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A CLASS OF IMPLICIT-EXPLICIT TWO-STEP RUNGE–KUTTA METHODS*

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Abstract. This work develops new implicit-explicit time integrators based on two-step Runge–Kutta methods. The class of schemes of interest is characterized by linear invariant preservation and high stage orders. Theoretical consistency, stability, and stiff convergence analyses are performed to reveal the excellent properties of these methods. The new framework offers extreme flexibility in the construction of partitioned integrators since no coupling conditions are necessary. Practical schemes of orders three, four, and six are constructed and are used to solve several test problems. Numerical results confirm the theoretical findings.

Key words. implicit-explicit methods, two-step Runge–Kutta, order reduction

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1. Introduction.

Many science and engineering problems require numerical simulations of multiphysics systems, i.e., systems driven by multiple simultaneous physical processes evolving at different time scales.

In this work we are concerned with solving systems that involve both stiff and nonstiff processes. They are modeled by the following system of ordinary differential equations (ODEs):

$$y'(t) = F(y) = f(y) + g(y)\,, \quad t_0 \le t \le t_F\,, \quad y(t_0) = y_0; \quad y(t) \in \mathbb{R}^N\,, \tag{1.1}$$

where f and g represent the nonstiff and the stiff components, respectively. Without loss of generality, we skip the explicit dependence of f and g on the time argument. Problems of the form (1.1) often arise from the spatial discretization of partial differential equations (PDEs) in the method of lines approach; in this case, y is the semidiscrete state. As an example consider advection-diffusion-reaction systems, where the advection is slow while the diffusion and chemistry are typically fast [22].

Another example is the semi-implicit time integration of PDEs, where g represents the linear part of the discretized spatial operator and f is its nonlinear part [9].

The best numerical solution strategy for a particular problem depends on its dynamics. For nonstiff processes, explicit time discretizations are the most efficient, due to their low cost per step. For stiff processes, explicit methods require prohibitively small time steps (limited by the fastest time scale in the system). In this case, implicit methods, designed such that their step sizes are not limited by stability considerations, are more efficient [11, 12]. The numerical solution of multiphysics systems (1.1) is challenging as neither purely explicit nor purely implicit methods are completely

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satisfactory. Explicit methods have restricted time steps (due to g), while implicit methods require the solution of (non)linear systems of equations that involve *all* the processes in the model.

The implicit-explicit (IMEX) approach alleviates these difficulties by combining an implicit scheme for the stiff component with an explicit scheme for the nonstiff component. The pair is chosen such that the overall discretization of (1.1) has the desired stability and accuracy properties. IMEX linear multistep (LM) methods have been proposed in [8, 14, 20] and IMEX Runge–Kutta (RK) schemes in [21, 2, 17]. The order of consistency of these methods is typically lower than five. High order IMEX RK methods are difficult to construct due to the large number of order conditions. IMEX LM methods have decreasing stability properties with increasing order.

General linear (GL) methods [3] represent a natural generalization of both RK and LM methods, as they use both internal stages and information from previous solution steps. Two-step Runge–Kutta (TSRK) methods are a subclass of GL methods that use the stage values from only one previous step [1, 16]. The added flexibility of using both internal and external stage information allows us to design algorithms with superior stability and accuracy properties.

This work proposes a new family of IMEX methods based on pairs of TSRK schemes. The order conditions and the stability properties of the resulting discretization are investigated. Practical IMEX TSRK methods are constructed and are used in numerical tests to illustrate the theoretical findings.

The remainder of the paper is organized as follows. Section 2 introduces the partitioned TSRK methods, and order conditions are derived in section 2.3. IMEX TSRK methods are proposed in section 3, and their stability properties are discussed in section 4. Practical IMEX TSRK methods are constructed in section 6 and are used in numerical tests in section 7. Conclusions are drawn in section 8.

2. Partitioned two-step Runge–Kutta methods.

2.1. TSRK methods. A TSRK method advances the numerical solution of (1.1) from t_n to $t_{n+1} = t_n + h$ as follows [16]:

$$\begin{aligned} Y_i^{[n]} &= (1-u_i)\, y_{n-1} + u_i\, y_{n-2} \\ &\quad + h \sum_{j=1}^{s} \left(a_{i,j}\, F\left(Y_j^{[n]}\right) + b_{i,j}\, F\left(Y_j^{[n-1]}\right) \right), \quad i = 1, \dots, s, \end{aligned} \tag{2.1a}$$

$$y_n = (1-\vartheta)\, y_{n-1} + \vartheta\, y_{n-2} + h \sum_{j=1}^{s} \left(v_j\, F\left(Y_j^{[n]}\right) + w_j\, F\left(Y_j^{[n-1]}\right) \right). \tag{2.1b}$$

The method (2.1) can be represented compactly by its tableau of coefficients [16]

$$\begin{array}{c|c|c} \mathbf{u} & \mathbf{A} & \mathbf{B} \\ \hline \vartheta & \mathbf{v}^T & \mathbf{w}^T \end{array}, \tag{2.2}$$

where $\mathbf{A} = (a_{i,j})_{1\le i,j\le s}$, $\mathbf{B} = (b_{i,j})_{1\le i,j\le s}$, $\mathbf{u} = (u_i)_{1\le i\le s}$, $\mathbf{v} = (v_i)_{1\le i\le s}$, $\mathbf{w} = (w_i)_{1\le i\le s}$, and ϑ is a scalar. In addition, the abscissa vector $\mathbf{c} = (c_i)_{1\le i\le s}$ describes the time points where stage approximations are computed.

The TSRK method (2.1) has *stage order* q [16] if the stage vectors $Y_j^{[n]}$ are order q approximations of the exact solution at $t_{n-1} + c_j h$,

$$Y_j^{[n]} = y(t_{n-1} + c_j h) + \mathcal{O}(h^{q+1}), \quad h \to 0, \quad j = 1, \dots, s.$$

According to [16], the necessary and sufficient condition for (2.1) to have stage order q is

$$\frac{\mathbf{c}^{\nu}}{\nu!} - \frac{(-1)^{\nu}}{\nu!}\mathbf{u} - \frac{\mathbf{A}\mathbf{c}^{\nu-1}}{(\nu-1)!} - \frac{\mathbf{B}(\mathbf{c}-\mathbf{e})^{\nu-1}}{(\nu-1)!} = 0\,, \quad \nu = 1,\dots,q\,, \tag{2.3}$$

where $\mathbf{e} = [1,\dots,1]^T \in \mathbb{R}^s$ and the power operator is applied componentwise. Note that the stage consistency condition ($\nu = 1$) determines the abscissa vector,

$$\mathbf{c} = (\mathbf{A}+\mathbf{B})\,\mathbf{e} - \mathbf{u}\,. \tag{2.4}$$

The TSRK method (2.1) has *order* p [16] if the final approximation y_{n_F} to the solution $y(t_F)$ is of (global) order p, that is,

$$y_{n_F} = y(t_F) + \mathcal{O}(h^p)\,, \quad h \to 0\,.$$

Consider a TSRK method (2.1) with stage order $q \ge p-1$. If the coefficients satisfy the additional conditions

$$\frac{1}{\nu!} - \frac{(-1)^{\nu}}{\nu!}\vartheta - \frac{\mathbf{v}^T\mathbf{c}^{\nu-1}}{(\nu-1)!} - \frac{\mathbf{w}^T(\mathbf{c}-\mathbf{e})^{\nu-1}}{(\nu-1)!} = 0\,, \quad \nu = 1,\dots,p\,, \tag{2.5}$$

then the method has order p [16].

2.2. Partitioned TSRK (PTSRK) methods. Consider the partitioned system of ODEs

$$y' = \begin{bmatrix} y_{\{1\}} \\ \vdots \\ y_{\{N\}} \end{bmatrix}' = \begin{bmatrix} f_{\{1\}}(y) \\ \vdots \\ f_{\{N\}}(y) \end{bmatrix} = \sum_{k=1}^{N} \begin{bmatrix} \mathbf{0} \\ f_{\{k\}}(y) \\ \mathbf{0} \end{bmatrix} = F(y) \tag{2.6}$$

with scalar quantities $y_{\{1\}},\dots,y_{\{N\}}$.

Each of the N ODEs for $y'_{\{k\}}$ is integrated using a different TSRK method:

$$\begin{array}{c|c|c} \mathbf{u}^{\{k\}} & \mathbf{A}^{\{k\}} & \mathbf{B}^{\{k\}} \\ \hline \vartheta^{\{k\}} & \left(\mathbf{v}^{\{k\}}\right)^T & \left(\mathbf{w}^{\{k\}}\right)^T \end{array}\,, \quad k = 1,\dots,N\,. \tag{2.7}$$

The coefficients of the methods (2.7) have to be coordinated such that the overall discretization of (2.6) has the desired accuracy and stability. We focus on families of methods (2.7) that have several particular characteristics which make them suitable for the integration of PDEs discretized in the method of lines.

Remark 2.1. The splitting of (2.6), (2.7) into scalar components does not restrict the generality of the discussion. All results in this section extend directly to systems of equations by selecting the component methods in (2.7) such that all components of a subsystem are discretized with the same scheme. For example, if the system (2.6) is partitioned into two vector subsystems with $y_{[1]} = [y_{\{1\}},\dots,y_{\{M\}}]^T$ and $y_{[2]} = [y_{\{M+1\}},\dots,y_{\{N\}}]^T$, then we apply a two way partitioned method by using (2.7) with $\mathbf{A}^{\{1\}} = \cdots = \mathbf{A}^{\{M\}} = \mathbf{A}^{[1]}$, $\mathbf{A}^{\{M+1\}} = \cdots = \mathbf{A}^{\{N\}} = \mathbf{A}^{[2]}$, and similarly for $\mathbf{B}$, ϑ, $\mathbf{u}$, $\mathbf{v}$, and $\mathbf{w}$.

Remark 2.2. Assume that the first L components of the system (2.6) are nonstiff, and the last $N-L$ components are stiff. Then the partitioned ODE (2.6) can be written in the additively split form (1.1):

$$f(y) = \sum_{k=1}^{L} \begin{bmatrix} \mathbf{0} \\ f_{\{k\}}(y) \\ \mathbf{0} \end{bmatrix}, \quad g(y) = \sum_{k=L+1}^{N} \begin{bmatrix} \mathbf{0} \\ f_{\{k\}}(y) \\ \mathbf{0} \end{bmatrix}.$$

Similarly, the system (1.1) can be written in the partitioned ODE form (2.6):

$$y = u + v, \quad \begin{bmatrix} u \\ v \end{bmatrix}' = \begin{bmatrix} f(u+v) \\ g(u+v) \end{bmatrix}.$$

Therefore numerical schemes (2.7) developed for the form (2.6) can be directly applied to systems (1.1) and vice versa.

