Super-Convergent Implicit-Explicit Peer Methods with Variable Step Sizes

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February 6, 2019

Dedicated to the Memory of Willem Hundsdorfer (1954 - 2017)

Abstract

Dynamical systems with sub-processes evolving on many different time scales are ubiquitous in applications. Their efficient solution is greatly enhanced by automatic time step variation. This paper is concerned with the theory, construction and application of IMEX-Peer methods that are super-convergent for variable step sizes and A-stable in the 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 super-convergent IMEX-Peer methods which keep their higher order for variable step sizes and exhibit favourable linear stability properties, we derive necessary and sufficient conditions on the nodes and coefficient matrices and apply an extrapolation approach based on already computed stage values. New super-convergent IMEX-Peer methods of order $s+1$ for $s=2,3,4$ stages are given as result of additional order conditions which maintain the super-convergence property independent of step size changes. Numerical experiments and a comparison to other super-convergent IMEX-Peer methods show the potential of the new methods when applied with local error control.

Keywords: implicit-explicit (IMEX) Peer methods; super-convergence; extrapolation; A-stability; variable step size; local error control

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1 Introduction

Many dynamical processes in engineering, physics, chemistry and other areas are modelled by large systems of ordinary differential equations (ODEs) of the form

$$u'(t) = F_0(u(t)) + F_1(u(t)), \tag{1}$$

where $F_0 : \mathbb{R}^m \to \mathbb{R}^m$ represents the non-stiff or mildly stiff part and $F_1 : \mathbb{R}^m \to \mathbb{R}^m$ gives the stiff part of the equation. Such problems often result from semi-discretized systems of partial differential equations with diffusion, advection and reaction terms. Instead of applying a single explicit or implicit method, an often more appropriate and efficient approach is to use the decomposition of the right-hand side by treating only the F_1 contribution in an implicit fashion. Thus, favourable stability properties of implicit schemes and the advantage of lower costs for explicit schemes are combined to enhance the overall computational efficiency. Since dynamical systems typically have sub-processes evolving on many different time scales, a good ODE integrator should come with some adaptive error control, making frequent step size changes over its own progress. In smooth regions, a few large steps should speed up the integration, whereas many small steps should be applied in non-smooth terrains. The resulting gains in efficiency can be up to factors of hundreds or more.

IMEX-Peer methods with variable step sizes have been successfully applied by Soleimani, Knoth, and Weiner [17] to fast-wave-slow-wave problems arising in weather prediction. The super-convergent IMEX-Peer methods recently developed by Soleimani and Weiner [18, 19] and Schneider, Lang, and Hundsdorfer [16] can in principle be applied with variable step sizes, but then they might lose their super-convergence property, especially for serious step size changes. Super-convergent explicit Peer methods for variable step sizes have first been constructed by Weiner, Schmitt, Podhaisky, and Jebens [21], exploiting special matrix structures. Another approach to construct such methods is the use of extrapolation as proposed by Schneider, Lang, and Hundsdorfer [16]. This idea goes back to Crouzeix [7] and was also used by Cardone, Jackiewicz, Sandu, and Zhang [5, 6] and later on by Braś, Izzo, and Jackiewicz [2] to construct implicit-explicit general linear and Runge-Kutta methods. The procedure can be easily extended to variable step sizes for IMEX-Peer methods.

In this paper, we use the extrapolation approach to construct new super-convergent IMEX-Peer methods that keep their higher order for variable step sizes and exhibit favourable linear stability properties, including A-stability of the implicit part. Additional order conditions on the nodes and coefficient matrices which maintain the super-convergence property independent of step size changes are derived for implicit, explicit and IMEX-Peer methods. We give formulas for new super-convergent IMEX-Peer methods of order $s+1$ for $s = 2, 3, 4$ stages. Stability regions are computed and compared to those of super-convergent IMEX-Peer methods for constant step sizes from Schneider, Lang, and Hundsdorfer [16]. Eventually, numerical results are presented for a Prothero-Robinson problem, the van der Pol oscillator, a one-dimensional Burgers equation with stiff diffusion and a one-dimensional advection-reaction problem with stiff reactions.

2 Implicit-Explicit Peer Methods with Variable Step Sizes

2.1 Super-convergent implicit Peer methods with variable step sizes

We apply the so-called Peer methods introduced by Schmitt, Weiner and co-workers [14, 15, 18] to solve initial value problems in the vector space $\mathbb{V}=\mathbb{R}^m, m\geq 1$,

$$u'(t)=F(u(t)),\quad u(0)=u_0\in\mathbb{V}\,. \tag{2}$$

The general form of an s-stage implicit Peer method with variable step sizes $\triangle t_n$ is

$$w_n=(P_n\otimes I)w_{n-1}+\triangle t_n(Q_n\otimes I)F(w_{n-1})+\triangle t_n(R_n\otimes I)F(w_n) \tag{3}$$

with the $m\times m$ identity matrix I, the $s\times s$ coefficient matrices $P_n=(p_{ij}(\sigma_n))$, $Q_n=(q_{ij}(\sigma_n))$, $R_n=(r_{ij}(\sigma_n))$, which depend on the step size ratio $\sigma_n:=\triangle t_n/\triangle t_{n-1}$, and approximations

$$w_n=[w_{n,1}^T,\ldots,w_{n,s}^T]^T\in\mathbb{V}^s,\quad w_{n,i}\approx u(t_n+c_i\triangle t_n). \tag{4}$$

Here, $\mathbb{V}^s=\mathbb{R}^{ms}$, $t_n=\triangle t_0+\ldots+\triangle t_{n-1}$, $n\geq 0$, and the nodes $c_i\in\mathbb{R}$ are such that $c_i\neq c_j$ if $i\neq j$, 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 introduced by Butcher [3]. 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 $p=s+1$ even for variable step sizes. For constant step sizes, such methods have been recently constructed by Soleimani and Weiner [18] and Schneider, Lang and Hundsdorfer [16]. 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, (3) simply reads

$$w_n=P_nw_{n-1}+\triangle t_nQ_nF(w_{n-1})+\triangle t_nR_nF(w_n)\,. \tag{5}$$

In what follows, we discuss requirements and desirable properties for the implicit Peer method (5).

Accuracy. Let $e=(1,\ldots,1)^T\in\mathbb{R}^s$. We assume pre-consistency, i.e., $P_ne=e$, 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 $w(t_n)=[u(t_n+c_i\triangle t_n)]\in\mathbb{V}^s$ in the implicit scheme (5):

$$r_n=w(t_n)-P_nw(t_{n-1})-\triangle t_nQ_nw'(t_{n-1})-\triangle t_nR_nw'(t_n)\,. \tag{6}$$

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 with the expressions

$$w_i(t_{n-1})=u\left(t_n+\frac{c_i-1}{\sigma_n}\triangle t_n\right),\quad i=1,\ldots,s, \tag{7}$$

gives

$$w(t_n) = e \otimes u(t_n) + \triangle t_n c \otimes u'(t_n) + \frac{1}{2}\triangle t_n^2 c^2 \otimes u''(t_n) + \dots \tag{8}$$

$$w(t_{n-1}) = e \otimes u(t_n) + \frac{\triangle t_n}{\sigma_n}(c-e) \otimes u'(t_n) + \frac{\triangle t_n^2}{2\sigma_n^2}(c-e)^2 \otimes u''(t_n) + \dots, \tag{9}$$

from which we obtain

$$r_n = \sum_{j\geq 1} \triangle t_n^j d_{n,j} \otimes u^{(j)}(t_n) \tag{10}$$

with

$$d_{n,j} = \frac{1}{j!}\left(c^j - \frac{1}{\sigma_n^j} P_n (c-e)^j - \frac{j}{\sigma_n^{j-1}} Q_n (c-e)^{j-1} - jR_n c^{j-1} \right). \tag{11}$$

A pre-consistent method is said to have stage order q if $d_{n,j} = 0$ for all σ_n and $j = 1, 2, \dots, q$. With the Vandermonde matrices

$$V_0 = \left(c_i^{j-1}\right), \qquad V_1 = \left((c_i - 1)^{j-1}\right), \qquad i, j = 1, \dots, s, \tag{12}$$

and $C = \mathrm{diag}(c_1, c_2, \dots, c_s)$, $D = \mathrm{diag}(1, 2, \dots, s)$, and $S_n = \mathrm{diag}(1, \sigma_n, \dots, \sigma_n^{s-1})$, the conditions for having stage order s for the implicit Peer method (5) for variable step sizes are

$$CV_0 - \frac{1}{\sigma_n} P_n (C-I) V_1 S_n^{-1} - Q_n V_1 D S_n^{-1} - R_n V_0 D = 0\,. \tag{13}$$

Since V_1 and D are regular, we have the relation

$$Q_n = \left((CV_0 - R_n V_0 D) S_n - \frac{1}{\sigma_n} P_n (C-I) V_1 \right) (V_1 D)^{-1}\,, \tag{14}$$

showing that Q_n is uniquely defined by the choice of P_n, R_n, the node vector c, and the step size ratio σ_n. Moreover, there is an easy way to achieve consistency for any choice of the step sizes $\triangle t_n$ by setting $P_n \equiv P$ and $R_n \equiv R$ with constant matrices P and R, and recomputing Q_n from (14) in each time step. In what follows, we will make use of this simplification and consider implicit Peer methods with variable step sizes $\triangle t_n$ of the form

$$w_n = P w_{n-1} + \triangle t_n Q_n F(w_{n-1}) + \triangle t_n R F(w_n) \tag{15}$$

with constant matrices P and R, and Q_n updated in each time step by

$$Q_n = \left((CV_0 - RV_0 D) S_n - \frac{1}{\sigma_n} P (C-I) V_1 \right) (V_1 D)^{-1}\,. \tag{16}$$

The matrix R is taken to be lower triangular with constant diagonal $r_{ii} = \gamma > 0$, $i = 1, \dots, s$, giving singly diagonally implicit methods.

