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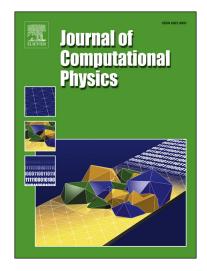
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Highlights

- Novel super-convergent IMEX-Peer methods with A-stable implicit part for s = 2, 3, 4 stages with order p = s + 1 are constructed.
 Several convergence theorems including the property of super-convergence are proved.
- Successful application of the new methods to well established test problems.

Extrapolation-Based Super-Convergent Implicit-Explicit Peer Methods with A-stable Implicit Part

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Abstract

In this paper, we extend the implicit-explicit (IMEX) methods of Peer type recently developed in [Lang, Hundsdorfer, J. Comp. Phys., 337:203–215, 2017] to a broader class of two-step methods that allow the construction of superconvergent IMEX-Peer methods with A-stable implicit part. IMEX schemes combine the necessary stability of implicit and low computational costs of explicit methods to efficiently solve systems of ordinary differential equations with both stiff and non-stiff parts included in the source term. To construct superconvergent IMEX-Peer methods with favourable stability properties, we derive necessary and sufficient conditions on the coefficient matrices and apply an extrapolation approach based on already computed stage values. Optimised super-convergent IMEX-Peer methods of order s+1 for s=2,3,4 stages are given as result of a search algorithm carefully designed to balance the size of the stability regions and the extrapolation errors. Numerical experiments and a comparison to other IMEX-Peer methods are included.

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Keywords: implicit-explicit (IMEX) Peer methods; super-convergence; extrapolation; A-stability

1 Introduction

Differential equations of the form $u' = F_0(u) + F_1(u)$, where F_0 is a non-stiff or mildly stiff part and F_1 is a stiff contribution, arise in many initial value problems. Such problems often result from semi-discretized systems of partial differential equations with diffusion, advection and reaction terms. Implicit-explicit (IMEX) methods use this decomposition by treating only the F_1 contribution in an implicit fashion. The advantage of lower costs for explicit schemes is combined with the favourable stability properties of implicit schemes to enhance the overall computational efficiency.

In this paper, we extend the IMEX methods of Peer type recently developed by Lang and Hundsdorfer [16] to a broader class of two-step methods that include function values from the previous step and thereby allow the construction of superconvergent IMEX-Peer methods with A-stable implicit part. Implicit Peer methods have been introduced by Schmitt, Weiner and co-workers [1, 17, 19] as a very comprehensive class of general linear methods. Such methods are described in detail by Butcher [4] and Jackiewicz [14]. Peer methods are characterized by their special feature that the approximations in all stages have the same order. They inherit good stability properties and an easy step size change in every time step from one-step methods without suffering from order reduction for stiff problems. The property that the Peer stage values have the same order of accuracy can be conveniently exploited to construct related explicit methods by using extrapolation. The combination of these implicit and explicit methods leads in a natural way to IMEX methods with the same order as the original implicit method. This idea was first used by Crouzeix [6] with linear multi-step methods of BDF type. Recently, Cardone, Jackiewicz, Sandu and Zhang [5] applied the extrapolation approach to diagonally implicit multistage integration methods and Lang and Hundsdorfer [16] to implicit Peer methods constructed by Beck, Weiner, Podhaisky and Schmitt [1]. IMEX-Peer methods are competitive alternatives to classic IMEX methods for large stiff problems. Higherorder IMEX Runge-Kutta methods are known to suffer from possible order reduction and serious efficiency loss for stiff problems. A detailed error analysis for increasingly stiff problems has been done by Boscarino [2], see also the references therein. Moreover, the increasing number of necessary coupling conditions makes their construction difficult. Kennedy and Carpenter gave general construction principles in the context of additive Runge-Kutta methods [15]. Boscarino designed an accurate third-order IMEX Runge-Kutta method with a better temporal order of convergence for stiff problems [3].

For a method with stage order q, it is possible to have convergence with order equal to q+1. This concept of super-convergence is discussed for Peer methods

applied to non-stiff problems by Weiner, Schmitt, Podhaisky and Jebens in [25] and in the book of Strehmel, Weiner and Podhaisky [24, Sect. 5.3]. It also holds for stiff problems as shown by Hundsdorfer [11]. Soleimani and Weiner [22] applied the concept of super-convergence to an optimally zero-stable subclass of implicit Peer methods, including also variable time step sizes. More recently, they have constructed super-convergent IMEX-Peer methods via a partitioning approach [23]. Some of their new methods have also an A-stable implicit part. The definition of the order (or order of consistency) of a method commonly used in Peer literature differs from the more comprehensive definition given in the book of Hairer, Nørsett and Wanner [10, Sect. III.8] for general linear methods, which also covers the super-convergence phenomenon. It uses the concept of quasi-consistency of Skeel, first introduced in [20]. Following this approach, we will slightly modify the usual criterion for having an extra order of convergence for Peer methods to construct super-convergent IMEX-Peer methods based on extrapolation.

The paper is organised as follows. In Section 2, we present the framework to obtain super-convergent IMEX-Peer methods, combining super-convergent implicit Peer methods with their corresponding explicit methods derived by extrapolation. We state necessary and sufficient conditions to ensure the super-convergence property for this combination. The construction of specific classes of methods is performed in Section 3. We first summarize all conditions and then design three new super-convergent IMEX-Peer methods for s=2,3,4 with favourable stability and accuracy properties. Stability regions are given and compared to those of IMEX-Peer methods from [16, 21]. Numerical results are presented in Section 4 for a Prothero-Robinson problem, a one-dimensional advection-reaction problem with stiff reactions, and a two-dimensional gravity wave problem, where selected advection and reaction terms lead to stiffness.

2 Implicit-Explicit Peer Methods Based on Extrapolation

2.1 Super-convergent implicit Peer methods

We apply the so-called Peer methods introduced by Schmitt, Weiner and co-workers [17, 18, 22] to solve initial value problems in the vector space $\mathbb{V} = \mathbb{R}^m, m \geq 1$,

$$u'(t) = F(u(t)), \quad u(0) = u_0 \in V.$$
 (1)

The general form of an s-stage implicit Peer method is

$$w_n = (P \otimes I)w_{n-1} + \Delta t(Q \otimes I)F(w_{n-1}) + \Delta t(R \otimes I)F(w_n)$$
 (2)

with $s \times s$ coefficient matrices $P = (p_{ij})$, $Q = (q_{ij})$, $R = (r_{ij})$, the $m \times m$ identity matrix I, and approximations

$$w_n = [w_{n,1}, \dots, w_{n,s}]^T \in \mathbb{V}^s, \quad w_{n,i} \approx u(t_n + c_i \triangle t),$$
(3)

where $t_n = n \triangle t$, $n \ge 0$, and the nodes $c_i \in \mathbb{R}$ are such that $c_i \ne c_j$ if $i \ne j$, and $c_s = 1$. Further, $F(w) = [F(w_i)] \in \mathbb{V}^s$ is the application of F to all components of $w \in \mathbb{V}^s$. The starting vector $w_0 = [w_{0,i}] \in \mathbb{V}^s$ is supposed to be given, or computed by a Runge-Kutta method, for example.

