

Extrapolation-Based Implicit-Explicit Peer Methods with Optimised Stability Regions

Jens Lang*

*Technische Universität Darmstadt
Dolivostraße 15, 64293 Darmstadt, Germany
lang@mathematik.tu-darmstadt.de*

Willem Hundsdorfer

*Center for Mathematics and Computer Science
P.O. Box 94079, 1090 GB Amsterdam, The Netherlands
Willem.Hundsdorfer@cw.nl*

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Abstract

In this paper we investigate an new class of implicit-explicit two-step methods of Peer type for systems of ordinary differential equations with both non-stiff and stiff parts included in the source term. An extrapolation approach based on already computed stage values with equally high consistency order is applied to construct such methods with strong stability properties. Optimised implicit-explicit Peer methods of order $p = 2, 3, 4$, 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 implicit-explicit methods are included.

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

1 Introduction

Many initial value problems arising in practice are in a 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. 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

*corresponding author

with the favorable stability properties of implicit schemes to enhance the overall computational efficiency.

To construct suitable IMEX methods it is convenient if an implicit method is available where all approximations have a high accuracy. Then a related explicit method can be found by using extrapolation, and 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 [3] with linear multistep methods of BDF type.

In this paper we will consider such IMEX methods based on implicit Peer methods. These methods introduced by Schmitt, Weiner and co-workers [1, 11, 12] are a very comprehensive class of general linear methods (GLMs) in which the approximations in all stages have the same order. Peer methods can be viewed as a natural generalization of linear multistep methods in the sense that each of the stages is a linear multistep method itself. Due to their multi-stage structure 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. IMEX-Peer methods are competitive alternatives to classic IMEX methods for large stiff problems. Higher order IMEX Runge-Kutta methods are known to suffer from possible order reduction and serious efficiency loss for stiff problems. Moreover, the increasing number of necessary coupling conditions makes their construction difficult.

Recently, the same extrapolation approach was used by Cardone, Jackiewicz, Sandu and Zhang [2] starting with diagonally implicit multistage integration methods (DIMSIMs). In those general linear methods the implicit internal stages are followed by explicit stages. Due to these explicit stages the linear stability properties of the resulting IMEX methods is less favourable than for the IMEX-Peer methods. Higher order IMEX-GLMs were constructed by Zhang, Sandu and Blaise [18], based on an earlier developed partitioned GLM framework of the same authors in [17].

In Section 2 of this paper we present the framework to obtain IMEX-Peer methods based on suitable implicit methods. The construction of specific classes of methods is performed in Section 3. Along with IMEX-BDF methods, which also fit in the Peer form, we will construct IMEX-Peer methods based on the implicit methods of order 3 and 4 that were developed by Beck, Weiner, Podhaisky and Schmitt [1]. Comparison of the stability regions of the methods shows promising results for the latter methods. This is confirmed in the numerical experiments in Section 5 for two advection-reaction problems with stiff reactions and a reaction-diffusion problem, where the diffusion leads to stiffness.

2 Implicit-Explicit Peer Methods Based on Extrapolation

2.1 Implicit Peer methods

To solve initial value problems in a vector space \mathbb{V} (e.g. $\mathbb{V} = \mathbb{R}^m, m \geq 1$),

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

we consider the so-called Peer methods introduced by Schmitt, Weiner and co-workers [11, 1]. An s -stage Peer method provides approximations

$$w_n = [w_{n,1}, \dots, w_{n,s}]^T \in \mathbb{V}^s, \quad w_{n,i} \approx u(t_n + c_i \Delta t), \quad (2)$$

with nodes $c_i \in \mathbb{R}$ such that $c_i \neq c_j$ if $i \neq j$, and $c_s = 1$. The starting vector $w_0 = [w_{0,i}] \in \mathbb{V}^s$ is supposed to be given, or computed from a Runge-Kutta method, for example.

Peer methods are general linear methods, based on the requirement that all approximations $w_{n,j}$ have the same order. Here, we will primarily aim at order $p = s$. With $s \times s$ coefficient matrices $P = (p_{ij})$, $Q = (q_{ij})$, $R = (r_{ij})$, and the $m \times m$ identity matrix I , the usual general form of the implicit methods of this Peer type is

$$w_n = (P \otimes I)w_{n-1} + \Delta t(Q \otimes I)F(w_{n-1}) + \Delta t(R \otimes I)F(w_n). \quad (3)$$

where $F(w) = [F(w_i)] \in \mathbb{V}^s$ is the application of F to all components of $w \in \mathbb{V}^s$. In the following, for an $s \times s$ -matrix we will use the same symbol for its Kronecker product with the identity matrix as mapping from the space \mathbb{V}^s to itself. Then, (3) simply reads

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

The matrix R is taken to be lower triangular, giving diagonally implicit methods, with diagonal R if parallelism is a special case of interest [12]. Implicit peer methods with good stability properties, i.e., $L(\alpha)$ -stability with large angles α , can be found by taking $Q = 0$ [1]. We will choose these methods to construct implicit-explicit peer methods based on extrapolation. Then the method reads

$$w_n = Pw_{n-1} + \Delta tRF(w_n). \quad (5)$$

Some requirements or desirable properties are briefly discussed here for the implicit method (5).

Zero-stability. The matrix P should be power bounded to have stability for the trivial problem $u'(t) = 0$. Let $\text{spr}(P)$ be the spectral radius of P . Since one eigenvalue of P will be equal to 1 for pre-consistency, the requirement of zero-stability means

$$\text{spr}(P) = 1 \text{ and eigenvalues with modulus 1 are not defective.} \quad (6)$$

This requirement was enforced by Schmitt, Weiner et al. by taking P such that one eigenvalue equals 1 and the others are 0. This choice, called optimal zero-stability, made the construction of methods more tractable. We will also look at methods that are strongly zero-stable, where P has one eigenvalue 1 and the other eigenvalues have modulus less than 1. This holds for example for the well-known BDF methods.