Remark 2.1. *Implicit Peer methods of the form (15) that are consistent of order s for constant time steps, i.e., $\triangle t_n = \triangle t$ and $Q_n = Q$, can be applied in a variable time-step environment without loss of their order of consistency by updating (the original) Q by Q_n from (16) in each time step. We will use this modification in the numerical comparisons for our recently developed methods in [16, 19].*

Stability. Applying the implicit method (15) to Dahlquist's test equation $y' = \lambda y$ with $\lambda \in \mathbb{C}$, gives the following recursion for the approximations w_n:

$$w_n = (I - z_n R)^{-1}(P + z_n Q_n) w_{n-1} =: M_{im}(z_n, \sigma_n) w_{n-1} \tag{17}$$

with $z_n := \sigma_n \sigma_{n-1} \cdots \sigma_1 z_0,\ z_0 = \triangle t_0 \lambda$. Hence,

$$w_n = M_{im}(z_n, \sigma_n) M_{im}(z_{n-1}, \sigma_{n-1}) \cdots M_{im}(z_1, \sigma_1) w_0\,. \tag{18}$$

The asymptotic behaviour of the matrix product is very difficult to analyse, see e.g. the discussion in Jackiewicz, Podhaisky, and Weiner [11, Sect. 1]. Here, we consider methods that are zero-stable for arbitrary step sizes and A-stable for constant step sizes. Zero stability requires the constant matrix $P = M_{im}(0, \sigma)$ to be power bounded to have stability for the trivial equation $u'(t) = 0$. We will derive methods for which the spectral radius of $M_{im}(z, \sigma)$ satisfies $\rho(M_{im}(z, \sigma)) \le 1$ for all $\sigma \in [\sigma_{min}, \sigma_{max}]$ with $0 \le \sigma_{min} < 1 \le \sigma_{max}$ and all $z \in \mathbb{C}$ with $\mathrm{Re}(z) \le 0$. Since for constant step sizes, $M_{im}(\infty, 1) = -R^{-1}Q(1)$ with $Q(1) \ne 0$, 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 $R^{-1}Q(\sigma)$ for $\sigma \in [\sigma_{min}, \sigma_{max}]$. Although we cannot prove boundedness of the matrix product in (18) for $n \to \infty$ and variable step sizes, the methods derived along the design principles described above performed always stable in our numerical applications for various step size patterns.

Super-convergence. Applying the convergence theory from multistep methods, stage order $q = s$ and zero stability yield convergence of order $p = s$ for variable step sizes with $0 \le \sigma_{min} < \sigma_n < \sigma_{max}$ and $\triangle t_n \le \triangle t_{max} := \max_{i=0,\dots,n} \triangle t_i$ demonstrated, e.g., in [1, 13]. Here, we are interested in using the degrees of freedom provided by the free parameters in P, R, and c to have convergence of 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 [20, Sect. 5.3] for non-stiff problems. Similar results for stiff systems were obtained by Hundsdorfer [9]. We follow the approach recently developed in Schneider, Lang, and Hundsdorfer [16] for having an extra order of convergence for Peer methods with constant step sizes to later discuss the property of super-convergence for IMEX-Peer methods based on extrapolation for variable step sizes.

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 [18]), we get the estimate $\|\varepsilon_n\| \le K(\|\varepsilon_0\| + \|r_1\| + \ldots + \|r_n\|)$. Together with stage order s, this gives the standard convergence result

$$\begin{aligned} \|\varepsilon_n\| \le K\|\varepsilon_0\| + K \left(\triangle t_1^{s+1} \|d_{1,s+1}\|_\infty + \ldots + \triangle t_n^{s+1} \|d_{n,s+1}\|_\infty \right) \times \\ \times \max_{0 \le t \le t_n} \|u^{(s+1)}(t)\| + \mathcal{O}\left(\triangle t_{max}^{s+1}\right)\,. \end{aligned} \tag{19}$$

Then we have the following

Theorem 2.1. *Assume the implicit Peer method (15) has stage order s and estimate (19) holds true for the global error with $\|\varepsilon_0\| = \mathcal{O}(\triangle t_0^s)$. Then the method is convergent of order $p = s$, i.e., the global error satisfies $\varepsilon_n = \mathcal{O}(\triangle t_{max}^s)$. Furthermore, if the initial values are of order $s+1$, $d_{i,s+1} \in range(I - P)$ and $\triangle t_{i-1} = (1 + \mathcal{O}(\triangle t_{max}))\triangle t_i$ for all $i = 1, \dots, n$, then the order of convergence is $p = s + 1$.*

Proof: The first statement follows directly from (19) with the estimate

$$\triangle t_1^{s+1}\|d_{1,s+1}\|_\infty + \ldots + \triangle t_n^{s+1}\|d_{n,s+1}\|_\infty \le (t_{n+1}-t_1)\triangle t_{max}^s \max_{i=1,\ldots,n}\|d_{i,s+1}\|_\infty\,.$$

Suppose that $d_{i,s+1} = (I-P)v_i$ with $v_i \in \mathbb{R}^s$. Since $I-P$ has an eigenvalue zero, v_i is not uniquely determined. To fix v_i, we choose the one with minimum Euclidean norm, i.e., $v_i = (I-P)^+ d_{i,s+1}$ with $(I-P)^+$ being the Moore-Penrose inverse. Let now

$$\bar{w}(t_i) := w(t_i) - \triangle t_i^{s+1} v_i \otimes u^{(s+1)}(t_i)\,. \tag{20}$$

Insertion of these modified solution values in the scheme (15) will give modified local errors

$$\begin{aligned} \bar{r}_i &= \bar{w}(t_i) - P\bar{w}(t_{i-1}) - \triangle t_i Q_i F(\bar{w}(t_{i-1})) - \triangle t_i RF(\bar{w}(t_i)) \\ &= r_i - \triangle t_i^{s+1} d_{i,s+1}\otimes u^{(s+1)}(t_i) - T(v_{i-1},v_i)\otimes u^{(s+1)}(t_i) + \mathcal{O}(\triangle t_i^{s+2})\,, \end{aligned} \tag{21}$$

where

$$T(v_{i-1},v_i) = \triangle t_i^{s+1} P v_i - \triangle t_{i-1}^{s+1} P v_{i-1}\,. \tag{22}$$

Next, we will show that $T(v_{i-1},v_i) = \mathcal{O}(\triangle t_{max})\triangle t_i^{s+1}$. From the assumption on the step sizes, $\triangle t_{i-1} = (1+\mathcal{O}(\triangle t_{max}))\triangle t_i$, we deduce $\sigma_i^{-1} = 1+\mathcal{O}(\triangle t_{max})$, which yields

$$\sigma_i^{-j} - \sigma_{i-1}^{-j} = \mathcal{O}(\triangle t_{max}) \quad \text{for all} \quad j \ge 1\,. \tag{23}$$