Peer methods belong to the class of general linear methods. All approximations have the same order, which gives the name of the methods. Here, we are interested in A-stable and super-convergent Peer methods with order of convergence p=s+1, recently constructed by Soleimani and Weiner in [22]. In the following, for an $s \times s$ matrix we will use the same symbol for its Kronecker product with the identity matrix as a mapping from the space \mathbb{V}^s to itself. Then, (2) simply reads

$$w_n = Pw_{n-1} + \Delta tQF(w_{n-1}) + \Delta tRF(w_n). \tag{4}$$

The matrix R is taken to be lower triangular with constant diagonal $r_{ii} = \gamma > 0$, $i=1,\ldots,s$, giving singly diagonally implicit methods. In what follows, we discuss requirements and desirable properties for the implicit method (4).

Accuracy. Let $e = (1, ..., 1)^T \in \mathbb{R}^s$. We assume pre-consistency, i.e., Pe = e, which means that for the trivial equation u'(t) = 0, we get solutions $w_{n,i} = 1$ provided that $w_{0,j} = 1, j = 1, \ldots, s$. The residual-type local errors result from inserting exact solution values $w(t_n) = [u(t_n + c_i \triangle t)] \in \mathbb{V}^s$ in the implicit scheme (4):

$$r_n = w(t_n) - Pw(t_{n-1}) - \triangle tQw'(t_{n-1}) - \triangle tRw'(t_n).$$
 (5)

Let $c = (c_1, \ldots, c_s)^T$ with point-wise powers $c^j = (c_1^j, \ldots, c_s^j)^T$. Then Taylor expansion gives

$$w(t_n) = e \otimes u(t_n) + \triangle tc \otimes u'(t_n) + \frac{1}{2} \triangle t^2 c^2 \otimes u''(t_n) + \dots$$
 (6)

$$w(t_{n-1}) = e \otimes u(t_n) + \triangle t(c-e) \otimes u'(t_n) + \frac{1}{2} \triangle t^2(c-e)^2 \otimes u''(t_n) + \dots, (7)$$

from which we obtain

$$r_n = \sum_{j \ge 1} \Delta t^j d_j \otimes u^{(j)}(t_n) \tag{8}$$

with

obtain
$$r_{n} = \sum_{j \geq 1} \triangle t^{j} d_{j} \otimes u^{(j)}(t_{n})$$

$$d_{j} = \frac{1}{j!} \left(c^{j} - P(c - e)^{j} - jQ(c - e)^{j-1} - jRc^{j-1} \right) .$$
(9)

A pre-consistent method is said to have stage order q if $d_j = 0$ for $j = 1, 2, \dots, q$. With the Vandermonde matrices

$$V_0 = (c_i^{j-1}), \qquad V_1 = ((c_i - 1)^{j-1}), \qquad i, j = 1, \dots, s,$$
 (10)

and the diagonal matrices $C = \operatorname{diag}(c_1, c_2, \dots, c_s), D = \operatorname{diag}(1, 2, \dots, s),$ the conditions for having stage order s with the implicit method (4) are

$$CV_0 - P(C - I)V_1 - QV_1D - RV_0D = 0. (11)$$

Since V_1 and D are regular, we have the relation

$$Q = (CV_0 - P(C - I)V_1 - RV_0D)(V_1D)^{-1}, (12)$$

showing that Q is uniquely defined by the choice of P, R, and the node vector c.

Stability. Applying the implicit method (4) to Dahlquist's test equation $y' = \lambda y$ with $\lambda \in \mathbb{C}$, gives the following recursion for the approximations w_n :

$$w_n = (I - zR)^{-1}(P + zQ)w_{n-1} =: M_{im}(z)w_{n-1}$$
(13)

with $z := \lambda \triangle t$. Hence, $w_n = M_{im}(z)^n w_0$. The matrix $P = M_{im}(0)$ should be power bounded to have stability for the trivial equation u'(t) = 0. This requirement of zero-stability is enforced by Schmitt, Weiner et. al by taking P such that one eigenvalue equals 1 (due to pre-consistency) and the others are 0. Such methods are called optimally zero-stable. We will also look at methods that are A-stable, i.e., the spectral radius of $M_{im}(z)$ satisfies $\rho(M_{im}(z)) \le 1$ for all $z \in \mathbb{C}$ with $\mathrm{Re}(z) \le 0$. Since $M_{im}(\infty) = R^{-1}Q$ with $Q \ne 0$, A-stability does not imply L-stability. To guarantee good damping properties for very stiff problems, we will aim at having a small spectral radius of $R^{-1}Q$.

Super-convergence. We are interested in using the degrees of freedom provided by the free parameters in P, R, and c to have convergence with order p=s+1 without raising the stage order further. This is discussed under the heading super-convergence in the book of Strehmel, Weiner and Podhaisky [24, Sect. 5.3] for non-stiff problems. It is related to the definition of order of consistency for general linear methods as given in [10, Sect. III.8]. Similar results for stiff systems can be found in [11]. According to the last paper, we will slightly modify the usual criterion for having an extra order of convergence for Peer methods to later construct super-convergent IMEX-Peer methods based on extrapolation.

Let $\varepsilon_n = w(t_n) - w_n$ be the global error. Under the standard stability assumption, where products of the transfer matrices are bounded in norm by a fixed constant K (see, e.g., Theorem 2 in [22]), we get the estimate $\|\varepsilon_n\| \leq K(\|\varepsilon_0\| + \|r_1\| + \ldots + \|r_n\|)$. Together with stage order s, this gives the standard convergence result

$$\|\varepsilon_n\| \le K \|\varepsilon_0\| + \Delta t^s t_n K \|d_{s+1}\|_{\infty} \max_{0 \le t \le t_n} \|u^{(s+1)}(t)\| + \mathcal{O}(\Delta t^{s+1}).$$
 (14)

Then we have the following

Theorem 2.1. Assume the implicit Peer method (4) has stage order s and estimate (14) holds true for the global error. Then the method is convergent of order p = s. Furthermore, if $d_{s+1} \in range(I - P)$ and the initial values are of order s + 1, then the order of convergence is p = s + 1.