Accuracy. Let $e = (1, \dots, 1)^T \in \mathbb{R}^s$. It will be assumed that

$$Pe = e. \quad (7)$$

This is the so-called pre-consistency condition, which means that for the trivial equation $u'(t) = 0$, we get solutions $w_{n,i} = 1$ provided that $w_{0,j} = 1$, $j = 1, \dots, s$. Inserting exact solution values $w(t_n) = [u(t_n + c_i \Delta t)] \in \mathbb{V}^s$ in the implicit scheme (5) gives the residual-type local errors

$$r_n = w(t_n) - Pw(t_{n-1}) - \Delta t R w'(t_n). \quad (8)$$

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

$$w(t_n) = e \otimes u(t_n) + \Delta t c \otimes u'(t_n) + \frac{1}{2} \Delta t^2 c^2 \otimes u''(t_n) + \dots \quad (9)$$

$$w(t_{n-1}) = e \otimes u(t_n) + \Delta t (c - e) \otimes u'(t_n) + \frac{1}{2} \Delta t^2 (c - e)^2 \otimes u''(t_n) + \dots, \quad (10)$$

from which we obtain

$$r_n = \sum_{j \geq i} \Delta t^j d_j \otimes u^{(j)}(t_n) \quad (11)$$

with

$$d_j = \frac{1}{j!} (c^j - P(c - e) - j R c^{j-1}). \quad (12)$$

The method is said to have (stage) order q if (7) holds and $d_j = 0$ for $j = 1, 2, \dots, q$. We will be interested in methods with (stage) order s . With the Vandermonde matrices $V_0 = (c_i^{j-1})$ and $V_1 = ((c_i - 1)^{j-1})$ for $i, j = 1, \dots, s$, $C = \text{diag}(c_1, c_2, \dots, c_s)$ and $D = \text{diag}(1, 2, \dots, s)$, the conditions for having stage order s with the implicit method (5) are

$$CV_0 - P(C - I)V_1 - RV_0 D = 0. \quad (13)$$

Remark 2.1 (superconvergence). *For a method with (stage) order q , it is possible to have convergence with order equal to $q + 1$. This is discussed under the heading super-convergence in the book of Strehmel, Weiner & Podhaisky ([15], Sect. 5.3) for non-stiff problems. It will also hold for stiff problems; see Hundsdorfer [7] for results with stiff linear systems.*

2.2 Extrapolation

Based on an implicit method with order s , a related explicit method can be found by extrapolation, leading to implicit-explicit methods. This is a well-known procedure for linear multistep methods, see for instance Crouzeix [3] or the review in the book of Hundsdorfer and Verwer ([9], Section IV.4.2). Recently this idea was also used with a class of general linear methods, the so-called diagonally implicit multistage integration methods (DIMSIMs), by Cardone, Jackiewicz, Sandu, and Zhang [2]. Here, we will use this extrapolation idea to obtain implicit-explicit Peer methods.

Having an implicit method, where all approximations $w_{n,j}$ have order s , we can obtain a corresponding explicit method by extrapolation using a Lagrange polynomial of degree $s - 1$, giving $\varphi(t_{n,i}) = \sum_j s_{ij} \varphi(t_{n-1,j}) + \mathcal{O}(\Delta t^s)$ for smooth functions φ , with $t_{n,i} = t_n + c_i \Delta t$. The extrapolation coefficients are $s_{ij} = \prod_{k \neq j} (c_i - c_k + 1) / (c_j - c_k)$.

We can apply this extrapolation with $\varphi(t) = F(u(t))$. Starting from the implicit method (5), this yields the explicit method

$$w_n = Pw_{n-1} + \Delta t \hat{Q} F(w_{n-1}), \quad (14)$$

with coefficient matrix $\hat{Q} = (\hat{q}_{ij})$ given by $\hat{Q} = RS$, where $S = (s_{ij})$. By the construction, all the stages have again order s , at least, so (14) is an explicit Peer method.

The extrapolation may be improved by using the last available information, whereby a value $\varphi(t_{n,i})$ is found as linear combination of some of the values $\varphi(t_{n-1,j})$ together with the most recent values $\varphi(t_{n,j})$, $j = 1, \dots, i - 1$, say

$$\varphi(t_{n,i}) = \sum_j s_{ij}^{(1)} \varphi(t_{n-1,j}) + \sum_{j \leq i-1} s_{ij}^{(2)} \varphi(t_{n,j}) + \mathcal{O}(\Delta t^s), \quad i = 1, \dots, s. \quad (15)$$

Setting $S_1 = (s_{ij}^{(1)})$, $S_2 = (s_{ij}^{(2)})$, this will lead to an explicit Peer method of the form

$$w_n = Pw_{n-1} + \Delta t \hat{Q} F(w_{n-1}) + \Delta t \hat{R} F(w_n) \quad (16)$$

with

$$\hat{Q} = RS_1, \quad \hat{R} = RS_2. \quad (17)$$

Note that \hat{R} is strictly lower triangular, since R is lower triangular and S_2 is strictly lower triangular.

Defining vectors $\Phi_m = [\varphi(t_{m,i})] \in \mathbb{V}^s$, the error vector for the extrapolation, $\delta_n = \Phi_n - S_1 \Phi_{n-1} - S_2 \Phi_n$, can be expanded in a Taylor series at t_n ,

$$\delta_n = (I - S_1 - S_2)e \otimes \varphi(t_n) + \sum_{j \geq 1} \frac{1}{j!} ((I - S_2)c^j - S_1(c - e)^j) \otimes \varphi^{(j)}(t_n) \Delta t^j. \quad (18)$$

Therefore, the conditions for order s reads

$$(I - S_2)c^j - S_1(c - e)^j = 0, \quad 0 \leq j \leq s - 1, \quad (19)$$

which is equivalent to the relation $S_1V_1 = (I - S_2)V_0$. The choice of a strictly lower triangular S_2 thus determines S_1 .

2.3 Implicit-Explicit Peer Methods

The combination of the related implicit and explicit methods (4), (16) can now be used to construct an implicit-explicit (IMEX) method for systems of the form

$$u'(t) = F_0(u(t)) + F_1(u(t)), \quad (20)$$

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

$$w_n = Pw_{n-1} + \Delta t \hat{Q}F_0(w_{n-1}) + \Delta t \hat{R}F_0(w_n) + \Delta t R F_1(w_n). \quad (21)$$

The extrapolation idea is used here only on the F_0 . 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.

Remark 2.2 (linearly implicit methods). *As a special case of (20), we can consider $F_0(u) = F(u) - Ju$, $F_1(u) = Ju$, with a Jacobian approximation $J \approx F'(u)$. This gives the linearly implicit Peer method*

$$w_n = Pw_{n-1} + \Delta t \hat{Q}F(w_{n-1}) + \Delta t \hat{R}F(w_n) - \Delta t \hat{Q}Jw_{n-1} + \Delta t (R - \hat{R})Jw_n. \quad (22)$$

By the above construction, leading to the IMEX scheme (21), all stages will be consistent of order s . However, since F_1 is linear here, it is possible that the order conditions are in fact a bit too strong.