Preservation of linear invariants. Preservation of linear invariants is an essential property for the integration of conservation laws [6, 7, 19]. For example, the numerical solution of the advection equation conserves the total mass of the system (to roundoff accuracy) if the space discretization is flux conservative, and the time discretization preserves linear invariants.

The family of TSRK methods (2.7) conserves linear invariants of the system if all the weights are equal to each other. Therefore of particular interest are methods which share the same theta,

$$\vartheta^{\{k\}} = \vartheta\,, \quad k = 1, \ldots, N\,, \tag{2.8}$$

and the same weight vectors,

$$\mathbf{v}^{\{k\}} = \mathbf{v}\,, \quad \mathbf{w}^{\{k\}} = \mathbf{w}\,, \quad k = 1, \ldots, N\,. \tag{2.9}$$

To be specific, consider a linear invariant of the ODE system (2.6),

$$\sum_{k=1}^{N} \mu_{\{k\}}\, f_{\{k\}}(y) = 0 \quad \forall\, y \quad \Rightarrow \quad \sum_{k=1}^{N} \mu_{\{k\}}\, y_{\{k\}}(t) = C = \text{constant} \quad \forall\, t\,.$$

Assume that all the previous numerical solutions preserve this invariant:

$$\sum_{k=1}^{N} \mu_{\{k\}}\, y_{\{k\},\ell} = C\,, \quad \ell = 0, \ldots, n-1\,.$$

From (2.1b), (2.8), and (2.9) it follows that the next step solution y_n also preserves the invariant.

Internal consistency. We consider the case where all individual methods (2.7) are stage consistent (2.4). Each method (2.7) computes stage values $Y^{[n]}_{\{k\}}$ that approximate the exact solution components $y_{\{k\}}(t_n + \mathbf{c}^{\{k\}}\, h)$ at abscissae $\mathbf{c}^{\{k\}} = (\mathbf{A}^{\{k\}} + \mathbf{B}^{\{k\}})\,\mathbf{e} - \mathbf{u}^{\{k\}}$. We call the method (2.7) internally consistent if all components $Y^{[n]}_{\{k\},i}$ of a stage vector approximate the exact solution at the same time moment, $t_n + c_i h$ for all k. Consequently, we focus on stage consistent methods which satisfy the simplifying assumption

$$\mathbf{u}^{\{k\}} = \mathbf{u}\,, \quad k = 1, \ldots, N\,, \tag{2.10}$$

and for which the abscissae of all N TSRK methods are equal:

$$\mathbf{c}^{\{k\}} = \left(\mathbf{A}^{\{k\}} + \mathbf{B}^{\{k\}}\right) \cdot \mathbf{e} - \mathbf{u} = \mathbf{c}\,, \quad k = 1, \ldots, N\,. \tag{2.11}$$

The class of methods under consideration. The class of partitioned TSRK (PTSRK) methods under consideration enjoys the properties of theta-consistency (2.8), u-consistency (2.10), linear conservation (2.9), and stage consistency (2.11). This class is characterized by the tableaux

$$\mathbf{c}^{\{k\}} = \mathbf{c}\,, \quad \begin{array}{c|c|c} \mathbf{u} & \mathbf{A}^{\{k\}} & \mathbf{B}^{\{k\}} \\ \hline \vartheta & \mathbf{v}^T & \mathbf{w}^T \end{array}\,, \quad k = 1, \ldots, N\,. \tag{2.12}$$

Partitioned methods in this family are written explicitly as follows:

(2.13a)

$$\begin{aligned} Y^{[n]}_{\{k\},i} &= (1-u_i)\, y_{\{k\},n-1} + u_i\, y_{\{k\},n-2} \\ &\quad + h \sum_{j=1}^{s} a^{\{k\}}_{i,j} f_{\{k\}} \left(Y^{[n]}_{\{1\},j}, \ldots, Y^{[n]}_{\{N\},j} \right) + h \sum_{j=1}^{s} b^{\{k\}}_{i,j} f_{\{k\}} \left(Y^{[n-1]}_{\{1\},j}, \ldots, Y^{[n-1]}_{\{N\},j} \right), \end{aligned}$$

(2.13b)

$$\begin{aligned} y_{\{k\},n} &= (1-\vartheta)\, y_{\{k\},n-1} + \vartheta\, y_{\{k\},n-2} \\ &\quad + h \sum_{j=1}^{s} v_j f_{\{k\}} \left(Y^{[n]}_{\{1\},j}, \ldots, Y^{[n]}_{\{N\},j} \right) + h \sum_{j=1}^{s} w_j f_{\{k\}} \left(Y^{[n-1]}_{\{1\},j}, \ldots, Y^{[n-1]}_{\{N\},j} \right), \\ k &= 1, \ldots, N\,. \end{aligned}$$

2.3. Order conditions for PTSRK methods. We follow the approach of Hairer and consider the set TP of P-trees [10, 13]. Each node of a P-tree carries a label (color) $\{1\}$ through $\{N\}$. For a P-tree $\tau \in TP$ we denote by $r(\tau)$ the label of its root, by $\rho(\tau)$ its number of vertices, and by $\alpha(\tau)$ the number of distinct monotonic labelings of the vertices of τ. A P-series has the form

$$\mathcal{P}(\phi, y) = \begin{bmatrix} \mathcal{P}_{\{1\}}(\phi, y) \\ \vdots \\ \mathcal{P}_{\{N\}}(\phi, y) \end{bmatrix} = \begin{bmatrix} \displaystyle\sum_{t \in TP \,\&\, r(t)=\{1\}} \phi(t)\, \alpha(t)\, F(t)(y)\, h^{\rho(t)}\, (\rho(t)!)^{-1} \\ \vdots \\ \displaystyle\sum_{t \in TP \,\&\, r(t)=\{N\}} \phi(t)\, \alpha(t)\, F(t)(y)\, h^{\rho(t)}\, (\rho(t)!)^{-1} \end{bmatrix},$$

where $\phi : TP \to \mathbb{R}$ is a real valued mapping and $F(t)(y)$ is the elementary differential associated with P-tree t and evaluated at y [10].

The following mappings are useful in the derivation. The step shift operator [13]

$$e(t) = 1\,, \quad e^{-1}(t) = (-1)^{\rho(t)} \quad \forall\, t \in TP$$

has the property that

$$y(t+h) \sim \mathcal{P}(e, y(t))\,, \quad y(t-h) \sim \mathcal{P}(e^{-1}, y(t))\,. \tag{2.14}$$

The derivative of a mapping ϕ with $\phi(\emptyset_{\{i\}}) = 1$ [13] is defined by

$$\phi'(\emptyset_{\{i\}}) = 0\,, \quad \phi'(\bullet_{\{i\}}) = 1\,, \quad \phi'(t) = \rho(t)\, \phi(t_1) \ldots \phi(t_k) \;\text{ for }\; t =_{\{i\}} [t_1, \ldots, t_k]$$

and has the property that

$$g \sim \mathcal{P}(\phi, y) \quad \Rightarrow \quad h\, f(g) \sim \mathcal{P}(\phi', y)\,.$$

The P-series coefficients of the stage solutions (2.13a) are defined recursively by

$$\begin{aligned} &\phi_i(\emptyset_{\{k\}}) = 1 \quad \text{for any } 1 \le k \le N\,, \\ &\phi_i(t) = u_i\,(-1)^{\rho(t)} + \sum_{j=1}^{s} a_{i,j}^{\{k\}}\,\phi_j'(t) + \sum_{j=1}^{s} b_{i,j}^{\{k\}}\,\left(e^{-1}\,\phi_j\right)'(t) \\ &\qquad \text{for } \rho(t) \ge 1 \text{ and } r(t) = \{k\}\,. \end{aligned} \tag{2.15}$$

Similarly, the P-series coefficients of the full solution (2.13b) are defined by

$$\begin{aligned} &\psi(\emptyset_{\{k\}}) = 1 \quad \text{for any } 1 \le k \le N\,, \\ &\psi(t) = \vartheta\,(-1)^{\rho(t)} + \sum_{j=1}^{s} v_j^{\{k\}}\,\phi_j'(t) + \sum_{j=1}^{s} w_j^{\{k\}}\,\left(e^{-1}\,\phi_j\right)'(t) \\ &\qquad \text{for } \rho(t) \ge 1 \text{ and } r(t) = \{k\}\,. \end{aligned} \tag{2.16}$$

We are now ready to state the main results of this section.

THEOREM 2.3 (order conditions for general PTSRK methods). *A PTSRK method has order p if and only if*

$$\psi(t) = 1 \quad \forall t \in TP \text{ with } \rho(t) \le p\,. \tag{2.17}$$

Proof. The exact solution has a P-series given by the step shift operator (2.14), $y(t_{n+1}) \sim \mathcal{P}(\psi, y(t_n))$. The PTSRK numerical solution obtained with an exact initialization has the P-series

$$y_{n+1} \sim \mathcal{P}(\psi, y(t_n))\,.$$

The method has order p if and only if the two series are equal up to order p, i.e., the local error is of order $p+1$. Therefore $\psi(t) = e(t)$ for all trees with $\rho(t) \le p$. ∎

Next, we study the order conditions for our class of PTSRK methods (2.12).

THEOREM 2.4 (order conditions for the special class of PTSRK methods (2.12)). *Consider a PTSRK method* (2.12) *which satisfies the internal stage consistency condition* (2.11). *The PTSRK method has order p and stage order $q \ge p-1$ if and only if each of the components methods has order $p^{\{k\}} = p$ and stage order $q^{\{k\}} \ge p-1$.*

Remark 2.5. In this case no "coupling" order conditions are needed. By "coupling" we mean order conditions in the form of nonlinear equations involving the coefficients of multiple methods. Such conditions are needed, for example, in the case of partitioned RK methods [11], as well as in the case of general PTSRK methods (2.17).

