t_{n+1} is not explicitly given. Indeed, since as shown below in peer methods all stages are computed with the same accuracy, any of them could be considered to provide a time-marching solution by appropriately adjusting the discrete grid. In this paper, for simplicity, we consider $c_s = 1$. In particular, we take

$$-1 \leq c_1 < c_2 < \dots < c_s = 1, \quad (2.3)$$

thus considering all nodes c_i within the interval $[-1, 1]$, and using the last stage $Y_{n,s}$ to obtain an approximation of the time-marching solution $y(t_{n+1})$.

For compactness, the coefficients of the peer method (2.2) can be grouped by introducing the matrices $A = (a_{ij})_{i,j=1}^s \in \mathbb{R}^{s \times s}$, $B = (b_{ij})_{i,j=1}^s \in \mathbb{R}^{s \times s}$ and $R =$

$(r_{ij})_{i,j=1}^s \in \mathbb{R}^{s \times s}$, which is strictly lower triangular, and the vector $c = (c_i)_{i=1}^s \in \mathbb{R}^s$. The method (2.2) can be expressed as

$$K_n = (A \otimes I_m)K_{n-1} + h(B \otimes I_m)F_{n-1} + h(R \otimes I_m)F_n, \quad n \geq 1, \tag{2.4}$$

being I_m the identity matrix of size m , and $K_n = (Y_{n,j})_{j=1}^s \in \mathbb{R}^{ms}$, $F_n = (f(t_{n,j}, Y_{n,j}))_{j=1}^s \in \mathbb{R}^{ms}$.

From formulation (2.2) or (2.4), note that function evaluations are required in correspondence of both the b_{ij} and r_{ij} coefficients in B and R , respectively. However, at each step $n = 1, \dots, N - 2$, once $Y_{n,j}$ is determined for a given j , the user can also compute $f(t_{n,j}, Y_{n,j})$. Indeed, this function evaluation is required at the current step and/or at the next step. Therefore, explicit s -stage peer methods require in general s function evaluations at each time step. Nevertheless, note that in some special cases, it may be possible to reduce the number of needed function evaluations. For instance, the choice $c_1 = 0, c_s = 1$, implies $Y_{n,s} = Y_{n+1,1}$, i.e., the first stage at the next step coincides with the last stage at the previous step. This can be exploited to reduce the number of function evaluations per step from s to $s - 1$. In the present manuscript, we focus on these mentioned special cases, which allow for a reduction in the computational cost of the methods. In this line, in recent works, Horváth et al. and Klinge et al. [21, 24] proposed to formulate explicit peer methods in such a way that s_r stages at the current time step correspond to stages already computed in the previous s_r time steps. In this way, at the current time step, only $s_e = s - s_r$ stages actually need to be computed. Subsequently, Calvo et al. in [6] proposed a further modification of the mentioned methods, so as to recover s_r stages only from the previous time step, without considering all the previous s_r time steps. Being explicit, such peer methods are characterized by small stability regions (see [6, Sec. 4]) and hence are unusable for stiff IVPs. In this paper, we aim to improve the stability properties of explicit peer methods by modifying them appropriately via the so-called singly TASE operators, leading to new linearly implicit peer methods. As shown below, by exploiting reused stages in this context when $s \geq 3$, it is possible to reduce not only the number of required function evaluations, but also the number of linear systems to be solved at each time step, compared to other existing linearly implicit peer methods.

The first TASE operators were introduced by Bassenne et al. in [4], and subsequently generalized by Calvo et al. in [8], to improve the stability properties of explicit RK methods. Then, these TASE operators have also been used to improve the stability properties of explicit two-step peer methods in [13, 26]. The use of the mentioned TASE operators on explicit peer methods (2.2) consists in modifying all the terms $f(t_{n-1,j}, Y_{n-1,j})$ and $f(t_{n,j}, Y_{n,j})$ as

$$T_p(hJ_{n-1}; \alpha) f(t_{n-1,j}, Y_{n-1,j}), \quad T_p(hJ_n; \alpha) f(t_{n,j}, Y_{n,j}),$$

with

$$T_p(hJ_n; \alpha) = \sum_{\ell=1}^p \beta_\ell (I_m - \alpha_\ell hJ_n)^{-1},$$

$$\alpha = (\alpha_\ell)_{\ell=1}^p \in \mathbb{R}^p, \quad \alpha_\ell \neq \alpha_q \text{ for } \ell \neq q, \alpha_\ell > 0, \tag{2.5}$$

being J_n the Jacobian of vector field of the problem (1.1) evaluated at (t_n, y_n) . Therefore, TASE operators lead to linearly implicit peer methods which, by assuming the invertibility of the coefficient matrices, require solving the following $s \cdot p$ linear systems at each step:

$$\begin{aligned} (I_m - \alpha_\ell h J_n) \chi &= \beta_\ell f(t_{n,j}, Y_{n,j}), \\ \chi &\in \mathbb{R}^m, \ell = 1, \dots, p, j = 1, \dots, s. \end{aligned} \quad (2.6)$$

Clearly, for the previous comments, at a given step n , the terms of type $T_p(hJ_{n-1}; \alpha) f(t_{n-1,j}, Y_{n-1,j})$ are already available from the previous step, and thus do not need to be computed. The operator T_p in (2.5), called TASE operator, is characterized by the coefficients $\alpha_\ell, \beta_\ell, \ell = 1, \dots, p$. The α_ℓ coefficients are free and can be selected to simultaneously obtain low error constants and good stability properties for the resulting linearly implicit method. The β_ℓ coefficients are all a priori fixed in such a way that, for small $h > 0$,

$$\begin{aligned} T_p(hJ_n; \alpha) &= I_m + \mathcal{O}(h^p) = I_m + k_p(\alpha)h^p J_n^p + \mathcal{O}(h^{p+1}), \\ k_p : \mathbb{R}^p &\rightarrow \mathbb{R}, k_p(\alpha) = (-1)^{p+1} \prod_{\ell=1}^p \alpha_\ell \neq 0. \end{aligned}$$

Indeed, this guarantees that if the starting explicit scheme has order p , then it maintains order p even after being modified by the TASE operator. We emphasize that the order of consistency of the methods stabilized by TASE operators is independent of the Jacobian J_n in T_p . That is, J_n can be replaced by an arbitrary matrix W , even a constant for all the numerical integration, without affecting the order of consistency of the methods, and this can allow to reduce their computational effort. However, stability is strongly affected by this choice, and it is generally studied under the assumption $W = J_n$.

Remark 1 In [13, 26], TASE operators T_p of the type (2.5) have been used to stabilize parallelizable explicit two-step peer methods, expressible in the form (2.4) with R corresponding to the zero matrix. This led to the derivation of linearly implicit peer methods with s stages and order $p = s = 2, 3, 4$, having good stability properties such as strong A-stability or strong $A(\theta)$ -stability (definitions of stability will be recalled in the next section). For the above analysis, see (2.6), such methods require the solution of p^2 linear systems at each step n , involving the p different coefficient matrices $(I_m - \alpha_\ell h J_n), \ell = 1, \dots, p$. In this paper, we introduce new linearly implicit peer methods characterized by a reduced computational cost, thanks to both the use of appropriate TASE operators and to the idea of reused stages when $s \geq 3$. Furthermore, the new numerical schemes will result in lower error constants and improved stability properties with respect to existing peer methods stabilized by TASE operators, such as L-stability or $L(\theta)$ -stability with θ close to 90° , leading to the efficient solution of highly stiff space discretized advection–diffusion–reaction problems.

3 A new family of linearly implicit two-step peer methods

The new two-step linearly implicit peer methods for stiff IVPs (1.1) we propose in this work read

$$\begin{aligned}
 Y_{n,i} = & \sum_{j=1}^s a_{ij} Y_{n-1,j} + h \sum_{j=1}^s b_{ij} T_p(hJ_{n-1}; d) f(t_{n-1,j}, Y_{n-1,j}) \\
 & + h \sum_{j=1}^{i-1} r_{ij} T_p(hJ_n; d) f(t_{n,j}, Y_{n,j}),
 \end{aligned}
 \tag{3.7}$$

$i = 1, \dots, s, n \geq 1$, where

$$\begin{aligned}
 T_p(hJ_n; d) &= \sum_{\ell=1}^p \beta_{p\ell} (dI_m - hJ_n)^{-\ell}, \quad d \in \mathbb{R}, \\
 \beta_{p\ell} &= (-1)^{\ell-1} \binom{p}{p-\ell} d^\ell, \quad \ell = 1, \dots, p.
 \end{aligned}
 \tag{3.8}$$

The new methods are obtained by combining the so-called singly TASE operators T_p in (3.8) (see [5]), with explicit two-step peer schemes in (2.2). As explained below and in Remark 2, this choice of T_p provides significant computational advantages, leading to achieving the same consistency order as other existing TASE operators at a lower cost. From now on, we denote the new methods (3.7)–(3.8) by STP (Singly TASE Peer). Note that the singly operator T_p in (3.8) depends on just one parameter d , since the $\beta_{p\ell}$ coefficients are all a priori fixed to guarantee that $T_p(hJ_n; d) = I_m + \mathcal{O}(h^p)$. Actually, with $\beta_{p\ell}$ fixed as in (3.8), we have that

$$T_p(hJ_n; d) = I_m + k_p(d)h^p J_n^p + \mathcal{O}(h^{p+1}), \quad k_p : \mathbb{R} \rightarrow \mathbb{R}, \quad k_p(d) = \frac{(-1)^{p+1}}{d^p} \neq 0.
 \tag{3.9}$$

As shown in the consistency analysis below in Section 3.1, in particular Propositions 1 and 2, and already mentioned in the previous section, thanks to this property, if the underlying explicit peer method has order of consistency p , then the order of consistency of the new method (3.7)–(3.8) also corresponds to p . Furthermore, we will show that the size of $k_p(d)$ in (3.8) can play a role in terms of the local truncation error of the method.

Remark 2 Note that, using a Horner-type algorithm, all terms of the type $T_p(hJ_n; d) f(t_{n,j}, Y_{n,j})$ in (3.7), with T_p as in (3.8), can be obtained by sequential solution of the following linear systems:

$$\begin{aligned}
 (dI_m - hJ_n) \chi^{[p]} &= \beta_{pp} f(t_{n,j}, Y_{n,j}), & \chi^{[p]} &\in \mathbb{R}^m, \\
 (dI_m - hJ_n) \chi^{[\ell]} &= \beta_{p\ell} f(t_{n,j}, Y_{n,j}) + \chi^{[\ell+1]}, & \chi^{[\ell]} &\in \mathbb{R}^m, \quad \ell = p-1, \dots, 1 \text{ with step } -1.
 \end{aligned}
 \tag{3.10}$$

Indeed, $\chi^{[1]}$ corresponds to $T_p(hJ_n; d)f(t_{n,j}, Y_{n,j})$. Therefore, each step involves the solution of $s \cdot p$ linear systems, similarly to existing peer methods combined with TASE operators, as explained in the previous section. However, recall that the linear systems of these latter methods involve p different coefficient matrices. Instead, for the new STP methods (3.7)–(3.8), the coefficient matrix of the linear systems is always the same, corresponding to $(dI_m - hJ_n)$ (see (3.10)). This allows to get methods with significantly improved efficiency, since in the implementation it is sufficient to compute at each step just one factorization, e.g. of LU type, for $(dI_m - hJ_n)$, then solving only triangular linear systems. Moreover, note that freezing J_n for several steps further reduces the computational cost, as it allows the factorization to be reused. We underline that, as mentioned and shown in the consistency analysis below in Section 3.1, freezing J_n does not affect the order of convergence of the methods. In numerical experiments, for the methods with singly TASE operators, we will use the algorithm described here.

As shown after the consistency and stability analysis below in Section 3.1, the concept of reused stages will allow to further improve the efficiency of the new STP methods (3.7)–(3.8), leading to a reduction in the number of linear systems to be solved at each step.

3.1 Consistency and stability analysis

To perform the consistency analysis of the new STP methods (3.7)–(3.8), for greater generality, let us replace the Jacobian in T_p with an arbitrary matrix W . Consider the definitions below, which are given following similar arguments to [29, Sec. 3].