The standard local consistency analysis for the IMEX-Peer method (21) with exact solution values $u(t_{n,i})$ yields for the residual-type local errors

$$r_n = E_{im} + \Delta t R E_{ex} + \mathcal{O}(\Delta t^{s+2}), \quad (23)$$

where $E_{im} = d_{s+1} \otimes u^{(s+1)}(t_n) \Delta t^{s+1}$ is the leading error term of the corresponding implicit Peer method with constant time steps. Replacing in (18) $\varphi(t)$ by $F_0(u(t))$ taken as function of t , we find for the leading error vector of the extrapolation,

$$E_{ex} = \frac{1}{s!} ((I - S_2)c^s - S_1(c - e)^s) \otimes \frac{d^s}{dt^s} F_0(u(t_n)) \Delta t^s. \quad (24)$$

Together with zero-stability of the implicit Peer method and standard arguments for multistep methods (see [6], Lemma 2.1), we have the following convergence result for the IMEX scheme (21):

Theorem 2.1. *Let the s -stage implicit Peer method (5) with coefficients (c, P, R) be zero-stable and consistent of order s for constant step size. Let the starting values satisfy $w_{0,i} - u(t_0 + c_i \Delta t) = \mathcal{O}(\Delta t^s)$, $i = 1, \dots, s$. Then the IMEX scheme (21) with $\hat{R} = RS_2$ and $\hat{Q} = R(I - S_2)V_0V_1^{-1}$ is convergent of order s for constant step size and arbitrary strictly lower triangular matrix S_2 .*

Eventually, we define the following two error constants for later use:

$$c_{im} = \|d_{s+1}\| = \left\| \frac{1}{(s+1)!} (c^{s+1} - P(c-e)^{s+1} - (s+1)Rc^s) \right\| \quad (25)$$

and

$$c_{ex} = \left\| \frac{1}{s!} \left((R - \hat{R})c^s - \hat{Q}(c-e)^s \right) \right\|. \quad (26)$$

with $\|\cdot\|$ being the Euclidean norm in \mathbb{R}^s . The first one is given by the implicit Peer method and the second one is related to the extrapolation process.

2.4 Stability of IMEX Peer Methods

We consider the general test equation

$$y'(t) = \lambda_0 y(t) + \lambda_1 y(t), \quad t \geq 0, \quad (27)$$

with complex parameters λ_0 and λ_1 . Define $z_i = h\lambda_i$, $i = 0, 1$. In what follows we adopt the notation to our schemes. Applying an IMEX-Peer method to (27) gives

$$Y^{n+1} = (I - z_0RS_2 - z_1R)^{-1}(P + z_0RS_1)Y^n. \quad (28)$$

This can be formalized to $Y^{n+1} = M(z_0, z_1)Y^n$. For given z_0 and z_1 , stability is ensured if

$$\rho(M(z_0, z_1)) < 1. \quad (29)$$

The stability function of the IMEX-Peer method is defined as the characteristic polynomial of the stability matrix $M(z_0, z_1)$:

$$\zeta(w, z_0, z_1) = \det(wI - M(z_0, z_1)). \quad (30)$$

Consequently, the IMEX-Peer method is stable for given $z_0, z_1 \in \mathbb{C}$ if all the roots $w_i(z_0, z_1)$, $i = 1, \dots, s$, of the stability function $\zeta(w, z_0, z_1)$ are inside the unit circle.

The higher order implicit Peer methods considered here are $L(\alpha)$ -stable with respect to the implicit part $z_1 \in \mathbb{C}$. Therefore, we introduce the sets

$$S_\beta = \left\{ z_0 \in \mathbb{C} : \begin{array}{l} (29) \text{ holds for any } z_1 \in \mathbb{C} \text{ with} \\ \operatorname{Re}(z_1) < 0 \text{ and } |\operatorname{Im}(z_1)| \leq \tan(\beta)|\operatorname{Re}(z_1)| \end{array} \right\}. \quad (31)$$

In order to compute these sets for specific angles β with $0 \leq \beta \leq \alpha$, we first define for fixed $y \in \mathbb{R}$,

$$S_{\beta,y} = \{z_0 \in \mathbb{C} : (29) \text{ holds for fixed } z_1 = -|y|/\tan(\beta) + y_1\} \quad (32)$$

and find then S_β from the intersection of all $S_{\beta,y}$, $y \in \mathbb{R}$, which follows from the maximum principle. The set $S_E := S_{\beta,0}$ is independent of β and corresponds to the stability region of the explicit method. Since $S_\alpha \subset S_E$, the goal is to construct IMEX-Peer methods for which S_E is large and $S_E \setminus S_\alpha$ is as small as possible for angles α that are close to $\pi/2$, whereas the error constant for the extrapolation, c_{ex} , is still of moderate size.

The boundary locus method can be used to compute the boundary of $S_{\beta,y}$:

$$\partial S_{\beta,y} = \{z_0 \in \mathbb{C} : \zeta(e^{\theta_1}, z_0, -|y|/\tan(\beta) + y_1) = 0, \theta \in [0, 2\pi)\}. \quad (33)$$

Varying the eigenvalues $w = e^{\theta_1}$ for fixed $z_1(y) = -|y|/\tan(\beta) + y_1, y \in \mathbb{R}$, allows to reformulate the eigenvalue problem $M(z_0, z_1)x = wx$ into an eigenvalue problem for $z_0(e^{\theta_1}, y)$, i.e., $G(e^{\theta_1}, z_1(y))x = z_0x$ with

$$G = (e^{\theta_1}\hat{R} + \hat{Q})^{-1}(e^{\theta_1}I - e^{\theta_1}z_1(y)R - P). \quad (34)$$

The set of all eigenvalues $z_0(e^{\theta_1}, y)$ contains the boundary of $S_{\beta,y}$. A similar approach was also successfully applied in [2] for DIMSIMs.

3 Construction of IMEX-Peer Methods

3.1 IMEX-Peer Methods with Equidistant Nodes

We will first consider IMEX Peer methods with equidistant nodes. A good candidate within this class are the IMEX-BDF methods introduced in [3, 16] and further analysed in [4]. Taken with s steps of length $\Delta t/s$, they can be reformulated as IMEX-Peer methods.