The definition of $d_{i,s+1}$ in (11) gives the polynomial representation $d_{i,s+1} = \sum_{j=0,\ldots,s+1} a_j \sigma^{-j}$ with σ-independent $a_j \in \mathbb{R}^s$ (see also (26) and (27) for more details). Hence, we have $d_{i,s+1} - d_{i,s} = \mathcal{O}(\triangle t_{max})$. Using $\triangle t_{i-1}^{s+1} = (1+\mathcal{O}(\triangle t_{max}))\triangle t_i^{s+1}$, we conclude that

$$\begin{aligned} T(v_{i-1},v_i) &= \triangle t_i^{s+1} P(v_i - v_{i-1}) + \mathcal{O}(\triangle t_{max})\triangle t_i^{s+1} \\ &= \triangle t_i^{s+1} P(I-P)^+(d_{i,s+1} - d_{i-1,s+1}) + \mathcal{O}(\triangle t_{max})\triangle t_i^{s+1} = \mathcal{O}(\triangle t_{max})\triangle t_i^{s+1}\,, \end{aligned} \tag{24}$$

which, due to (10), reveals $\bar{r}_i = \mathcal{O}(\triangle t_{max}\triangle t_i^{s+1})$ in (21). This yields, in the same way as above, $\|\bar{\varepsilon}_n\| = \|\bar{w}(t_n) - w_n\| \le K\|\varepsilon_0\| + \mathcal{O}(\triangle t_{max}^{s+1})$. Since $\|\bar{\varepsilon}_n - \varepsilon_n\| \le \triangle t_n^{s+1}\|v_n\|_\infty \|u^{(s+1)}(t_n)\|$ and $\|\varepsilon_0\| = \mathcal{O}(\triangle t_0^{s+1})$, this shows convergence of order $s+1$ for the global errors ε_n. □

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. Therefore, up to a constant there is a unique vector $v \in \mathbb{R}^s$ such that $(I-P^T)v = 0$. Then we have

$$d_{i,s+1} \in \text{range}\,(I-P) \quad \text{iff} \quad v^T d_{i,s+1} = 0 \quad \text{for all } i = 1,\ldots,n\,. \tag{25}$$

Since $d_{i,s+1}$ depends on σ_i, these equations have to be satisfied for all σ_i. In the following, we will drop the index i and examine $v^T d_{s+1}(\sigma)$ as a function of σ. From (11), we find

$$d_{s+1}(\sigma) = \frac{1}{(s+1)!}\left(c^{s+1} - \frac{1}{\sigma^{s+1}}P(c-e)^{s+1} - \frac{s+1}{\sigma^s}Q(\sigma)(c-e)^s - (s+1)Rc^s\right), \tag{26}$$

where $Q(\sigma)$ is taken from (16) with $\sigma_n = \sigma$. Replacing Q, using the definition of S_n, and separating all powers of σ, we eventually get the polynomial representation

$$v^T d_{s+1}(\sigma) = h_0 + \sum_{j=1}^{s} \tilde{v}_{s+1-j}^T\,\tilde{c}_{s+1-j}\sigma^{-j} + h_{s+1}\sigma^{-(s+1)} \tag{27}$$

with the σ-independent coefficients

$$h_0 = \frac{1}{(s+1)!} v^T \left(c^{s+1} - (s+1) R c^s \right), \tag{28}$$

$$\tilde{v}^T = \frac{1}{s!} v^T (R V_0 - C V_0 D^{-1}), \tag{29}$$

$$\tilde{c} = V_1^{-1} (c-e)^s, \tag{30}$$

$$h_{s+1} = \frac{1}{(s+1)!} v^T (C-I) V_1 \tilde{D} V_1^{-1} (c-e)^s. \tag{31}$$

Here, $\tilde{D} := (s+1)D^{-1} - I$. Note that we have used the relation $v^T P = v^T$ to eliminate P in (31). With $h_j := \tilde{v}_{s+1-j}^T \, \tilde{c}_{s+1-j}$ for $j = 1, \ldots, s$, condition (25) can be fulfilled by adding the $s+2$ additional equations $h_j \equiv 0$ to the consistency conditions in order to achieve super-convergence for variable step sizes. The special structure of the coefficients $\tilde{c}_{s+1-j}$ allows the following statement.

Lemma 2.1. *Assume $c_1, \ldots, c_{s-1} < 1$ with $s \geq 2$, $c_i \neq c_j$ for $i \neq j$, and $c_s = 1$. Then, $\tilde{c}_1 = 0$ and $\tilde{c}_2, \ldots, \tilde{c}_s \neq 0$.*

Proof: The conditions on c_i guarantee the regularity of the Vandermonde matrix V_1. Let $x_i := c_i - 1$, $i = 1 \ldots, s$. Then, we have $x^s = (c-e)^s$ and $V_1 = (x_i^{j-1})$, $i, j = 1, \ldots, s$. From (30), we deduce $V_1 \tilde{c} = x^s$. The choice $c_s = 1$ yields $x_s = 0$ and hence $\tilde{c}_1 = 0$ from the last equation. Further, assumption $c_i < 1$ gives $x_1, \ldots, x_{s-1} < 0$. This allows division by x_i, resulting in the linear equations

$$\begin{pmatrix} 1 & x_1 & \cdots & x_1^{s-2} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{s-1} & \cdots & x_{s-1}^{s-2} \end{pmatrix} \begin{pmatrix} \tilde{c}_2 \\ \vdots \\ \tilde{c}_s \end{pmatrix} = \begin{pmatrix} x_1^{s-1} \\ \vdots \\ x_{s-1}^{s-1} \end{pmatrix}. \tag{32}$$

Now, let us consider the polynomial of order $s-1$,

$$p(x) = x^{s-1} - \sum_{k=0}^{s-2} \tilde{c}_{k+2} \, x^k. \tag{33}$$

Then, $p(x_i) = 0$ is the i-th row of system (32) and hence $x_1, \ldots, x_{s-1}$ are the $s-1$ roots of p, i.e., $p(x) = (x - x_1) \cdots (x - x_{s-1})$. The theorem of Vieta shows

$$-\tilde{c}_{s+1-j} = (-1)^j \kappa_j \quad \text{with} \quad \kappa_j = \sum_{1 \leq i_1 < i_2 < \cdots < i_j \leq s-1} x_{i_1} \cdots x_{i_j}, \; j = 1, \ldots, s-1. \tag{34}$$

Since $x_i < 0$ for all $i = 1, \ldots, s-1$, we observe that all products in the sum have the same number of factors which have one and the same sign, i.e., the sums cannot vanish. More precisely, $\mathrm{sgn}(\kappa_j) = (-1)^j$ and hence $\mathrm{sgn}(\tilde{c}_{s+1-j}) = -1$, which proves the statement. $\square$

We are now ready to formulate additional simplified conditions for the super-convergence of implicit Peer methods when they are applied with variable step sizes.

Theorem 2.2. *Assume the implicit Peer method (15) has stage order s and estimate (19) holds true for the global error with $\|\varepsilon_0\| = \mathcal{O}\left(\triangle t_0^{s+1}\right)$. Let $\triangle t_{i-1} = (1+\mathcal{O}(\triangle t_{max}))\triangle t_i$ for all $i = 1,\ldots,n$. Then the method is convergent of order $p = s+1$, i.e., the global error satisfies $\varepsilon_n = \mathcal{O}\left(\triangle t_{max}^{s+1}\right)$, if for all $v \in \mathbb{R}^s$ with $(I-P^T)v = 0$, the following additional conditions are satisfied:*

$$v^T(C-I)V_1\tilde{D}V_1^{-1}(c-e)^s = 0, \tag{35}$$

$$v^T\left(c^j - jRc^{j-1}\right) = 0, \quad j = 2,\ldots,s+1. \tag{36}$$

Proof: Condition $v^T d_{s+1}(\sigma) = 0$ requires $h_j = 0$ for $j = 0,\ldots,s+1$ in (27). Observe that $h_s = 0$ is always satisfied since $c_s = 1$ and hence $\tilde{c}_1 = 0$. The property $\tilde{c}_j \neq 0$ for $j = 2,\ldots,s$, leads to $\tilde{v}_j^T = 0$, which is equivalent to $v^T(c^j - jRc^{j-1}) = 0$. The remaining conditions follow directly from $h_0 = h_{s+1} = 0$. □

2.2 Super-convergent explicit Peer methods for variable steps sizes

Super-convergent explicit Peer methods for variable step sizes with a special structure of the matrix P have first been constructed by Weiner, Schmitt, Podhaisky, and Jebens [21]. A convenient way to construct such methods for more general P is the use of extrapolation as proposed by Schneider, Lang, and Hundsdorfer [16]. This idea goes back to Crouzeix [7] and was also used by Cardone, Jackiewicz, Sandu, and Zhang [6] to construct implicit-explicit diagonally implicit multistage integration methods. The procedure can be easily extended to variable step sizes.

Assume that all approximations $w_{n,j}$ obtained from method (15) have stage order s. Then, we can use w_{n-1} and most recent values $w_{n,j}$, $j = 1,\ldots,i-1$, already available for the computation in the i-th stage, to extrapolate $F(w_n)$ by

$$F(w_n) = E_{1,n}F(w_{n-1}) + E_{2,n}F(w_n) + \mathcal{O}\left(\tau_n^s\right), \tag{37}$$

where $\tau_n = \max\left(\triangle t_{n-1}, \triangle t_n\right)$ and the $s\times s$-matrices $E_{1,n}$ and $E_{2,n}$ of extrapolation coefficients depend on the step size ratio σ_n. Here, $E_{2,n}$ is a strictly lower triangular matrix. Replacing $F(w_n)$ in (15) gives the explicit method

$$w_n = Pw_{n-1} + \triangle t_n(Q_n + RE_{1,n})F(w_{n-1}) + \triangle t_n RE_{2,n}F(w_n). \tag{38}$$

Note that $RE_{2,n}$ is strictly lower triangular since R is lower triangular. We will discuss consistency and super-convergence of this explicit method.