Proof. As explained by Hairer and Wanner [13] the stage order of the method constrains the stage P-series coefficients (2.15). Under the internal consistency assumption (2.11) the partitioned method has stage order q if and only if

$$\phi_i(t) = c_i^{\rho(t)} \quad \forall\, t \in TP\,:\; \rho(t) \le q\,.$$

Note that the coefficient ϕ_i is the same for all P-trees with a given number of nodes, regardless of their structure and regardless of the labeling (color) of their nodes. From the composition of P-series it holds that

$$\phi_i'(t) = \rho(t)\,c_i^{\rho(t)-1}\,, \quad \left(e^{-1}\phi_i\right)(t) = (1-c_i)^{\rho(t)}\,, \quad \left(e^{-1}\phi_i\right)'(t) = \rho(t)\,(1-c_i)^{\rho(t)-1}\,.$$

From (2.15) we infer that the PTSRK method has stage order q if and only if

$$c_i^\nu = u_i\,(-1)^\nu + \sum_{j=1}^{s} a_{i,j}^{\{k\}}\,\nu\,c_j^{\nu-1} + \sum_{j=1}^{s} b_{i,j}^{\{k\}}\,\nu\,(1-c_i)^{\nu-1} \qquad (2.18)$$
$$\forall\ t \text{ with } 1 \le \nu = \rho(t) \le q \text{ and } r(t) = k = 1,\dots,N\,.$$

We note that (2.18) is the stage order condition (2.3) for the $\{k\}$th component TSRK method. Therefore an internally consistent PTSRK method has stage order q (2.15) *if and only if* each of the component methods has stage order q.

Consider now the case where $q \ge p-1$. From (2.16) and (2.17) the PTSRK method has order p if and only if

$$1 = \vartheta\,(-1)^\nu + \sum_{j=1}^{s} v_j^{\{k\}}\,\nu\,c_j^{\nu-1} + \sum_{j=1}^{s} w_j^{\{k\}}\,\nu\,(1-c_i)^{\nu-1} \qquad (2.19)$$
$$\forall\ t \text{ with } 1 \le \nu = \rho(t) \le p \text{ and } r(t) = k = 1,\dots,N\,.$$

Equation (2.19) is the order condition (2.5) for the $\{k\}$th component method. Therefore an internally consistent PTSRK method with stage order $q \ge p-1$ has order p *if and only if* each of the component methods has order p. □

The above stability and consistency results lead to the following convergence theorem.

THEOREM 2.6 (convergence for the special class of PTSRK methods (2.12)). *Consider the class* (2.12) *of PTSRK methods which satisfy the internal stage consistency condition* (2.11). *If*

- *each individual method is zero stable,*
- *the starting values are of order p,*
- *each component method has order p,*
- *each component method has stage order $q \ge p-1$,*

then the numerical solution converges with order p,

$$y_n - y(t_n) = \mathcal{O}(h^p) \quad \forall\, n\,.$$

Proof. Application of (2.7) to the test equation $y' = 0$ shows that the partitioned method is zero-stable if and only if each of the component methods is zero-stable. This and the order result of Theorem 2.4 imply convergence with order p. □

A direct proof of Theorem 2.6 following the approach of Jackiewicz [16] that is not based on P-trees is given in [23].

3. IMEX TSRK methods. IMEX TSRK methods are PTSRK methods (2.12) with a two way splitting

$$\mathbf{A}^{\{1\}} = \mathbf{A}\,, \quad \mathbf{A}^{\{2\}} = \widehat{\mathbf{A}}\,, \quad \mathbf{B}^{\{1\}} = \mathbf{B}\,, \quad \mathbf{B}^{\{2\}} = \widehat{\mathbf{B}}\,,$$

where $\mathbf{A}$, $\mathbf{B}$ are the coefficients of an explicit TSRK method, and $\widehat{\mathbf{A}}$, $\widehat{\mathbf{B}}$ are the coefficients of an implicit one. Moreover, $\widehat{\mathbf{A}}$ is lower triangular, with $\widehat{\mathbf{A}}_{i,i} = \gamma$ for all stages $i = 1, \ldots, s$. An IMEX TSRK method applied to (1.1) reads

$$
\begin{aligned}
\text{(3.1a)}\quad Y_i^{[n]} &= (1-u_i)\, y_{n-1} + u_i\, y_{n-2} + h \sum_{j=1}^{i-1} a_{i,j}\, f\left(Y_j^{[n]}\right) + h \sum_{j=1}^{s} b_{i,j}\, f\left(Y_j^{[n-1]}\right) \\
&\quad + h \sum_{j=1}^{i-1} \widehat{a}_{i,j}\, g\left(Y_j^{[n]}\right) + h\gamma\, g\left(Y_i^{[n]}\right) + h \sum_{j=1}^{s} \widehat{b}_{i,j}\, g\left(Y_j^{[n-1]}\right) , \\
\text{(3.1b)}\quad y_n &= (1-\vartheta)\, y_{n-1} + \vartheta\, y_{n-2} \\
&\quad + h \sum_{j=1}^{s} v_j\, (f+g)\left(Y_j^{[n]}\right) + h \sum_{j=1}^{s} w_j\, (f+g)\left(Y_j^{[n-1]}\right) .
\end{aligned}
$$

4. Stability aspects. Application of the TSRK method (2.2) to the linear scalar test equation

$$y' = \zeta\, y$$

leads to a stability matrix of the form

$$
\text{(4.1)}\qquad \mathbf{M}(z) = \begin{bmatrix} 1-\vartheta + z\mathbf{v}^T\mathbf{S}(z)(\mathbf{e}-\mathbf{u}) & \vartheta + z\mathbf{v}^T\mathbf{S}(z)\mathbf{u} & \mathbf{w}^T + z\mathbf{v}^T\mathbf{S}(z)\mathbf{B} \\ 1 & 0 & \mathbf{0} \\ z\mathbf{S}(z)(\mathbf{e}-\mathbf{u}) & z\mathbf{S}(z)\mathbf{u} & z\mathbf{S}(z)\mathbf{B} \end{bmatrix},
$$

with $z = h\,\zeta$ and $\mathbf{S}(z) = (\mathbf{I}_s - z\mathbf{A})^{-1}$ (see [16, p. 95]). The method is linearly stable if the spectral radius of the stability matrix (4.1) is less than or equal to one. The stability region of the method is defined as

$$\mathcal{S} = \{ z \in \mathbb{C} \ :\ \rho(M(z)) \le 1 \} .$$

4.1. Linear stability of the partitioned method. To assess the stability of the IMEX method (3.1), i.e., to study how the stability properties of the two methods combine when used in tandem, we consider the linear scalar test problem

$$
\text{(4.2)}\qquad y' = \zeta\, y + \eta\, y \ , \quad \{\text{where } f(y) = \zeta\, y \ ,\ \ g(y) = \eta\, y\} .
$$

We denote the nonstiff and the stiff complex variables by $z = h\,\zeta$ and $x = h\,\eta$, respectively. The method (3.1) applied to the scalar test equation (4.2) gives

$$
\begin{bmatrix} y_n \\ y_{n-1} \\ Y^{[n]} \end{bmatrix} = \mathbf{M}(x,z) \cdot \begin{bmatrix} y_{n-1} \\ y_{n-2} \\ Y^{[n-1]} \end{bmatrix}
$$

with

$$
\text{(4.3)}\qquad \mathbf{M}(x,z) = \begin{bmatrix} \mathbf{M}_{1,1}(x,z) & \mathbf{M}_{1,2}(x,z) & \mathbf{M}_{1,3}(x,z) \\ 1 & 0 & \mathbf{0}_{1\times s} \\ \mathbf{S}(x,z)\,(\mathbf{e}-\mathbf{u}) & \mathbf{S}(x,z)\,\mathbf{u} & \mathbf{S}(x,z)\,\left(z\,\mathbf{B} + x\,\widehat{\mathbf{B}}\right) \end{bmatrix},
$$

where

$$
\begin{aligned}
\mathbf{S}(x,z) &= \left(\mathbf{I_s} - z\,\mathbf{A} - x\,\widehat{\mathbf{A}}\right)^{-1} , \\
\mathbf{M}_{1,1}(x,z) &= (1-\vartheta) + (z\,\mathbf{v} + x\,\widehat{\mathbf{v}})^T\ \mathbf{S}(x,z)\,(\mathbf{e}-\mathbf{u})\,, \\
\mathbf{M}_{1,2}(x,z) &= \vartheta + (z\,\mathbf{v} + x\,\widehat{\mathbf{v}})^T\ \mathbf{S}(x,z)\,\mathbf{u}\,, \\
\mathbf{M}_{1,3}(x,z) &= (z\,\mathbf{v} + x\,\widehat{\mathbf{v}})^T\ \mathbf{S}(x,z)\ \left(z\,\mathbf{B} + x\,\widehat{\mathbf{B}}\right) + z\,\mathbf{w}^T + x\,\widehat{\mathbf{w}}^T .
\end{aligned}
$$

Theoretical results about the spectral radius of the matrix (4.3) are difficult to obtain. Instead, the joint stability is analyzed numerically as follows. Define a desired stiff stability region $\mathcal{S} \subset \mathbb{C}$, for example, $\mathcal{S}_\alpha = \{x \in \mathbb{C}^- \ : \ |\mathrm{Im}(x)| \le \tan(\alpha)\,|\mathrm{Re}(x)|\}$ for $A(\alpha)$-stability, and compute numerically the constrained nonstiff stability region:

$$\mathcal{N}_\alpha = \{z \in \mathbb{C} \ : \ \rho(M(x,z)) \le 1 \quad \forall\, x \in \mathcal{S}_\alpha\} \ . \tag{4.4}$$

If the $\mathcal{N}_\alpha$ is not degenerate (contains an open subset of the left half plane), then the IMEX combined stability is considered acceptable.

Nonlinear (algebraic) stability of the TSRK methods can be treated in the general linear method framework following [3, 4]. To the best of our knowledge, no extension of the algebraic stability to partitioned or IMEX methods is available at this time.

5. Convergence aspects. In this section we investigate the convergence and possible order reduction of IMEX TSRK methods with the help of several standard test problems. We consider an infinite "region of interest" in the complex plane

$$\mathcal{R} = \{z \in \mathbb{C} \ : \ \mathrm{Re}(z) \le z_0 < 0\,, \quad |\mathrm{Im}(z)| \le \alpha\,|\mathrm{Re}(z)|\,, \quad \alpha \ge 0\} \tag{5.1}$$

that contains all the eigenvalues of the stiff Jacobian $h\,g_y$.

5.1. Semilinear problems. Consider the split ODE

$$y' = \underbrace{\mu\, y}_{g(y)} + f(y)\ , \quad \mathrm{Re}(\mu) < 0\ , \quad y(t_0) = y_0\,, \tag{5.2}$$

where the stiff part $g(y) = \mu y$ is linear with $\mu \in \mathcal{R}$ (5.1), and the nonstiff part $f(y)$ is nonlinear. We assume that $f(y)$ is continuously differentiable and that its Jacobian is uniformly bounded in a vicinity of the solution, $\|\mathbf{f}_{\mathbf{y}}(y)\| \le L_f$ with $L_f = \mathcal{O}(1)$ of moderate size. This assumption is slightly stronger than Lipschitz continuity, and L_f plays the role of the Lipschitz constant.