Definition 1 Let $m = 1$ in (1.1), and $y(t)$ sufficiently smooth. The residuals of the STP method (3.7)–(3.8) are defined as

$$\delta_{n,i} := y(t_{n,i}) - \sum_{j=1}^s a_{ij}y(t_{n-1,j}) - h \sum_{j=1}^s b_{ij}T_p(h w; d)y'(t_{n-1,j}) - h \sum_{j=1}^{i-1} r_{ij}T_p(h w; d)y'(t_{n,j}), \quad (3.11)$$

$i = 1, \dots, s$, where w is an arbitrary constant related to W .

Definition 2 The STP method (3.7)–(3.8) has order of consistency p if, for small $h > 0$,

$$\delta_{n,i} = \mathcal{O}(h^{p+1}), \quad \forall i = 1, \dots, s,$$

with $\delta_{n,i}$ as in (3.11).

Therefore, it follows from Definition 2 that all stages must be at least of order p .

Proposition 1 Let $\zeta_{0,i} = 1 - \sum_{j=1}^s a_{ij}$ and, for each $k \geq 1$,

$$\zeta_{k,i} = \frac{c_i^k}{k!} - \sum_{j=1}^s a_{ij} \frac{(c_j - 1)^k}{k!} - \sum_{j=1}^s b_{ij} \frac{(c_j - 1)^{k-1}}{(k - 1)!} - \sum_{j=1}^{i-1} r_{ij} \frac{c_j^{k-1}}{(k - 1)!}.$$

The STP method (3.7)–(3.8) is consistent of order p if $\zeta_{k,i} = 0$, for all $k = 0, \dots, p$ and $i = 1, \dots, s$. Furthermore, with $k_p(d)$ as in (3.9), if the method has order p , the main local truncation error constants read

$$\tilde{\zeta}_i^{[1]} = \zeta_{p+1,i}, \quad \tilde{\zeta}_i^{[2]} = - \left(\sum_{j=1}^s (b_{ij} + r_{ij}) \right) k_p(d), \quad i = 1, \dots, s. \quad (3.12)$$

Proof By Taylor expansion, the residuals in (3.11) read, for $i = 1, \dots, s$,

$$\delta_{n,i} = \zeta_{0,i} y(t_n) + \sum_{k=1}^p \zeta_{k,i} y^{(k)}(t_n) h^k + \zeta_{p+1,i} y^{(p+1)}(t_n) h^{p+1} - \left(\sum_{j=1}^s (b_{ij} + r_{ij}) \right) k_p(d) w^p y'(t_n) h^{p+1} + \mathcal{O}(h^{p+2}), \quad (3.13)$$

with $\zeta_{k,i} = 0, k = 0, \dots, p$, by assumption. According to Definition 2, this concludes the proof. \square

Proposition 2 Let $\zeta_{k,i} = 0$ for $k = 0, \dots, p^*, i = 1, \dots, s$, with $p^* \neq p$, being $\zeta_{k,i}$ as in statement of Proposition 1. Then:

1. If $p^* < p$, the STP method (3.7)–(3.8) has order of consistency p^* , and its main local truncation error constants are given by $\tilde{\zeta}_i^{[1]} = \zeta_{p^*+1,i}, i = 1, \dots, s$.
2. If $p^* > p$, the STP method (3.7)–(3.8) has order of consistency p , and its main local truncation error constants are given by $\tilde{\zeta}_i^{[2]} = - \left(\sum_{j=1}^s (b_{ij} + r_{ij}) \right) k_p(d), i = 1, \dots, s$.

Proof Similarly to Proposition 1, by Taylor expansion, if $p^* < p$ the residuals in (3.11) read

$$\delta_{n,i} = \zeta_{0,i} y(t_n) + \sum_{k=1}^{p^*} \zeta_{k,i} y^{(k)}(t_n) h^k + \zeta_{p^*+1,i} y^{(p^*+1)}(t_n) h^{p^*+1} + \mathcal{O}(h^{p^*+2}), \quad i = 1, \dots, s,$$

with $\zeta_{k,i} = 0, k = 0, \dots, p^*$, by assumption. According to Definition 2, this concludes the proof in the first case. Instead, if $p^* > p$, the residuals in (3.11) can be expressed as in (3.13), with $\zeta_{k,i} = 0$ for $k = 0, \dots, p + 1$, since $p^* > p$ by assumption. According to Definition 2, this concludes the proof in the second case. \square

Conditions $\zeta_{k,i} = 0, k = 0, \dots, p^*, i = 1, \dots, s$, guarantee order p^* for the underlying explicit peer method (see e.g. [29, p. 611]). Therefore, by Propositions 1 and 2, when the underlying explicit peer scheme has order $p^* \geq p$, the STP method has order p . This is natural due to property (3.9) of the operator T_p in (3.8), which also makes the role of w in (3.11) irrelevant for consistency. Note that to minimize the size of the STP error, it is convenient to choose d in (3.8) so as to minimize the size of $k_p(d)$. However, when choosing the d parameter, it is important to also take into account the stability properties of the STP method.

To perform the stability analysis, we apply the STP method (3.7)–(3.8) on the standard linear equation

$$\frac{d}{dt} y(t) = \lambda y(t), \quad \lambda \in \mathbb{C}, \operatorname{Re}(\lambda) < 0,$$

leading to

$$K_n = M(z)K_{n-1}, \text{ with } M(z) = (I_s - zT_p(z; d)R)^{-1}(A + zT_p(z; d)B) \in \mathbb{R}^{s \times s}, \quad (3.14)$$

where we have used the matrix notation introduced in Sect. 2, and $z = h\lambda$. The stability function of the linearly implicit STP method (3.7)–(3.8) is therefore given by the spectral radius $\rho(M(z))$. Let us define in the left complex half-plane the cone region

$$\mathcal{S}(\theta) := \{z \in \mathbb{C} \text{ with } \operatorname{Re}(z) < 0 \text{ s.t. } |\arg(-z)| \leq \theta\}, \quad \theta \in [0, \pi/2]. \quad (3.15)$$

According to, e.g., [26, p. 161], the method is said to be the following:

- A(θ)-stable for a given $\theta \in [0, \pi/2]$ if $\rho(M(z)) \leq 1$ for all $z \in \mathcal{S}(\theta)$;
- strongly A(θ)-stable if it is A(θ)-stable and also, for $z \in \mathbb{R}$, $\tilde{\mu} := \lim_{z \rightarrow -\infty} \rho(M(z)) < 1$
- L(θ)-stable if it is strongly A(θ)-stable with $\tilde{\mu} = 0$

When $\rho(M(z)) = 1$, the corresponding eigenvalue must be simple. To avoid redundancy, we shall omit reiterating this point in subsequent references to the stability of the methods.

Note that the case $\theta = \pi/2$ means that the stability condition of the method occurs in the whole left complex half-plane. In this situation, the above definitions are actually called, respectively, A-stability, strong A-stability, and L-stability. Clearly, among the mentioned properties, L-stability or L(θ)-stability with θ as close as possible to $\pi/2$ are the preferable ones for dealing with advection-reaction-diffusion problems, since they are generally characterized by a spectrum that can cover a large part of the left complex half-plane, and in addition can have a solution with highly stiff components.

A peer method is said to be zero-stable, which guarantees the equivalence between convergence and consistency, if an eigenvalue μ_i of $M(0) = A$ (see (3.14)) is 1, all other eigenvalues μ_j , $j = 1, \dots, s$, $j \neq i$, are such that $|\mu_j| \leq 1$, and those with modulus one are simple elementary divisors. To avoid zero-stability issues, in this work, we consider optimally zero-stable methods (see, e.g., [29, Sec. 3]), i.e., we choose A such that one eigenvalue is 1 (A always has at least one unit eigenvalue due to the preconsistency condition $\zeta_{0,i} = 0$ in Propositions 1 or 2) and all others are 0.

Let

$$p_C(\mu; z) = d_s(z)\mu^s + d_{s-1}(z)\mu^{s-1} + \dots + d_1(z)\mu + d_0(z), \quad (3.16)$$

be the characteristic polynomial of $M(z)$ in (3.14), where $z \in \mathbb{C}$, $\operatorname{Re}(z) < 0$. Note that, being functions of z , the d_i coefficients of the polynomial p_C are complex. The

$A(\theta)$ -stability condition can then be expressed as

$$\mu_i(z) := \text{roots}(p_C(\mu; z)) \in C_{0,1}, \quad \forall z \in S(\theta), \quad i = 1, \dots, s, \tag{3.17}$$

denoting $C_{0,1}$ the unit circle (with center at the origin and radius one), and being $S(\theta)$ defined in (3.15). Remember that the eigenvalues on the boundary of $C_{0,1}$ must be simple. To study the stability condition (3.17), the following two criteria from [22, p. 111] and [17, p. 194], respectively, can be exploited.

Proposition 3 Schur criterion. *Let*

$$\begin{aligned} p(\mu) &= d_s \mu^s + d_{s-1} \mu^{s-1} + \dots + d_1 \mu + d_0, \quad d_i \in \mathbb{C}, \text{ and} \\ \bar{p}(\mu) &= \bar{d}_0 \mu^s + \bar{d}_1 \mu^{s-1} + \dots + \bar{d}_{s-1} \mu + \bar{d}_s, \end{aligned}$$

where, for each i , \bar{d}_i is the complex conjugate of d_i . Also, let

$$p_1(\mu) = \frac{1}{\mu} (\bar{p}(0)p(\mu) - p(0)\bar{p}(\mu)),$$

which has a degree at most $s - 1$. Then, $p(\mu)$ is a Schur polynomial, i.e., it has all roots inside $C_{0,1}$, if and only if

$$|\bar{p}(0)| > |p(0)|, \text{ and } p_1(\mu) \text{ is a Schur polynomial.}$$

Therefore, the use of the Schur criterion on the polynomial $p_C(\mu; z)$ in (3.16) allows the study of the $A(\theta)$ -stability of the new STP methods (3.7)–(3.8). Actually, in the case $\theta = \pi/2$, if the roots $\mu_i(z)$ are analytic functions of z , by the maximum principle, it is sufficient to verify the Schur criterion for $z = \iota \cdot \text{Im}(z)$, and not for all $z = \text{Re}(z) + \iota \cdot \text{Im}(z) \in \mathbb{C}$ with $\text{Re}(z) < 0$ (see, e.g., [22, p. 111]), denoting ι the imaginary unit.

Proposition 4 Routh-Hurwitz criterion. *Consider a polynomial*

$$q(\gamma) = \tilde{g}_0 \gamma^s + g_0 \gamma^{s-1} + \tilde{g}_1 \gamma^{s-2} + g_1 \gamma^{s-3} + \dots + \hat{g}_{\lfloor \frac{s}{2} \rfloor}, \quad \tilde{g}_i, g_i \in \mathbb{R}, \quad \tilde{g}_0 \neq 0, \tag{3.18}$$

where $\hat{g}_{\lfloor \frac{s}{2} \rfloor} = g_{\frac{s-1}{2}}$ for s odd and $\hat{g}_{\lfloor \frac{s}{2} \rfloor} = \tilde{g}_{\frac{s}{2}}$ for s even. From it, define the vectors of length s

$$\begin{aligned} g^{[0]} &= (g_0, g_1, \dots, g_{s-1}), \quad g^{[1]} = (0, g_0, \dots, g_{s-2}), \dots, \quad g^{[s-1]} = (0, \dots, 0, g_0), \quad g_i = 0 \text{ for } i > \frac{s-1}{2}, \\ \tilde{g}^{[0]} &= (\tilde{g}_0, \tilde{g}_1, \dots, \tilde{g}_{s-1}), \quad \tilde{g}^{[1]} = (0, \tilde{g}_0, \dots, \tilde{g}_{s-2}), \dots, \quad \tilde{g}^{[s-1]} = (0, \dots, 0, \tilde{g}_0), \quad \tilde{g}_i = 0 \text{ for } i > \frac{s}{2}. \end{aligned}$$

Finally, consider the matrix H having as rows, in order, the vectors $g^{[0]}$, $\tilde{g}^{[0]}$, $g^{[1]}$, $\tilde{g}^{[1]}$, \dots , $g^{[s-1]}$, and $\tilde{g}^{[s-1]}$. The polynomial $q(\gamma)$ in (3.18) has all roots with negative real part if and only if

$$\tilde{g}_0 \Delta_n > 0 \quad \forall \text{ odd } n, \quad \Delta_n > 0 \quad \forall \text{ even } n, \quad n = 1, \dots, s,$$

being Δ_n the determinant of the submatrix obtained by selecting the first n rows and columns of H .