Accuracy. Taylor expansion with exact values $F(w(t_n))$ gives for the residual-type error vector

$$\begin{aligned}\delta_n &= F(w(t_n)) - E_{1,n}F(w(t_{n-1})) - E_{2,n}F(w(t_n)) \\ &= \sum_{j\geq 0}\frac{\triangle t_n^j}{j!}\left((I-E_{2,n})c^j - \frac{1}{\sigma_n^j}E_{1,n}(c-e)^j\right)\otimes\frac{d^j}{dt^j}F(u(t_n))\,.\end{aligned} \tag{39}$$

Then, the residual-type local error of the explicit Peer method (38) reads

$$r_n = \sum_{j\geq 1}\triangle t_n^j\left(d_{n,j} + Rl_{n,j-1}\right)\otimes u^{(j)}(t_n) \tag{40}$$

with

$$l_{n,j} = \frac{1}{j!}\left((I-E_{2,n})c^j - \frac{1}{\sigma_n^j}E_{1,n}(c-e)^j\right). \tag{41}$$

We can achieve stage order s, if the underlying implicit Peer method has stage order s, i.e., $d_{n,j}=0$ for all σ_n and $j=1,\ldots,s$, and if we choose

$$E_{1,n} = (I-E_2)V_0S_nV_1^{-1} \tag{42}$$

with a constant $s\times s$-matrix E_2 and $S_n=\mathrm{diag}(1,\sigma_n,\ldots,\sigma_n^{s-1})$ as defined above. This gives $l_{n,j}=0$ for all σ_n and $j=0,\ldots,s-1$ and eventually $r_n=\mathcal{O}(\triangle t_n^{s+1})$.

Super-convergence. Under standard stability assumptions as for the implicit method, we derive the global error estimate for the explicit Peer method defined in (38),

$$\begin{aligned}\|\varepsilon_n\| \le K\|\varepsilon_0\| + K\left(\triangle t_1^{s+1}\|d_{1,s+1}+Rl_{1,s}\|_\infty + \ldots + \triangle t_n^{s+1}\|d_{n,s+1}+Rl_{n,s}\|_\infty\right)\times \\ \times \max_{0\le t\le t_n}\|u^{(s+1)}(t)\| + \mathcal{O}\left(\triangle t_{max}^{s+1}\right). \end{aligned}\tag{43}$$

Analogously, we have

Theorem 2.3. *Assume the implicit Peer method (15) has stage order s and estimate (43) holds true for the global error with $\|\varepsilon_0\|=\mathcal{O}(\triangle t_0^s)$. Then the explicit method (38) is convergent of order $p=s$, i.e., the global error satisfies $\varepsilon_n=\mathcal{O}(\triangle t_{max}^s)$. Furthermore, if the initial values are of order $s+1$, $(d_{i,s+1}+Rl_{i,s})\in range(I-P)$ and $\triangle t_{i-1}=(1+\mathcal{O}(\triangle t_{max}))\triangle t_i$ for all $i=1,\ldots,n$, then the order of convergence is $p=s+1$.*

Proof: Replacing $d_{i,s+1}$ by $d_{i,s+1}+Rl_{i,s}$ in the proof of Theorem 2.1 gives the desired result.□

Thus, super-convergence for variable step sizes is achieved if for all $i=1,\ldots,n$, it holds

$$v^T(d_{i,s+1}+Rl_{i,s})=0 \text{ with } v\in\mathbb{R}^s \text{ such that } (I-P^T)v=0. \tag{44}$$

If the underlying implicit method is already super-convergent, the conditions simplify to $v^TRl_{i,s}=0$. Next, we will study the $l_{i,s}$ as functions of σ and derive sufficient conditions for order $s+1$.

From (41) and (42), we get

$$l_s(\sigma) = \frac{1}{s!}(I-E_2)\left(c^s - \frac{1}{\sigma^s}V_0S(\sigma)V_1^{-1}(c-e)^s\right). \tag{45}$$

The investigation of the product $v^T(d_{s+1}(\sigma)+Rl_s(\sigma))$ yields the following

Theorem 2.4. *Assume the explicit Peer method (38) has stage order s and estimate (43) holds true for the global error with $\|\varepsilon_0\|=\mathcal{O}\left(\triangle t_0^{s+1}\right)$. Let $\triangle t_{i-1}=(1+\mathcal{O}(\triangle t_{max}))\triangle t_i$ for all $i=1,\ldots,n$. Then the method is convergent of order $p=s+1$, i.e., the global error satisfies $\varepsilon_n=\mathcal{O}\left(\triangle t_{max}^{s+1}\right)$, if for all $v\in\mathbb{R}^s$ with $(I-P^T)v=0$, the following additional conditions are satisfied:*

$$v^T(C-I)V_1\tilde{D}V_1^{-1}(c-e)^s=0, \tag{46}$$

$$v^T\left(c^j - jRE_2c^{j-1}\right)=0, \quad j=2,\ldots,s+1. \tag{47}$$

Proof: The proof follows the same way as demonstrated in the proof of Theorem 2.1. The coefficients of $\sigma^{-s}, \ldots, \sigma^{-1}$ are again expressed as products $\tilde{v}_1\tilde{c}_1, \ldots, \tilde{v}_s\tilde{c}_s$ with

$$\tilde{c} = V_1^{-1}(c-e)^s \quad \text{and} \quad \tilde{v}^T = \frac{1}{s!}v^T(RE_2V_0 - CV_0D^{-1}).$$

Due to $\tilde{c}_j \neq 0$ for $j = 2, \ldots, s$, we have $\tilde{v}_j^T = 0$ and hence $v^T(c^j - jRE_2c^{j-1}) = 0$. The other condition remains unchanged. □

We would like to conclude with the following observation: If we start with a super-convergent implicit Peer method for variable step sizes, i.e., the additional conditions in Theorem 2.2 are already fulfilled, then (46) disappears and (47) changes to $v^TR(E_2 - I)c^{j-1} = 0$. This can be rewritten to $v^TR(E_2 - I)CV_0 = 0$. Since $R(E_2 - I)$ and V_0 are regular matrices, C must be singular to satisfy (47) for $v \neq 0$. That means, one of the nodes c_i must be zero, because we always assume $c_i \neq c_j$. We will discuss this point later.

2.3 Super-convergent IMEX-Peer methods with variable step sizes

We now apply the implicit and explicit methods (15) and (38) to systems of the form

$$u'(t) = F_0(u(t)) + F_1(u(t))\,, \tag{48}$$

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

$$w_n = Pw_{n-1} + \triangle t_n \left(\hat{Q}_nF_0(w_{n-1}) + \hat{R}F_0(w_n) + Q_nF_1(w_{n-1}) + RF_1(w_n)\right), \tag{49}$$

where $\hat{Q}_n = Q_n + RE_{1,n}$, $\hat{R} = RE_2$, and extrapolation is used only on F_0. Combining the local consistency analysis for both the explicit and implicit method, the residual-type local errors for the IMEX-Peer methods have the form

$$r_n = \sum_{j\geq 1} \triangle t_n^j \left(d_{n,j} \otimes u^{(j)}(t_n) + R\,l_{n,j-1} \otimes \frac{d^j}{dt^j}F_0(u(t_n))\right). \tag{50}$$