Proof. The first statement follows directly from (14). Suppose that $d_{s+1} = (I - P)v$ with $v \in \mathbb{R}^s$, and let

$$\bar{w}(t_n) := w(t_n) - \triangle t^{s+1} v \otimes u^{(s+1)}(t_n).$$
 (15)

Insertion of these modified solution values in the scheme (4) will give modified local errors

$$\bar{r}_{n} = \bar{w}(t_{n}) - P\bar{w}(t_{n-1}) - \triangle tQF(\bar{w}(t_{n-1})) - \triangle tRF(\bar{w}(t_{n}))
= r_{n} - \triangle t^{s+1}d_{s+1} \otimes u^{(s+1)}(t_{n}) + \mathcal{O}(\triangle t^{s+2}),$$
(16)

which, due to (8), reveals $\bar{r}_n = \mathcal{O}(\triangle t^{s+2})$. For $\bar{\varepsilon}_n = \bar{w}(t_n) - w_n$ this yields, in the same way as above, $\|\bar{\varepsilon}_n\| \le K \|\varepsilon_0\| + \mathcal{O}(\triangle t^{s+1})$. Since $\|\bar{\varepsilon}_n - \varepsilon_n\| \le \triangle t^{s+1} \|v\|_{\infty} \|u^{(s+1)}(t_n)\|$ and $\|\varepsilon_0\| = \mathcal{O}(\triangle t^{s+1})$, this shows convergence of order s+1 for the global errors ε_n . \square

Recall that the range of I-P consists of the vectors that are orthogonal to the null space of $I-P^T$. If the method is zero-stable, then this null space has dimension one. So up to a constant there is a unique vector $v \in \mathbb{R}^s$ such that $(I-P^T)v=0$. Then we have

$$d_{s+1} \in \operatorname{range}(I - P) \quad \text{iff} \quad v^T d_{s+1} = 0. \tag{17}$$

We fix v by $v^T e = 1$ and set $P = ev^T$ to ensure pre-consistency (Pe = e), optimal zero-stability and $(I - P^T)v = 0$. In this way, P is determined by the vector v, which has to satisfy the conditions

$$v^T e = 1$$
 and $v^T d_{s+1} = 0$ (18)

to achieve super-convergence of order s+1.

A closer inspection of the global error ε_n reveals that the condition $P^j d_{s+1} = 0$ for all $j \geq s-1$ is also an appropriate way to construct super-convergent Peer methods. This approach has been used by Schmitt, Weiner et al. [18, 25] for explicit and implicit schemes. There is a strong relation to (17), which can be stated in the following

Theorem 2.2. (1) Let $P^j d_{s+1} = 0$ for all $j \geq s-1$ and $eig(P) = \{1, \lambda_2, \dots, \lambda_s\}$ with $|\lambda_i| < 1, i = 2, \dots, s$, i.e., the Peer method is zero-stable. Then, d_{s+1} lies in the range of I-P. (2) Suppose d_{s+1} lies in the range of I-P and $eig(P) = \{1, 0, \dots, 0\}$, i.e., the Peer method is optimally zero-stable. Then $P^j d_{s+1} = 0$ for all $j \geq s-1$.

Proof: Due to the spectra of P in both cases, there is a regular matrix S such that

$$P = S^{-1} \begin{pmatrix} 1 & 0 \\ 0 & J \end{pmatrix} S =: S^{-1} \hat{P} S, \qquad (19)$$

where $J \in \mathbb{R}^{(s-1)\times(s-1)}$ consists of certain Jordan blocks. (1) Using this form, the assumption on powers of P reads $S^{-1}\hat{P}^{j}Sd_{s+1} = 0$ for $j \geq s-1$, from which follows

that the first component of the vector Sd_{s+1} vanishes. Then, the solvability of the equation $(I-P)x = S^{-1}(I-\hat{P})Sx = d_{s+1}$ reduces to the question whether $I_{s-1} - J$ with I_{s-1} being the unit matrix in $\mathbb{R}^{(s-1)\times(s-1)}$ is invertible. This is indeed the case, since it is an upper triangular matrix with values $1-\lambda_i \neq 0, i=2,\ldots,s$ on the diagonal. (2) In this case, the assumption gives the existence of an $x \in \mathbb{R}^s$ such that $(I-P)x = d_{s+1}$. Using (19), we have $(I-\hat{P})Sx = Sd_{s+1}$, which shows that the first component of the vector Sd_{s+1} vanishes. Since $I-\hat{P}$ is a strictly upper diagonal matrix, we deduce $P^jd_{s+1} = S^{-1}\mathrm{diag}(1,0,\ldots,0)Sd_{s+1} = 0$ for $j \geq s-1$.

Remark 2.1. The second statement in Theorem 2.2 does not hold, if the Peer method is zero-stable, but not optimally zero-stable. In this case, there exist superconvergent Peer methods which do not satisfy the conditions $P^jd_{s+1} = 0$ for all $j \geq s-1$. An example is the new IMEX-Peer4s method constructed in Section 3.

2.2 Extrapolation

In [16], Lang and Hundsdorfer have applied extrapolation to an implicit method of the form (4) with Q=0 and order s to find a related explicit method and eventually construct IMEX-Peer methods of order s with good stability properties. This procedure is well-known from linear multistep methods, see for instance Crouzeix [6] or the review in the book of Hundsdorfer and Verwer [13, Sect. IV.4.2]. It was also used by Cardone, Jackiewicz, Sandu, and Zhang [5] to construct implicit-explicit diagonally implicit multistage integration methods. Here, we will extend this extrapolation idea to obtain super-convergent IMEX-Peer methods of order s+1, where the implicit method is A-stable and the stability region of the overall method is optimised.

Starting with an implicit method (4), where all approximations $w_{n,j}$ have order s, we can obtain a corresponding explicit method by extrapolation of $F(w_n)$ with order s. Using w_{n-1} and most recent values $w_{n,j}, j = 1, \ldots, i-1$, available in the ith-stage with 1 < i < s, gives

$$F(w_n) = S_1 F(w_{n-1}) + S_2 F(w_n) + \mathcal{O}(\triangle t^s), \qquad (20)$$

where the extrapolation coefficients are collected in the $s \times s$ -matrices S_1 and S_2 . Note that S_2 is strictly lower triangular. Applied in (4), this leads to an explicit method of the form

$$w_n = Pw_{n-1} + \Delta t \hat{Q} F(w_{n-1}) + \Delta t \hat{R} F(w_n), \qquad (21)$$

with $\hat{Q} = Q + RS_1$ and the strictly lower triangular matrix $\hat{R} = RS_2$, since R is lower triangular. In what follows, we discuss properties and the issue of super-convergence for this explicit method.