By (3.17), for stability, we need all the roots $\mu_i(z)$ of $p_C(\mu; z)$ to be in $\mathcal{C}_{0,1}$. Using the Möbius transformation $\mu \rightarrow \gamma$, $\gamma = \frac{\mu+1}{\mu-1}$, $\mu \neq 1$, we move from the μ -unit circle to the γ -left-complex-half-plane (see [7, p. 8]). Therefore, the stability condition becomes

$$\gamma_i(z) := \text{roots } (q_S(\gamma; z)) \in \mathcal{S}\left(\frac{\pi}{2}\right), \quad \forall z \in \mathcal{S}(\theta), \quad i = 1, \dots, s,$$

being

$$q_S(\gamma; z) := (\gamma - 1)^s p_C\left(\frac{\gamma + 1}{\gamma - 1}; z\right) = \tilde{g}_0(z)\gamma^s + g_0(z)\gamma^{s-1} + \dots + \hat{g}_{\lfloor \frac{s}{2} \rfloor}(z), \quad \gamma \neq 1, \tag{3.19}$$

with p_C defined in (3.16), and denoting $\mathcal{S}(\frac{\pi}{2})$ the left complex half-plane. Again, the values of $\gamma_i(z)$ on the boundary of the region must be simple. Being functions of z , the coefficients of the polynomial q_S are complex. However, for $z \in \mathbb{R}$, $z < 0$, $q_S(\gamma; z)$ in (3.19) turns out to have only real coefficients, and then we can use the Routh-Hurwitz criterion, which allows to investigate whether its roots $\gamma_i(z)$ are in $\mathcal{S}(\frac{\pi}{2})$, and hence whether the roots $\mu_i(z)$ of $p_C(\mu; z)$ in (3.16) are in $\mathcal{C}_{0,1}$. Therefore, the Routh-Hurwitz criterion allows to investigate the $A(0)$ -stability (since to use it we assume $z \in \mathbb{R}$) of the STP methods (3.7)–(3.8), which is a necessary condition for $A(\theta)$ -stability for any θ .

3.2 Reuse of the stages

In accordance with Remark 2, the new STP methods (3.7)–(3.8) require less computational effort than existing peer methods based on TASE operators. For the derivation of s -stage STP methods up to order $p = 4$, which is performed in the next sections, in the case $s \geq 3$, we appropriately reuse some stages to further improve their efficiency according to the following definition, which is the analogue of [6, Def. 2] for explicit two-step peer methods.

Definition 3 STP methods with reused stages. Consider the s -stage STP method (3.7)–(3.8). It has s_r reused stages and thus $s_e = s - s_r$ effective stages if

$\exists s_r$ pairs of indices $(i_1, j_1), (i_2, j_2), \dots, (i_{s_r}, j_{s_r})$, with $1 \leq i_k, j_\ell \leq s \ \forall 1 \leq k, \ell \leq s_r$, such that:

- $\forall k \neq \ell, i_k \neq i_\ell$ and $j_k \neq j_\ell$.
- $\forall k, \ell, i_k \neq j_\ell$.
- $c_{i_k} = c_{j_k} - 1$, and $Y_{n,i_k} = Y_{n-1,j_k}$, for $k = 1, \dots, s_r$.

From now on, such a method will be referred to as STPR (singly TASE peer with reused stages).

The pairs (i_k, j_k) in Definition 3 mean that the i_k -th stage at step n corresponds to the j_k -th stage at step $n - 1$, and therefore, it does not need to be computed being already available. Let us note that, in view of Definition 3, if the i_k -th stage is reused, then $b_{i_k j} = r_{i_k j} = 0$ for all $j = 1, \dots, s$, in (3.7). Also, if at step n , the i_k -th stage

is reused, and corresponds to the j_k -th stage at step $n - 1$, i.e., $Y_{n,i_k} = Y_{n-1,j_k}$, then $a_{i_k j_k} = 1$, and $a_{i_k j} = 0$ for all $j \neq j_k$, and $c_{i_k} = c_{j_k} - 1$. Using the matrices with the coefficients of the methods, this translates into

$$e_{i_k}^T B = e_{i_k}^T R = (0, \dots, 0)^T \in \mathbb{R}^s, \text{ and } e_{i_k}^T A = e_{j_k}^T, \quad c_{i_k} = c_{j_k} - 1, \quad k = 1, \dots, s_r,$$

being e_k the column vector with all zeros, and one in position k .

To clarify the construction of the new STPR methods and discuss their computational cost, we give below two examples corresponding to $s = 3, 4$, respectively, with $s_e = 2$.

Example 1 Case $s=3$ with $s_r = 1$ and $s_e = 2$.

Note that, in principle, we have six possible choices for constructing such a method according to Definition 3: for $i_1 = 1, j_1 = 2$ or $j_1 = 3$; for $i_1 = 2, j_1 = 1$ or $j_1 = 3$; for $i_1 = 3, j_1 = 1$ or $j_1 = 2$. However, let us immediately observe that the cases $(i_1, j_1) = (2, 1), (3, 1), (3, 2)$ are not admissible. Indeed, they would lead to selecting $c_k > c_\ell$ with $k < \ell$, thus violating assumption (2.3). The remaining three cases allow to get peer methods with the following c_i coefficients and reused stages:

- $(i_1, j_1) = (1, 2)$, leading to $c = (c_2 - 1, c_2, 1)^T$, with c_2 free, and thus $Y_{n,1} = Y_{n-1,2} \forall n \geq 1$;
- $(i_1, j_1) = (1, 3)$, leading to $c = (0, c_2, 1)^T$, with c_2 free, and thus $Y_{n,1} = Y_{n-1,3} \forall n \geq 1$;
- $(i_1, j_1) = (2, 3)$, leading to $c = (c_1, 0, 1)^T$, with c_1 free, and thus $Y_{n,2} = Y_{n-1,3} \forall n \geq 1$.

Denoting for brevity $\hat{f}_{n,j} = T_p(hJ_n; d)f(t_{n,j}, Y_{n,j})$, we report below in full the methods obtained with the last two choices, respectively:

$$\begin{aligned} Y_{n,1} &= Y_{n-1,3}, \\ Y_{n,2} &= a_{21}Y_{n-2,3} + a_{22}Y_{n-1,2} + a_{23}Y_{n-1,3} + \\ &\quad h \left(b_{21}\hat{f}_{n-2,3} + b_{22}\hat{f}_{n-1,2} + (b_{23} + r_{21})\hat{f}_{n-1,3} \right), \\ Y_{n,3} &= a_{31}Y_{n-2,3} + a_{32}Y_{n-1,2} + a_{33}Y_{n-1,3} + \\ &\quad h \left(b_{31}\hat{f}_{n-2,3} + b_{32}\hat{f}_{n-1,2} + (b_{33} + r_{31})\hat{f}_{n-1,3} \right) + hr_{32}\hat{f}_{n,2}, \end{aligned} \tag{3.20}$$

$$\begin{aligned} Y_{n,1} &= a_{11}Y_{n-1,1} + a_{12}Y_{n-2,3} + a_{13}Y_{n-1,3} + \\ &\quad h \left(b_{11}\hat{f}_{n-1,1} + b_{12}\hat{f}_{n-2,3} + b_{13}\hat{f}_{n-1,3} \right), \\ Y_{n,2} &= Y_{n-1,3}, \\ Y_{n,3} &= a_{31}Y_{n-1,1} + a_{32}Y_{n-2,3} + a_{33}Y_{n-1,3} + \\ &\quad h \left(b_{31}\hat{f}_{n-1,1} + b_{32}\hat{f}_{n-2,3} + (b_{33} + r_{32})\hat{f}_{n-1,3} \right) + hr_{31}\hat{f}_{n,1}. \end{aligned} \tag{3.21}$$

This allows to observe that, in general, if the i_k -th stage at step n corresponds to the j_k -stage at step $n - 1$, then the coefficients $b_{i_j k}$ and $r_{i_i k}$, for all $i = 1, \dots, s$, multiply the same quantities. We can therefore consider $r_{i_i k} = 0$, $i = 1, \dots, s$, leading to a reduction in the number of coefficients of the methods. Additionally, note that if in method (3.21) we exchange the first two rows and columns of the coefficient matrices A , B and R , and c_1 with c_2 , we obtain an equivalent numerical scheme, which also has the same structure as (3.20). Therefore, by suitably reordering the stages, the cases $(i_1, j_1) = (1, 3)$ and $(i_1, j_1) = (2, 3)$ lead to analogous methods, and we can consider only one of them.

From Example 1, it is clear that reusing stages allows to reduce the number of linear systems to be solved. Indeed, for, e.g., method (3.20), since the first stage is reused, we do not need to compute $T_p(hJ_n; d)f(t_{n,1}, Y_{n,1})$. In general, for STPR methods with at least one reused stage, the number of linear systems to be solved at each step is $s_e \cdot p$, with $s_e < s$, and not $s \cdot p$ as it happens for existing peer methods combined with TASE operators. Actually, contrary to the latter methods, that to reach order $p \leq 4$ using $s = p$ stages, in the next sections, we show that it is possible to construct STPR methods up to order $p = 4$ with only two effective stages ($s_e = 2$).

Remark 3 Note that, in view of the considerations expressed in Example 1, we can assume the following for Definition 3 without loss of generality, similarly to [6, p. 78]:

$$\begin{aligned} r_{i_i k} &= 0, \quad i = 1, \dots, s, \quad k = 1, \dots, s_r, \\ i_1 &= 1, \dots, i_{s_r} = s_r < j_k, \quad \forall k = 1, \dots, s_r. \end{aligned}$$

That is, we eliminate unnecessary coefficients and assume that the reused stages are always the first s_r , since a different choice would lead to equivalent methods. This also leads to

$$j_1 < \dots < j_{s_r},$$

since otherwise it would happen that $c_k > c_\ell$ with $k < \ell$, violating assumption (2.3). Finally, note that according to the definition, we cannot reuse more than $s/2$ stages. That is, $s_r \leq s/2$, and thus $s_e = s - s_r \geq s_r$.

Example 2 Case $s=4$ with $s_r = 2$ and $s_e = 2$.

In view of Definition 3 and Remark 3, we consider $(i_1, j_1) = (1, 3)$ and $(i_2, j_2) = (2, 4)$. That is, we have

$$c = (c_3 - 1, 0, c_3, 1)^T, \text{ and so } Y_{n,1} = Y_{n-1,3}, \quad Y_{n,2} = Y_{n-1,4}.$$

Using the same notation as in Example 1, this method reads in full

$$\begin{aligned}
 Y_{n,1} &= Y_{n-1,3}, \\
 Y_{n,2} &= Y_{n-1,4}, \\
 Y_{n,3} &= a_{31}Y_{n-2,3} + a_{32}Y_{n-2,4} + a_{33}Y_{n-1,3} + a_{34}Y_{n-1,4} + \\
 &\quad h \left(b_{31}\hat{f}_{n-2,3} + b_{32}\hat{f}_{n-2,4} + b_{33}\hat{f}_{n-1,3} + b_{34}\hat{f}_{n-1,4} \right), \\
 Y_{n,4} &= a_{41}Y_{n-2,3} + a_{42}Y_{n-2,4} + a_{43}Y_{n-1,3} + a_{44}Y_{n-1,4} + \\
 &\quad h \left(b_{41}\hat{f}_{n-2,3} + b_{42}\hat{f}_{n-2,4} + b_{43}\hat{f}_{n-1,3} + b_{44}\hat{f}_{n-1,4} \right) + hr_{43}\hat{f}_{n,3}.
 \end{aligned} \tag{3.22}$$

4 STP methods of order two

This section is devoted to the derivation of two-stage STP methods of order two. We show that it is possible to fix the coefficients of the methods in order to obtain L -stability and low error constants.