Super-convergence. In order to construct super-convergent IMEX-Peer methods of order $s+1$ for variable step sizes, we have to impose consistency of order s and ensure that for all $v \in \mathbb{R}^s$ with $(I - P^T)v = 0$ it holds

$$v^Td_{s+1}(\sigma) = 0 \quad \text{and} \quad v^TR\,l_s(\sigma) = 0 \tag{51}$$

for all σ. We have the following

Theorem 2.5. *Let the s-stage implicit Peer method (15) defined by the coefficients (c, P, Q_n, R), with Q_n from (16), be zero-stable and suppose its stage order is equal to s. Let the initial values satisfy $w_{0,i} - u(t_0 + c_i\triangle t_0) = \mathcal{O}(\triangle t_0^{s+1})$, $i = 1, \ldots, s$, and $\triangle t_{i-1} = (1 + \mathcal{O}(\triangle t_{max}))\,\triangle t_i$, $i = 1, \ldots, n$. Then the IMEX-Peer method (49) is convergent of order $s+1$, i.e., the global error satisfies $\varepsilon_n = \mathcal{O}(\triangle t_{max}^{s+1})$, if for all $v \in \mathbb{R}^s$ with $(I - P^T)v = 0$, the following additional conditions are satisfied:*

$$v^T(C - I)V_1\tilde{D}V_1^{-1}(c-e)^s = 0, \tag{52}$$

$$v^T\left(c^j - jRc^{j-1}\right) = 0, \quad j = 2, \ldots, s+1, \tag{53}$$

$$v^TR(E_2 - I)c^{j-1} = 0, \quad j = 2, \ldots, s+1. \tag{54}$$

Proof: Suppose $d_{i,s+1} = (I-P)v_{d,i}$ and $R\,l_{i,s} = (I-P)v_{l,i}$ with $v_{d,i}, v_{l,i} \in \mathbb{R}^s$. Again, we fix these vectors by setting $v_{d,i} = (I-P)^+ d_{i,s+1}$ and $v_{l,i} = (I-P)^+ Rl_{i,s}$ with $(I-P)^+$ being the Moore-Penrose inverse. Let now

$$\bar{w}(t_i) = w(t_i) - \triangle t_i^{s+1} v_{d,i} \otimes u^{(s+1)}(t_i) - \triangle t_i^{s+1} v_{l,i} \otimes \frac{d^s}{dt^s} F_0(u(t_i))\,. \tag{55}$$

Inserting these modified values in (49) gives the modified residual-type local errors

$$\begin{aligned} \bar{r}_i \;&=\; \bar{w}(t_i) - P\bar{w}(t_{i-1}) - \triangle t_i \hat{Q}_i F_0(\bar{w}(t_{i-1})) - \triangle t_i \hat{R} F_0(\bar{w}(t_i)) \\ &\quad - \triangle t_i Q_i F_1(\bar{w}(t_{i-1})) - \triangle t_i R F_1(\bar{w}(t_i))\,, \end{aligned} \tag{56}$$

which can be rearranged to

$$\begin{aligned} \bar{r}_i \;&=\; \bar{w}(t_i) - P\bar{w}(t_{i-1}) - \triangle t_i Q_i F(\bar{w}(t_{i-1})) - \triangle t_i R F(\bar{w}(t_i)) \\ &\quad + \triangle t_i R \left(F_0(\bar{w}(t_i)) - E_{1,i} F_0(\bar{w}(t_{i-1})) - E_2 F_0(\bar{w}(t_i))\right)\,. \end{aligned} \tag{57}$$

Then, Taylor expansions yields

$$\begin{aligned} \bar{r}_i \;&=\; r_i - \triangle t_i^{s+1} d_{i,s+1} \otimes u^{(s+1)}(t_i) - \triangle t_i^{s+1} R\,l_{i,s} \otimes \frac{d^s}{dt^s} F_0(u(t_i)) \\ &\quad + T(v_{d,i-1}, v_{d,i}) \otimes u^{(s+1)}(t_i) + T(v_{l,i-1}, v_{l,i}) \otimes \frac{d^s}{dt^s} F_0(u(t_i)) + \mathcal{O}(\triangle t_i^{s+2}) \end{aligned} \tag{58}$$

with $T(\cdot,\cdot)$ and r_i as defined in (22) and (50), respectively. The same arguments as in the proof of Theorem 2.1 show $\bar{r}_i = \mathcal{O}(\triangle t_{max} \triangle t_i^{s+1})$ and eventually the convergence of order $s+1$ for the global errors $\varepsilon_n = w(t_n) - w_n$. □

The $2s+1$ additional conditions (52)-(54) are quite demanding. We have already mentioned the fact that (54) requests that one of the nodes c_i, $i \neq s$, must be zero. In this case, the method delivers two vectors, $w_{n-1,s}$ and $w_{n,i}$ with a certain i, that approximate $u(t_n)$. We note that the difference of these approximations is used in the extrapolation process as an additional degree of freedom. The matrix $E_{1,n}$ in (42) is still well defined. However, it is not always possible to construct such methods at all or with good stability properties in particular. In many practical applications, it might be sufficient that the explicit method has the property of super-convergence for variable step sizes and the implicit method is only super-convergent for constant step sizes. We have constructed such methods as well. They have to fulfill the following additional conditions for all $v \in \mathbb{R}^s$ with $(I - P^T)v = 0$ and for all σ:

$$v^T d_{s+1}(1) = 0 \quad \text{and} \quad v^T(d_{s+1}(\sigma) + Rl_s(\sigma)) = 0. \tag{59}$$

Due to the second condition for $\sigma = 1$, the first one can be replaced by the often simpler requirement $v^T Rl_s(1) = 0$. Using Theorem 2.4 and the definition of Rl_s, we find the explicit relations

$$v^T R(I - E_2)\left(c^s - V_0 V_1^{-1}(c-e)^s\right) = 0, \tag{60}$$

$$v^T (C - I) V_1 \tilde{D} V_1^{-1} (c-e)^s = 0, \tag{61}$$

$$v^T \left(c^j - jRE_2 c^{j-1}\right) = 0, \quad j = 2, \ldots, s+1. \tag{62}$$

Compared to (52)-(54), the number of conditions has been significantly reduced. Moreover, since condition (54) disappeared, the restriction $c_i = 0$ for a certain i is no longer necessary.

2.4 Stability of super-convergent IMEX-Peer methods

We consider the usual split scalar test equation

$$y'(t) = \lambda_0 y(t) + \lambda_1 y(t), \quad t \geq 0, \tag{63}$$

with complex parameters λ_0 and λ_1. Applying an IMEX-Peer method (49) to (63) gives the recursion

$$w_n = \left(I - z_0^{(n)}\hat{R} - z_1^{(n)}R\right)^{-1}\left(P + z_0^{(n)}\hat{Q}_n + z_1^{(n)}Q_n\right) w_{n-1} =: M_n(z_0^{(n)}, z_1^{(n)}) w_{n-1} \tag{64}$$

with $z_i^{(n)} = \triangle t_n \lambda_i$, $i = 0, 1$. As for the implicit method itself, an analysis of matrix products formed by $M_1 M_2 \cdots M_n$ would be far too complicated. Therefore, we restrict ourselves to constant step sizes and require

$$\rho(M(z_0, z_1)) \leq 1 \tag{65}$$

with $z_i = \triangle t \lambda_i$, $i = 0, 1$. Then, the stability regions of the IMEX-Peer method applied with constant step sizes are defined by the sets

$$\mathbb{S}_\alpha = \{z_0 \in \mathbb{C} : (65) \text{ holds for any } z_1 \in \mathbb{C} \text{ with } |\mathrm{Im}(z_1)| \leq -\tan(\alpha) \cdot \mathrm{Re}(z_1)\} \tag{66}$$

in the left-half complex plane for $\alpha \in [0^\circ, 90^\circ]$. Further, we define the stability region of the corresponding explicit method (with constant step sizes) as

$$\mathbb{S}_E = \{z_0 \in \mathbb{C} : \rho(M(z_0, 0)) \leq 1\} \tag{67}$$

with the stability matrix $M(z_0, 0) = (I - z_0\hat{R})^{-1}(P + z_0\hat{Q})$. Efficient numerical algorithms to compute $\mathbb{S}_\alpha$ and $\mathbb{S}_E$ are extensively described in [6, 12].

Our goal is to construct IMEX-Peer methods for which $\mathbb{S}_E$ is large and $\mathbb{S}_E \backslash \mathbb{S}_\alpha$ is as small as possible for angles α that are close to 90°. We will construct super-convergent IMEX-Peer methods with A-stable implicit part for constant step sizes, i.e., the stability region $\mathbb{S}_{90^\circ}$ is non-empty. Concerning variable step sizes, we follow the design principles already stated in the stability discussion in Section 2.1.

2.5 Practical Issues

Starting procedure. In order to execute the first step of the IMEX-Peer method (49), we have to choose t_1, $\triangle t_0$, $\triangle t_1$, and need to approximate the s initial values $w_{0,i} \approx u(t_1 - (1 - c_i)\triangle t_0)$. For this, we apply a suitable integration method with continuous output, e.g. a Runge-Kutta or BDF scheme, on the interval $[t_0, t_0 + \tau]$ with $\tau > 0$. The accuracy of the continuous numerical solution $\tilde{w}(t)$ can be controlled by standard step size control or by choosing τ sufficiently small. Denoting the minimum and maximum component of the node vector c by c_{min} and c_{max}, respectively, we require

$$t_1 - (1 - c_{min})\triangle t_0 = t_0 \quad \text{and} \quad t_1 - (1 - c_{max})\triangle t_0 = t_0 + \tau. \tag{68}$$

This linear system for t_1 and $\triangle t_0$ has the unique solution

$$t_1 = t_0 + \frac{1 - c_{min}}{c_{max} - c_{min}}\tau \quad \text{and} \quad \triangle t_0 = \frac{1}{c_{max} - c_{min}}\tau. \tag{69}$$

The initial values are now taken from

$$w_{0,i} := \tilde{w}(t_1 - \triangle t_0 + c_i \triangle t_0) = \tilde{w}\left(t_0 + \frac{c_i - c_{min}}{c_{max} - c_{min}}\tau\right),\ i = 1, \ldots, s. \tag{70}$$

Note that $w_{0,i} = u_0$ for index i with $c_i = c_{min}$. Eventually, we set $\triangle t_1 = \triangle t_0$.