Starting at $t = t_{n-1}$ with approximate solutions $u_{n-1-i/s} \approx u(t_{n-1} - i\Delta t/s)$ for $i = 0, \dots, s-1$, we have for s (constant) steps of the s -step IMEX-BDF method:

$$k = 1, \dots, s : \quad \sum_{i=0}^s a_i u_{n-1-\frac{i-k}{s}} = \frac{\Delta t}{s} e_s^T S \begin{pmatrix} F_0(u_{n-2+\frac{k}{s}}) \\ \vdots \\ F_0(u_{n-1+\frac{k-1}{s}}) \end{pmatrix} + \frac{\Delta t}{s} F_1(u_{n-1+\frac{k}{s}}) \quad (35)$$

with $e_s = (0, \dots, 0, 1)^T \in \mathbb{R}^s$ and $S = (s_{ij}) = V_0 V_1^{-1}$ defined by the normalized vector $c = (0, 1, \dots, s-1)^T$. In order to obtain the standard form of a Peer method,

we set

$$w_{n-1} = \begin{pmatrix} u_{n-2+\frac{1}{s}} \\ u_{n-2+\frac{2}{s}} \\ \vdots \\ u_{n-1} \end{pmatrix} \quad \text{and} \quad w_n = \begin{pmatrix} u_{n-1+\frac{1}{s}} \\ u_{n-1+\frac{2}{s}} \\ \vdots \\ u_n \end{pmatrix}. \quad (36)$$

This yields

$$A_2 w_n = -A_1 w_{n-1} + \frac{\Delta t}{s} B_1 F_0(w_{n-1}) + \frac{\Delta t}{s} B_2 F_0(w_n) + \frac{\Delta t}{s} F_1(w_n) \quad (37)$$

with the matrices

$$A_1 = \begin{pmatrix} a_s & a_{s-1} & \cdots & a_1 \\ 0 & a_s & \cdots & a_2 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_s \end{pmatrix}, \quad A_2 = \begin{pmatrix} a_0 & 0 & \cdots & 0 \\ a_1 & a_0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ a_{s-1} & a_{s-2} & \cdots & a_0 \end{pmatrix} \quad (38)$$

and

$$B_1 = \begin{pmatrix} s_{s1} & s_{s2} & \cdots & s_{ss} \\ 0 & s_{s1} & \cdots & s_{s,s-1} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & s_{s1} \end{pmatrix}, \quad B_2 = \begin{pmatrix} 0 & 0 & \cdots & 0 \\ s_{ss} & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ s_{s2} & \cdots & s_{ss} & 0 \end{pmatrix}. \quad (39)$$

In Table 1, the coefficients of the BDF methods for $s = 2, 3, 4$ are provided. Note that A_2 is invertible since always $a_0 \neq 0$. The coefficients of the equivalent IMEX-Peer method are then determined by the following Lemma:

Lemma 3.1. *An s -stage IMEX-BDF method (35) with s steps of length $\Delta t/s$ is equivalent to an s -stage IMEX-Peer (21) with nodes $c = (1/s, 2/s, \dots, 1)^T$ and coefficient matrices*

$$P = -A_2^{-1} A_1, \quad \hat{Q} = (1/s) A_2^{-1} B_1, \quad \hat{R} = (1/s) A_2^{-1} B_2, \quad \text{and} \quad R = (1/s) A_2^{-1}. \quad (40)$$

IMEX-BDF methods have proven to work very well and therefore they are a good target for general IMEX-Peer methods with $p = s$.

Example 3.1. *Exemplarily, the (peer-)coefficients of the IMEX-BDF3 method with three steps of length $\Delta t/3$ are given. The node vector $c = (0, 1, 2)$ yields $e_3^T S = (1, -3, 3)$. Thus, the matrices in (21) are:*

$$P = \begin{pmatrix} \frac{2}{11} & -\frac{9}{11} & \frac{18}{11} \\ \frac{36}{121} & -\frac{140}{121} & \frac{225}{121} \\ \frac{450}{1331} & -\frac{1629}{1331} & \frac{2510}{1331} \end{pmatrix}, \quad R = \begin{pmatrix} \frac{2}{11} & 0 & 0 \\ \frac{36}{121} & \frac{2}{11} & 0 \\ \frac{450}{1331} & \frac{36}{121} & \frac{2}{11} \end{pmatrix}, \quad (41)$$

$$\hat{Q} = \begin{pmatrix} \frac{2}{11} & -\frac{6}{11} & \frac{6}{11} \\ \frac{36}{121} & -\frac{86}{121} & \frac{42}{121} \\ \frac{450}{1331} & -\frac{954}{1331} & \frac{404}{1331} \end{pmatrix}, \quad \hat{R} = \begin{pmatrix} 0 & 0 & 0 \\ \frac{6}{11} & 0 & 0 \\ \frac{42}{121} & \frac{6}{11} & 0 \end{pmatrix}. \quad (42)$$

The eigenvalues of P are 1 and $(-119 \pm 27\sqrt{39}i)/2662$.

s	a_0	a_1	a_2	a_3	a_4	α
2	$\frac{3}{2}$	-2	$\frac{1}{2}$			90.00°
3	$\frac{11}{6}$	-3	$\frac{3}{2}$	$-\frac{1}{3}$		86.03°
4	$\frac{25}{12}$	-4	3	$-\frac{4}{3}$	$\frac{1}{4}$	73.35°

Table 1: Coefficients and stability values for $L(\alpha)$ -stability of BDF methods for $s = 2, 3, 4$.

3.2 General IMEX-Peer Methods

3.2.1 The case $s = 2$

The two-stage singly implicit methods (5) with order two form a one-parameter family, with free parameter c_1 , say. The choice $c_1 = 1/2$ produces the above implicit BDF2 method with step-size $\Delta t/2$. Note that requiring optimal zero stability, with P having a single eigenvalue one and the other zero, yields a completely defined method. However, this would exclude interesting methods, such as the BDF2 method.