4.1 STPs2p2: two-stage L -stable STP method of order two

Consider the STP method (3.7)–(3.8), with $s = p = 2$. By Proposition 1, to get order two we impose $\zeta_{k,i} = 0$ for $k = 0, 1, 2, i = 1, 2$. With this choice, the error constants of the method are given by (3.12). Furthermore, to simplify the structure of the method, we set $a_{12} = a_{22} = c_1 = 0$. In view of the optimal zero-stability condition recalled in Sect. 3, which is necessary for convergence, the coefficients of the STP method are thus as follows:

$$A = \begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ 0 & 2 - r_{21} \end{pmatrix}, \quad R = \begin{pmatrix} 0 & 0 \\ r_{21} & 0 \end{pmatrix}, \quad c = (0, 1)^T.$$

By (3.14), the stability matrix of the considered STP method reads

$$M(z) = \begin{pmatrix} \frac{2+\tilde{z}}{2} & \frac{\tilde{z}}{2} \\ 1 + \frac{1}{2}r_{21}\tilde{z}(2+\tilde{z}) & \frac{1}{2}(4+r_{21}(-2+\tilde{z}))\tilde{z} \end{pmatrix}, \quad \text{with } \tilde{z} = zT_2(z; d).$$

To set the remaining free coefficients r_{21} and d , we impose $\lim_{z \rightarrow -\infty} \rho(M(z)) = 0$ for $z \in \mathbb{R}$, which is a necessary condition of $L(\theta)$ -stability. This leads to

$$r_{21} = 1, \quad d = \frac{1}{2}.$$

Let us denote the two-stage second-order method thus constructed by STPs2p2.

Theorem 1 *The STPs2p2 method is L -stable.*

Proof To prove the result, we use the Schur criterion (see Proposition 3). The characteristic polynomial of $M(z)$ is

$$p_C(\mu; z) = \mu^2 + \frac{-2 + 13z - 25z^2 + 12z^3}{2(1 - 2z)^4} \mu + \frac{z(1 - 7z + 12z^2)}{2(1 - 2z)^4}. \tag{4.23}$$

Its roots are $\mu_i(z) = \frac{\mu_i^{\text{num}}(z)}{4(1-2z)^4}$, $i = 1, 2$, being $\mu_i^{\text{num}}(z)$ some coefficients depending on z . Therefore, the poles of $\mu_i(z)$ do not reside in the left complex half-plane, i.e., the roots $\mu_i(z)$ are analytic functions for $z \in \mathbb{C}$ with $\text{Re}(z) < 0$. By the maximum principle, it is therefore sufficient to verify the Schur criterion only for $z = \iota z_{\text{im}}$, denoting $z_{\text{im}} = \text{Im}(z) \in \mathbb{R}$.

Let us thus consider $p_C(\mu; \iota z_{\text{im}})$ in (4.23) and compute $\bar{p}_C(\mu; \iota z_{\text{im}})$. The first Schur condition reads

$$|\bar{p}_C(0; \iota z_{\text{im}})| - |p_C(0; \iota z_{\text{im}})| = \frac{4 + 63z_{\text{im}}^2 + 359z_{\text{im}}^4 + 880z_{\text{im}}^6 + 1024z_{\text{im}}^8}{4(1 + 4z_{\text{im}}^2)^4} > 0.$$

Note that it is satisfied for every value of $z_{\text{im}} (\in \mathbb{R})$. Then, we compute

$$p_{C1}(\mu; \iota z_{\text{im}}) = \frac{1}{\mu} (\bar{p}_C(0; \iota z_{\text{im}}) p_C(\mu; \iota z_{\text{im}}) - p_C(0; \iota z_{\text{im}}) \bar{p}_C(\mu; \iota z_{\text{im}})) = \tilde{d}_1(z_{\text{im}}) \mu + \tilde{d}_0(z_{\text{im}}), \tag{4.24}$$

being

$$\begin{aligned} \tilde{d}_1(z_{\text{im}}) &= \frac{4 + 63z_{\text{im}}^2 + 359z_{\text{im}}^4 + 880z_{\text{im}}^6 + 1024z_{\text{im}}^8}{4(1 + 4z_{\text{im}}^2)^4}, \\ \tilde{d}_0(z_{\text{im}}) &= -\frac{(1 + 7z_{\text{im}}^2)(4 + 33z_{\text{im}}^2 + 16z_{\text{im}}^4)}{4(1 + 4z_{\text{im}}^2)^4} + \iota \left(-\frac{z_{\text{im}}(2 + 39z_{\text{im}}^2 + 196z_{\text{im}}^4 + 192z_{\text{im}}^6)}{2(1 + 4z_{\text{im}}^2)^4} \right). \end{aligned}$$

The second Schur condition, i.e., $|\bar{p}_{C1}(0; \iota z_{\text{im}})| > |p_{C1}(0; \iota z_{\text{im}})|$, corresponds to

$$\frac{65z_{\text{im}}^4 + 1503z_{\text{im}}^6 + 13632z_{\text{im}}^8 + 61496z_{\text{im}}^{10} + 149504z_{\text{im}}^{12} + 206848z_{\text{im}}^{14} + 131072z_{\text{im}}^{16}}{2(1 + 4z_{\text{im}}^2)^8} > 0.$$

Therefore, the recursive Schur criterion is satisfied. This concludes the proof of the theorem. □

Finally, from (3.12), we calculate the error constants that characterize the second stage, which being $c_2 = 1$ provides the time-marching solution:

$$|\tilde{\zeta}_2^{[1]}| = 0.33333, \quad |\tilde{\zeta}_2^{[2]}| = 8.$$

Also, we report below the two-norm of the error terms of the STPs2p2 method:

$$\|(\tilde{\zeta}_i^{[1]})_{i=1}^2\|_2 = 0.34359, \quad \|(\tilde{\zeta}_i^{[2]})_{i=1}^2\|_2 = 8.9443.$$

4.2 STPs2p2_{minerr}: two-stage L-stable STP method of order two with minimum error

Consider the STP method (3.7)–(3.8), with $s = p = 2$. Compared to STPs2p2, in this case, we require $\zeta_{k,i} = 0$ also for $k = 3$, i.e., for $k = 0, 1, 2, 3, i = 1, 2$. That is, we impose order three for the underlying explicit peer method. In this way, according to Proposition 2, we obtain order two for the STP method. However, its error constants are only given by $\zeta_i^{[2]}$, $i = 1, 2$, and not also by $\zeta_i^{[1]}$, $i = 1, 2$, as in STPs2p2. Using the optimal zero-stability condition, this leads to

$$A = \begin{pmatrix} \frac{(-3+c_1)c_1^2}{(-1+c_1)^3} & \frac{-1+3c_1}{(-1+c_1)^3} \\ \frac{(-3+c_1)c_1^2}{(-1+c_1)^3} & \frac{-1+3c_1}{(-1+c_1)^3} \end{pmatrix}, \quad B = \begin{pmatrix} \frac{c_1^2}{(-1+c_1)^2} & \frac{c_1}{(-1+c_1)^2} \\ \frac{2-5c_1+9c_1^2+c_1^3-c_1^4}{6(-1+c_1)^2} & \frac{-5+17c_1-15c_1^2+11c_1^3-2c_1^4}{6(-1+c_1)^2c_1} \end{pmatrix},$$

$$R = \begin{pmatrix} 0 & 0 \\ \frac{(-1+c_1)(-5+(-2+c_1)c_1)}{6c_1} & 0 \end{pmatrix}, \quad c = (c_1, 1)^T. \tag{4.25}$$

The stability matrix of the considered STP method is, by (3.14),

$$M(z) = \begin{pmatrix} \frac{c_1^2(-3+c_1-\tilde{z}+c_1\tilde{z})}{(-1+c_1)^3} & \frac{-1-c_1(-3+\tilde{z})+c_1^2\tilde{z}}{(-1+c_1)^3} \\ m_{21} & m_{22} \end{pmatrix}, \quad \text{with } \tilde{z} = zT_2(z; d), \tag{4.26}$$

where

$$m_{21} = \frac{-2\tilde{z} + c_1^5\tilde{z}^2 - 4c_1^4\tilde{z}(1 + \tilde{z}) - c_1\tilde{z}(8 + 5\tilde{z}) + 2c_1^3(3 + 7\tilde{z}) + 2c_1^2(-9 + 4\tilde{z}^2)}{6(-1 + c_1)^3},$$

$$m_{22} = -\frac{6 + 4\tilde{z} + 36c_1^2\tilde{z} + 4c_1^3(-4 + \tilde{z})\tilde{z} - c_1^4(-2 + \tilde{z})\tilde{z} + 5\tilde{z}^2 - 2c_1(9 + 13\tilde{z} + 4\tilde{z}^2)}{6(-1 + c_1)^3}. \tag{4.27}$$

Imposing $\lim_{z \rightarrow -\infty} \rho(M(z)) = 0$ for $z \in \mathbb{R}$, for $L(\theta)$ -stability, leads to

$$c_1 = c_1^* = -0.43115945733712047, \quad d = d^* = 0.5533230647436219.$$

As explained, we have reduced the number of error terms compared to the previously derived STPs2p2 method. Therefore, the new second-order scheme here constructed is denoted by STPs2p2_{minerr}.

Theorem 2 *The STPs2p2_{minerr} method is L-stable.*

Proof The characteristic polynomial of $M(z)$ reads

$$p_C(\mu; z) = \mu^2 + d_1(z)\mu + d_0(z), \tag{4.28}$$

being

$$d_1(z) = \frac{\tilde{a}_0 + \tilde{a}_1 z + \tilde{a}_2 z^2 + \tilde{a}_3 z^3}{6(-1 + c_1^*)(d^* - z)^4}, \quad d_0(z) = \frac{\tilde{b}_1 z + \tilde{b}_2 z^2 + \tilde{b}_3 z^3}{6(-1 + c_1^*)(d^* - z)^4}, \quad (4.29)$$

where

$$\begin{aligned} \tilde{a}_0 &= 0.80492, & \tilde{a}_1 &= -4.6815, & \tilde{a}_2 &= 7.9231, & \tilde{a}_3 &= -3.1102, \\ \tilde{b}_1 &= -0.33237, & \tilde{b}_2 &= 2.1024, & \tilde{b}_3 &= -3.2567. \end{aligned}$$

Its roots are of the type $\mu_i(z) = \frac{\mu_i^{\text{num}}(z)}{12(-1+c_1^*)(d^*-z)^4}$, $i = 1, 2$. Therefore, the roots $\mu_i(z)$ are analytic functions for $z \in \mathbb{C}$ with $\text{Re}(z) < 0$, and we can simplify the study by considering $z = \iota z_{\text{im}}$ ($z_{\text{im}} \in \mathbb{R}$), similarly to Theorem 1. The Schur conditions read

$$\begin{aligned} |\tilde{p}_C(0; \iota z_{\text{im}})| - |p_C(0; \iota z_{\text{im}})| &= \frac{\tilde{\ell}_0 + \tilde{\ell}_2 z_{\text{im}}^2 + \tilde{\ell}_4 z_{\text{im}}^4 + \tilde{\ell}_6 z_{\text{im}}^6 + \tilde{\ell}_8 z_{\text{im}}^8}{36(-1 + c_1^*)^2 (d^{*2} + z_{\text{im}}^2)^4} > 0, \\ |\tilde{p}_{C1}(0; \iota z_{\text{im}})| - |p_{C1}(0; \iota z_{\text{im}})| &= \frac{\tilde{r}_4 z_{\text{im}}^4 + \tilde{r}_6 z_{\text{im}}^6 + \tilde{r}_8 z_{\text{im}}^8 + \tilde{r}_{10} z_{\text{im}}^{10} + \tilde{r}_{12} z_{\text{im}}^{12} + \tilde{r}_{14} z_{\text{im}}^{14} + \tilde{r}_{16} z_{\text{im}}^{16}}{1296(-1 + c_1^*)^4 (d^{*2} + z_{\text{im}}^2)^8} > 0, \end{aligned}$$

where $\tilde{\ell}_0 = 0.64790$, $\tilde{\ell}_2 = 8.3542$, $\tilde{\ell}_4 = 39.215$, $\tilde{\ell}_6 = 79.695$, $\tilde{\ell}_8 = 73.736$, $\tilde{r}_4 = 10.045$, $\tilde{r}_6 = 190.39$, $\tilde{r}_8 = 1.4045 \cdot 10^3$, $\tilde{r}_{10} = 5.0997 \cdot 10^3$, $\tilde{r}_{12} = 9.8867 \cdot 10^3$, $\tilde{r}_{14} = 1.104 \cdot 10^4$, $\tilde{r}_{16} = 5.4370 \cdot 10^3$, with p_{C1} obtained from p_C in (4.28)–(4.29) using formula (4.24). Both Schur conditions are satisfied. \square

From the first statement of Proposition 2, we finally compute the terms representing the error of the method:

$$|\tilde{\zeta}_2^{[2]}| = 4.2833, \quad \|(\tilde{\zeta}_i^{[2]})_{i=1}^2\|_2 = 4.3012.$$

For brevity, we will refer to STPs2p2_{minerr} as STPs2p2_{me} in the following.