Step size selection. We extend the approach proposed by Soleimani, Knoth, and Weiner in [17] to locally approximate $\triangle t_n^s u^{(s)}(t_n)$, which mimics the leading error term of an embedded solution of order $s-1$. Let $F = F_0 + F_1$ and define

$$est := \triangle t_n \sum_{i=1}^{s} \left(\alpha_i F(w_{n,i}) + \beta_i F(w_{n-1,i})\right) \tag{71}$$

with α and β determined through

$$\alpha^T = \delta(s-1)!\, e_s^T V_0^{-1} \quad \text{and} \quad \beta^T = (1-\delta)\sigma_n^{s-1}(s-1)!\, e_s^T V_1^{-1}, \tag{72}$$

where $e_s^T = (0, \ldots, 0, 1)$ and $\delta \in [0,1]$ is chosen as a weighting factor. Then Taylor expansion of the exact solution shows the desired property:

$$\begin{aligned}
&\triangle t_n \sum_{i=1}^{s} \left(\alpha_i u'(t_n + c_i \triangle t_n) + \beta_i u'\left(t_n + \frac{c_i - 1}{\sigma_n}\triangle t_n\right)\right) \\
&= \triangle t_n \Bigg((\alpha^T e) u'(t_n) + \ldots + \frac{\triangle t_n^{s-1}}{(s-1)!}(\alpha^T c^{s-1}) u^{(s)}(t_n) \qquad (73) \\
&\quad + (\beta^T e) u'(t_n) + \ldots + \frac{\triangle t_n^{s-1}}{\sigma_n^{s-1}(s-1)!}(\beta^T (c-e)^{s-1}) u^{(s)}(t_n)\Bigg) + \mathcal{O}(\triangle t_n^{s+1}) \\
&= \triangle t_n^s u^{(s)}(t_n) + \mathcal{O}(\triangle t_n^{s+1}). \qquad (74)
\end{aligned}$$

In our numerical experiments, we have discovered that the use of old function values, i.e., $\delta = 0$ in (72), works quite reliable for stiff and very stiff problems. For mildly stiff problems, the choice $\delta = 1$ often leads to a slightly better performance. For our examples in Section 4, we will present results for $\delta = 0$.

The new step size is computed by

$$\triangle t_{new} = \min\left(1.2, \max\left(0.8, 0.9\, err^{-1/s}\right)\right) \triangle t_n \tag{75}$$

with the weighted relative maximum error

$$err = \max_{i=1,\ldots,m} \frac{|est_i|}{atol\ +\ rtol\,(\delta|w_{n,s,i}| + (1-\delta)|w_{n-1,s,i}|)}. \tag{76}$$

In order to reach the time end point T with a step of averaged normal length, we adjust after each step size $\triangle t_{new}$ to $\triangle t_{new} = (T - t_n)/\lfloor(1 + (T - t_n)/\triangle t_{new})\rfloor$.

Given an overall tolerance TOL, the step is accepted and the computation is continued with $\triangle t_{n+1} = \triangle t_{new}$, if $err \le TOL$. Otherwise, the step is rejected and repeated with $\triangle t_n = \triangle t_{new}$.

3 Construction of super-convergent IMEX-Peer methods with variable step sizes

3.1 The case $s = 2$

First, we have a negative result. With $c_1 = 0$, $c_2 = 1$, and pre-consistency $Pe = e$, the coefficient matrices are

$$c = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad P = \begin{pmatrix} p_1 & 1-p_1 \\ p_2 & 1-p_2 \end{pmatrix}, \quad R = \begin{pmatrix} \gamma & 0 \\ r_{21} & \gamma \end{pmatrix}, \quad E_2 = \begin{pmatrix} 0 & 0 \\ e_{21} & 0 \end{pmatrix}. \tag{77}$$

The first condition (52) for super-convergence reads $(-1/2, 0)\, v = 0$, which gives, up to scaling, $v = (0,1)^T$. Then, (53) reduces to $1 - 2\gamma = 1 - 3\gamma = 0$, which is not possible for any γ.

Next we try to find methods that satisfy (60)-(62) with $c_1 \neq 0$. There are indeed candidates with $c_1 = 2/3$, $p_2 = 0$, $e_{12} = 3/(4\gamma)$, and $r_{21} = 3/4 - 2\gamma$. The remaining parameters p_1 and γ are chosen such that the implicit part is A-stable and the stability regions of the IMEX-method are optimized. Good results are obtained for the following method:

$$c = \begin{pmatrix} \frac{2}{3} \\ 1 \end{pmatrix}, \quad P = \begin{pmatrix} -\frac{19}{20} & \frac{39}{20} \\ 0 & 1 \end{pmatrix}, \quad R = \begin{pmatrix} \frac{17}{20} & 0 \\ -\frac{19}{20} & \frac{17}{20} \end{pmatrix}, \quad E_2 = \begin{pmatrix} 0 & 0 \\ \frac{15}{17} & 0 \end{pmatrix}. \tag{78}$$

We will refer to this method as IMEX-Peer2sve.

IMEX-	$\lvert\mathbb{S}_{90^\circ}\rvert$	x_{max}	$\lvert\mathbb{S}_{0^\circ}\rvert$	y_{max}	$\rho(R^{-1}Q)$	c_{im}	c_{ex}
Peer2s	2.15	-1.41	4.47	1.21	0.128	$2.37\,10^{-1}$	$3.23\,10^{-1}$
Peer2sve	$6.68\,10^{-5}$	$-5.68\,10^{-3}$	0.14	0.36	0.863	$1.94\,10^{-1}$	$2.83\,10^{-1}$
Peer3s	2.67	-1.58	6.11	1.69	0.552	$1.24\,10^{-1}$	$1.68\,10^{-1}$
Peer3sv	0.11	-0.25	0.55	0.43	0.254	$2.29\,10^{-1}$	$1.43\,10^{-1}$
Peer4s	1.07	-1.45	4.39	1.00	0.542	$6.42\,10^{-2}$	$1.17\,10^{-1}$
Peer4sve	1.66	-1.68	3.11	0.92	0.118	$2.02\,10^{-2}$	$3.37\,10^{-2}$
Peer4sv	$1.34\,10^{-3}$	$-4.05\,10^{-2}$	0.63	0.67	0.632	$7.47\,10^{-2}$	$6.75\,10^{-2}$

Table 1: Size of stability regions $\mathbb{S}_{90^\circ}$ and $\mathbb{S}_{0^\circ}$, $x_{max}(\mathbb{S}_{90^\circ})$ at the negative real axis, $y_{max}(\mathbb{S}_{0^\circ})$ 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 super-convergent IMEX-Peer methods, including those from [16].

3.2 The cases $s = 3$ and $s = 4$

In order to construct super-convergent methods for variable step sizes, we have to satisfy conditions (52)-(54) for all $v \in \mathbb{R}^s$ with $(I - P^T)v = 0$ and one of the nodes c_i being zero.

A surprisingly simple choice is $c_1 = 0$ and $v = e_1$, which yields the validity of (53) and (54). Then, equation (52) yields one condition for the remaining nodes. We find $c_2 = 0.5$ for $s = 3$ and $c_3 = (5c_2 - 1)/(10c_2 - 5)$ for $s = 4$. Furthermore, the first row of P is e_1, which goes along with pre-consistency. The value of c_3 and the remaining coefficients of P, R and E_2 are chosen in such a way that the implicit Peer methods are A-stable and the IMEX-Peer methods exhibit good stability properties and moderate error constants. This has been done using the Matlab-routine *fminsearch*, where we included the desired properties in the objective function and used random start values for the remaining degrees of freedom. Different combinations of weights in the objective function have been employed to select promising candidates which were then tested in various problems. We will refer to the methods finally selected as IMEX-Peer3sv and IMEX-Peer4sv.

We have also constructed a 4-stage IMEX-Peer method, denoted by IMEX-Peer4sve, with the property that the explicit method is super-convergent for variable step sizes and the implicit method is only super-convergent for constant step sizes. In this case, conditions (60)-(62) must be satisfied, where c_i, $i = 1, 2, 3$, are still free parameters. We set $v = e_s$, which gives (61) since then $v^T(C - I) = 0$. The additional degrees of freedom in the nodes allow us to achieve greater stability regions and smaller error constants compared to IMEX-Peer4sv. The method found is optimally zero-stable, i.e., one eigenvalue of P equals one (due to pre-consistency) and the others are zero.