In order to find an IMEX method, where the explicit method has a larger stability region, we start with the implicit BDF2 method with step size $\Delta t/2$ and then apply extrapolation with a strictly lower triangular $S_2 = (s_{ij}^{(2)}) \neq 0$, say $s_{21}^{(2)} = \mu \neq 0$. Note that $\mu = 2$ recovers the IMEX-BDF2 method from above. A careful study of the stability matrix revealed that the largest interval $(-\beta_R, 0)$ of the real negative axis in the stability region is obtained if μ is the smallest root of the polynomial $\mu^2 - 20\mu + 20$, i.e., $\mu = \mu^* = 10 - 4\sqrt{5} \approx 1.0557$ with real stability boundary $\beta_R \approx 5.38$. Choosing μ equal to this optimal μ^* gives a stability region which is pinched off at the real point $x^* \approx -2.54$. Taking μ a bit larger, for example $\mu = \mu^* + 1/10$, gives a better shaped stability region, as shown in Figure 1. The coefficients of the resulting IMEX-Peer2 method are

$$c = \begin{pmatrix} \frac{1}{2} \\ 1 \end{pmatrix}, \quad P = \begin{pmatrix} -\frac{1}{3} & \frac{4}{3} \\ -\frac{4}{9} & \frac{13}{9} \end{pmatrix}, \quad R = \begin{pmatrix} \frac{1}{3} & 0 \\ \frac{4}{9} & \frac{1}{3} \end{pmatrix}, \quad S_2 = \begin{pmatrix} 0 & 0 \\ \mu & 0 \end{pmatrix}, \quad (43)$$

accomplished with $\hat{R} = RS_2$ and $\hat{Q} = R(I - S_2)V_0V_1^{-1}$.

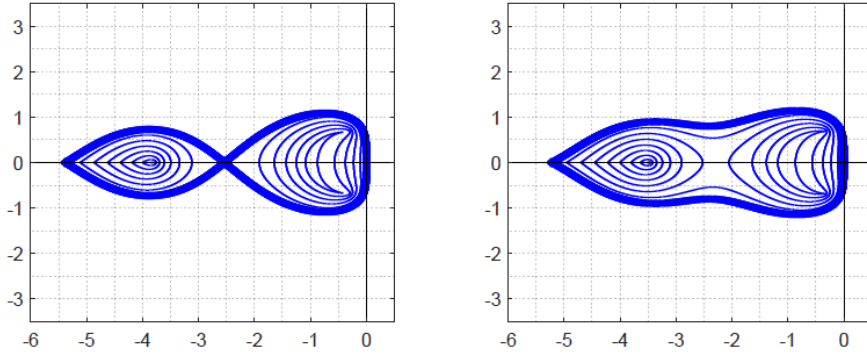


Figure 1: IMEX-Peer2 method. Implicit method with $c_1 = \frac{1}{2}$, i.e., BDF2 with $\Delta t/2$. Plots of the stability regions of the corresponding explicit methods with $s_{21}^{(2)} = \mu \neq 0$; left panel with optimal $\mu = \mu^* = 10 - 4\sqrt{5}$, right panel with $\mu = \mu^* + \frac{1}{10}$.

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

To ensure good stability of the implicit Peer method with three or four stages, we start with superconvergent singly-implicit methods of order $p = s$ for constant step size and optimal zero-stability, developed by Beck, Weiner, Podhaisky and Schmitt ([1], Table 3) for large stiff ODE systems. These methods are $L(\alpha)$ -stable with angles 86.1° and 83.2° , and possess relatively small error constants. The nodes are selected such that $0 < c_1 < c_2 < \dots < c_s = 1$. The free parameters are then the $d = s(s-1)/2$ inputs of the matrix S_2 .

As a design criterion, we would like to balance between optimal stability regions S_α and small error constants c_{ex} for the extrapolation. The latter one is very important since extrapolation has to be done forward in time, i.e., future values are approximated outside the range of given time points, which might cause relatively large errors. We expect that optimizing S_α results also in reasonably shaped stability regions S_E of the explicit methods.

Eventually, we perform an optimization over the parameter space $p \in \mathbb{R}^d$ to compute

$$p^* = \operatorname{argmin}\{-|S_\alpha| + 1.5 \cdot 10^s |c_{ex} - c_0|\}, \quad (44)$$

where c_{ex} is defined in (26) and c_0 corresponds to the extrapolation based on the s most recently computed stage values, i.e.,

$$w_{n-1}^{(j+1)}, \dots, w_{n-1}^{(s)} = w_n^{(0)}, w_n^{(1)}, \dots, w_n^{(j)}, \quad j = 0, \dots, s-1. \quad (45)$$

We have $c_0 = 4.1082 \cdot 10^{-2}, 4.2632 \cdot 10^{-3}$ for $s = 3, 4$, respectively. The corresponding parameter vector p_0 is taken as initial guess for the routine *fminsearch* implemented

in MATLAB. This gives the parameters

$$\begin{aligned} p_{21} &= 4.6617853424698374 \cdot 10^0, & p_{31} &= 3.3696230360366979 \cdot 10^0, \\ p_{32} &= 5.6686050026329915 \cdot 10^{-1}, \end{aligned} \quad (46)$$

for the IMEX-Peer3 method and

$$\begin{aligned} p_{21} &= 4.0913830614894255 \cdot 10^0, & p_{31} &= -1.2244427616780204 \cdot 10^1, \\ p_{32} &= 5.7564397758588521 \cdot 10^0, & p_{41} &= 1.0587962913073733 \cdot 10^1, \\ p_{42} &= -7.7409749651373776 \cdot 10^0, & p_{43} &= 4.1019377658951353 \cdot 10^0, \end{aligned} \quad (47)$$

for the IMEX-Peer4 method. We set $s_{ij}^{(2)} = p_{ij}$ to define S_2 in each case.

The resulting values for the stability regions S_α and S_E as well as for the error constants are collected in Table 2. For comparison, we also show the values for the IMEX-BDF methods. It can be observed that (i) the error constants for the extrapolation are comparable, (ii) the sizes of the stability regions differ only moderately, and (iii) the IMEX-Peer methods has a significantly larger interval (up to a factor two) on the negative real axis included in the stability region. More details are visible in Figure 2.

Method	α	$ S_\alpha $	x_{max}	$ S_E $	x_{max}	c_{im}	c_{ex}
IMEX-BDF2	90.0°	6.28	-2.67	6.98	-2.67	$7.05 \cdot 10^{-2}$	$2.11 \cdot 10^{-1}$
IMEX-BDF3	86.0°	7.27	-2.86	9.65	-2.86	$8.93 \cdot 10^{-3}$	$3.57 \cdot 10^{-2}$
IMEX-BDF4	73.4°	7.30	-2.84	9.92	-2.84	$8.91 \cdot 10^{-4}$	$4.45 \cdot 10^{-3}$
IMEX-Peer2	90.0°	7.44	-4.86	8.53	-5.22	$7.05 \cdot 10^{-2}$	$2.78 \cdot 10^{-1}$
IMEX-Peer3	86.1°	8.28	-3.07	10.68	-3.07	$8.20 \cdot 10^{-3}$	$3.58 \cdot 10^{-2}$
IMEX-Peer4	83.2°	4.64	-3.57	9.36	-3.57	$3.43 \cdot 10^{-4}$	$4.27 \cdot 10^{-3}$

Table 2: Size of stability regions S_α and S_E , x_{max} at the negative real axis and error constants for IMEX-BDF and IMEX-Peer methods with $s = 2, 3, 4$.