5 STP and STPR methods of order three

In this section, we derive two methods of order three: the first is a two-stage STP method; the second is a method STPR with two effective stages. We fix their coefficients so that both methods are $L(\theta)$ -stable with θ close to $\pi/2$.

5.1 STPs2p3: two-stage $L(\theta)$ -stable STP method of order three

Consider the STP method (3.7)–(3.8), with $s = 2$ and $p = 3$. By Proposition 1, to get order three, we impose $\zeta_{k,i} = 0$ for $k = 0, 1, 2, 3$, $i = 1, 2$. Using the optimal zero-stability condition, A, B, R , and c are therefore as in (4.25). Also, the stability matrix

has the same expression as in (4.26)–(4.27). However, in this case, $\tilde{z} = zT_3(z; d)$. Imposing $\lim_{z \rightarrow -\infty} \rho(M(z)) = 0$ for $z \in \mathbb{R}$ leads to

$$c_1 = c_1^* = -0.4311594573371182, \quad d = d^* = 0.36888204316241346.$$

Let us denote the two-stage third-order method thus constructed by STPs2p3.

Using the Schur criterion similarly to the previous section, it can be shown that STPs2p3 is not L-stable. In fact, the second Schur condition in this case reads

$$\frac{\tilde{r}_4 z_{im}^4 + \tilde{r}_6 z_{im}^6 + \dots + \tilde{r}_{24} z_{im}^{24}}{1296(-1 + c_1^*)^4(d^{*2} + z_{im}^2)^{12}} > 0, \quad \tilde{r}_4 = -8.6604 \cdot 10^{-6}, \quad \tilde{r}_6 = -3.7094 \cdot 10^{-4}, \quad \tilde{r}_{24} = 5.437 \cdot 10^3.$$

Note that, for z_{im} close to zero, the above condition is not satisfied due to the negativity of \tilde{r}_4 (and \tilde{r}_6). However, below, we prove that STPs2p3 is $L(0)$ -stable. In particular, we will show that it is $L(\theta)$ -stable with $\theta = 89^\circ$.

Theorem 3 *The STPs2p3 method is $L(0)$ -stable.*

Proof In accordance with the Routh-Hurwitz criterion (see Proposition 4 and the observations below it), from $M(z)$, we compute the characteristic polynomial $p_C(\mu; z)$, and then $q_S(\gamma; z)$ through (3.19),

$$q_S(\gamma; z) = \tilde{g}_0(z)\gamma^2 + g_0(z)\gamma + \tilde{g}_1(z), \quad z \in \mathbb{R}, \quad z < 0,$$

being

$$\begin{aligned} \tilde{g}_0(z) &= \frac{\tilde{a}_1 z + \tilde{a}_2 z^2 + \tilde{a}_3 z^3 + \tilde{a}_4 z^4 + \tilde{a}_5 z^5 + \tilde{a}_6 z^6}{6(-1 + c_1^*)(d^* - z)^6}, \\ g_0(z) &= \frac{\tilde{b}_0 + \tilde{b}_1 z + \tilde{b}_2 z^2 + \tilde{b}_3 z^3 + \tilde{b}_4 z^4 + \tilde{b}_5 z^5 + \tilde{b}_6 z^6}{3(-1 + c_1^*)(d^* - z)^6}, \\ \tilde{g}_1(z) &= \frac{\tilde{c}_0 + \tilde{c}_1 z + \tilde{c}_2 z^2 + \tilde{c}_3 z^3 + \tilde{c}_4 z^4 + \tilde{c}_5 z^5 + \tilde{c}_6 z^6}{6(-1 + c_1^*)(d^* - z)^6}, \end{aligned}$$

where

$$\begin{aligned} \tilde{a}_1 &= 0.021635, \quad \tilde{a}_2 = -0.35002, \quad \tilde{a}_3 = 2.3543, \quad \tilde{a}_4 = -7.9818, \quad \tilde{a}_5 = 13.346, \quad \tilde{a}_6 = -8.5870, \\ \tilde{b}_0 &= -0.021635, \quad \tilde{b}_1 = 0.36084, \quad \tilde{b}_2 = -2.5222, \quad \tilde{b}_3 = 9.4740, \quad \tilde{b}_4 = -20.019, \quad \tilde{b}_5 = 21.900, \quad \tilde{b}_6 = -8.5870, \\ \tilde{c}_0 &= -0.043271, \quad \tilde{c}_1 = 0.66431, \quad \tilde{c}_2 = -4.1454, \quad \tilde{c}_3 = 13.180, \quad \tilde{c}_4 = -22.089, \quad \tilde{c}_5 = 18.875, \quad \tilde{c}_6 = -8.5870. \end{aligned}$$

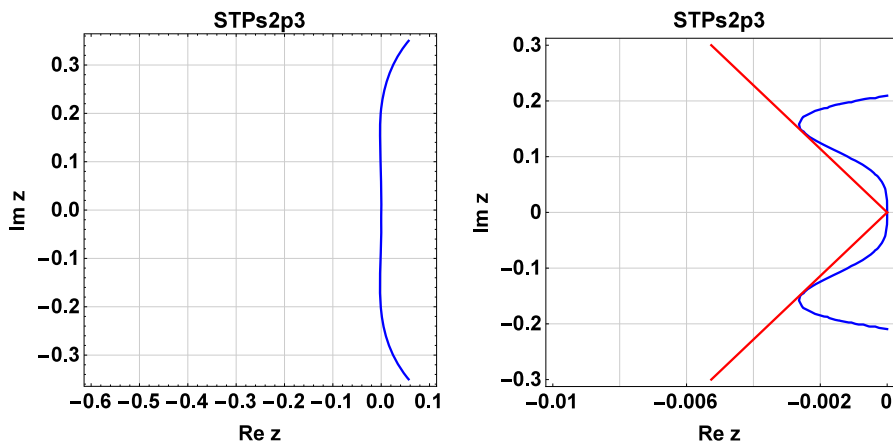


Fig. 1 Contour of the stability region of the STPs2p3 method (zoom near the origin on the right). It is $L(\theta)$ -stable with $\theta = 89^\circ$

The Routh-Hurwitz conditions read

$$\Delta_2(z) = g_0(z)\tilde{g}_1(z) = \frac{1}{18(-1 + c_1^*)^2(d^* - z)^{12}} \left(\sum_{\substack{i=0 \\ i \text{ even}}}^{12} \tilde{\ell}_i^e z^i - \sum_{\substack{i=1 \\ i \text{ odd}}}^{11} \tilde{\ell}_i^o z^i \right) > 0,$$

$$\tilde{g}_0(z)\Delta_1(z) = \tilde{g}_0(z)g_0(z) = \frac{1}{18(-1 + c_1^*)^2(d^* - z)^{12}} \left(\sum_{\substack{i=2 \\ i \text{ even}}}^{12} \tilde{r}_i^e z^i - \sum_{\substack{i=1 \\ i \text{ odd}}}^{11} \tilde{r}_i^o z^i \right) > 0,$$

where $\tilde{\ell}_i^e, \tilde{\ell}_i^o, \tilde{r}_i^e, \tilde{r}_i^o$ are all positive coefficients. Therefore, the Routh-Hurwitz conditions are satisfied for all $z < 0$. □

By Theorem 3, we conclude that the STPs2p3 method is $L(\theta)$ -stable for some $\theta > 0$. Actually, as shown in Fig. 1, in this case, $\theta = 89^\circ$, i.e., it is very close to the optimal value $\pi/2$.

From (3.12), we finally report below the terms representing the error of the STPs2p3 method:

$$|\tilde{\zeta}_2^{[1]}| = 0.20159, \quad |\tilde{\zeta}_2^{[2]}| = 26.126, \quad \|(\tilde{\zeta}_i^{[1]})_{i=1}^2\|_2 = 0.20174, \quad \|(\tilde{\zeta}_i^{[2]})_{i=1}^2\|_2 = 26.235.$$

5.2 STPR_s2p3: $L(\theta)$ -stable STPR method of order three with two effective stages

Consider here a three-stage STP method (3.7)–(3.8) of order three, with one reused stage. In this way, we have two effective stages, and as shown below, there are some free coefficients available that can be set to obtain lower error constants than those of STPs2p3. In particular, consider the STPR method (3.20) with $p = 3$, requiring it to

be of order three, i.e., imposing the conditions $\zeta_{k,i} = 0$ for $k = 0, 1, 2, 3, i = 1, 2, 3$, via Proposition 1. With optimal zero-stability, this leads to

$$A = \begin{pmatrix} 0 & 0 & 1 \\ 0 & \frac{6b_{23}-6(1+b_{23})c_2+c_2^3}{2-3c_2+c_2^3} & \frac{2+6b_{23}(-1+c_2)+3c_2}{2-3c_2+c_2^3} \\ 0 & \frac{6b_{23}-6(1+b_{23})c_2+c_2^3}{2-3c_2+c_2^3} & \frac{2+6b_{23}(-1+c_2)+3c_2}{2-3c_2+c_2^3} \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 0 & 0 \\ \frac{-b_{23}(-1+c_2)^2+c_2}{c_2(2+c_2)} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \end{pmatrix},$$

$$R = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & \frac{(-1+c_2)(-14-6b_{23}+6b_{33}+c_2+c_2^2)}{6(1+c_2)} & 0 \end{pmatrix}, \quad c = (0, c_2, 1)^T,$$

where

$$b_{22} = \frac{1}{6} \left(6 + \frac{10}{-1+c_2} + \frac{3b_{23}}{c_2} + \frac{2+9b_{23}}{2+c_2} \right),$$

$$b_{31} = \frac{5+6c_2(-2+b_{33}+c_2-b_{33}c_2)-(1+2c_2)(6b_{23}-6(1+b_{23})c_2+c_2^3)/(2+c_2)}{6c_2(1+c_2)},$$

$$b_{32} = \frac{-5+(9-6b_{33})c_2-(6b_{23}-6(1+b_{23})c_2+c_2^3)(1+c_2(4+c_2))/(-2+c_2+c_2^2)}{6c_2}.$$

Let us denote by STPRs_e2p3 the family of third-order methods, with two effective stages, thus obtained.

To fix the remaining free coefficients, we proceed as follows: first, we consider the values of b_{23}, b_{33}, c_2, d which are solutions of $\lim_{z \rightarrow -\infty} \rho(M(z)) = 0$ for $z \in \mathbb{R}$, where $M(z)$ is the stability matrix of the method (see (3.14)); then, we check whether these coefficients satisfy the Routh-Hurwitz criterion. In this way, we obtain a set of quadruples (b_{23}, b_{33}, c_2, d) leading to L(θ)-stability. Figure 2 shows the obtained results. In particular, we report the values of the stability angle θ and the error terms for each quadruple, for which d is taken as representative. From (3.12), given $k_p(d)$ in (3.9), a good choice to get low errors certainly consists of high d . However, we also want a large θ . From Fig. 2, note that the best method is therefore the one to which the marker “X” is linked, having coefficients

$$\begin{aligned} b_{23} &= 0.713048140270401, & b_{33} &= 0.410109327703551, \\ c_2 &= 0.574644329399715, & d &= 0.565384615384615. \end{aligned} \tag{5.30}$$

For it, $\theta = 89.05^\circ$ (see Fig. 3 (left)), and the terms representing the error are

$$|\tilde{\zeta}_3^{[1]}| = 0.060243, \quad |\tilde{\zeta}_3^{[2]}| = 1.7339, \quad \|(\tilde{\zeta}_i^{[1]})_{i=1}^3\|_2 = 0.070423, \quad \|(\tilde{\zeta}_i^{[2]})_{i=1}^3\|_2 = 4.4399.$$

Remark 4 In Fig. 2, we have not reported the results obtained for all quadruples (b_{23}, b_{33}, c_2, d) leading to L(θ)-stability. For example, there are also coefficients that yield methods with $\theta < 10^\circ$, which however we are not interested in. Also, although

a formal proof is not given, using the Routh-Hurwitz criterion (see Proposition 2), we have analytically verified that all the STPR_{s_e}2p3 methods considered to get Fig. 2 are L(0)-stable. In this regard, we show in Fig. 3 (right) that the Routh-Hurwitz conditions are satisfied by choosing the coefficients in (5.30). We finally mention that it is not possible to construct STPR_{s_e}2p3 methods that are L-stable, i.e., with $\theta = \pi/2$.

