Transformed implicit-explicit DIMSIMs with strong stability preserving explicit part

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Abstract. For many systems of differential equations modeling problems in science and engineering, there are often natural splittings of the right hand side into two parts, one of which is non-stiff or mildly stiff, and the other part is stiff. Such systems can be efficiently treated by a class of implicit-explicit (IMEX) diagonally implicit multistage integration methods (DIMSIMs), where the stiff part is integrated by an implicit formula, and the non-stiff part is integrated by an explicit formula. We will construct methods where the explicit part has strong stability preserving (SSP) property, and the implicit part of the method is A-, or L-stable. We will also investigate stability of these methods when the implicit and explicit parts interact with each other. To be more precise, we will monitor the size of the region of absolute stability of the IMEX scheme, assuming that the implicit part of the method is A-, or L-stable. Finally we furnish examples of SSP IMEX DIMSIMs up to the order four with good stability properties.

Key words. IMEX methods, SSP property, general linear methods, DIMSIMs, stability analysis, construction of highly stable methods

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1 Introduction

Many practical problems in science and engineering are modeled by large systems of ordinary differential equations (ODEs) which arise from discretization in space of partial differential equations (PDEs) by finite difference methods, finite elements or finite volume methods, or pseudospectral methods. For such systems there are often natural splittings of the right hand sides of the differential systems into two parts, one of which is non-stiff or mildly stiff, and suitable for explicit time integration, and the other part is stiff, and suitable for implicit time integration. Such systems can be written in the form

$$\begin{aligned} &y'(t) = f\big(y(t)\big) + g\big(y(t)\big), \quad t \in [t_0, T], \\ &y(t_0) = y_0 \in \mathbb{R}^m, \end{aligned} \tag{1.1}$$

$f : \mathbb{R}^m \to \mathbb{R}^m$, $g : \mathbb{R}^m \to \mathbb{R}^m$, where $f(y)$ represents the non-stiff processes, for example advection, and $g(y)$ represents stiff processes, for example diffusion or chemical reaction, in semidiscretization of advection-diffusion-reaction equations [14].

In this paper we will analyze methods, where the non-stiff part $f(y)$ is treated by the explicit general linear method (GLM) and the stiff part $g(y)$ by the implicit GLM, with the same abscissa vector $\mathbf{c} = [c_1, \ldots, c_s]^T \in \mathbb{R}^s$, and the coefficients

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right] \in \mathbb{R}^{(s+r)\times(s+r)}, \quad \left[\begin{array}{c|c} \mathbf{A}^* & \mathbf{U} \\ \hline \mathbf{B}^* & \mathbf{V} \end{array}\right] \in \mathbb{R}^{(s+r)\times(s+r)},$$

We assume that both methods have the same coefficients matrices $\mathbf{U}$ and $\mathbf{V}$, and that $\mathbf{A}$ is strictly lower triangular, and $\mathbf{A}^*$ is lower triangular with the same element $\lambda > 0$ on the diagonal. Denote the components of $\mathbf{A}$, $\mathbf{A}^*$, $\mathbf{U}$, $\mathbf{B}$, $\mathbf{B}^*$, and $\mathbf{V}$ by a_{ij}, a^*_{ij}, u_{ij}, b_{ij}, b^*_{ij}, and v_{ij}. Then on the uniform grid $t_n = t_0 + nh$, $n = 0, 1, \ldots, N$, $Nh = T - t_0$, the IMEX GLMs are defined by

$$\begin{aligned} Y_i^{[n+1]} &= h\sum_{j=1}^{i-1} a_{ij} f\big(Y_j^{[n+1]}\big) + h\sum_{j=1}^{i} a^*_{ij} g\big(Y_j^{[n+1]}\big) + \sum_{j=1}^{r} u_{ij} y_j^{[n]}, \ i = 1, 2, \ldots, s, \\ y_i^{[n+1]} &= h\sum_{j=1}^{s} \Big(b_{ij} f\big(Y_j^{[n+1]}\big) + b^*_{ij} g\big(Y_j^{[n+1]}\big)\Big) + \sum_{j=1}^{r} v_{ij} y_j^{[n]}, \quad i = 1, 2, \ldots, r, \end{aligned} \tag{1.2}$$