Accuracy. With exact values $F(w(t_n)) \in \mathbb{V}^s$, the residual-type error vector for the extrapolation can be expanded by Taylor series at t_n :

$$\delta_{n} = F(w(t_{n})) - S_{1}F(w(t_{n-1})) - S_{2}F(w(t_{n}))
= \sum_{j>0} \frac{1}{j!} \left((I - S_{2})c^{j} - S_{1}(c - e)^{j} \right) \otimes \frac{d^{j}}{dt^{j}} F(u(t_{n})) \triangle t^{j}.$$
(22)

The conditions for order s read

$$(I - S_2)c^j - S_1(c - e)^j = 0, \quad 0 \le j \le s - 1,$$
 (23)

which can be reformulated to $S_1 = (I - S_2)V_0V_1^{-1}$. Thus, the choice of a strictly lower triangular S_2 determines S_1 .

Using the expression for δ_n , the conditions for stage order s of the implicit method, and (23), we derive for the residual-type local error of the explicit method (21) the form

$$r_n = \Delta t^{s+1} (d_{s+1} + R l_s) \otimes u^{(s+1)}(t_n) + \mathcal{O}(\Delta t^{s+2})$$
 (24)

with

$$l_s = \frac{1}{s!} \left((I - S_2)c^s - S_1(c - e)^s \right). \tag{25}$$

Thus, by construction, all the stages have again order s, at least, so (21) is an explicit Peer method.

Super-convergence. First, we proceed as for the implicit method under the standard stability assumption. With stage order s of the implicit method (4) and order s of the extrapolation in (20), we analogously get the convergence result for the global error of the explicit method defined in (21),

$$\|\varepsilon_n\| \le K \|\varepsilon_0\| + \Delta t^s t_n K \|d_{s+1} + R l_s\|_{\infty} \max_{0 < t < t_n} \|u^{(s+1)}(t)\| + \mathcal{O}(\Delta t^{s+1}).$$
 (26)

Then we have the following

Theorem 2.3. Assume the implicit Peer method (4) has stage order s, conditions (23) for the extrapolation are satisfied, and estimate (26) holds true for the global error. Then the explicit Peer method (21) is convergent of order p=s. Furthermore, if $(d_{s+1} + R l_s) \in range(I - P)$ and the initial values are of order s+1, then the order of convergence is p=s+1.

Proof: The first statement follows directly from (26). Replacing d_{s+1} by $d_{s+1} + R l_s$ in the proof of Theorem 2.1 gives the desired result.

With this result, we can conclude, in the same way as above for the implicit method, that super-convergence is achieved if

$$v^T(d_{s+1} + R l_s) = 0$$
 with $v \in \mathbb{R}^s$ such that $(I - P^T)v = 0$. (27)

If the implicit Peer method is already super-convergent, this simplifies to $v^T R l_s = 0$.

2.3 Super-convergent IMEX-Peer methods

Combining the related implicit and explicit methods (4) and (21) yields an IMEX method for systems of the form

$$u'(t) = F_0(u(t)) + F_1(u(t)), (28)$$

where F_0 will represent the non-stiff or mildly stiff part, and F_1 gives the stiff part of the equation. The resulting IMEX scheme is

$$w_n = Pw_{n-1} + \Delta t \hat{Q} F_0(w_{n-1}) + \Delta t \hat{R} F_0(w_n) + \Delta t Q F_1(w_{n-1}) + \Delta t R F_1(w_n), \quad (29)$$

where the extrapolation is used only on F_0 . Here, $\hat{Q} = Q + RS_1$ and $\hat{R} = RS_2$. For non-stiff problems, this IMEX method will have order s for any decomposition $F = F_0 + F_1$. However, for stiff problems it should be required that the derivatives of $\varphi_k(t) = F_k(u(t))$, k = 0, 1, are bounded by a moderate constant which is not affected by the stiffness parameters, such as the spatial mesh width h for semi-discrete systems obtained from PDEs.

With exact solution values $u(t_{n,i})$, standard local consistency analysis for the IMEX-Peer method (29) gives for the residual-type local errors

$$r_n = E_{im} + \triangle tR E_{ex} + \mathcal{O}\left(\triangle t^{s+2}\right) , \qquad (30)$$

with

$$E_{im} = \triangle t^{s+1} d_{s+1} \otimes u^{(s+1)}(t_n) \quad \text{and} \quad E_{ex} = \triangle t^s l_s \otimes \frac{d^s}{dt^s} F_0(u(t_n)). \tag{31}$$

Therefore, by standard convergence arguments, we have the following

Theorem 2.4. Let the s-stage implicit Peer method (4) with coefficients (c, P, Q, R), Q defined in (12), be zero-stable and suppose its stage order is equal to s. Let the initial values satisfy $w_{0,i} - u(t_0 + c_i \triangle t) = \mathcal{O}(\triangle t^s)$, $i = 1, \ldots, s$. Then the IMEX-Peer method (29) with $\hat{R} = RS_2$ and $\hat{Q} = Q + R(I - S_2)V_0V_1^{-1}$ is convergent of order s for constant step size and arbitrary strictly lower triangular matrix S_2 .

Combining the requirements for super-convergence of order s+1 stated above for the explicit and implicit Peer methods we have

Theorem 2.5. Let the assumptions of Theorem 2.4 be fulfilled and the IMEX-Peer method (29) be convergent of order s. If the initial values are of order s+1, $d_{s+1} \in range(I-P)$ and $Rl_s \in range(I-P)$, then the order of convergence is s+1.