6 STPR method of order four

In this section, we derive a fourth-order L(θ)-stable STPR method with two effective stages.

6.1 STPR_{s_e}2p4: L(θ)-stable STPR method of order four with two effective stages

Consider a four-stage STP method (3.7)–(3.8) of order four, with two reused stages. Therefore, we have two effective stages. In particular, let us consider the STPR method (3.22) with $p = 4$, requiring it to be of order four, i.e., imposing the conditions $\zeta_{k,i} = 0$ for $k = 0, 1, 2, 3, 4, i = 1, 2, 3, 4$, via Proposition 1. With the optimal zero-stability

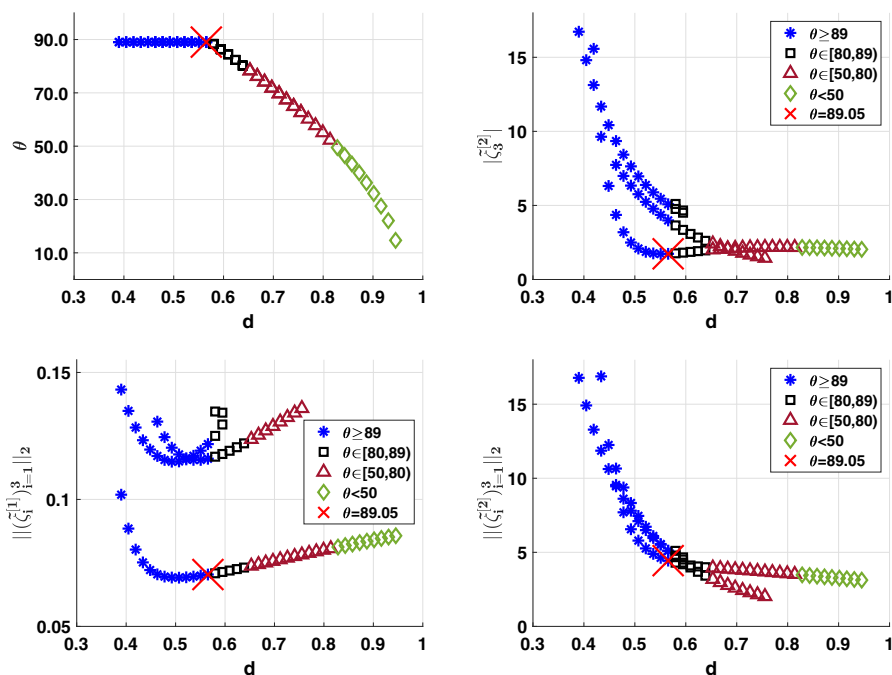


Fig. 2 In all plots, each point is related to a quadruple (b_{23}, b_{33}, c_2, d) leading to L(θ)-stability for the STPR_{s_e}2p3 methods. We take d (on the x -axis) as the representative of each quadruple and report (on the y -axis): the corresponding value of the angle θ (top left); the maximum in absolute value of the error terms in the calculation of the time-marching solution (top right); the two-norm of the error terms (bottom). The marker “X” is related to the coefficients in (5.30)

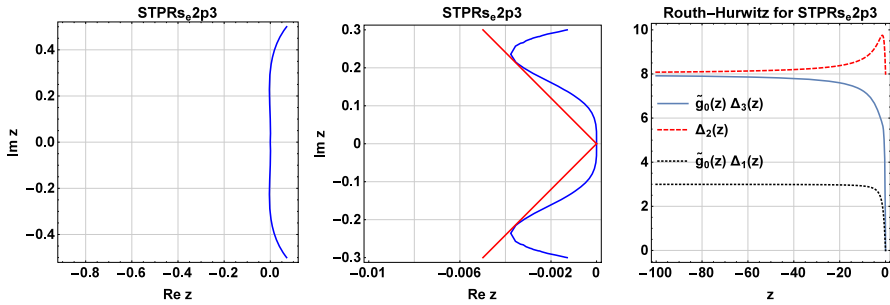


Fig. 3 All plots refer to the method $STPRs_e2p3$ with coefficients in (5.30), that is $L(\theta)$ -stable with $\theta = 89.05^\circ$. Contour of its stability region (left and center, where there is zoom near the origin). Verification of the related Routh-Hurwitz conditions (right)

condition, we then fix some coefficients of the method; $a_{32}, a_{33}, b_{41}, c_3$, and d remain free. We denote by $STPRs_e2p4$ the family of fourth-order methods, with two effective stages, thus obtained.

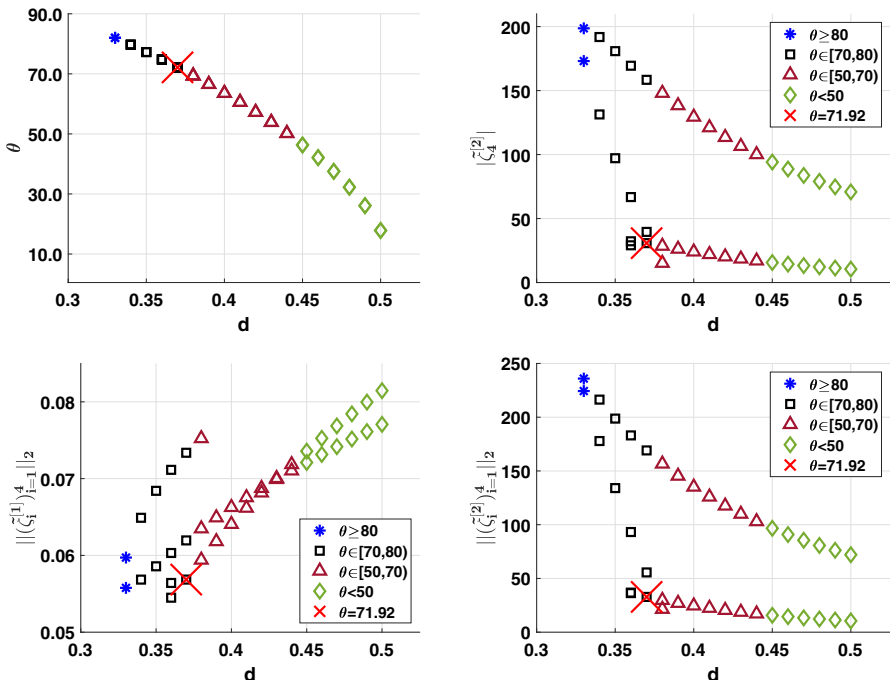


Fig. 4 In all plots, each point is related to a set of coefficients leading to $L(\theta)$ -stability for the STPR methods of order four. We take d (on the x -axis) as the representative of each set and report (on the y -axis): the corresponding value of the angle θ (top left); the maximum in absolute value of the error terms in the calculation of the time-marching solution (top right); the two-norm of the error terms (bottom). The marker “X” is related to the coefficients in (6.31)

To set the remaining free coefficients, we proceed as done for $STPR_{s_e}2p3$, i.e., we require that $\lim_{z \rightarrow -\infty} \rho(M(z)) = 0$ for $z \in \mathbb{R}$, being $M(z)$ the stability matrix of the method, and also the $L(0)$ -stability. The results obtained are summarized in Fig. 4. Note that the method with a good balance between large θ and low error terms is the one to which the marker “X” is linked, having coefficients

$$\begin{aligned}
 a_{31} &= 0, & a_{32} &= 0.2333839654228104, & a_{33} &= -1.329408591758657, \\
 a_{34} &= 1.061102430400786, & a_{41} &= 0, & a_{42} &= 0.283079997799902, \\
 a_{43} &= -1.612488589558559, & a_{44} &= 2.926457428127916, & b_{31} &= -0.311454549578532, \\
 b_{32} &= 1.105856866808153, & b_{33} &= -1.887616777039025, & b_{34} &= 1.306361697460386, \\
 b_{41} &= -0.925343695916987, & b_{42} &= 3.008305707932430, & b_{43} &= -4.437693982127162, \\
 b_{44} &= 2.491777709348757, & r_{43} &= 0.439794877459440, & c_3 &= 0.562018989978237.
 \end{aligned}
 \tag{6.31}$$

This method is $L(\theta)$ -stable, with $\theta \approx 72^\circ$ (see Fig. 5 (left)). The terms representing its error are

$$|\tilde{\zeta}_4^{[1]}| = 0.054961, \quad |\tilde{\zeta}_4^{[2]}| = 30.779, \quad \|(\tilde{\zeta}_i^{[1]})_{i=1}^4\|_2 = 0.056852, \quad \|(\tilde{\zeta}_i^{[2]})_{i=1}^4\|_2 = 32.813.$$

Similarly to $STPR_{s_e}2p3$ (see Remark 4), we do not report in Fig. 4 coefficients leading to $L(\theta)$ -stability with $\theta < 10^\circ$. Also, we show numerically the verification of the Routh-Hurwitz conditions for the coefficients in (6.31) (see Fig. 5 (right)).

7 Numerical experiments

In this section, we perform numerical experiments on advection–diffusion–reaction problems.

Remark 5 Note that, based on the previous analysis, we selected specific coefficients for the new methods to ensure $L(\theta)$ -stability while balancing a large θ and low error

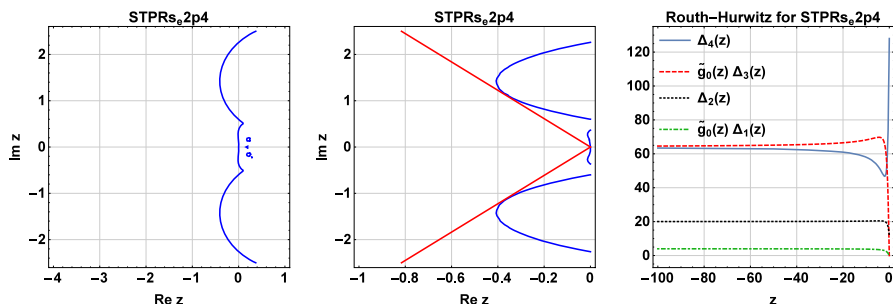


Fig. 5 All plots refer to the method $STPR_{s_e}2p4$ with coefficients in (6.31), that is $L(\theta)$ -stable with $\theta = 71.92^\circ$. Contour of its stability region (left and center, where there is zoom near the origin). Verification of the related Routh-Hurwitz conditions (right)

constants. As shown in the numerical experiments below, these choices perform well for the selected advection–diffusion–reaction problems. In any case, by exploiting the analysis presented in the paper, the user can adjust the parameters according to the problem at hand. For example, one may favor a larger θ at the cost of slightly higher errors, or, when a large stability angle is not necessary, reduce θ to achieve lower errors. Actually, in problems dominated by advection, where the eigenvalues of the Jacobian matrix are purely imaginary or have an imaginary part much stronger than the real part, it may be necessary to employ fully L-stable methods, i.e., L(θ)-stable methods with $\theta = \pi/2$, to avoid constraints on the time step size for stability reasons. Therefore, in such situations, it is advisable to use the second-order STP methods derived in Sect. 4, as they possess this property.

Below, we compare the performance of the new STP and STPR methods proposed in this manuscript with linearly implicit schemes recently introduced in the literature, of peer and RK type, the latter based on the use of singly preconditioners. In particular, for the comparison, we consider the following linearly implicit methods.

- SRKTP: the RK methods based on Singly TASE operators, proposed in [5], of order $p = 2, 3, 4$
- TTP: the Peer methods based on the TASE operators (2.5), proposed in [13], of order $p = 2, 3$
- SEPPP: the Stabilized Explicit (Parallelizable) Peer methods of order $p = 2, 3, 4$, proposed in [26]

For SRKTP methods, we used as underlying explicit RK schemes those reported in [4, Appendix A].

All these methods require the solution of linear systems with coefficient matrices of the type $(I_m - h\alpha J_n)$, with $\alpha > 0$. In the experiments, we also consider the case of frozen Jacobian (i.e., we replace J_n with a constant W matrix for all numerical integration), since as observed this does not alter the consistency order of the methods and lowers their computational cost. For the solution of linear systems, in the implementation, we compute LU factorizations of the coefficient matrices. By doing so, we solve triangular linear systems at each step.