THEOREM 5.1 (convergence of IMEX TSRK methods applied to semilinear test problem). *Consider the IMEX TSRK method* (3.1) *of order p, stage order q for the explicit component, and stage order $\widehat{q}$ for the implicit component. Assume that the implicit component is linearly stable and that the spectral radius of the implicit stability matrix* (4.3) *is bounded uniformly in the infinite "region of interest"* (5.1),

$$\rho\left(\widehat{\mathbf{M}}(z)\right) \le \rho_0 < 1 \quad \forall\, z \in \mathcal{R}\,.$$

Then the IMEX method (3.1) *is convergent with order* $\min(p, q, \widehat{q})$ *for any μ. This convergence order holds uniformly for all levels of stiffness, i.e., for any $h\mu \in \mathcal{R}$.*

It is convenient to construct IMEX TSRK methods (3.1) with $\widehat{q} = q = p$, as such methods do not suffer from order reduction on the semilinear problem (5.2).

Proof. The method (3.1) applied to (5.2) reads

$$\begin{aligned} Y^{[n]} &= (\mathbf{e} - \mathbf{u})\; y_{n-1} + \mathbf{u}\, y_{n-2} \\ &\quad + h\,\mathbf{A}\, f^{[n]} + h\,\mathbf{B}\, f^{[n-1]} + h\,\mu\,\widehat{\mathbf{A}}\, Y^{[n]} + h\,\mu\,\widehat{\mathbf{B}}\, Y^{[n-1]}\,, \end{aligned} \tag{5.3a}$$

$$\begin{aligned} y_n &= (1 - \vartheta)\, y_{n-1} + \vartheta\, y_{n-2} \\ &\quad + h\,\mathbf{v}^T\, f^{[n]} + h\,\mathbf{w}^T\, f^{[n-1]} + h\,\mu\,\mathbf{v}^T\, Y^{[n]} + h\,\mu\,\mathbf{w}^T\, Y^{[n-1]}\,, \end{aligned} \tag{5.3b}$$

where $f^{[j]} = f(Y^{[j]})$ and $g^{[j]} = g(Y^{[j]})$. Consider the global errors

$$\Delta y_n = y_n - y(t_n)\ , \quad \Delta Y^{[n]} = Y^{[n]} - y\,(t_{n-1} + \mathbf{c}\,h)\ . \tag{5.4}$$

Write the stage equation (5.3a) in terms of the exact solution and global errors,

$$\begin{aligned}\Delta Y^{[n]} &= -y\,(t_{n-1}+\mathbf{c}\,h) + (\mathbf{e}-\mathbf{u})\; y(t_{n-1}) + \mathbf{u}\,y(t_{n-2}) + (\mathbf{e}-\mathbf{u})\;\Delta y_{n-1} + \mathbf{u}\,\Delta y_{n-2}\\ &\quad + h\,\mathbf{A}\,f\,(t_{n-1}+\mathbf{c}\,h) + h\,\mathbf{B} f\,(t_{n-2}+\mathbf{c}\,h) + h\,\mathbf{A}\,\Delta f^{[n]} + h\,\mathbf{B}\,\Delta f^{[n-1]}\\ &\quad + h\,\mu\,\widehat{\mathbf{A}}\,\Delta Y^{[n]} + h\,\mu\,\widehat{\mathbf{B}}\,\Delta Y^{[n-1]} + h\,\mu\,\widehat{\mathbf{A}}\,y\,(t_{n-1}+\mathbf{c}\,h) + h\,\mu\,\widehat{\mathbf{B}}\,y\,(t_{n-2}+\mathbf{c}\,h)\;,\end{aligned}$$

where $f(t) = f(\,y(t)\,)$ and $\Delta f^{[n]} = f^{[n]} - f(t_n+\mathbf{c}h)$. Using the stage order conditions of the implicit component

$$\begin{aligned}y\,(t_{n-1}+\mathbf{c}\,h) &= (\mathbf{e}-\mathbf{u})\; y(t_{n-1}) + \mathbf{u}\,y(t_{n-2}) + h\,\widehat{\mathbf{A}}\,f\,(t_{n-1}+\mathbf{c}\,h) + h\,\widehat{\mathbf{B}} f\,(t_{n-2}+\mathbf{c}\,h)\\ &\quad + h\,\mu\,\widehat{\mathbf{A}}\,y\,(t_{n-1}+\mathbf{c}\,h) + h\,\mu\,\widehat{\mathbf{B}} y\,(t_{n-2}+\mathbf{c}\,h) + \mathcal{O}\left(h^{\widehat{q}+1}\right),\end{aligned}$$

one obtains

$$\begin{aligned}\left(\mathbf{I}-h\,\mu\,\widehat{\mathbf{A}}\right)\,\Delta Y^{[n]} &= (\mathbf{e}-\mathbf{u})\;\Delta y_{n-1} + \mathbf{u}\,\Delta y_{n-2} + h\,\mu\,\widehat{\mathbf{B}}\,\Delta Y^{[n-1]}\\ &\quad + h\,\mathbf{A}\,\Delta f^{[n]} + h\,\mathbf{B}\,\Delta f^{[n-1]} - h\,(\widehat{\mathbf{A}}-\mathbf{A})\,f\,(t_{n-1}+\mathbf{c}\,h)\\ &\quad - h\,(\widehat{\mathbf{B}}-\mathbf{B})\,f\,(t_{n-2}+\mathbf{c}\,h) + \mathcal{O}\left(h^{\widehat{q}+1}\right)\;.\end{aligned} \tag{5.5}$$

Taylor series expansions about t_{n-1} yield

$$\phi\,(t_{n-1}+\mathbf{c}\,h) = \sum_{k=0}^{\infty} \frac{h^k\mathbf{c}^k}{k!}\phi^{(k)}(t_{n-1})\,; \qquad \phi\,(t_{n-2}+\mathbf{c}\,h) = \sum_{k=0}^{\infty} \frac{h^k(\mathbf{c}-\mathbf{e})^k}{k!}\phi^{(k)}(t_{n-1})\,.$$

These expansions and the stage order conditions (2.3) of the implicit component give

$$\begin{aligned}\widehat{\mathbf{A}}\,f\,(t_{n-1}+\mathbf{c}\,h) + \widehat{\mathbf{B}}\,f\,(t_{n-2}+\mathbf{c}\,h) &= \sum_{k=0}^{\infty}\frac{h^k}{k!}\left(\widehat{\mathbf{A}}\mathbf{c}^k + \widehat{\mathbf{B}}(\mathbf{c}-\mathbf{e})^k\right) f^{(k)}(t_{n-1})\\ &= \sum_{k=0}^{\infty}\frac{h^k}{k!}\left(\frac{\mathbf{c}^{k+1}+(-1)^k\mathbf{u}}{k+1}\right) f^{(k)}(t_{n-1}) + \mathcal{O}\left(h^{\widehat{q}}\right)\;.\end{aligned}$$

Similarly, the solution Taylor expansions and the explicit stage order conditions yield

$$\mathbf{A}\,f\,(t_{n-1}+\mathbf{c}\,h) + \mathbf{B}\,f\,(t_{n-2}+\mathbf{c}\,h) = \sum_{k=0}^{\infty}\frac{h^k}{k!}\left(\frac{\mathbf{c}^{k+1}+(-1)^k\mathbf{u}}{k+1}\right) f^{(k)}(t_{n-1}) + \mathcal{O}\left(h^{q}\right)\;.$$

Since the explicit and implicit methods share the same $\mathbf{c}$ and $\mathbf{u}$, inserting the above relations in (5.5) leads to

$$\begin{aligned}\Delta Y^{[n]} &= \widehat{\mathbf{S}}(z)\;(\mathbf{e}-\mathbf{u})\;\Delta y_{n-1} + \widehat{\mathbf{S}}(z)\,\mathbf{u}\,\Delta y_{n-2} + z\,\widehat{\mathbf{S}}(z)\,\widehat{\mathbf{B}}\,\Delta Y^{[n-1]}\\ &\quad + h\,\widehat{\mathbf{S}}(z)\,\mathbf{A}\,\Delta f^{[n]} + h\,\widehat{\mathbf{S}}(z)\,\mathbf{B}\,\Delta f^{[n-1]} + \mathcal{O}\left(h^{\min(q,\widehat{q})+1}\right)\cdot\widehat{\mathbf{S}}(z)\,,\end{aligned} \tag{5.6}$$

where $z = h\mu$ and $\widehat{\mathbf{S}}(z) = (\mathbf{I} - z\,\widehat{\mathbf{A}})^{-1}$. Note that h and $z = h\mu$ are allowed to vary independently.

Inserting the exact solution in (5.3b) and using the order p condition, then subtracting the numerical solution (5.3b), leads to the following equation for the global error:

$$\begin{aligned}\Delta y_n &= (1-\vartheta)\,\Delta y_{n-1} + \vartheta\,\Delta y_{n-2} + z\,\mathbf{v}^T\,\Delta Y^{[n]} + z\,\mathbf{w}^T\,\Delta Y^{[n-1]}\\ &\quad + h\,\mathbf{v}^T\,\Delta f^{[n]} + h\,\mathbf{w}^T\,\Delta f^{[n-1]} + \mathcal{O}\left(h^{p+1}\right)\;.\end{aligned}$$

After using (5.6) and rearranging the expression we obtain

$$
\begin{aligned}
(5.7)\quad \Delta y_n = &\Big((1-\vartheta) + z\,\mathbf{v}^T\,\widehat{\mathbf{S}}(z)\,(\mathbf{e}-\mathbf{u})\Big)\,\Delta y_{n-1} + \Big(\vartheta + z\,\mathbf{v}^T\,\widehat{\mathbf{S}}(z)\Big)\,\Delta y_{n-2}\\
&+ z\,\Big(\mathbf{w}^T + z\,\mathbf{v}^T\,\widehat{\mathbf{S}}(z)\,\widehat{\mathbf{B}}\Big)\,\Delta Y^{[n-1]}\\
&+ \mathbf{v}^T\,\Big(\mathbf{I} + z\,\widehat{\mathbf{S}}(z)\,\mathbf{A}\Big)\,h\,\Delta f^{[n]} + \mathbf{w}^T\,\Big(\mathbf{I} + z\,\widehat{\mathbf{S}}(z)\,\mathbf{B}\Big)\,h\,\Delta f^{[n-1]}\\
&+ \mathcal{O}\left(h^{p+1}\right) + \mathcal{O}\left(h^{\min(q,\widehat{q})+1}\right)\cdot z\widehat{\mathbf{S}}(z)\,.
\end{aligned}
$$

We have that the poles of $\widehat{\mathbf{S}}(z)$ are in the right half of the complex plane. The functions $\widehat{\mathbf{S}}(z)$, $z\widehat{\mathbf{S}}(z)$ are holonomic on $\mathcal{R}$ with $\widehat{\mathbf{S}}(z)\to\mathbf{0}$ and $z\widehat{\mathbf{S}}(z)\to\widehat{\mathbf{A}}^{-1}\widehat{\mathbf{B}}$ when $z\to\infty$. Consequently the functions are uniformly bounded on the region of interest, $\|\widehat{\mathbf{S}}(z)\|\le\beta_1$ and $\|z\widehat{\mathbf{S}}(z)\|\le\beta_2$ for any $z\in\mathcal{R}$. The error term $\mathcal{O}\left(h^{\min(q,\widehat{q})+1}\right)$ in (5.7) has a constant that is independent of z.