Proof. Suppose $d_{s+1} = (I - P)v_d$ and $R l_s = (I - P)v_l$ with $v_d, v_l \in \mathbb{R}^s$, and let

$$\bar{w}(t_n) = w(t_n) - \Delta t^{s+1} v_d \otimes u^{(s+1)}(t_n) - \Delta t^{s+1} v_l \otimes \frac{d^s}{dt^s} F_0(u(t_n)). \tag{32}$$

Inserting these values in (29) gives the modified residual-type local errors

$$\bar{r}_{n} = \bar{w}(t_{n}) - P\bar{w}(t_{n-1}) - \Delta t \hat{Q} F_{0}(\bar{w}(t_{n-1})) - \Delta t \hat{R} F_{0}(\bar{w}(t_{n}))
- \Delta t Q F_{1}(\bar{w}(t_{n-1})) - \Delta t R F_{1}(\bar{w}(t_{n})),$$
(33)

which can be rearranged to

$$\bar{r}_n = \bar{w}(t_n) - P\bar{w}(t_{n-1}) - \triangle tQF(\bar{w}(t_{n-1})) - \triangle tRF(\bar{w}(t_n)) + \triangle tR(F_0(\bar{w}(t_n)) - S_1F_0(\bar{w}(t_{n-1})) - S_2F_0(\bar{w}(t_n))).$$
(34)

Taylor expansions gives

$$\bar{r}_n = r_n - \triangle t^{s+1} d_{s+1} \otimes u^{(s+1)}(t_n) - \triangle t^{s+1} R l_s \otimes \frac{d^s}{dt^s} F_0(u(t_n)) + \mathcal{O}(\triangle t^{s+2})$$
 (35)

with r_n as defined in (30). This shows $\bar{r}_n = \mathcal{O}(\triangle t^{s+2})$. Then, the same arguments as in the proof of Theorem 2.1 give convergence of order s+1 for the global errors $\varepsilon_n = w(t_n) - w_n$.

Let $d_{s+1} \in \text{range}(I-P)$ and $R l_s \in \text{range}(I-P)$. Then, with the unique vector $v \in \mathbb{R}^s$ such that $(I-P^T)v = 0$ and $v^T e = 1$ it holds

$$y \in \text{range}(I - P) \quad \text{iff} \quad v^T y = 0$$
 (36)

with $y = d_{s+1}$, $R l_s$. Setting $P = ev^T$, we enforce pre-consistency, optimal zero-stability and $(I - P^T)v = 0$. Furthermore, P is fully determined by the vector v. We will use this simplifying construction to find suitable super-convergent IMEX-Peer methods for s = 2, 3. To enrich the space of suitable matrices P for s = 4, we only request zero-stability and follow the approach discussed in Theorem 2.5 with d_{s+1} , $R l_s \in \text{range}(I - P)$ to achieve super-convergence.

2.4 Stability of IMEX-Peer methods

In order to discuss stability properties of the IMEX-Peer method (29), we consider the split scalar test equation

$$y'(t) = \lambda_0 y(t) + \lambda_1 y(t), \quad t \ge 0, \tag{37}$$

with complex parameters λ_0 and λ_1 . Applying an IMEX-Peer method to (37) gives the recursion

$$w_{n+1} = (I - z_0 R S_2 - z_1 R)^{-1} (P + z_0 Q + z_0 R S_1 + z_1 Q) w_n =: M(z_0, z_1) w_n$$
 (38)

with $z_i = h\lambda_i, i = 0, 1$. Therefore, stability is ensured if

$$\rho(M(z_0, z_1)) < 1. \tag{39}$$

The stability regions of the IMEX-Peer method for $\alpha \in [0^{\circ}, 90^{\circ}]$ are defined by the sets

$$\mathbb{S}_{\alpha} = \{ z_0 \in \mathbb{C} : (39) \text{ holds for any } z_1 \in \mathbb{C} \text{ with } |\operatorname{Im}(z_1)| \le -\tan(\alpha) \cdot \operatorname{Re}(z_1) \}$$
 (40)

in the left-half complex plane. Further, we define the stability region of the corresponding explicit method as

$$S_E = \{ z_0 \in \mathbb{C} : \rho(M(z_0, 0)) < 1 \}$$
(41)

with the stability matrix $M(z_0, 0) = (I - z_0 R S_2)^{-1} (P + z_0 Q + z_0 R S_1)$. Efficient numerical algorithms to compute \mathbb{S}_{α} and \mathbb{S}_E are extensively described in [5, 16].

Since $\mathbb{S}_{\alpha} \subset \mathbb{S}_{E}$, the goal is to construct IMEX-Peer methods for which \mathbb{S}_{E} is large and $\mathbb{S}_{E} \setminus \mathbb{S}_{\alpha}$ is as small as possible for angles α that are close to 90°. In what follows, we will use the additional degrees of freedom provided by introducing the terms $\triangle tQF(w_{n-1})$ in the implicit method to construct super-convergent IMEX-Peer methods with a non-empty stability region $\mathbb{S}_{90^{\circ}}$, i.e., the underlying implicit Peer method is A-stable.

3 Construction of Super-Convergent IMEX-Peer Methods Based on Extrapolation

We will first summarize the conditions on the coefficients of the methods derived in the previous sections and give a procedure for the construction of super-convergent IMEX-Peer methods with favourable stability properties for s = 2, 3, 4.

Implicit method. An s-stage implicit Peer method is determined by the coefficient matrices $P, Q, R \in \mathbb{R}^{s \times s}$, and the node vector $c \in \mathbb{R}^s$. We look for singly diagonally implicit methods, i.e., R is taken to be lower triangular with a constant $\gamma > 0$ on the diagonal. Stage order s is imposed through, see (12),

$$Q = (CV_0 - P(C - I)V_1 - RV_0D)(V_1D)^{-1}.$$
(42)

The matrix P is chosen such that the method is pre-consistent, (optimally) zero-stable, and super-convergent. More precisely, we set

- (1) $P = ev^T$ with $v \in \mathbb{R}^s$ and $v^T e = 1$ for s = 2, 3,
- (2) P such that the method is zero-stable for s=4.

In both cases, super-convergence is obtained by satisfying $v^T d_{s+1} = 0$ with d_{s+1} defined in (9) and v such that $(I - P^T)v = 0$. Note that the special choice of P in (1) yields an optimally zero-stable method, whereas for case (2) the property of zero-stability has to be incorporated in the search algorithm. We were not able to