4 Comparison of Stability Regions

Here we compare the stability regions of the IMEX-Peer and IMEX-BDF methods to those of the IMEX-DIMSIM methods developed and tested by Cardone et al. [2]. There, the authors first selected an implicit DIMSIM method with suitable stability and order properties, and then obtained the explicit component through an optimization procedure that maximized the combined stability region of the pair. They applied this methodology to construct IMEX pairs of orders one to four. In

contrast, we took also care on the error constants for the underlying extrapolation process. The stability regions S_β for varying angle β and methods with $s = 2, 3, 4$, are shown in Figure 2.

It is obvious that the two-step methods of Peer type allow the construction of higher-order extrapolation-based IMEX schemes with larger stability regions. Whereas the IMEX-DIMSIM2 scheme is still competitive with respect to absolute size, the other two IMEX-DIMSIM schemes suffer clearly from small stability regions. For these methods, we expect stability problems for larger time steps, which is indeed confirmed by our numerical experiments. In Figure 3, we have collected the values for the size of stability regions S_β with $\beta = \alpha, 75^\circ, 60^\circ, 45^\circ, 30^\circ, 15^\circ$ and the absolute value of the left-most point $x_{max} \in S_E$ on the negative real axis.

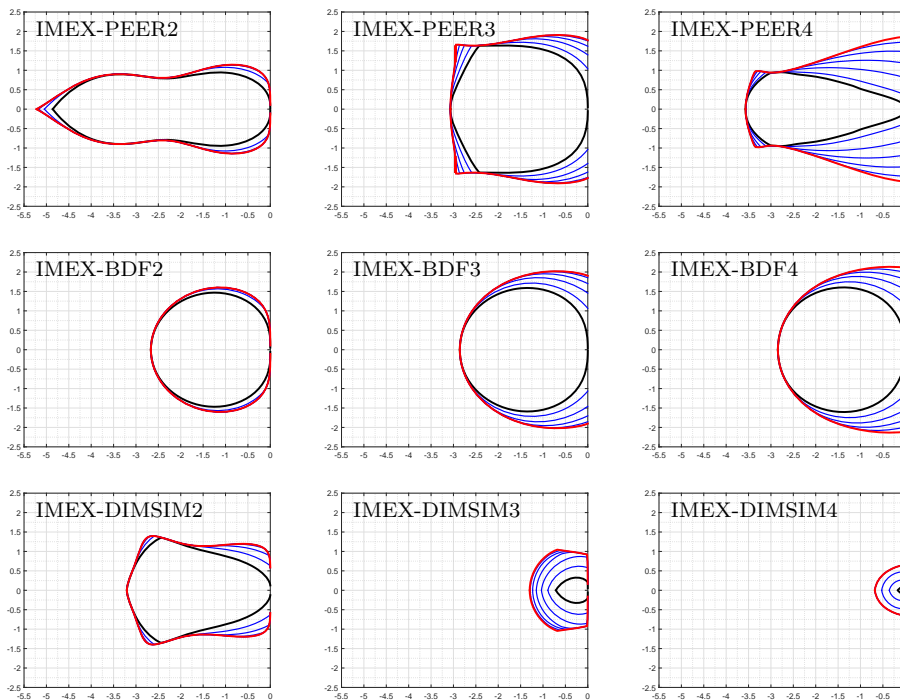


Figure 2: Top to bottom: stability regions S_α (black line), S_β for $\beta = 75^\circ, 60^\circ, 45^\circ, 30^\circ, 15^\circ$ (blue lines), and S_0 (red line) for IMEX-PEER(s), IMEX-BDF(s), and IMEX-DIMSIM(s) methods, $s = 2, 3, 4$ (left to right).

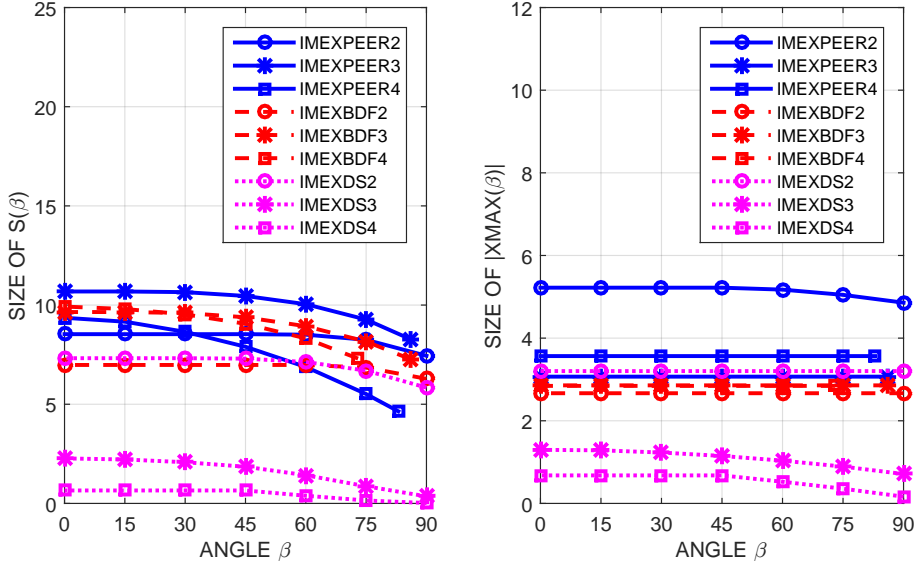


Figure 3: Size of stability regions S_β for $\beta = \alpha, 75^\circ, 60^\circ, 45^\circ, 30^\circ, 15^\circ$ (left panel) and $|x_{max}|$ on the negative real axis (right panel) for IMEX-PEER(s), IMEX-BDF(s), and IMEX-DIMSIM(s) methods, $s = 2, 3, 4$.