From the mean value theorem,

$$\Delta f^{[n]} = \mathbf{f_y}^{[n]}\,\Delta Y^{[n]}\,,\quad \Delta f^{[n-1]} = \mathbf{f_y}^{[n-1]}\,\Delta Y^{[n-1]}\,,$$

where the Jacobians are evaluated at some intermediate point.

From (5.6) and (5.7) we obtain the error recurrence

$$
(5.8)\qquad \begin{bmatrix}\Delta y_n\\ \Delta y_{n-1}\\ \Delta Y^{[n]}\end{bmatrix} = \widetilde{\mathbf{M}}(z)\cdot\begin{bmatrix}\Delta y_{n-1}\\ \Delta y_{n-2}\\ \Delta Y^{[n-1]}\end{bmatrix} + h\,\widetilde{\mathbf{P}}(z)\cdot\begin{bmatrix}\Delta Y^{[n]}\\ \Delta Y^{[n-1]}\end{bmatrix} + \mathcal{O}\left(h^r\right)\,,
$$

with $r=\min(q,\widehat{q},p)+1$ and

$$
\widetilde{\mathbf{M}}(z) = \begin{bmatrix} 1-\vartheta + z\,\mathbf{v}^T\,\widehat{\mathbf{S}}(z)\,(\mathbf{e}-\mathbf{u}) & \vartheta + z\,\mathbf{v}^T\,\widehat{\mathbf{S}}(z)\,\mathbf{u} & z\,\Big(\mathbf{w}^T + z\,\mathbf{v}^T\,\widehat{\mathbf{S}}(z)\,\widehat{\mathbf{B}}\Big)\\ 1 & 0 & 0\\ \widehat{\mathbf{S}}(z)\,(\mathbf{e}-\mathbf{u}) & \widehat{\mathbf{S}}(z)\,\mathbf{u} & z\,\widehat{\mathbf{S}}(z)\,\widehat{\mathbf{B}}\end{bmatrix},
$$

$$
\widetilde{\mathbf{P}}(z) = \begin{bmatrix} \widehat{\mathbf{S}}(z)\,\mathbf{A}\,\mathbf{f_y}^{[n]} & \widehat{\mathbf{S}}(z)\,\mathbf{B}\,\mathbf{f_y}^{[n-1]}\\ 0 & 0\\ \mathbf{v}^T\,\Big(\mathbf{I} + z\,\widehat{\mathbf{S}}(z)\,\mathbf{A}\Big)\,\mathbf{f_y}^{[n]} & \mathbf{w}^T\,\Big(\mathbf{I} + z\,\widehat{\mathbf{S}}(z)\,\mathbf{B}\Big)\,\mathbf{f_y}^{[n-1]}\end{bmatrix}.
$$

From the uniform boundedness of $\mathbf{f_y}$ and $z\widehat{\mathbf{S}}(z)$ it follows that $\|\widetilde{\mathbf{P}}(z)\|\le\beta_3$ for any $z\in\mathcal{R}$ where the bound is of moderate size $\beta_3=\mathcal{O}(1)$.

The following error recurrence is obtained by combining (5.6) and (5.8):

$$
(5.9)\quad (\mathbf{I}-\mathcal{O}(h))\begin{bmatrix}\Delta y_n\\ \Delta y_{n-1}\\ \Delta Y^{[n]}\end{bmatrix} = \Big(\widetilde{\mathbf{M}}(h\mu) + \mathcal{O}(h)\Big)\cdot\begin{bmatrix}\Delta y_{n-1}\\ \Delta y_{n-2}\\ \Delta Y^{[n-1]}\end{bmatrix} + \mathcal{O}\left(h^r\right)\,.
$$

Assume that a one-step, order p method is used to initialize both the step and the stage solutions of the TSRK method [16, section 6.2]. The error starting values are $e_0=0$, $e_1=\mathcal{O}(h^p)$, and $E^{[1]}=\mathcal{O}(h^p)$. The error amplification matrix $\widetilde{\mathbf{M}}(z)$ is similar to the stability function (4.3) of the implicit method for any finite nonzero z, $\widetilde{\mathbf{M}}(z)\sim\widehat{\mathbf{M}}(z)$. Therefore its spectral radius is uniformly bounded below one for all

$z = h\mu \in \mathcal{R}$. For small enough step sizes the matrix $(\mathbf{I} - \mathcal{O}(h))^{-1}\,(\widetilde{\mathbf{M}}(h\mu) + \mathcal{O}(h))$ also has a spectral radius that is uniformly bounded below one for all $z = h\mu$ of interest. All the constants for the $\mathcal{O}(h)$ terms are given by the Lipschitz constant of the nonstiff nonlinear term and are therefore order one. The step size restriction is not too stringent. By standard numerical ODE arguments [11], (5.9) implies convergence of global errors to zero at a rate $\|\Delta y_n\| = \mathcal{O}\left(h^{r-1}\right) = \mathcal{O}\left(h^{\min(p,q,\widehat{q})}\right)$. ∎

5.2. Singular perturbation analysis. Consider the singular perturbation test problem [12]

$$\begin{bmatrix} y \\ z \end{bmatrix}' = \begin{bmatrix} f(y,z) \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ \varepsilon^{-1}\, g(y,z) \end{bmatrix}, \quad t_0 \le t \le t_F\,, \quad \begin{bmatrix} y \\ z \end{bmatrix}(t_0) = \begin{bmatrix} y_0 \\ z_0 \end{bmatrix}, \tag{5.10}$$

where the sub-Jacobian g_z is invertible in a vicinity of the solution. Consequently, there is a locally unique solution $z = G(y)$ that satisfies $g\,(y, G(y)) = 0$. For $\varepsilon \to 0$ the system (5.10) reduces to the index-1 differential algebraic equation

$$\begin{bmatrix} y' \\ 0 \end{bmatrix} = \begin{bmatrix} f(y,z) \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ g(y,z) \end{bmatrix}, \quad \begin{bmatrix} y \\ z \end{bmatrix}(t_0) = \begin{bmatrix} y_0 \\ G(y_0) \end{bmatrix}, \tag{5.11}$$

and the differential variable evolves according to the nonstiff reduced ODE,

$$y' = f\,(y, G(y))\,, \quad t_0 \le t \le t_F\,, \quad y(t_0) = y_0\,. \tag{5.12}$$

Of particular interest are IMEX TSRK pairs where the implicit component is stiffly accurate,

$$\mathbf{v} = \widehat{\mathbf{A}}^T\,\mathbf{e}_s\,, \quad \mathbf{w} = \widehat{\mathbf{B}}^T\,\mathbf{e}_s\,, \quad \vartheta = \mathbf{u}^T\,\mathbf{e}_s\,, \tag{5.13a}$$

and, in addition, it satisfies

$$\rho(\widehat{\mathbf{A}}^{-1}\,\widehat{\mathbf{B}}) < 1\,. \tag{5.13b}$$

Stiffly accurate methods are characterized by $\mathbf{v}^T\,\widehat{\mathbf{A}}^{-1} = \mathbf{e}_s^T$, c_s=1, and

$$\mathbf{w}^T = \mathbf{v}^T\,\widehat{\mathbf{A}}^{-1}\,\widehat{\mathbf{B}}, \tag{5.13c}$$

$$\vartheta = \mathbf{v}^T\,\widehat{\mathbf{A}}^{-1}\mathbf{u}, \quad 1 - \vartheta = \mathbf{v}^T\,\widehat{\mathbf{A}}^{-1}(\mathbf{1} - \mathbf{u})\,. \tag{5.13d}$$

From (4.1) the stiff stability matrix at infinity is

$$\widehat{\mathbf{M}}(\infty) = \begin{bmatrix} 1 - \vartheta - \mathbf{v}^T\widehat{\mathbf{A}}^{-1}(\mathbf{1} - \mathbf{u}) & \vartheta - \mathbf{v}^T\widehat{\mathbf{A}}^{-1}\mathbf{u} & \mathbf{w}^T - \mathbf{v}^T\,\widehat{\mathbf{A}}^{-1}\,\widehat{\mathbf{B}} \\ 1 & 0 & 0 \\ -\widehat{\mathbf{A}}^{-1}(\mathbf{1} - \mathbf{u}) & -\widehat{\mathbf{A}}^{-1}\mathbf{u} & \widehat{\mathbf{A}}^{-1}\,\widehat{\mathbf{B}} \end{bmatrix}. \tag{5.14}$$

For stiffly accurate schemes, (5.13b) and (5.13c) imply that $\rho(\widehat{\mathbf{M}}(\infty)) = \rho(\widehat{\mathbf{A}}^{-1}\,\widehat{\mathbf{B}}) < 1$.

The IMEX TSRK method (3.1) applied to (5.10) reads

$$Y^{[n]} = (\mathfrak{1} - \mathfrak{u})\,y_{n-1} + \mathfrak{u}\,y_{n-2} + h\,\mathfrak{A}\,f^{[n]} + h\,\mathfrak{B}\,f^{[n-1]}, \tag{5.15a}$$

$$Z_i^{[n]} = (\mathfrak{1} - \mathfrak{u})\,z_{n-1} + \mathfrak{u}\,z_{n-2} + h\,\varepsilon^{-1}\,\widehat{\mathfrak{A}}\,g^{[n]} + h\,\varepsilon^{-1}\,\widehat{\mathfrak{B}}\,g^{[n-1]}\,, \tag{5.15b}$$

$$y_n = (1 - \vartheta)\,y_{n-1} + \vartheta\,y_{n-2} + h\,\mathfrak{v}^T f^{[n]} + h\,\mathfrak{w}^T f^{[n-1]}\,, \tag{5.15c}$$

$$z_n = (1 - \vartheta)\,z_{n-1} + \vartheta\,z_{n-2} + h\,\varepsilon^{-1}\,\mathfrak{v}^T g^{[n]} + h\,\varepsilon^{-1}\,\mathfrak{w}^T g^{[n-1]}\,. \tag{5.15d}$$

We denote the Kronecker products of coefficients by Gothic letters, e.g., $\mathfrak{A} = \mathbf{A} \otimes \mathbf{I}$ for an appropriately sized identity matrix in (5.15a), and so on. We use the notation $f^{[n]} = [f^T(Y_1^{[n]}, Z_1^{[n]}) \dots f^T(Y_s^{[n]}, Z_s^{[n]})]^T$; $g^{[n]}$ is defined similarly.