IMEX-Peer2s, $s = 2$, optimally zero-stable										
c_1	0.591977499693304	p_{11}	1 000105410515050							
c_2	1.00000000000000000	p_{12}	2.082167419515352							
γ	0.969486340522434	p_{21}	-1.082167419515352							
r_{21}	-1.007885680522306	p_{22}	2.082167419515352							
s_{21}	0.819167640511257									
IMEX-Peer3s, $s = 3$, optimally zero-stable										
c_1	0.173922498101250	p_{11}	-0.516269158723393							
c_2	0.584759944717930	p_{12}	2.301256858880021							
c_3	1.0000000000000000	p_{13}	-0.784987700156628							
γ	0.456150901216430	p_{21}	-0.516269158723393							
r_{21}	0.271188675194957	p_{22}	2.301256858880021							
r_{31}	0.099808771568803	p_{23}	-0.784987700156628							
r_{32}	0.395734854902157	p_{31}	-0.516269158723393							
s_{21}	1.5000000000000000	p_{32}	2.301256858880021							
s_{31}	0.204731875658678	p_{33}	-0.784987700156628							
s_{32}	1.3200000000000000									
IME	X-Peer4s, $s = 4$, zero-stab	ole								
c_1	-0.926697334544583	p_{11}	0.164346920652337							
c_2	0.180751924024702	p_{12}	1.941408294648193							
c_3	0.850343633101352	$-p_{13}$	-2.764059964877189							
c_4	1.0000000000000000	p_{14}	1.658304749576660							
γ	0.413154106969917	p_{21}	0.424734281438207							
r_{21}	1.186201415903827	p_{22}	1.133423589655944							
r_{31}	1.327861645060559	p_{23}	-0.792340606563880							
r_{32}	0.525143168803633	p_{24}	0.234182735469729							
r_{41}	1.324984727912657	p_{31}	0.562642125818718							
r_{42}	0.576558985833141	p_{32}	0.131525283967289							
r_{43}	0.071014878172581	p_{33}	2.162128869126546							
s_{21}	3.884803988586850	p_{34}	-1.856296278912553							
s_{31}	-3.053336552626494	p_{41}	0.589388877693458							
s_{32}	2.821635541838257	p_{42}	-0.169092459871472							
s ₄₁	-3.555025951383727	p_{43}	3.071031564759426							
s_{42}	2.895140468767150	p_{44}	-2.491327982581412							
s_{43}	0.162040780709875									

Table 1: Coefficients of the super-convergent s-stage IMEX-Peer methods IMEX-Peer2s, IMEX-Peer3s, and IMEX-Peer4s for s=2,3,4 with $S_2=(s_{ij})$.

find suitable methods within the setting (1) for s=4. Further, for the nodes $c_i \in \mathbb{R}$, we use $c_i \in (0,1]$ for s=2,3 and $c_i \in (-1,1]$ for s=4.

Explicit method. The extrapolation is uniquely defined by the choice of the matrices S_1 and S_2 in (20). Order s is guaranteed by setting, see (23),

$$S_1 = (I - S_2)V_0V_1^{-1}. (43)$$

So the entries of $S_2 \in \mathbb{R}^{s \times s}$ are free parameters. Super-convergence is obtained by satisfying $v^T R l_s = 0$ with l_s defined in (25) and v such that $(I - P^T)v = 0$.

IMEX-	α	$ \mathbb{S}_{\alpha} $	x_{max}	$\rho(R^{-1}Q)$	$ \mathbb{S}_E $	y_{max}	c_{im}	c_{ex}
Peer2s	90.0°	2.15	-1.41	1.2810^{-1}	4.47	1.21	$2.37 10^{-1}$	3.2310^{-1}
Peer3s	90.0°	2.67	-1.58	5.5210^{-1}	6.11	1.69	1.2410^{-1}	1.6810^{-1}
Peer4s	90.0°	1.07	-1.45	5.4210^{-1}	4.39	1.00	6.4210^{-2}	1.1710^{-1}
Peer2	90.0°	7.44	-4.86	0.00	8.53	0.40	7.0510^{-2}	2.7810^{-1}
Peer3	86.1°	8.28	-3.07	0.00	10.68	1.78	8.2010^{-3}	3.5810^{-2}
Peer4	83.2°	4.64	-3.57	0.00	9.36	1.90	3.4310^{-4}	4.2710^{-3}
Peer3a	90.0°	2.87	-1.69	1.6010^{-3}	5.19	1.75	1.4610^{-1}	1.9010^{-1}
Peer4a	90.0°	2.65	-1.73	1.2410^{-1}	3.53	1.15	8.9710^{-2}	1.4110^{-1}

Table 2: Size of stability regions \mathbb{S}_{α} and \mathbb{S}_{E} , x_{max} at the negative real axis, y_{max} at the positive imaginary axis, spectral radius of $R^{-1}Q$, and error constants $c_{im} = |d_{s+1}|$ and $c_{ex} = |R l_s|$ for IMEX-Peer methods with s = 2, 3, 4, including those from [16, 21].

Construction principles. We start with the search for a super-convergent implicit Peer method along the following design criteria:

A-stability,
$$\rho(R^{-1}Q)$$
 is close to zero, $||P||_F$, $||Q||_F$, $||R||_F$, $|d_{s+1}|$ are small.

This is done using the MATLAB-routine *fminsearch*, where we include the desired properties in the objective function and use random start values for the remaining degrees of freedom. Different combinations of weights in the objective function are employed to select promising candidates which are then used for a subsequent extrapolation. The latter aims at finding parameters in S_2 such that we have the following properties:

large stability regions \mathbb{S}_E and $\mathbb{S}_{90^{\circ}}$, $||S_1||_F$, $||S_2||_F$, $||R||_s$ are small.

Again fminsearch is used with different combinations of weights in the objective function. Following this approach, we have found new super-convergent IMEX-Peer methods for s=2,3,4. The coefficients of the methods for c,P,R and $S_2=(s_{ij})$ are given in Table 1.

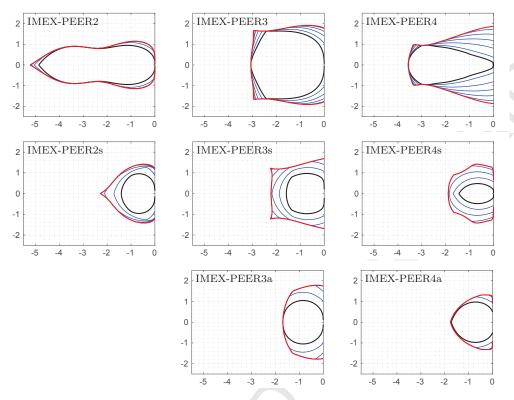


Figure 1: Stability regions \mathbb{S}_{α} (black line), \mathbb{S}_{β} for $\beta = 75^{\circ}, 60^{\circ}, 45^{\circ}, 30^{\circ}, 15^{\circ}$ (blue lines), and \mathbb{S}_{0} (red line) for IMEX-Peer-methods with s = 2, 3, 4 (left to right). We have $\alpha = 90^{\circ}$, i.e., A-stability of the underlying implicit method, for all methods except IMEX-Peer3 ($\alpha = 86.1^{\circ}$) and IMEX-Peer4 ($\alpha = 83.3^{\circ}$).