5 Numerical Experiments

5.1 Linear Advection-Reaction Problem

A first PDE problem for accuracy test is a linear advection-reaction system from [8]. The equations are

$$\partial_t u + \alpha_1 \partial_x u = -k_1 u + k_2 v + s_1, \quad (48)$$

$$\partial_t v + \alpha_2 \partial_x v = k_1 u - k_2 v + s_2 \quad (49)$$

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

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

and with the following initial and boundary conditions:

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

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 [8] 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. Accurate initial values are computed by the variable step-size code ODE15S with high tolerances. We have used step sizes $\Delta t = 10^{-3}, 5 \cdot 10^{-4}, 2.5 \cdot 10^{-4}, 10^{-4}$ and compared the numerical values at the final time $T = 1$ with an accurate reference solution in the l_2 -vector norm as in [2]. The results are plotted in Figure 4.

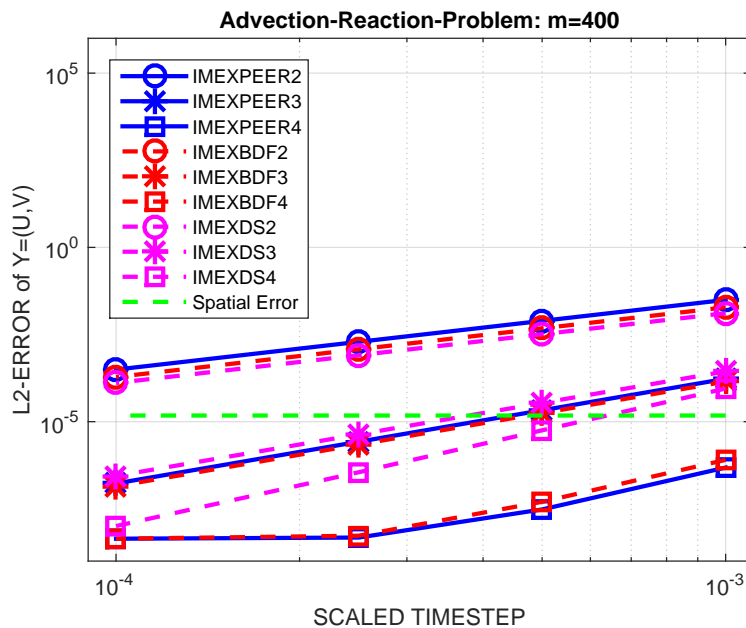


Figure 4: Advection-Reaction-Problem: Temporal l_2 -errors at $T = 1$ of the total concentration vs. scaled step sizes, $m = 400$. Comparison of IMEX-Peer, IMEX-BDF and IMEX-DIMSIM methods.

All second-order and third-order methods show their classical orders and perform nearly identical for this problem. For the IMEX-DIMSIM4 method we observe order four, but the larger error constant compared to the IMEX-Peer4 and IMEX-BDF4 scheme is apparent. The similar asymptotic behavior for the latter shows an order reduction, which was also observed in [8] as an inherent issue for very high-accuracy computations. However, this effect appears on a level far below the spatial discretization error.

5.2 Nonlinear Adsorption-Desorption Problem

The problem is taken from [8]. Let u and v be the dissolved and adsorbed concentration, respectively, satisfying the equations

$$\partial_t u + a \partial_x u = \kappa(v - \phi(u)), \quad (50)$$

$$\partial_t v = -\kappa(v - \phi(u)) \quad (51)$$

for $0 < x < 1$ and $0 < t \leq T$, with $\phi(u) = k_1 u / (1 + k_2 u)$. The initial values are set to zero, $u_0 = v_0 = 0$, and an oscillatory inflow condition is taken to get some smooth variations in the solution, along with the shocks:

$$\begin{aligned} u(0, t) &= 1 - \cos^2(6\pi t) && \text{if } a > 0, \\ u(1, t) &= 0 && \text{if } a < 0. \end{aligned}$$

The parameters are $\kappa = 10^6$, $k_1 = 50$, $k_2 = 100$, $T = 1.25$, and the velocity is set to

$$a = -\frac{3}{\pi} \arctan(100(t - 1)),$$

giving approximately $a = 1.5$ for $t < 1$ (adsorption phase) and $a = -1.5$ for $t > 1$ (desorption phase).

We use the WENO5 scheme for the spatial discretization from Shu ([14], formulas (2.58) – (2.63) with parameter $\varepsilon = 10^{-12}$) on a uniform (cell centered) grid, $x_i = (i - \frac{1}{2})\Delta x$, $i = 1, \dots, m$, with mesh width $\Delta x = 1/m$. This WENO5 spatial scheme provides high accuracy in smooth regions together with good monotonicity properties near shocks. We set $m = 800$ and note that in this case the spatial error is $1.2 \cdot 10^{-3}$.

In the IMEX methods, the advection term is treated explicitly and the stiff relaxation term implicitly, where a Newton method is efficiently performed at each spatial node separately. As in [8] the starting values for the methods are taken as $w_0 = 0$. We have used step sizes $\Delta t = 2^{-j} \Delta x$, $j = 1, \dots, 5$, and compared the numerical values of the total concentration, $u + v$, at the final time $t = T$ with an accurate reference solution in the discrete l_1 -norm ($\|v\|_1 = h \sum_i |v_i|$), see Figure 5.

As before, the results for the IMEX schemes with $s = 2, 3$, largely coincide. We note that the IMEX-BDF2 and IMEX-DIMSIM3 method did not converge for the largest time step. We clearly observe stability problems for IMEX-DIMSIM4, which can be explained by the relatively small stability region of the underlying explicit methods. The method needs small time steps to prevent instabilities, and even then the error behavior favors the other fourth-order methods. IMEX-Peer4 and IMEX-BDF4 gave nearly identical results with an increasing order reduction which was already visible in the first test problem. In view of the spatial error, temporal errors below 10^{-4} are of less importance for the total PDE error, however.