Taking the limit $\varepsilon \to 0$ in (5.15) gives

$$Y^{[n]} = (\mathfrak{1} - \mathfrak{u})\, y_{n-1} + \mathfrak{u}\, y_{n-2} + h\, \mathfrak{A}\, f^{[n]} + h\, \mathfrak{B}\, f^{[n-1]}, \tag{5.16a}$$

$$g^{[n]} = -\left(\widehat{\mathbf{A}}^{-1}\, \widehat{\mathbf{B}} \otimes \mathbf{I}\right) g^{[n-1]}\,, \tag{5.16b}$$

$$y_n = (1 - \vartheta)\, y_{n-1} + \vartheta\, y_{n-2} + h\, \mathfrak{v}^T f^{[n]} + h\, \mathfrak{w}^T f^{[n-1]}\,, \tag{5.16c}$$

$$0 = \mathfrak{v}^T g^{[n]} + \mathfrak{w}^T g^{[n-1]} = \left((\mathbf{w}^T - \mathbf{v}^T\, \widehat{\mathbf{A}}^{-1}\, \widehat{\mathbf{B}}) \otimes \mathbf{I}\right) g^{[n-1]}\,. \tag{5.16d}$$

Equation (5.16b) defines the stage values $Z_i^{[n]}$. If the initial conditions and the initial stages are consistent, then (5.16b) implies by induction

$$g^{[0]} = 0 \quad \Rightarrow \quad g^{[n]} = 0 \quad \forall \text{ steps } n \geq 1\,. \tag{5.17}$$

Equation (5.16b) can be replaced with the algebraic constraints $g(Y_i^{[n]}, Z_i^{[n]}) = 0$ or $Z_i^{[n]} = G(Y_i^{[n]})$ for $i = 1, \dots, s$. Note that if (5.13b) holds, the small numerical errors in the solution of the nonlinear algebraic equation at each step are damped out. The value of the residual $g^{[n]} \to 0$ for $n \to \infty$ even for inconsistent initial values ($g^{[0]} \neq 0$). Since $g^{[n]} = 0$, (5.16d) is also satisfied. Moreover, if (5.13c) holds, then (5.16d) is satisfied identically.

Equations (5.16a) and (5.16c) represent the application of the explicit method to the nonstiff reduced ODE (5.12). By the convergence theory of TSRK methods [16], the global errors are

$$\Delta y_n = y_n - y(t_n) = \mathcal{O}\left(h^p\right)\,, \quad \Delta Y^{[n]} = Y^{[n]} - y(t_{n-1} + \mathbf{c}h) = \mathcal{O}\left(h^q\right)\,. \tag{5.18}$$

Solving for $g^{[n]}$ in (5.15b),

$$h\, \varepsilon^{-1}\, g^{[n]} = -\widehat{\mathfrak{A}}^{-1}\, \widehat{\mathfrak{B}}\, \left(h\, \varepsilon^{-1}\, g^{[n-1]}\right) + \widehat{\mathfrak{A}}^{-1}\, \left(Z^{[n]} - (\mathfrak{1} - \mathfrak{u})\, z_{n-1} - \mathfrak{u}\, z_{n-2}\right)\,,$$

and replacing it in (5.15d) leads to

$$\begin{aligned} z_n = {} & (1 - \vartheta - \mathfrak{v}^T\, \widehat{\mathfrak{A}}^{-1} (\mathfrak{1} - \mathfrak{u}))\, z_{n-1} + (\vartheta - \mathfrak{v}^T\, \widehat{\mathfrak{A}}^{-1} \mathfrak{u})\, z_{n-2} \\ & + \cancelto{0}{\left(\mathfrak{w}^T - \mathfrak{v}^T\, \widehat{\mathfrak{A}}^{-1}\, \widehat{\mathfrak{B}}\right)}\, h\, \varepsilon^{-1}\, g^{[n-1]} + \mathfrak{v}^T\, \widehat{\mathfrak{A}}^{-1}\, Z^{[n]}\,. \end{aligned} \tag{5.19}$$

We assume that (5.13c) holds, as it is a necessary condition for the singular perturbation limit $\varepsilon \to 0$ of (5.19) to exist. Insert the exact solution in (5.15b) and use the stage order conditions of the implicit method to obtain

$$\begin{aligned} h\, z'\, (t_{n-1} + \mathbf{c}h) = {} & \widehat{\mathfrak{A}}^{-1}\, \left(z(t_{n-1} + \mathbf{c}h) - (\mathfrak{1} - \mathfrak{u})\, z(t_{n-1}) - \mathfrak{u}\, z(t_{n-2})\right) \\ & - h\, \widehat{\mathfrak{A}}^{-1}\, \widehat{\mathfrak{B}}\, z'\, (t_{n-2} + \mathbf{c}h) + \mathcal{O}\left(h^{\widehat{q}+1}\right)\,. \end{aligned} \tag{5.20}$$

Use the exact solution in (5.15d) and the order conditions of the implicit method,

$$\begin{aligned} z(t_n) = {} & (1 - \vartheta)\, z(t_{n-1}) + \vartheta\, z(t_{n-2}) \\ & + h\, \mathfrak{v}^T\, z'\, (t_{n-1} + \mathbf{c}h) + h\, \mathfrak{w}^T\, z'\, (t_{n-2} + \mathbf{c}h) + \mathcal{O}\left(h^{p+1}\right)\,. \end{aligned} \tag{5.21}$$

Inserting (5.20) into (5.21) leads to

$$\begin{aligned} z(t_n) &= (1-\vartheta-\mathfrak{v}^T\widehat{\mathfrak{A}}^{-1}(\mathfrak{1}-\mathfrak{u}))\,z(t_{n-1})+(\vartheta-\mathfrak{v}^T\widehat{\mathfrak{A}}^{-1}\mathfrak{u})\,z(t_{n-2}) \\ &\quad+\mathfrak{v}^T\,\widehat{\mathfrak{A}}^{-1}\,z(t_{n-1}+\mathbf{c}h) \\ &\quad+h\cancelto{0}{\left(\mathfrak{w}^T-\mathfrak{v}^T\,\widehat{\mathfrak{A}}^{-1}\,\widehat{\mathfrak{B}}\right)}\,z'\,(t_{n-2}+\mathbf{c}h)+\mathcal{O}\left(h^{\min(p,\widehat{q})+1}\right). \end{aligned} \tag{5.22}$$

Consider the global errors

$$\Delta z_n = z_n - z(t_n)\,, \quad \Delta Z^{[n]} = Z^{[n]} - z(t_n+\mathbf{c}h)\,.$$

Subtracting (5.22) from (5.19) yields the global error recurrence

$$\begin{aligned} \Delta z_n &= \left(1-\vartheta-\mathfrak{v}^T\,\widehat{\mathfrak{A}}^{-1}(\mathfrak{1}-\mathfrak{u})\right)\,\Delta z_{n-1}+(\vartheta-\mathfrak{v}^T\,\widehat{\mathfrak{A}}^{-1}\mathfrak{u})\,\Delta z_{n-2} \\ &\quad+\mathfrak{v}^T\,\widehat{\mathfrak{A}}^{-1}\,\Delta Z^{[n]}+\mathcal{O}\left(h^{\min(p,\widehat{q})+1}\right), \end{aligned} \tag{5.23}$$

Let L_G be the Lipschitz constant of the function $G(\cdot)$. From (5.17) and (5.18),

$$\left\|\Delta Z^{[n]}\right\| = \left\|G\left(Y^{[n]}\right)-G\left(y(t_{n-1}+\mathbf{c}h)\right)\right\| \le L_G\,\left\|\Delta Y^{[n]}\right\| = \mathcal{O}\left(h^{\min(p,q)}\right).$$

The recurrence (5.23) becomes

$$\begin{aligned} \Delta z_n &= \left(1-\vartheta-\mathfrak{v}^T\,\widehat{\mathfrak{A}}^{-1}(\mathfrak{1}-\mathfrak{u})\right)\,\Delta z_{n-1}+(\vartheta-\mathfrak{v}^T\,\widehat{\mathfrak{A}}^{-1}\mathfrak{u})\,\Delta z_{n-2} \\ &\quad+\mathcal{O}\left(h^{\min(p,q,\widehat{q}+1)}\right). \end{aligned} \tag{5.24}$$

If $\rho(\widehat{\mathbf{M}}(\infty)) < 1$ in (5.14), assumption (5.13b) implies that

$$\rho\left(\begin{bmatrix} 1-\vartheta-\mathbf{v}^T\widehat{\mathbf{A}}^{-1}(\mathbf{1}-\mathbf{u}) & \vartheta-\mathbf{v}^T\widehat{\mathbf{A}}^{-1}\mathbf{u} \\ 1 & 0 \end{bmatrix}\right) < 1\,.$$

In this case, the error iteration (5.24) converges and

$$\Delta z_n = \mathcal{O}\left(h^{\min(p-1,q-1,\widehat{q})}\right).$$

If (5.13d) holds, e.g., if the method is stiffly accurate, then (5.24) reduces to

$$\Delta z_n = \mathfrak{v}^T\,\widehat{\mathfrak{A}}^{-1}\,\Delta Z^{[n]}+\mathcal{O}\left(h^{\min(p,\widehat{q})+1}\right) = \mathcal{O}\left(h^{\min(p,q,\widehat{q}+1)}\right).$$

We have established the following.