$n = 0, 1, \ldots, N-1$. Here, $Y_i^{[n+1]}$ are approximations of stage order q to $y(t_n + c_i h)$, i.e.,

$$Y_i^{[n+1]} = y(t_n + c_i h) + O(h^{q+1}), \quad i = 1, 2, \ldots, s, \tag{1.3}$$

and $y_i^{[n]}$ are approximations of order p to the linear combinations of the derivatives of the solution y at the point t_n, i.e.,

$$y_i^{[n]} = \sum_{k=0}^{p} q_{ik} h^k y^{(k)}(t_n) + O(h^{p+1}), \quad i = 1, 2, \ldots, r, \tag{1.4}$$

where y is the solution to (1.1). These IMEX methods were introduced in [28] and further investigated in [8].

Putting

$$y^{[n+1]} = \begin{bmatrix} y_1^{[n+1]} \\ \vdots \\ y_r^{[n+1]} \end{bmatrix}, \quad y^{[n]} = \begin{bmatrix} y_1^{[n]} \\ \vdots \\ y_r^{[n]} \end{bmatrix}, \quad Y^{[n+1]} = \begin{bmatrix} Y_1^{[n+1]} \\ \vdots \\ Y_s^{[n+1]} \end{bmatrix},$$

$$f\big(Y^{[n+1]}\big) = \begin{bmatrix} f\big(Y_1^{[n+1]}\big) \\ \vdots \\ f\big(Y_s^{[n+1]}\big) \end{bmatrix}, \quad g\big(Y^{[n+1]}\big) = \begin{bmatrix} g\big(Y_1^{[n+1]}\big) \\ \vdots \\ g\big(Y_s^{[n+1]}\big) \end{bmatrix},$$

the method (1.2) can be written in a more compact form

$$\begin{aligned} Y^{[n+1]} &= h(\mathbf{A} \otimes \mathbf{I}) f\big(Y^{[n+1]}\big) + h(\mathbf{A}^* \otimes \mathbf{I}) g\big(Y^{[n+1]}\big) + (\mathbf{U} \otimes \mathbf{I}) y^{[n]}, \\ y^{[n+1]} &= h(\mathbf{B} \otimes \mathbf{I}) f\big(Y^{[n+1]}\big) + h(\mathbf{B}^* \otimes \mathbf{I}) g\big(Y^{[n+1]}\big) + (\mathbf{V} \otimes \mathbf{I}) y^{[n]}, \end{aligned} \tag{1.5}$$

$n = 0, 1, \ldots, N-1$, $\mathbf{I} \in \mathbb{R}^m$, and the relation (1.4) takes the form

$$y^{[n]} = \sum_{k=0}^{p} \mathbf{q}_k h^k y^{(k)}(t_n) + O(h^{p+1}), \tag{1.6}$$

with the vectors $\mathbf{q}_0, \mathbf{q}_1, \ldots, \mathbf{q}_s$ given by

$$\mathbf{q}_0 = \begin{bmatrix} q_{1,0} \\ \vdots \\ q_{r,0} \end{bmatrix}, \quad \mathbf{q}_1 = \begin{bmatrix} q_{1,1} \\ \vdots \\ q_{r,1} \end{bmatrix}, \quad \ldots, \quad \mathbf{q}_p = \begin{bmatrix} q_{1,p} \\ \vdots \\ q_{r,p} \end{bmatrix}.$$