The coefficients of all new methods for c, P, R, and E_2 are given in Table 2 and Table 3. Values for the stability regions as well as other constants are collected in Table 1. More details on the stability regions are shown in Figure 1. Obviously, the new property of super-convergence for variable step sizes comes with significantly smaller stability regions, except for IMEX-Peer4sve which even slightly improves S_{90° of IMEX-Peer4s.

4 Numerical examples

We will present results for two ODE and two PDE problems. In order to guarantee that errors of the initial values do not affect the computations, unknown initial values as well as reference solutions Y at the final time are computed by ODE15S from MATLAB with sufficiently high tolerances. In the comparisons, the global errors are computed by $err = \max_i |Y_i - \hat{Y}_i|/(1 + |Y_i|)$, where $\hat{Y}$ is the numerical approximation.

All calculations have been done with Matlab-Version R2017a on a Latitude 7280 with an i5-7300U Intel processor at 2.7 GHz.

4.1 Prothero-Robinson Problem

In order to study the rate of convergence under stiffness and changing step sizes, we consider the Prothero-Robinson type equation used in [16, 17],

$$y' = \begin{pmatrix} 0 \\ y_1 + y_2 - \sin(t) \end{pmatrix} + \begin{pmatrix} -10^6(y_1 - \cos(t)) + 10^3(y_2 - \sin(t)) - \sin(t) \\ 0 \end{pmatrix}, \tag{79}$$

where $t \in [0, 5]$. The first term is treated explicitly and the second implicitly. Initial values are taken from the analytic solution $y(t) = (\cos(t), \sin(t))$. For constant step sizes $\triangle t = 0.05/i$, $i = 1, \ldots, 6$, we consider the σ-dependent sequences

$$\triangle t_i = \triangle t_{i-1}\, \sigma^{(-1)^i}, \quad i = 2, \ldots, N \tag{80}$$

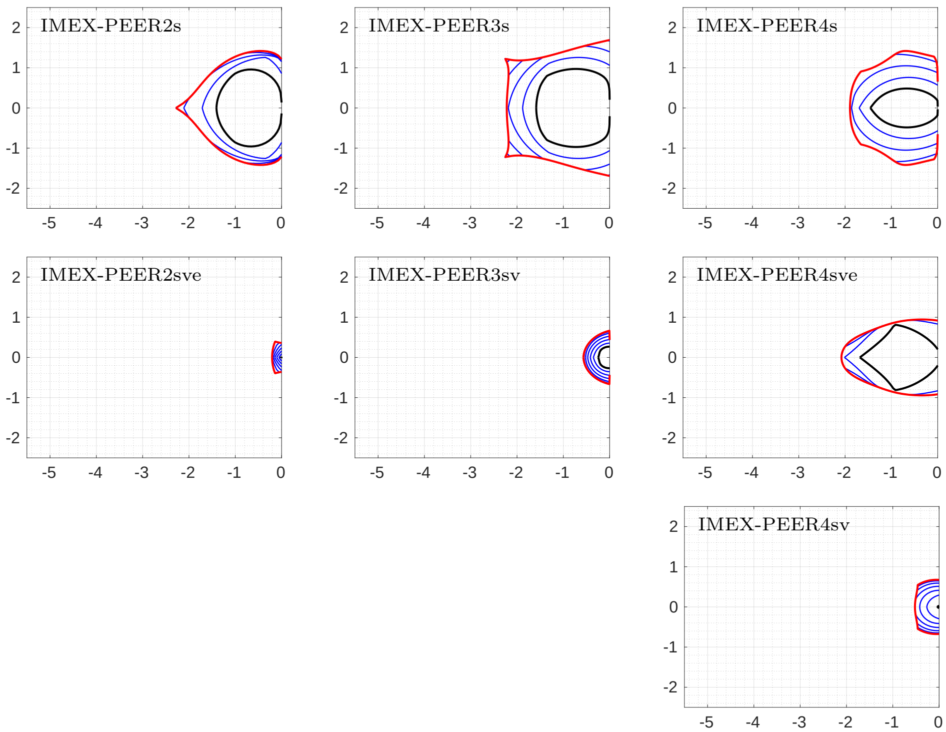

Figure 1: Stability regions $\mathbb{S}_{90^\circ}$ (black line), $\mathbb{S}_\beta$ for $\beta = 75^\circ, 60^\circ, 45^\circ, 30^\circ, 15^\circ$ (blue lines), and $\mathbb{S}_{0^\circ}$ (red line) for super-convergent IMEX-Peer methods with $s = 2, 3, 4$ (left to right).

with $\triangle t_1 = 2\triangle t/(1+\sigma)$ and $N = T/\triangle t$. Results for $\sigma = 1.0, 1.1, 1.2$ are shown in Figure 2. Since the 4-stage methods become instable for $\sigma = 1.2$, these results are omitted. One can nicely see that all new methods keep their order of convergence observed for constant step sizes and, therefore, perform quite robust with respect to changing the step size. This is, of course, not the case for the methods that are only super-convergent for constant step sizes.

4.2 Van der Pol Oscillator

Next we consider the well known stiff van der Pol oscillator

$$y' = \begin{pmatrix} y_2 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 10^6\left((1-y_1^2)y_2 - y_1\right) \end{pmatrix} \tag{81}$$

with $y_1(0) = 2$, $y_2(0) = 0$, and $t \in [0, 2]$. The first term is treated explicitly and the second implicitly. This singularly perturbed problem challenges any code and its efficient solution requires a step size adaptation over several orders of magnitude, see e.g. [8] and the discussions therein. The tolerances are $atol = rtol = 10^{-3-i}$, $i = 0, 1, \ldots, 4$ and the calculations are started with initial step $\tau = atol$ for all methods. The results are shown and discussed in Figure 3.

IMEX-Peer3sv, $s=3$			
c_1	0.000000000000000	p_{11}	1.000000000000000
c_2	0.500000000000000	p_{12}	0.000000000000000
c_3	1.000000000000000	p_{13}	0.000000000000000
γ	0.690969692535085	p_{21}	1.009534846612963
r_{21}	0.351562922857064	p_{22}	−0.000125189884283
r_{31}	0.346024253990984	p_{23}	−0.009409656728680
r_{32}	0.328884660689640	p_{31}	0.927244072163109
e_{21}	1.454929231059714	p_{32}	−0.000247968521087
e_{31}	−6.099201725139450	p_{33}	0.073003896357977
e_{32}	3.157746208382228		

IMEX-Peer4sv, $s=4$			
c_1	0.000000000000000	p_{11}	1.000000000000000
c_2	−1.598239239549169	p_{12}	0.000000000000000
c_3	0.523829503832339	p_{13}	0.000000000000000
c_4	1.000000000000000	p_{14}	0.000000000000000
γ	0.681884472048995	p_{21}	1.000204745561481
r_{21}	1.292744499701930	p_{22}	−0.000195233457439
r_{31}	1.074957286644128	p_{23}	−0.000009518220959
r_{32}	−0.054028162784565	p_{24}	0.000000006116916
r_{41}	4.064480810437903	p_{31}	1.169763235411655
r_{42}	1.031994574173631	p_{32}	−0.169740581681421
r_{43}	−0.534558192336057	p_{33}	−0.000025123517333
e_{21}	−0.153830152235951	p_{34}	0.000002469787099
e_{31}	0.065444441626366	p_{41}	1.915153835547942
e_{32}	−0.976514386415223	p_{42}	−0.244331567248295
e_{41}	−0.234155732816782	p_{43}	−0.671042624270695
e_{42}	−2.535629358626096	p_{44}	0.000220355971049
e_{43}	1.477107513945526		

Table 2: Coefficients of IMEX-Peer3sv and IMEX-Peer4sv which are super-convergent for variable step sizes. Here, $E_2 = (e_{ij})$.

IMEX-Peer4sve, $s=4$, optimally zero-stable			
c_1	−0.868838855210029	p_{11}	0.000000000000000
c_2	−0.253884413463736	p_{12}	0.316402904545681
c_3	0.754504864110948	p_{13}	1.127642509582261
c_4	1.000000000000000	p_{14}	−0.444045414127942
γ	0.473861788489939	p_{21}	0.000000000000000
r_{21}	0.732961380396538	p_{22}	0.000000000000000
r_{31}	−2.472299983846101	p_{23}	−0.017465269321373
r_{32}	0.077358285702625	p_{24}	1.017465269321373
r_{41}	−1.603925020256191	p_{31}	0.000000000000000
r_{42}	−2.797576519478004	p_{32}	0.000000000000000
r_{43}	−0.278164642408456	p_{33}	0.000000000000000
e_{21}	−0.183287385063759	p_{34}	1.000000000000000
e_{31}	5.974911797174020	p_{41}	0.000000000000000
e_{32}	−2.556627399170977	p_{42}	0.000000000000000
e_{41}	2.456065798975378	p_{43}	0.000000000000000
e_{42}	−2.032396276261657	p_{44}	1.000000000000000
e_{43}	1.255044479285407		

Table 3: Coefficients of IMEX-Peer4sve which is optimally zero-stable, super-convergent for variable step sizes in the explicit part and for constant step sizes in the implicit part. Here, $E_2 = (e_{ij})$.