THEOREM 5.2 (IMEX TSRK on index-1 DAEs). *Consider an IMEX TSRK method* (3.1) *of order p, explicit stage order q, and implicit stage order $\widehat{q}$, and whose implicit part satisfies* (5.13c) *and $\rho(\widehat{\mathbf{M}}(\infty)) < 1$. The application of this IMEX TSRK method to the reduced problem* (5.16) *gives solutions with global errors*

$$y_n - y(t_n) = \mathcal{O}\left(h^p\right), \quad z_n - z(t_n) = \mathcal{O}\left(h^{\min(p-1,q-1,\widehat{q})}\right).$$

In addition, if (5.13d) *holds, then*

$$z_n - z(t_n) = \mathcal{O}\left(h^{\min(p,q,\widehat{q}+1)}\right).$$

The last equation holds for IMEX TSRK methods with a stiffly accurate implicit component.

In particular it is advantageous to construct IMEX TSRK methods with a stiffly accurate implicit part, $q = p$, and $\widehat{q} \in \{p-1, p\}$.

6. Construction of practical IMEX TSRK methods. In this section we construct practical IMEX TSRK schemes with order $p = s + 1$ and stage order $\widehat{q} = q = s$. The relatively large number of stages is necessary to be able to enforce the desired stability properties.

We consider two strategies to construct IMEX pairs. The first starts with an existing implicit TSRK method with appropriate stability properties (e.g., A- or L-stability) and develops the explicit component. This simplifies the construction procedure, but places significant restrictions on the IMEX pairs one can obtain; for example, most A-stable TSRK methods currently available in the literature impose $\mathbf{u} = 0$ for simplicity, which limits the stability of the IMEX pair. We use this approach to develop a sixth order IMEX TSRK pair (see Appendix E in the supplementary material). The second strategy is to build simultaneously both the implicit and the explicit components of the IMEX TSRK pair. We construct pairs of orders three and four with $\mathbf{u} \neq 0$, and with implicit components that are both stiffly accurate and $A(\alpha)$-stable (see Appendices C and D in the supplementary material).

In both strategies a two-step optimization process is employed to search for the best method coefficients. First, we explore the parameter space using the genetic algorithm function `ga` in the MATLAB optimization toolbox. The best member of this process is then taken as the starting point for the MATLAB `fminsearch` routine, which locally refines the solution and provides a sufficient number of accurate digits.

6.1. A third order, two stages IMEX pair. Third order IMEX TSRK methods with two stages are specified by the abscissa vector $\mathbf{c} = [c_1, c_2]$ and the tableaux of coefficients

$$\begin{array}{c|cc|cc} u_1 & \lambda & & \widehat{b}_{11} & \widehat{b}_{12} \\ u_2 & \widehat{a}_{21} & \lambda & \widehat{b}_{21} & \widehat{b}_{22} \\ \hline \vartheta & v_1 & v_2 & w_1 & w_2 \end{array}\,, \qquad \begin{array}{c|cc|cc} u_1 & & & b_{11} & b_{12} \\ u_2 & a_{21} & & b_{21} & b_{22} \\ \hline \vartheta & v_1 & v_2 & w_1 & w_2 \end{array}\,, \tag{6.1}$$

where all the variables are real parameters. We impose the abscissa values $\mathbf{c} = [0, 1]^T$, the order conditions (2.19), the stage order conditions (2.18), and the stiff accuracy condition (5.13a) to constrain the coefficients. The resulting family of third order IMEX TSRK pairs depends on four free parameters $u_1, u_2, \widehat{a}_{21}, a_{21}$. The implicit component is

$$\begin{array}{c|cc|cc} u_1 & \frac{5-u_2}{12} & & \frac{u_1}{2} & \frac{u_2+6u_1-5}{12} \\ u_2 & \widehat{a}_{21} & \frac{5-u_2}{12} & \frac{5u_2-1}{12} & \frac{2u_2-2\widehat{a}_{21}+2}{3} \\ \hline u_2 & \widehat{a}_{21} & \frac{5-u_2}{12} & \frac{5u_2-1}{12} & \frac{2u_2-2\widehat{a}_{21}+2}{3} \end{array}\,,$$

and the explicit component is

$$\begin{array}{c|cc|cc} u_1 & & & \frac{u_1}{2} & \frac{u_1}{2} \\ u_2 & a_{21} & & \frac{u_2-1}{2} & \frac{3+u_2-2a_{21}}{2} \\ \hline u_2 & \widehat{a}_{21} & \frac{5-u_2}{12} & \frac{5u_2-1}{12} & \frac{2u_2-2\widehat{a}_{21}+2}{3} \end{array}\,.$$

The optimization procedure could not find any feasible points for A-stability, so we relaxed this restriction by requiring $A(\alpha)$-stability with $\alpha = 75°$. The resulting method is called IMEX TSRK(2,3), and its coefficients are given in Appendix B of the supplementary material. The stability regions for each component and for the combined method are shown in Figure G.1 of the supplementary material.

6.2. A fourth order, three stages IMEX pair. We impose the abscissa values $\mathbf{c} = [0, 1/2, 1]^T$, the order conditions (2.19), the stage order conditions (2.18), and the stiff accuracy condition (5.13a) to constrain the coefficients. A family of fourth order, third stage order IMEX TSRK pairs is obtained with nine degrees of freedom. We choose $u_1, u_2, u_3, \lambda, a_{21}, a_{31}, a_{32}, \widehat{a}_{21}, \widehat{a}_{31}$ as the free parameters. The resulting IMEX pair has the implicit component

$$\begin{array}{c|ccc|ccc}
u_1 & \lambda & & & \frac{u_1}{6} & \frac{2u_2}{3} & \frac{u_1}{6} - \lambda \\
u_2 & \widehat{a}_{21} & \lambda & & \frac{5+4u_2-24\lambda}{24} & -\frac{2}{3} + \frac{2u_2}{3} + 3\lambda & \frac{23}{24} - \widehat{a}_{21} + \frac{u_2}{6} - 3\lambda \\
u_3 & \widehat{a}_{31} & \frac{4}{3} - 4\lambda & \lambda & \frac{\vartheta+6\lambda-1}{6} & \frac{2}{3} + \frac{2\vartheta}{3} - 4\lambda & -\frac{5}{6} - \widehat{a}_{31} + \frac{\vartheta}{6} + 6\lambda \\
\hline
u_3 & \widehat{a}_{31} & \frac{4}{3} - 4\lambda & \lambda & \frac{\vartheta+6\lambda-1}{6} & \frac{2}{3} + \frac{2\vartheta}{3} - 4\lambda & -\frac{5}{6} - \widehat{a}_{31} + \frac{\vartheta}{6} + 6\lambda
\end{array}$$

and the explicit component

$$\begin{array}{c|ccc|ccc}
u_1 & & & & \frac{u_1}{6} & \frac{2u_2}{3} & \frac{u_1}{6} \\
u_2 & a_{21} & & & \frac{5+4u_2}{24} & -\frac{2}{3} + \frac{2u_2}{3} & \frac{23}{24} - a_{21} + \frac{u_2}{6} \\
u_3 & a_{31} & a_{32} & & \frac{\vartheta-6a_{32}+7}{6} & -\frac{10}{3} + 3a_{32} + \frac{2\vartheta}{3} & \frac{19}{6} - a_{31} + 3a_{32} + \frac{\vartheta}{6} \\
\hline
u_3 & \widehat{a}_{31} & \frac{4}{3} - 4\lambda & \lambda & \frac{\vartheta+6\lambda-1}{6} & \frac{2}{3} + \frac{2\vartheta}{3} - 4\lambda & -\frac{5}{6} - \widehat{a}_{31} + \frac{\vartheta}{6} + 6\lambda
\end{array}.$$

We impose $A(\alpha)$-stability with $\alpha = 75^\circ$. The optimized method is called IMEX TSRK(3,4), and its coefficients are given in Appendix C of the supplementary material. The stability regions for each component and for the combined method are shown in Figure G.1 of the supplementary material.

6.3. A sixth order, five stages IMEX pair. This method is characterized by $s = 5$, $p = 6$, and $q = 5$. The implicit part is taken from [1] and is L-stable. The coefficients $\mathbf{A}$ are obtained by numerical optimization. All method coefficients $\mathbf{c}, \mathbf{u}, \mathbf{A}, \mathbf{B}, \widehat{\mathbf{A}}, \widehat{\mathbf{B}}, \vartheta, \mathbf{v}$, and $\mathbf{w}$ are given in Appendix F of the supplementary material for completeness. The region of stability for this method is shown in Figure H.1 of the supplementary material.

7. Numerical tests. We now illustrate the convergence properties of the proposed IMEX TSRK schemes with the help of several test problems. The advection-reaction PDE displays stiffness in one additive component of the right-hand side and helps in investigating the convergence behavior and the possible order reduction of various methods. The larger shallow water model is used in coastal and environmental engineering and helps in comparing the accuracy and relative efficiency of different IMEX time integration schemes. In addition, numerical results for the stiff Van der Pol equation are presented in Appendix F of the supplementary material.

The advantage of IMEX RK and IMEX LM schemes over fully explicit or fully implicit schemes applied to separable problems (1.1) has been well established [21, 5, 14]. These results, however, do not show a clear favorite: different IMEX schemes perform best on different problems. We compare the new IMEX TSRK schemes with the following RK and multistep IMEX methods from the literature:

- the second and third order IMEX RK methods $ARS(2,2,2)$ and $ARS(3,4,3)$, respectively, from Ascher, Ruuth, and Spiteri [21];
- the fourth and fifth order methods $ARK4(3)6L[2]SA$ and $ARK5(4)8L[2]SA$, named here $KC(5,6,4)$ respectively $KC(7,8,5)$, from Kennedy and Carpenter [5];
- the IMEX LM methods of orders 2–5 from Hundsdorfer and Ruuth [14].

Here we use the naming of these methods proposed in [14].

For each of the test cases below, a reference solution was computed with the MATLAB `ode15s` routine with the very tight tolerances $\text{atol} = \text{rtol} = 2.22045 \cdot 10^{-14}$. The initial steps needed by multistep methods and TSRK methods are also calculated by `ode15s` with the same tolerance settings. All numerical errors are measured at the final simulation times against the corresponding reference solutions. All the experiments are performed on a workstation with 4 Intel Xeon E5-2630 processors running Linux Kernel 3.8.4.