Furthermore, since the considered peer methods are two-step schemes and some of them include negative nodes, the initialization proceeds as follows: starting from $y_0 = y(t_0)$, we compute a reference solution at $t_1 = t_0 + h$, along with the stages values $Y_{1,i}$ for $i = 1, \dots, s$. From them, we then apply the peer method. These stages, that are computed using the W-method of order $p = 4$ proposed in [18], serve as an approximation of the solution over the interval $[t_0, t_2 = t_0 + 2h]$, given that $-1 \leq c_i \leq 1$ ($i = 1, \dots, s$) by (2.3). For the sake of comparison, when measuring the CPU times employed by the methods, both for the peer and RK schemes, we therefore start from the second time step.

The properties of the above methods, and of the new numerical schemes introduced in this paper, are summarized in Table 1. As can be observed, the new singly peer methods generally have better stability than the other schemes, and lower error constants and computational cost, in terms of LU factorizations and/or linear systems solution when exploiting reused stages (i.e., for order $p = 3, 4$). This will be

Table 1 Properties of the linearly implicit RK and peer methods considered in the experiments; p denotes the order of consistency, $\tilde{\mu}$ denotes the absolute value of the limit of the stability function at infinity, θ denotes the $A(\theta)$ -stability angle, $|k_p|$ denotes the size of the error constant of the TASE operator, s_e denotes the number of effective stages (thus, $s_e = s$ for SRKT p , TP p and SEPP p), n_{sys} denotes the number of linear systems to solve at each step, and nLU denotes the number of LU factorization computed at each step

Method	p	Stability	$\tilde{\mu}$	θ	$ k_p $	s_e	n_{sys}	nLU
SRKT2		Strong A-stability	0.5	90	4	2	4	1
TP2		Strong A-stability	0.58	90	12	2	4	2
SEPP2	2	Strong A-stability	0.5	90	2.67	2	4	2
STPs2p2		L-stability	0	90	4	2	4	1
STPs2p2 _{me}		L-stability	0	90	3.27	2	4	1
SRKT3		L(θ)-stability	0	88.99	6.64	3	9	1
TP3		Strong A(θ)-stability	0.79	88.98	231	3	9	3
SEPP3	3	Strong A(θ)-stability	0.69	89.4	20.80	3	9	3
STPs2p3		L(θ)-stability	0	89	19.92	2	6	1
STPR _{s_e} 2p3		L(θ)-stability	0	89.05	5.53	2	6	1
SRKT4		Strong A(θ)-stability	0.27	87.17	39.45	4	16	1
SEPP4	4	Strong A(θ)-stability	0.9	32.62	85.96	4	16	4
STPR _{s_e} 2p4		L(θ)-stability	0	71.92	53.36	2	8	1

confirmed in numerical experiments that have been performed on a laptop with the following specifications: 8 GB of RAM, a 64-bit operating system, and a processor AMD Ryzen 7 3700U with Radeon Vega Mobile Graphics, running at 2.30 GHz. All codes were executed using the MATLAB version R2023b. For each test problem, given by a system of ordinary differential equations resulting from the semi-discretization of PDEs with finite differences, a reference solution has been computed using the MATLAB `ode15s` function, with tolerance set to `eps`. For each used method, the (absolute) errors have been calculated at the last time grid point, using the infinity norm, exploiting this reference solution. Also, we have calculated the estimated order of convergence p_{est} by the formula

$$p_{est}(h) = \frac{\log(\text{err}(2h)) - \log(\text{err}(h))}{\log(2)},$$

being $\text{err}(h)$ the above error obtained using step size h .

7.1 Burgers equation

The Burgers equation is a well-known (nonlinear) PDE that arises in various areas of applied mathematics and physics. In conservative form, it reads

$$\frac{\partial u}{\partial t} = \epsilon \frac{\partial^2 u}{\partial x^2} - \frac{1}{2} \frac{\partial u^2}{\partial x}, \quad \epsilon > 0, \quad (x, t) \in [x_0, x_{\text{end}}] \times [t_0, t_{\text{end}}] \quad (7.32)$$

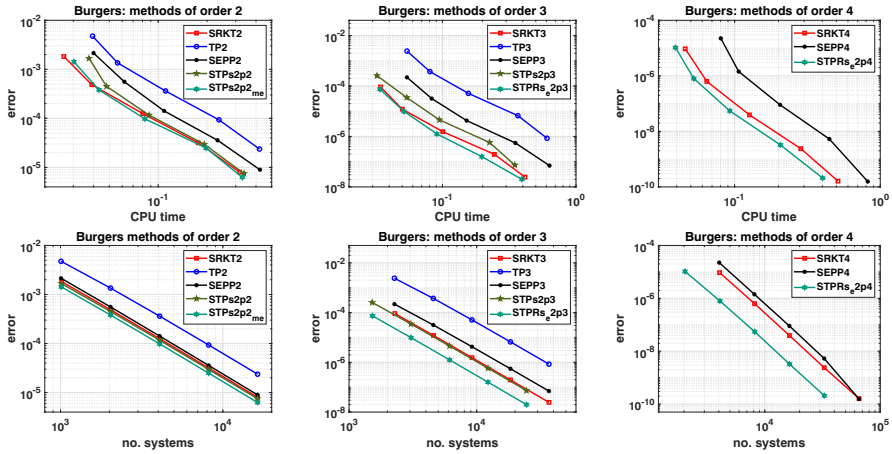


Fig. 6 CPU time vs error (top) and number of triangular linear systems solved (bottom), as the step size h varies, for the 2nd-, 3rd-, and 4th-order methods in the case of exact Jacobian, for the Burgers equation ($\Delta x \approx 0.05, \epsilon = 0.01$)

(see, e.g., [8, Subsec. 3.2]). Here, experiments are done taking $x_0 = 0, x_{\text{end}} = 2\pi, t_0 = 0, t_{\text{end}} = 2, \epsilon = 0.01$, periodic boundary conditions and initial condition $u(x, 0) = \sin(x)$. Furthermore, we have performed the semi-discretization using order-four finite differences, selecting space step size $\Delta x = x_{\text{end}}/2^7 \approx 0.05$. The numerical results are reported in Figs. 6 and 7 and Tables 2, 3, and 4.

In Fig. 6, we present the errors obtained for all the considered methods of order $p = 2, 3, 4$, evaluated over a range of time step sizes given by $h = t_{\text{end}}/2^i$, with $i = 7, \dots, 11$, and the corresponding CPU time (top) and the number of (triangular) linear systems solved (bottom). Note that the number of linear systems solved is a reliable indicator of the computational cost, as evidenced by the similarity between the top and bottom graphs. However, with them, we do not take into account the number of LU factorizations which also affects the cost, as shown below. From the results, it is evident that the newly proposed STP and STPR methods are more efficient than the other numerical schemes used for comparison. Indeed, at a given time step size, they

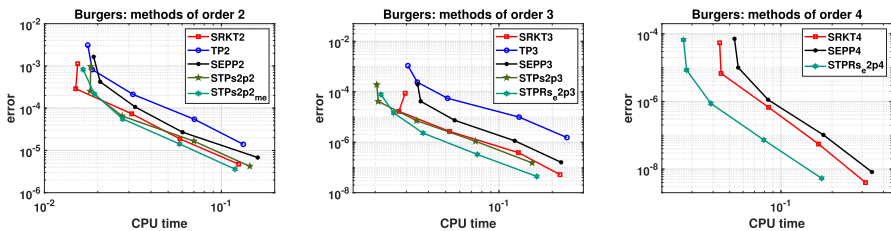


Fig. 7 CPU time vs error, as the step size h varies, for the 2nd-, 3rd-, and 4th-order methods in the case of frozen Jacobian, for the Burgers equation ($\Delta x \approx 0.05, \epsilon = 0.01$)

Table 2 Errors (and estimated order p_{est} in round brackets) for the methods of order 2 in the case of exact Jacobian, for the Burgers equation ($\Delta x \approx 0.05$, $\epsilon = 0.01$)

h	SRKT2	TP2	SEPP2	STPs2p2	STPs2p2 _{me}
1.56e-02	1.83e-03 (-)	4.75e-03 (-)	2.15e-03 (-)	1.67e-03 (-)	1.43e-03 (-)
7.81e-03	4.86e-04 (1.91)	1.35e-03 (1.81)	5.58e-04 (1.94)	4.50e-04 (1.90)	3.80e-04 (1.91)
3.91e-03	1.25e-04 (1.96)	3.61e-04 (1.91)	1.42e-04 (1.98)	1.17e-04 (1.95)	9.79e-05 (1.96)
1.95e-03	3.17e-05 (1.98)	9.33e-05 (1.95)	3.57e-05 (1.99)	2.96e-05 (1.97)	2.48e-05 (1.98)
9.77e-04	8.00e-06 (1.99)	2.37e-05 (1.98)	8.97e-06 (1.99)	7.47e-06 (1.99)	6.26e-06 (1.99)

generally achieve lower errors while requiring fewer computations. This advantage is particularly evident for the STPR methods of order $p = 3$ and $p = 4$, where the reuse of stages leads to a substantial reduction in the number of linear systems to be solved. Figure 6 is complemented by Tables 2, 3, and 4, which report the error values and the estimated order of convergence, for $h = t_{\text{end}}/2^i$, $i = 7, \dots, 11$. All methods show the expected order of convergence. In confirmation of previous comments, also note, e.g., that the STPR method of order $p = 3$ achieves significantly lower errors than the other schemes for the same values of h .

Finally, in the same setting as Figs. 6, 7 reports errors versus CPU times when using frozen Jacobian evaluated at the first grid point. As expected, this strategy leads to reduced computing times for all methods. In this scenario, the advantages of the new STPR methods become even more evident. This is mainly due to the fact that, with frozen Jacobian, the dominant computational cost arises from solving triangular linear systems at each time step, as the LU factorization of the coefficient matrices is performed only once. Since STPR methods exploit reuse of stages, they require fewer linear systems to solve compared to other methods, such as SRKT. On the other hand, when the Jacobian is updated at each step, the LU factorizations play a role in terms of cost. In such cases, STPR and SRKT methods perform a comparable number of LU factorizations, as both require one per step (see Table 1).

Table 3 Errors (and estimated order p_{est} in round brackets) for the methods of order 3 in the case of exact Jacobian, for the Burgers equation ($\Delta x \approx 0.05$, $\epsilon = 0.01$)

h	SRKT3	TP3	SEPP3	STPs2p3	STPR _{se} 2p3
1.56e-02	9.13e-05 (-)	2.41e-03 (-)	2.19e-04 (-)	2.56e-04 (-)	7.40e-05 (-)
7.81e-03	1.20e-05 (2.92)	3.72e-04 (2.69)	3.16e-05 (2.80)	3.47e-05 (2.88)	9.79e-06 (2.92)
3.91e-03	1.54e-06 (2.96)	5.09e-05 (2.87)	4.24e-06 (2.90)	4.53e-06 (2.94)	1.26e-06 (2.96)
1.95e-03	1.95e-07 (2.98)	6.64e-06 (2.94)	5.50e-07 (2.95)	5.79e-07 (2.97)	1.59e-07 (2.98)
9.77e-04	2.45e-08 (2.99)	8.47e-07 (2.97)	6.99e-08 (2.98)	7.30e-08 (2.99)	1.99e-08 (2.99)

Table 4 Errors (and estimated order p_{est} in round brackets) for the methods of order 4 in the case of exact Jacobian, for the Burgers equation ($\Delta x \approx 0.05$, $\epsilon = 0.01$)

h	SRKT4	SEPP4	STPR _{sc} 2p4
1.56e-02	9.38e-06 (-)	2.24e-05 (-)	1.04e-05 (-)
7.81e-03	6.29e-07 (3.90)	1.43e-06 (3.98)	7.96e-07 (3.71)
3.91e-03	3.92e-08 (4.00)	9.06e-08 (3.98)	5.47e-08 (3.86)
1.95e-03	2.38e-09 (4.04)	5.30e-09 (4.10)	3.26e-09 (4.07)
9.77e-04	1.61e-10 (3.88)	1.56e-10 (5.08)	2.09e-10 (3.96)

7.2 Burgers equation with discontinuous initial condition

Here, we again focus on the Burgers equation (7.32), with periodic conditions, and use order-four finite differences for the space discretization. However, now, we choose a discontinuous initial condition:

$$\begin{cases} u(x, 0) = 1 & \text{if } x \in [0, \pi], \\ u(x, 0) = 0 & \text{if } x \in (\pi, 2\pi]. \end{cases}$$