In this paper we will investigate the class of IMEX diagonally implicit multistage integration methods (DIMSIMs). These are schemes with $p = q = r = s$, where the coefficient matrix $\mathbf{U} = \mathbf{I}$, and $\mathbf{V}$ is a rank one matrix of the form $\mathbf{V} = \mathbf{e}\mathbf{v}^T$, $\mathbf{e} = [1, \ldots, 1]^T \in \mathbb{R}^s$, $\mathbf{v} = [v_1, \ldots, v_s]^T \in \mathbb{R}^s$, with $\mathbf{v}^T\mathbf{e} = 1$. It was proved in [3] (see also [18]) that for given $\mathbf{A}$, $\mathbf{A}^*$, and $\mathbf{V}$ the explicit method and the implicit method has order p and stage order $q = p$ if the coefficients matrices $\mathbf{B}$ and $\mathbf{B}^*$ are computed from the formulas

$$\mathbf{B} = \mathbf{B}_0 - \mathbf{A}\mathbf{B}_1 - \mathbf{V}\mathbf{B}_2 + \mathbf{V}\mathbf{A}, \quad \mathbf{B}^* = \mathbf{B}_0 - \mathbf{A}^*\mathbf{B}_1 - \mathbf{V}\mathbf{B}_2 + \mathbf{V}\mathbf{A}^*, \tag{1.7}$$

where $\mathbf{B}_0$, $\mathbf{B}_1$, and $\mathbf{B}_2$, are $s \times s$ matrices defined by

$$\mathbf{B}_0 = \left[\frac{\int_0^{1+c_i} \phi_j(x)dx}{\phi_j(c_j)}\right], \quad \mathbf{B}_1 = \left[\frac{\phi_j(1+c_i)}{\phi_j(c_j)}\right], \quad \mathbf{B}_2 = \left[\frac{\int_0^{c_i} \phi_j(x)dx}{\phi_j(c_j)}\right],$$

$i, j = 1, 2, \ldots, s$, and $\phi_i(x)$ are defined by

$$\phi_i(x) = \prod_{j=1, j\neq i}^{s} (x - c_j), \quad i = 1, 2, \ldots, s.$$

It was also proved in [28] that if the explicit and implicit methods have order p and stage order $q = p$, then the same is true for the resulting IMEX scheme defined by (1.5).

The methods investigated in this paper are also applicable to the hyperbolic systems with relaxation considered, for example, in [19, 21], and they compare favorably with IMEX Runge-Kutta (RK) methods for these problems. In the stiff limit the IMEX RK schemes, considered for example in [21] converge, but their order drops to $p = 1$, while all IMEX DIMSIMs constructed in this paper achieve the expected order of convergence, and no order reduction occurs. This is confirmed in Section 5 by numerical experiments on the shallow water equation.

The organization of the remainder of the paper is as follows. In Section 2 we will review various stability concepts of explicit, implicit, and IMEX schemes. In particular, we will recall the definition of strong stability preserving (SSP) property of explicit methods, absolute stability, and definitions of regions of absolute stability, of explicit, implicit, and the resulting IMEX methods. In Section 3 we define transformed IMEX methods. In Section 4 we describe the construction of SSP transformed IMEX schemes of order $p = 1$, 2, 3, and 4. In Section 5 the results of some numerical experiments are presented.

2 Stability analysis of IMEX DIMSIMs

2.1 SSP property of the explicit part

We recall first the concept of SSP property of explicit methods following the presentation in [10]. To define this property we assume that the discretization of the problem (1.1) with $g \equiv 0$, by the forward Euler method

$$y_{n+1} = y_n + hf(y_n), \quad n = 0, 1, \ldots, N-1,$$

satisfies the inequality

$$\|y_{n+1}\| \leq \|y_n\|, \quad n = 0, 1, \ldots, N-1, \tag{2.1}$$

in some norm or semi-norm $\| \cdot \|$, if the time step h is restricted by the condition

$$h \leq h_{FE}. \tag{2.2}$$

It is then of interest to construct higher order numerical methods for (1.1) with $g \equiv 0$, which preserve the property (2.1) under the time step restrictions

$$h \leq \mathcal{C} \cdot h_{FE}, \tag{2.3}$$

where $\mathcal{C} \geq 0$ is some constant. Numerical schemes for (1.1) with $g \equiv 0$, which preserve the property (2.1) under the condition (2.3) are called SSP methods, and the maximal constant $\mathcal{C}$ in (2.3) is called SSP coefficient. To compare numerical methods with different number of stages s we also define, following [9, 10, 20], the effective SSP coefficient $\mathcal{C}_{eff}$ by the relation $\mathcal{C}_{eff} = \mathcal{C}/s$.