7.1. Advection-reaction system. This test case is borrowed from [14] and is described by the following PDE system:

$$\partial_t \begin{bmatrix} y \\ z \end{bmatrix} = -\partial_x \begin{bmatrix} \alpha_1 y \\ \alpha_2 z \end{bmatrix} + \begin{bmatrix} -k_1 & k_2 \\ k_1 & -k_2 \end{bmatrix} \cdot \begin{bmatrix} y \\ z \end{bmatrix} + \begin{bmatrix} s_1 \\ s_2 \end{bmatrix}, \quad (t,x) \in [0,1] \times [0,1], \tag{7.1}$$

with parameters $\alpha_1 = 1$, $\alpha_2 = 0$, $k_1 = 10^6$, $k_2 = 2 \cdot 10^6$, $s_1 = 0$, $s_2 = 1$, and with the following initial and boundary values:

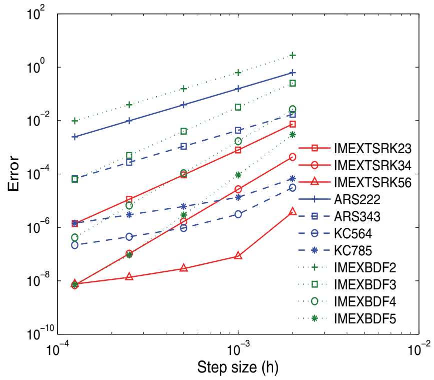
$$y(x,0) = 1 + s_2 x, \quad z(x,0) = \frac{k_1}{k_2} y(x,0) + \frac{1}{k_2} s_2, \quad y(0,t) = 1 - \sin(12t)^4.$$

The space discretization is done with fourth order finite differences in the interior and third order upwind biased finite differences at the borders of the spatial domain. The space grid consists of 400 uniformly distributed nodes. We treat the nonstiff advection term explicitly and the stiff reaction term implicitly.

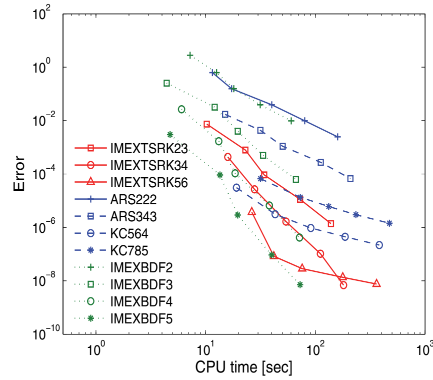
For all the schemes tested, the solutions are computed with different fixed time steps. They are compared against the MATLAB reference solution at the final time. The errors in L_1-norms are plotted against the time step in Figure 1(a). We observe that $ARS(3,4,3)$ shows the same second order behavior $ARS(2,2,2)$. Both KC schemes suffer from significant order reduction. However, the IMEX backward differentiation formula (IMEX BDF) schemes, IMEX TSRK(2,3), and IMEX TSRK(3,4) do not exhibit order reduction. For the same step size, IMEX TSRK schemes yield much smaller errors than IMEX BDF schemes of the same order. The sixth order scheme IMEX TSRK(5,6) does not show the theoretical order, but has the advantage of high accuracy compared to other schemes under the same step size.

In Figure 1(b) the errors are plotted as functions of CPU time (in seconds) with the same sequence of time step sizes used in the convergence results. Among all the third order schemes, IMEX TSRK(2,3) shows the highest efficiency. For fourth order ones, IMEX TSRK(3,4) and IMEX BDF4 almost coincide; KC(5,6,4) leads for the low accuracy part and lags behind for higher accuracy (errors smaller than 10^{-6}).

7.2. Shallow water equations. *Semi-implicit time integration* has become popular in the numerical weather and climate prediction communities, e.g., as an effective way to treat gravity waves. Semi-implicit integration uses an IMEX scheme, with the implicit method applied to the linearized right-hand side operator and the explicit method applied to the remaining nonlinear part [9].



(a) Solution errors versus time step h.



(b) Solution errors versus CPU time.

FIG. 1. *Work-precision diagrams for IMEX TSRK, IMEX RK, and IMEX BDF schemes applied to the advection-reaction problem* (7.1). *The solution errors are measured at the final time in the L_1-norm.*

In this test we solve the two-dimensional shallow water equations using a semi-implicit integration approach. The shallow water system under consideration is

$$\begin{aligned} \partial_t H &= -\partial_x(uH) - \partial_y(vH) \\ \partial_t(uH) &= -\partial_x\Big(u^2H + \frac{1}{2}gH^2\Big) - \partial_y(uvH) \\ \partial_t(vH) &= -\partial_x(uvH) - \partial_y\Big(v^2H + \frac{1}{2}gH^2\Big) \end{aligned} \tag{7.2}$$

on the unit square domain $(x, y) \in [0, 1] \times [0, 1]$. Here H is the fluid height and u and v are the flow velocity components. The initial conditions at $t_0 = 0$ are

$$u(t_0, x, y) = 0\,, \quad v(t_0, x, y) = 0\,, \quad H(t_0, x, y) = 1 + \exp(-\|(x, y) - (c_1, c_2)\|_2^2)\,, \tag{7.3}$$

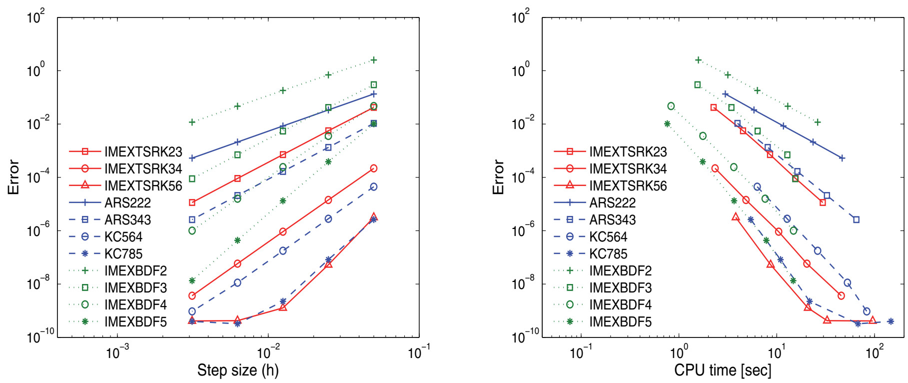
where the Gaussian height profile is described by $c_1 = 1/3$ and $c_2 = 2/3$. Furthermore, the local gravity constant is $g = 9.81$ $[m/sec^2]$. Reflective boundary conditions are used for velocity terms, and free-slip boundary conditions are used for height. The initial condition produces traveling waves that suffer multiple reflections at the boundaries.

A second order finite difference scheme is used for space discretization. The resulting semidiscrete ODE system is

$$\frac{\mathrm{d}}{\mathrm{d}t}U(t) = F_{\rm swe}\,(U(t)) = \underbrace{J_{\rm swe}\big(U(t)\big)\cdot U(t)}_{g(U(t))} + \underbrace{F_{\rm swe}(U(t)) - g\,(U(t))}_{f(U(t))}\,, \tag{7.4}$$

where $U(t)$ is the discrete counterpart of the vector of unknowns (H, uH, vH). Denote by $J_{\rm swe} = \partial F_{\rm swe}/\partial U$ the Jacobian of the discretized shallow water operator. We split the right-hand side of (7.4) into a stiff part g and a nonstiff part f. Here g is a nonlinear function in $U(t)$. The numerical solution of the implicit part of the method uses a simplified Newton iteration that requires only a single factorization of $\mathbf{I} - h\lambda J_{swe}(U_n)$ per step. Here U_n is the numerical approximation to $U(t_n)$. Note that a semi-implicit approach can be obtained similarly by choosing a linear stiff part, i.e., a splitting of the form $g(U) = J_{\text{swe}}(U_n) \cdot (U(t) - U_n)$ on each step $t \in [t_n, t_{n+1}]$.

The system is integrated from $t_0 = 0$ to $t_F = 1$ [second] with a sequence of step sizes that starts with $h = 0.05$ [seconds]; the step size is halved for each subsequent run. The Jacobian is updated only once in each time step for all methods tested. The errors in L_1-norms are plotted against the time step size in Figure 2(a) and against the CPU time in Figure 2(b). Figure 2(a) reveals that all the schemes display the theoretical orders of convergence. IMEX RK methods yield the smallest errors for a given time step. However, IMEX TSRK are slightly superior to both IMEX RK and IMEX BDF in terms of efficiency. To achieve the same order, IMEX TSRK requires fewer stages than IMEX RK, and the performance gap between the two families gets larger as the order increases. IMEX BDF methods have the lowest cost per time step; however, the larger number of time steps attenuates this advantage. In general, high order IMEX schemes are more efficient than low order ones. But for a specific order, the selection of one IMEX family is not a clear cut choice. The efficiency is highly dependent on implementation, and the relative performance is likely to vary for different problems. Intrinsic method properties such as stability, accuracy, and lack of order reduction become even more important in the context of complex multiphysics systems, for which IMEX schemes are designed.



(a) Solution errors versus step size. (b) Solution errors versus CPU time.

Fig. 2. *Work-precision diagrams for IMEX TSRK, IMEX RK, and IMEX BDF schemes applied to the shallow water equations* (7.2). *The solution errors are measured at the final time in the L_1-norm.*

8. Conclusions. This paper develops a new family of implicit-explicit (IMEX) time integrators based on pairs of two-step Runge–Kutta (TSRK) methods. The class of schemes of interest is characterized by stage consistency (same abscissae) and linear invariant preservation (same weights). The study of order conditions for partitioned TSRK methods reveals that, in the case of high stage orders, no additional coupling conditions need to be satisfied. Therefore this framework offers extreme flexibility in pairing implicit and explicit methods. We construct three practical IMEX TSRK methods, of orders three, four, and six, respectively. In the first two cases the implicit parts are stiffly accurate. The sixth order method uses an L-stable implicit component from the literature. The corresponding explicit parts have been constructed so as to maximize their stability properties; their coefficients were found via a numerical optimization approach. A convergence analysis for the Prothero–Robinson problem shows that the effective order of IMEX schemes in the case of stiffness equals the stage order of the explicit part; a slight order reduction (from p to $q = p - 1$) is expected in the general case, but it can be avoided in principle by using explicit methods with $q = p$.

Numerical examples include an advection-reaction system, the Van der Pol equation, and a semi-implicit integration of shallow water equations. Representative existing IMEX schemes of RK and linear multistep (LM) types are included for comparison. The results show that IMEX TSRK methods have favorable properties for stiff problems, while IMEX RK methods suffer from severe order reduction. The larger shallow water test shows that the IMEX TSRK methods are competitive in terms of accuracy and efficiency with the currently available families of methods.

The new framework allows us to obtain IMEX schemes of order p and stage order $p - 1$ using only $s = p - 1$ stages. For $p \geq 4$ this is an advantage over existing IMEX RK schemes. The proposed framework offers extreme flexibility in the construction of new partitioned methods, since no coupling conditions are necessary.

An important ingredient of efficient implementations for large multiphysics simulations is step size adaptivity. In order to realize the full potential of IMEX TSRK methods, future work will focus on the construction of schemes in this family with error estimation and adaptive time steps.

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