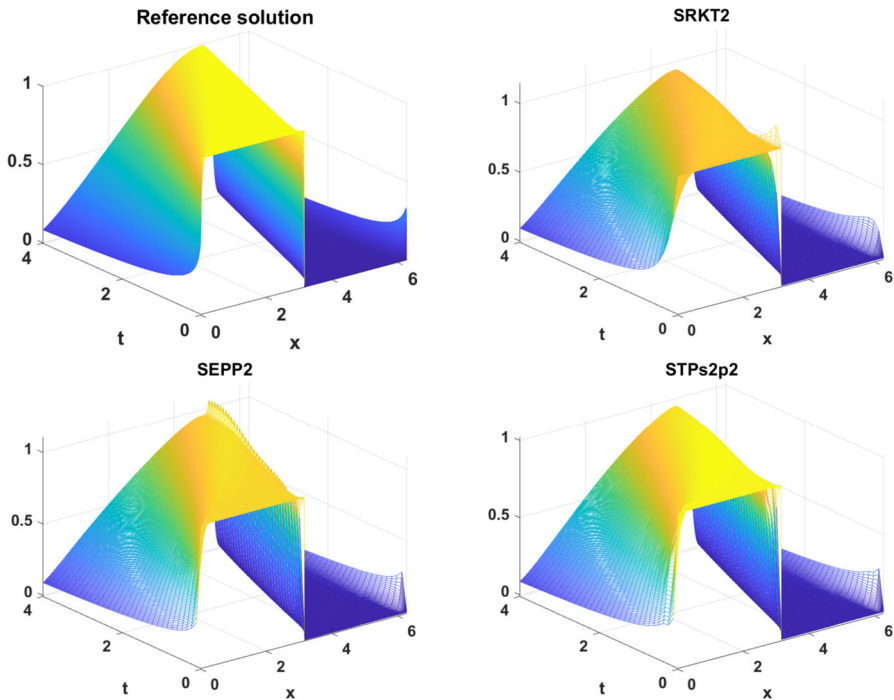


Fig. 8 Solution of the Burgers equation by the methods ode15s, SRKT2, SEPP2, and STPs2p2, with step size $h = 0.125$ and discontinuous initial condition ($\Delta x \approx 0.01$, $\epsilon = 0.025$)

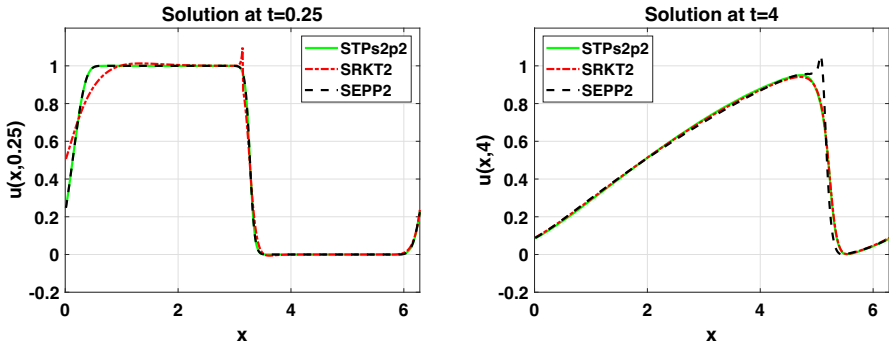


Fig. 9 Solution of the Burgers equation at $t = 0.25$ and $t = 4$ by the methods STPs2p2, SRKT2, and SEPP2, with step size $h = 0.125$ and discontinuous initial condition ($\Delta x \approx 0.01$, $\epsilon = 0.025$)

Also, we now select $\epsilon = 0.025$ and $\Delta x = x_{\text{end}}/2^9 \approx 0.01$. In this setting, the semi-discrete problem exhibits increased stiffness compared to the previous subsection. As discussed, e.g., in [8, Subsec. 3.2], this may require the use of $L(\theta)$ -stable methods.

Figures 8 and 9, that show the solutions obtained using several second-order methods with time step size $h = 0.125$ ($t_{\text{end}} = 4$), confirm this. Indeed, while the SRKT2 and SEPP2 methods, that are both strongly A-stable but not L-stable (see Table 1), exhibit instability at some x , the L-stable STPs2p2 scheme successfully captures the behavior of the solution. Therefore, although the second-order STP methods proposed in this work do not exhibit significant improvements in accuracy or computing times with respect to the other schemes considered for comparison, as shown in the previous subsection, they provide advantages in terms of stability.

7.3 KdV equation

Here, we consider the Korteweg-De Vries (KdV) equation,

$$\frac{\partial u}{\partial t} = -6u \frac{\partial u}{\partial x} - \frac{\partial^3 u}{\partial x^3}, \quad (x, t) \in [x_0, x_{\text{end}}] \times [t_0, t_{\text{end}}].$$

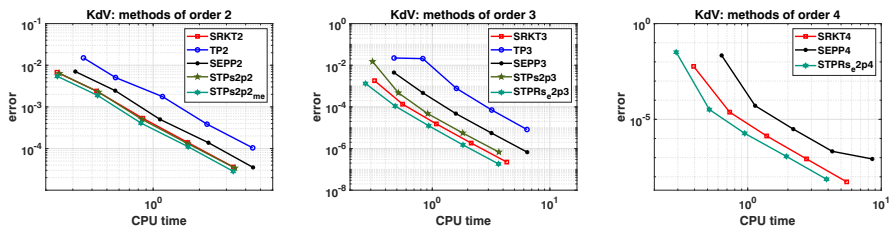


Fig. 10 CPU time vs error, as the step size h varies, for the 2nd-, 3rd-, and 4th-order methods in the case of exact Jacobian, for the KdV equation ($\Delta x = 0.25$)

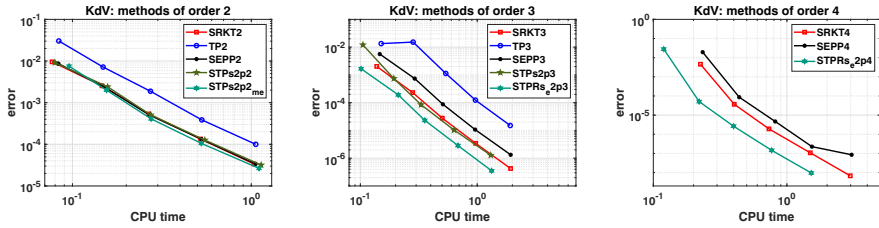


Fig. 11 CPU time vs error, as the step size h varies, for the 2nd-, 3rd-, and 4th-order methods in the case of frozen Jacobian, for the KdV equation ($\Delta x = 0.25$)

taking $x_0 = -10$, $x_{\text{end}} = 10$, periodic boundary conditions, and, according to [14, Sec. 3], initial condition

$$u(x, 0) = \frac{5}{2} \operatorname{sech}^2\left(\frac{\sqrt{5}}{2}(x + 5)\right).$$

For the spatial discretization, we choose finite differences of order two.

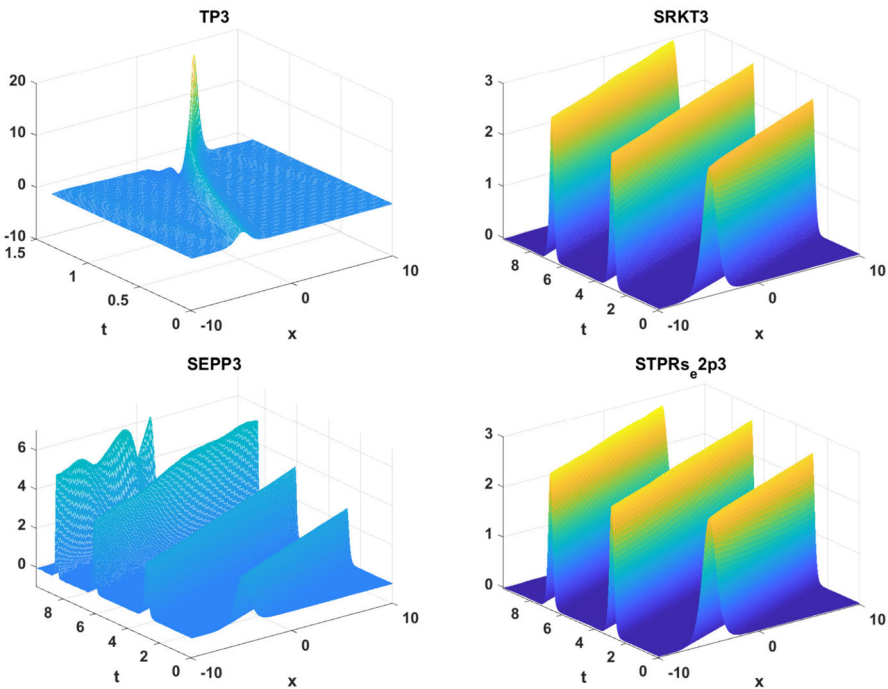


Fig. 12 Solution of the KdV equation by the methods TP3, SRKT3, SEPP3, and STP_s2p₃, respectively, using frozen Jacobian, with time step size $h \approx 0.01$ ($\Delta x = 0.1$)

First, we solve the problem for $t_0 = 0$, $t_{\text{end}} = 2$, using $h = t_{\text{end}}/2^i$, $i = 11, \dots, 15$, selecting $\Delta x = 0.25$. The results, reported in Figs. 10 and 11, correspond respectively to the cases of using exact Jacobian and frozen Jacobian evaluated at the first time grid point, following the same approach as before. In both scenarios, these results confirm the better efficiency of the new STP and STPR methods compared to the other schemes.

Finally, we evaluate the stability of some methods when applied with a frozen Jacobian. Indeed, while this can significantly reduce computational costs, it may also alter the stability properties of the methods, which are analyzed under the assumption of using an exact Jacobian. Let us therefore increase the stiffness of the semi-discretized problem by choosing $\Delta x = 0.1$, applying as an example some of the considered third-order methods. Note, from Table 1, that all the considered third-order methods are either strongly $A(\theta)$ -stable or $L(\theta)$ -stable, with θ close to 90° . This makes them suitable for problems whose Jacobian has eigenvalues lying close to the imaginary axis, as in this case. However, Fig. 12 shows that, for time step size $h = 10/2^{10} \approx 0.01$, the TP3 and SEPP3 methods exhibit instability when using a frozen Jacobian. Instead, the SRKT3 and STPR_{s_e2p3} schemes remain stable. This suggests that the latter methods have good stability properties even by using an inexact Jacobian.

8 Conclusions

In this work, we have proposed a new family of two-step peer methods for the solution of large and stiff IVPs arising from the space discretization of nonlinear advection–diffusion–reaction PDEs. The new methods combine two key ingredients: the employment of singly TASE operators, leading to strong stability properties such as L -stability or $L(\theta)$ -stability with θ close to 90° , and the reuse of previously computed stages, which significantly reduces the number of linear system to solve at each time step, compared to recently developed linearly implicit RK and peer schemes. We have derived methods of the new class up to order $p = 4$, showing through several numerical experiments their good performance compared to other recently introduced schemes, in terms of error, stability, and computational cost.

Several works can be done starting from this paper. For instance, one could develop a variable step size implementation of the proposed methods. Additionally, the idea of reused stages could be extended to other classes of numerical schemes. Another interesting line of investigation would be the analysis of the stability properties of such methods when using an inexact Jacobian.

Acknowledgements The author G. P. thanks GNCS-INdAM.

Author contribution The authors G. P. and L. R. contributed equally to conceptualization, methodology, software, validation, formal analysis, investigation, resources, data curation, original draft, review and editing, visualization, supervision, project administration, and funding acquisition.

Funding Open access funding provided by Università degli Studi di Napoli Federico II within the CRUI-CARE Agreement. This work has been supported by: the GNCS-INdAM Project; the Italian Ministry of University and Research (MUR), through the PRIN PNRR 2022 Projects P20228C2PP (CUP:

F53D23010020001 “BAT-MEN” and P2022WC2ZZ (CUP: E53D23018030001) “MatForPat”; the Spanish Project PID2022–141385NB–I00 of Ministerio de Ciencia e Innovación.

Declarations

Conflict of interest The authors declare no competing interests.

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