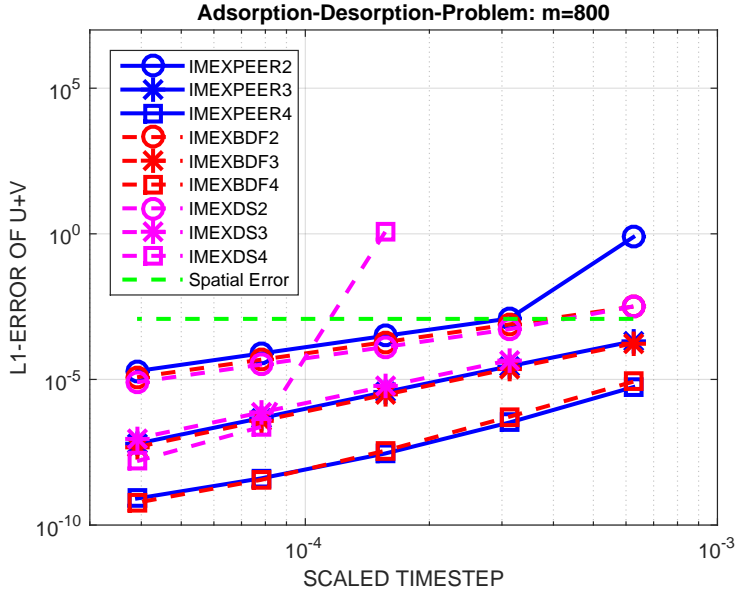


Figure 5: Adsorption-Desorption-Problem: Temporal discrete l_1 -errors of the total concentration vs. scaled step sizes, $m = 800$. Comparison of IMEX-Peer, IMEX-BDF and IMEX-DIMSIM methods.

5.3 The Schnakenberg Problem

A classical example of a two-dimensional reaction-diffusion equations for testing numerical algorithms is the Schnakenberg system [13, 9]. The equations read

$$\partial_t u = D_1 \nabla^2 u + \kappa(a - u + u^2 v), \quad (52)$$

$$\partial_t v = D_2 \nabla^2 v + \kappa(b - u^2 v), \quad (53)$$

where u and v denote the concentration of activator and inhibitor, respectively. We follow the setup in [9] and take $D_1 = 0.05$, $D_2 = 1$, $\kappa = 100$, $a = 0.1305$, $b = 0.7695$, $T = 1$. The solution is computed on the unit square domain $\Omega = (0, 1)^2$ with the initial conditions

$$u(x, y, 0) = a + b + 10^{-3} \exp\left(-100 * \left(\left(x - \frac{1}{3}\right)^2 + \left(y - \frac{1}{2}\right)^2\right)\right),$$

$$v(x, y, 0) = \frac{b}{(a + b)^2}.$$

and homogeneous Neumann boundary conditions.

For the spatial discretization, we apply second-order finite differences on a uniform (cell centered) grid, $(x_i = (i - \frac{1}{2})h, y_j = (j - \frac{1}{2})h)$, $i, j = 1, \dots, m$, with mesh width $h = 1/m$, where $m = 400$ has been taken.

Here, we treat the reaction explicitly and the diffusion implicitly. Accurate initial values are computed by the variable step-size code ODE15S with high tolerances. We have used step sizes $\Delta t = 2^{3-j}/m, j = 1, \dots, 5$, and compared the numerical values at the final time $t = T$ with an accurate reference solution in the discrete l_2 -norm, ($\|v\|_2 = \sqrt{h \sum_i |v_i|^2}$), see Figure 6.

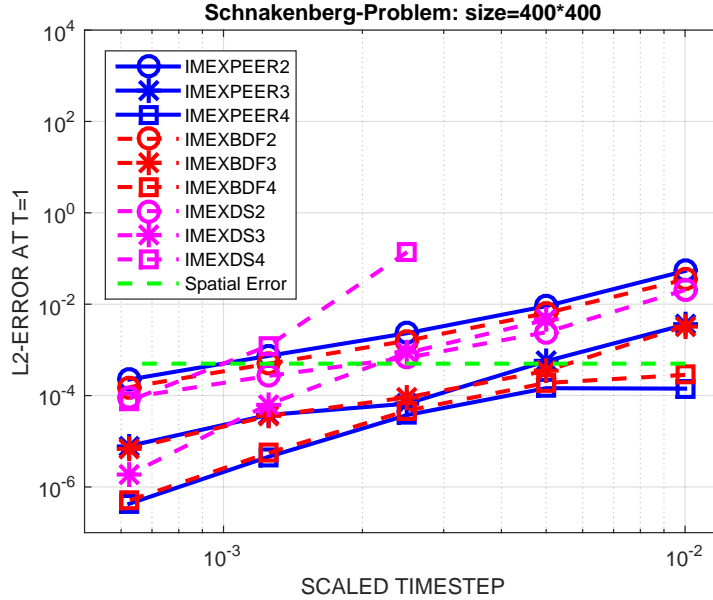


Figure 6: Schnakenberg-Problem: Temporal discrete l_2 -errors at $T = 1$ vs. scaled step sizes, $m = 400$. Comparison of IMEX-Peer, IMEX-BDF and IMEX-DIMSIM methods.

The second-order IMEX methods perform well and show their classical order. IMEX-DIMSIM2 produced the best results due to a smaller error constant. The higher order IMEX-DIMSIM schemes failed for larger time steps, whereas IMEX-DIMSIM4 gave again unsatisfactory results at all. A further time, Peer and BDF methods delivered nearly identical numerical solutions. Both showed a somehow unpredictable behavior for larger time steps, but in this case they are still more efficient than the DIMSIM schemes.

6 Conclusion

We have developed a new family of s -stage implicit-explicit Peer methods, starting with $L(\alpha)$ -stable implicit Peer methods with order $p = s$ and applying an extrapolation of the same order to preserve the order of convergence. The well-known IMEX-BDF(s) methods applied with constant step size $\Delta t/s$ fit into this frame-

work when they are considered as s -stage Peer methods with equidistant nodes and step size Δt . We gave the corresponding formula to convert. We examined the linear stability properties of these IMEX methods to construct new IMEX-Peer methods of order $p = 2, 3, 4$, with optimally balanced size of stability regions and error constants for the underlying extrapolation. A detailed comparison with the recently proposed IMEX-DIMSIM methods [2] showed a significant improvement of the stability properties and a better performance of the higher-order methods for three numerical test problems.

We are planning to extend this work to a variable step size environment and to include other classes of implicit Peer methods, e.g., those with strictly diagonal matrix R to allow an efficient parallelisation. We will also consider linearly implicit Peer methods of higher order $p \geq 4$ as developed in [10] and successfully applied in [5] to large scale PDE problems within an adaptive Rothe approach. There are $L(\alpha)$ -stable methods of this type with reasonable large angles α and small error constants available up to order $p = 8$, which give them a clear advantage over higher order BDF methods.

7 Acknowledgement

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