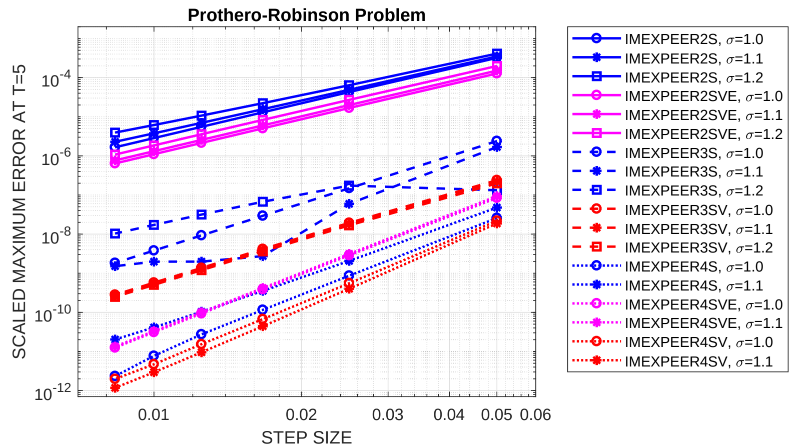

Figure 2: Prothero-Robinson Problem: Scaled maximum errors at $T = 5$ vs. time step sizes for $\sigma = 1.0, 1.1, 1.2$. All new methods perform quite robust with respect to changes of the step sizes.

4.3 Burgers Problem

The first PDE problem is taken from [4], see also [19] for further numerical results with super-convergent IMEX-Peer methods. We consider

$$\partial_t u = 0.1\, \partial_{xx} u + u \partial_x u + \varphi(t,x), \quad -1 \le x \le 1,\ 0 \le t \le 2 \tag{82}$$

with initial value $u(0,x) = \sin(\pi(x+1))$ and homogeneous Dirichlet boundary conditions. The source term is defined through

$$\varphi(t,x) = r(x)\sin(t), \quad r(x) = \begin{cases} 0, & -1 \le x \le -1/3 \\ 3(x+1/3), & -1/3 \le x \le 0 \\ 3(2/3-x)/2, & 0 \le x \le 2/3 \\ 0, & 2/3 \le x \le 1. \end{cases} \tag{83}$$

The spatial discretization is done by finite differences with $\triangle x = 1/2500$. We treat the diffusion implicitly and all other terms explicitly.

We have used tolerances $atol = rtol = 10^{-2-i}$, $i = 0, 1, \ldots, 5$ and initial step sizes $\tau = \sqrt{atol}$. The results are plotted and discussed in Figure 4.

4.4 Linear Advection-Reaction Problem

A second PDE problem for an accuracy test is the linear advection-reaction system from [10]. The equations are

$$\partial_t u + \alpha_1\, \partial_x u = -k_1 u + k_2 v + s_1\,, \tag{84}$$
$$\partial_t v + \alpha_2\, \partial_x v = k_1 u - k_2 v + s_2 \tag{85}$$

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

$$\alpha_1 = 1,\ \alpha_2 = 0,\ k_1 = 10^6,\ k_2 = 2k_1,\ s_1 = 0,\ s_2 = 1,$$

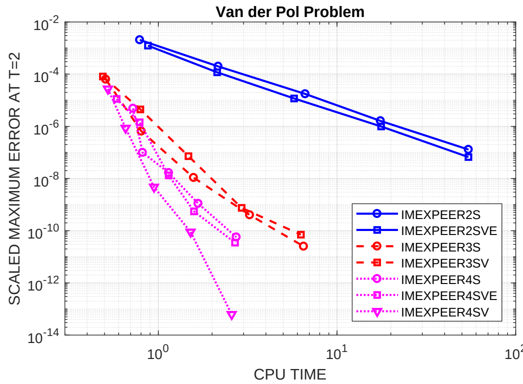

Figure 3: Van der Pol Oscillator: Scaled maximum errors at $T = 2$ vs. computing time. For the 2- and 3-stage methods, the differences are moderate. IMEX-Peer4sv shows a clear improvement over the other 4-stage methods.

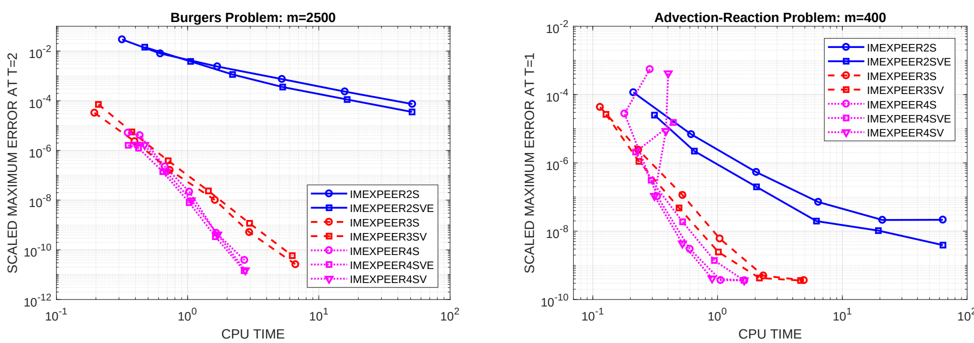

Figure 4: Burgers and Advection-Reaction Problem: Scaled maximum errors vs. computing time. For the Burgers problem, no significant improvement can be observed. In several cases, the better performance of the new methods for the advection-reaction problem is obvious. All 4-stage methods run for low tolerances at their stability limit, which is related to $\triangle t \approx 4\,10^{-4}$. The order reduction of higher order methods for small time steps was already observed in [10] and [12] as an inherent issue for very high-accuracy computations.

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 [10] and gives rise to a spatial error of $1.5\,10^{-5}$. In the IMEX setting, the reaction is treated implicitly and all other terms explicitly.

We have used tolerances $atol = rtol = 10^{-3-i}$, $i = 0, 1, \ldots, 5$ and an initial step size $\tau = 10^{-3}$ for all runs. The results are plotted and discussed in Figure 4.

5 Conclusion

We have developed a new class of s-stage super-convergent IMEX-Peer methods with A-stable implicit part, which maintain their super-convergence order of $s+1$ for variable step sizes. A-stability is important to solve problems with function contributions that have large imaginary eigenvalues in the spectrum of their Jacobian. Applying the idea of extrapolation and studying the σ-dependent coefficients in the local error representations, we first derived additional conditions for implicit and explicit Peer methods, which are then combined to state $2s+1$ corresponding conditions for IMEX-Peer methods. An interesting theoretical result is that one of the nodes must be zero. Such methods exist for $s>2$. We designed new methods for $s=3,4$. However, the new property of super-convergence for variable step sizes reduces the scope for achieving good stability properties, resulting in significantly smaller stability regions compared to the super-convergent IMEX-Peer methods from [16]. We also constructed methods for $s=2,4$ having an explicit part that is super-convergent for variable step sizes, whereas the implicit part is only super-convergent for constant steps. In all cases, we employed the MATLAB-routine *fminsearch* with varying objective functions and starting values to find suitable methods with stability regions as large as possible, good damping properties for very stiff problems and small error constants.

We have implemented our newly designed methods with local error control based on linear combinations of old function evaluations to approximate the leading error term of an embedded solution of order $s-1$. From our observations made for four numerical examples, we can draw the following conclusions: (i) The new methods perform quite robust with respect to changing the step size and, as expected, show their theoretical order at the same time. (ii) For problems that demand a fast step size adaptation over several orders of magnitudes, like the van der Pol oscillator, the new methods have the potential to perform better. (iii) For problems that can be integrated with moderate step size changes, like the Burgers problem, super-convergence for constant step sizes is still sufficient to profit from the additional order and possibly from the larger stability regions.

6 Acknowledgement

J. Lang was supported by the German Research Foundation within the collaborative research center TRR154 "Mathematical Modeling, Simulation and Optimisation Using the Example of Gas Networks" (DFG-SFB TRR154/2-2018, TP B01) and the Graduate Schools Computational Engineering (DFG GSC233) and Energy Science and Engineering (DFG GSC1070).

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