The characterization of SSP coefficient for GLMs was discovered by Spijker [26]. To describe this characterization for GLMs defined by the abscissa vector $\mathbf{c}$ and coefficient matrices $\mathbf{A}$, $\mathbf{U}$, $\mathbf{B}$, and $\mathbf{V}$, consider the relations

$$\begin{array}{ll} (\mathbf{I} + \gamma\mathbf{A})^{-1}\mathbf{U} \geq 0, & \mathbf{I} - (\mathbf{I} + \gamma\mathbf{A})^{-1} \geq 0, \\ \mathbf{V} - \gamma\mathbf{B}(\mathbf{I} + \gamma\mathbf{A})^{-1}\mathbf{U} \geq 0, & \gamma\mathbf{B}(\mathbf{I} + \gamma\mathbf{A})^{-1} \geq 0, \end{array} \tag{2.4}$$

where $\gamma \geq 0$ is a constant, and where these inequalities should be interpreted componentwise. Then it was demonstrated by Izzo and Jackiewicz [16], using the results by Spijker [26], that the SSP coefficient is given by

$$\mathcal{C} = \mathcal{C}(\mathbf{c}, \mathbf{A}, \mathbf{U}, \mathbf{B}, \mathbf{V}) = \sup\Big\{\gamma \in \mathbb{R} : \ \gamma \text{ satisfies } (2.4)\Big\}. \tag{2.5}$$

It follows from this relation that SSP coefficient $\mathcal{C}$ can be computed by solving the minimization problem

$$F(\gamma) := -\gamma \longrightarrow \min, \tag{2.6}$$

with a very simple objective function $F(\gamma) = -\gamma$, subject to the nonlinear constrains (2.4). This process will be illustrated in Section 4.

2.2 Absolute stability of the implicit part

DIMSIMs investigated in the literature have so-called RK stability property, i.e., their stability function $p^*(w,z)$ assumes the form

$$p^*(w,z) = w^{s-1}(w - R(z)),$$

where $R(z)$ is an approximation of order p to the exponential function $\exp(z)$. However, this stability requirement is quite restrictive and does not, in general, permit the construction of IMEX schemes with A- or L-stable implicit part and SSP explicit part, and, for this reason, we do not enforce RK stability of implicit methods in this paper. But we will still refer to the resulting implicit formulas as DIMSIMs.

In order to construct methods with A- or L-stable implicit part, we will apply the the well known Schur criterion ([24]) in combination with the maximum principle. Let us recall that the polynomial

$$\phi_k(w) = c_k w^k + c_{k-1} w^{k-1} + \cdots + c_1 w + c_0$$

where c_i are complex coefficients, with $c_k \neq 0$ and $c_0 \neq 0$, is said to be a Schur polynomial if all of its roots w_i, $i = 1, 2, \ldots, k$, are inside of the unit circle, that is $|w_i| < 1$, for all $i = 1, 2, \ldots, k$. Define the following two polynomials

$$\widehat{\phi}_k(w) = \overline{c}_0 w^k + \overline{c}_1 w^{k-1} + \cdots + \overline{c}_{k-1} w + \overline{c}_k,$$

and

$$\phi_{k-1}(w) = \frac{1}{w}\left(\widehat{\phi}(0)\phi(w) - \phi(0)\widehat{\phi}(w)\right),$$

where $\overline{c}_i$ represents the complex conjugate of the coefficient c_i, $i = 0, 1, \ldots, k$, and let us remark that the polynomial $\phi_{k-1}(w)$ has degree at most $k - 1$. The Schur recursive criterion is based on the following result.