The resulting values for the stability regions \mathbb{S}_{α} and \mathbb{S}_{E} as well as other constants are collected in Table 2. For comparison, we also show the values for the IMEX-Peer methods tested in [16] (IMEX-Peer2, IMEX-Peer3, IMEX-Peer4) and in [21] (IMEX-Peer3a, IMEX-Peer4a), where IMEX-Peer-3a is nearly super-convergent in the implicit part. It can be observed that super-convergence comes with (i) smaller stability regions and (ii) significantly larger error constants for higher order. However, the convergence is one order higher and A-stability of the implicit method pays off for problems with eigenvalues on the imaginary axis as can be seen from our numerical experiments. More details on the stability regions are shown in Figure 1.

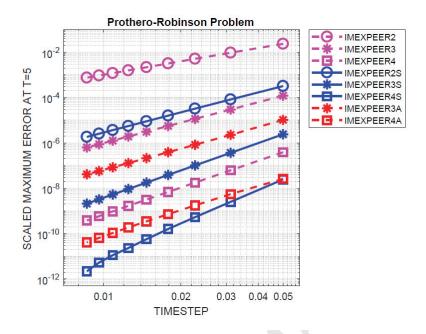


Figure 2: Prothero-Robinson Problem: Scaled maximum errors at T=5 vs. time step sizes. Comparison of IMEX-Peer methods. The convergence orders derived from a least squares fit are: 1.95, 2.94, 2.99, 3.14, 4.00, 3.94, 3.68, 5.21 (top to bottom).

4 Numerical Experiments

4.1 Prothero-Robinson Problem

In order to study the rate of convergence under stiffness, we consider the Prothero-Robinson type equation used in [21],

$$y' = \begin{pmatrix} 0 \\ y_1 + y_2 - \sin(t) \end{pmatrix} + \begin{pmatrix} -10^6 (y_1 - \cos(t)) + 10^3 (y_2 - \sin(t)) - \sin(t) \\ 0 \end{pmatrix}, \quad (44)$$

where $t \in [0, 5]$. The first term is treated explicitly and the second implicitly. Initial values are taken from the analytic solution $y(t) = (\cos(t), \sin(t))$. The error of the approximate solution Y is calculated at the final time T = 5 in the scaled maximum norm, i.e., $err = \max_{i=1,2} |Y_i - y_i|/(1 + |y_i|)$. The values for $\Delta t = 5/(100 + 60i)$, $i = 0, \ldots, 8$ are shown in Figure 2.

All methods show their theoretical order of convergence quite nicely. The smaller error constants of the IMEX-Peer(s) methods for s=3,4 compared to the superconvergent IMEX-Peer methods with the same order are also visible.

4.2 Linear Advection-Reaction Problem

A second PDE problem for an accuracy test is the linear advection-reaction system from [12]. The equations are

$$\partial_t u + \alpha_1 \, \partial_x u = -k_1 u + k_2 v + s_1 \,, \tag{45}$$

$$\partial_t v + \alpha_2 \, \partial_x v = k_1 u - k_2 v + s_2 \tag{46}$$

for 0 < x < 1 and $0 < t \le 1$, with parameters

$$\alpha_1 = 1$$
, $\alpha_2 = 0$, $k_1 = 10^6$, $k_2 = 2k_1$, $k_1 = 0$, $k_2 = 1$,

and with the following initial and boundary conditions:

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

Note that there are no boundary conditions for v since α_2 is set to be zero.

Fourth-order finite differences on a uniform mesh consisting of m=400 nodes are applied in the interior of the domain. At the boundary we can take third-order upwind biased finite differences, which here does not affect an overall accuracy of four [12] and gives rise for a spatial error of $1.5 \cdot 10^{-5}$.

In the IMEX setting, the reaction is treated implicitly and all other terms explicitly. In order to guarantee that errors of the initial values do not affect the computations, accurate initial values are computed by ODE15s from MATLAB with high tolerances. We have used step sizes $\Delta t = (4, 2, 1, 0.5, 0.25, 0.1, 0.05, 0.025) \cdot 10^{-3}$, and compared the numerical values at the final time T=1 with an accurate reference solution in the l_2 -vector norm ($||v||^2 = \sum_i v_i^2$) as used in [16]. The results are plotted in Figure 3.

All methods show their theoretical orders, but the larger error constants of the super-convergent IMEX-Peer schemes compared to the IMEX-Peer(s) family are again apparent. The 3-stage methods and IMEX-Peer4 still deliver satisfactory results for the largest time step, $\Delta t = 4 \cdot 10^{-3}$, whereas the others fail. The similar asymptotic behaviour of the higher-order methods shows order reduction for smaller time steps, which was also observed in [12] as an inherent issue for very high-accuracy computations. However, this effect appears on a level far below the spatial discretization error.

4.3 Nonlinear Two-Dimensional Gravity Waves

This problem is taken from [21]. Let u(x, z) be the velocity of the gravity waves with x and z denoting the horizontal and vertical coordinates in m, respectively. The gravity waves are generated by a localized region of a non-divergent forcing in a stratified shear flow. The horizontal background wind (in m s⁻¹) is given by

$$u_0(z) = 5 + \frac{z}{1000} + 0.4\left(5 - \frac{z}{1000}\right)\left(5 + \frac{z}{1000}\right)$$

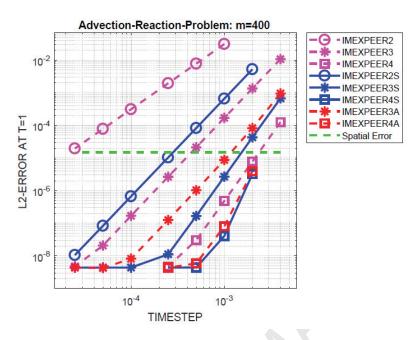


Figure 3: Advection-Reaction-Problem: l_2 -errors at T=1 of the total concentration vs. time step sizes, m=400. Comparison of IMEX-Peer methods. To keep clarity for the other methods, results for the 4-stage methods applied with $\Delta t \leq 10^{-4}$ are not shown. The corresponding errors stagnate at $4 \cdot 10^{-9}$. Further missing results correspond to failures or unstable numerical solutions.

and the waves are forced by the curl of a non-divergent stream function (in $\rm m^2\,s^{-1})$

$$\psi(x,z,t) = \psi_0 \left(\frac{\pi x}{L_x}\right) \sin(\omega t) \exp\left[-\left(\frac{\pi x}{L_x}\right)^2 - \left(\frac{\pi z}{L_z}\right)^2\right].$$

The parameters used here are $\psi_0 = 80 \text{ m}^2 \text{ s}^{-1}$, $L_x = 10 \cdot 10^3 \text{ m}$ and $L_z = 2.5 \cdot 10^3 \text{ m}$. The governing system of equations reads

$$\frac{Du}{Dt} + \frac{\partial P}{\partial x} = -\frac{\partial \psi}{\partial z} + \frac{u_0(z) - \bar{u}(z, t)}{\tau}, \qquad (47)$$

$$\frac{Dw}{Dt} + \frac{\partial P}{\partial z} = b + \frac{\partial \psi}{\partial x}, \tag{48}$$

$$\frac{Db}{Dt} + N^2 w = 0, (49)$$

$$\frac{DP}{Dt} + c_s^2 \left(\frac{\partial u}{\partial x} + \frac{\partial w}{\partial z} \right) = 0, \tag{50}$$

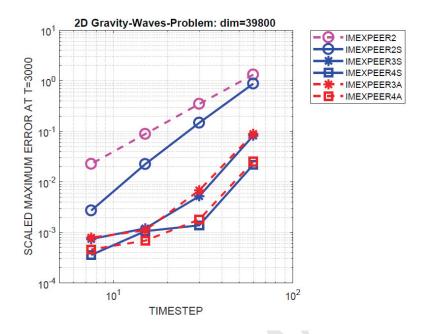


Figure 4: Nonlinear Two-Dimensional Gravity Waves: Scaled maximum errors at $T=3000\,\mathrm{s}$ taken over all system components vs. time step sizes. Comparison of IMEX-Peer methods.

with horizontally averaged mean flow \bar{u} , $x \in [-15 L_x, 15 L_x]$, $z \in [-2 L_z, 2 L_z]$ and $t \in [0 \text{ s}, 3000 \text{ s}]$. The constants are

$$\omega = 0.005 \, \mathrm{s}^{-1}, \quad N = 0.02 \quad \text{and} \quad c_s = 350 \, \mathrm{m \, s}^{-1} \quad \text{(speed of sound)}.$$

For the spatial discretization, we set

$$\delta_{nx}f(x) = \frac{f(x + n\Delta x/2) - f(x - n\Delta x/2)}{n\Delta x},$$

$$\langle f(x)\rangle^{nx} = \frac{f(x + n\Delta x/2) + f(x - n\Delta x/2)}{2},$$

$$\psi_x = \frac{\psi(x + \Delta x, z, t) - \psi(x, z, t)}{\Delta x},$$

$$\psi_z = \frac{\psi(x, z + \Delta z, t) - \psi(x, z, t)}{\Delta z}$$

and obtain the semi-discretized system of ODEs

$$\frac{\partial u}{\partial t} + \frac{1}{2}\delta_{2x}(u^2) + \langle \langle w \rangle^x \delta_z u \rangle^z - \frac{u_0(z) - \bar{u}(z, t)}{\tau} + \psi_z + K\Delta_h u = -\delta_x P$$
 (51)

$$\frac{\partial w}{\partial t} + \langle \langle u \rangle^z \delta_x w \rangle^x + \frac{1}{2} \delta_{2z}(w^2) - \psi_x + K \Delta_h w = -\delta_z P + b \qquad (52)$$

$$\frac{\partial b}{\partial t} + \langle \langle u \rangle^z \delta_x b \rangle^x + \langle \langle w \rangle^z \delta_z b \rangle^z + K \Delta_h b = -N^2 w \tag{53}$$

$$\frac{\partial P}{\partial t} + \langle u \delta_x P \rangle^x + \langle w \delta_z P \rangle^z = -c_s^2 (\delta_x u + \delta_z w),$$
(54)

where $K = 4.69 \cdot 10^{-4} \,\mathrm{s}^{-1}$. We add a fourth-derivative hyper-diffusion term

$$\Delta_h := \left((\Delta x \delta_x)^2 + (\Delta z \delta_z)^2 \right)^2$$

to prevent nonlinear instability and to impose a simple parametrization of turbulent mixing. In our calculation, we have used $m_x = 100$ and $m_z = 100$ nodes for the spatial grid. This yields a system of dimension 39800. A reference solution is computed by Matlab's ODE15s with high precision. For more details, we refer to [21], see also [7].

We identify the right hand side of (51)–(54) as the stiff part of the ODE system, which is treated implicitly. The eigenvalues of its Jacobian are all complex and lie approximately in [-7i, 7i]. This especially shows that A-stability is necessary for a stable computation of the gravity waves. It also explains why the methods IMEX-Peer3 and IMEX-Peer4 [16] with $\alpha < 90^{\circ}$, i.e., the implicit method is not A-stable, fail for this problem and are not shown in Figure 4. We have used step sizes $\Delta t = 60, 30, 15, 7.5 \,\mathrm{s}$ and compared the numerical values at the final time $T = 3000 \,\mathrm{s}$ with an accurate reference solution y_{ref} in the scaled maximum norm, i.e., we set $err = \max_{i=1,...,n} |y_i - y_{ref,i}|/(1 + |y_{ref,i}|)$, see Figure 4.

The super-convergent IMEX-Peer2s clearly shows its additional order. IMEX-Peer3s and (the nearly super-convergent) IMEX-Peer3a deliver almost identical results due to their similar error constants, whereas super-convergence can only be observed for larger time steps. Both 4-stage IMEX-Peer methods show an unpredictable behaviour, but give the smallest errors. Similar results are presented in [21].

5 Conclusion

We have developed a new family of s-stage IMEX-Peer methods, applying the idea of extrapolation from [5, 16] to a broader class of implicit Peer methods which also include function values from the previous step. These additional degrees of freedom

allow the construction of super-convergent IMEX-Peer methods of order s+1 with A-stable implicit part. A-stability is important to solve problems with function contributions that have large imaginary eigenvalues in the spectrum of their Jacobians. We analysed the property of super-convergence and gave sufficient conditions for it. These conditions are motivated by the definition of the order of consistency for general linear methods and are more general as those commonly used in Peer literature. Linear stability properties were carefully examined to derive new super-convergent s-stage IMEX-Peer methods with order p=s+1 for s=2,3,4. We employed the MATLAB-routine fminsearch with varying objective functions and starting values to find suitable methods with sufficiently large stability regions and small error constants. However, the new properties, super-convergence and A-stability, go along with significantly smaller stability regions and larger error constants, compared to the IMEX-Peer methods from [16].

In a detailed comparison with recently proposed IMEX-Peer methods in [16, 21], the new methods showed their super-convergence property and performed better in many cases. They gave equally well results for a two-dimensional gravity wave problem used in [21] to demonstrate the importance of A-stability of the implicit part, whereas the higher-order methods from [16] failed due to their lack of this property. In future work, we will extend our construction principles to variable step size sequences with local error control. This is especially important when it comes to solve real-life applications with often largely varying time scales, see e.g. [8, 9] for linearly implicit Peer methods with variable step sizes.

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