Theorem 2.1 *(J. Schur [24]) The polynomial $\phi_k(w)$ is a Schur polynomial if and only if*

$$\big|\widehat{\phi}_k(0)\big| > \big|\phi_k(0)\big|,$$

and $\phi_{k-1}(w)$ is a Schur polynomial.

To analyze stability properties of implicit methods it is convenient to multiply stability function of these methods by the polynomial factor $(1-\lambda z)^s$. The resulting stability polynomial $p^*(w,z)$ takes then the form

$$p^*(w,z) = (1-\lambda z)^s w^s - p_1(z)w^{s-1} + p_2(z)w^{s-2} + \cdots + (-1)^s p_s(z), \quad (2.7)$$

where $p_1(z), p_2(z), \ldots, p_s(z)$ are polynomials of degree less than or equal to s. To construct implicit formulas whose stability polynomial (2.7) is a Schur polynomial in the left half of the complex plane, we will force all the roots $w_j = w_j(z)$, $j = 1,2,\ldots,r$, of $p^*(w,z)$ to have no poles for $Re(z) \le 0$. Since these roots are analytic functions of z for $Re(z) \le 0$, they fall inside the unit circle for $Re(z) \le 0$ if and only if they are inside the unit circle for the values of z on the imaginary axis. In other words, by the maximum principle (compare [4]), it follows that $|w_j(z)| < 1$, $j = 1,2,\ldots,r$, for all $z \in \mathbb{C}$ with $Re(z) \le 0$, if and only if $|w_j(iy)| < 1$, $j = 1,2,\ldots,r$, for all $y \in \mathbb{R}$.

For methods with number of stages $s = r$, the stability polynomial $p^*(w,z)$ has degree r and the conditions given by the recursive Schur criterion are the following

$$\big|\widehat{\phi}_r(0)\big| - \big|\phi_r(0)\big| > 0, \quad \big|\widehat{\phi}_{r-1}(0)\big| - \big|\phi_{r-1}(0)\big| > 0, \quad \ldots, \quad \big|\widehat{\phi}_1(0)\big| - \big|\phi_1(0)\big| > 0.$$

Let us define the quantities

$$a_k := \big|\widehat{\phi}_{r-k}(0)\big| - \big|\phi_{r-k}(0)\big|, \quad k = 0,1,\ldots,r-1.$$

Each a_k depends on z, and when it is evaluated at $z = iy$, $y \in \mathbb{R}$, it results to be a polynomial in the unknown y with real coefficients, of the form

$$a_k(iy) = \sum_{j=0}^{r2^k} m_{kj} y^{2j}, \quad k = 0,1,\ldots,r-1,$$

with $m_{kj} \in \mathbb{R}$ for all $k = 0,1,\ldots,r-1$ and $j = 1,2,\ldots,r2^k$. Thus, a sufficient condition to ensure the A-stability of the corresponding method is to force

$$m_{kj} \ge 0, \quad k = 1,2,\ldots,r, \quad j = 1,2,\ldots,r2^k, \quad (2.8)$$

where for each k at least one m_{kj}, $j = 0, 1, \dots, r2^k$, has to be strictly positive.

To construct methods which are L-stable we have to enforce the condition that the polynomials $p_1(z), p_2(z), \dots, p_s(z)$ appearing in (2.7) have degrees strictly less than s.

2.3 Absolute stability of the IMEX method

We will discuss next absolute stability. To analyze absolute stability properties of IMEX GLMs (1.5) we will use the test equation

$$y'(t) = \lambda_0 y(t) + \lambda_1 y(t), \quad t \geq 0, \tag{2.9}$$

where λ_0 and λ_1 are complex parameters. Here, $\lambda_0 y(t)$ corresponds to the non-stiff part and $\lambda_1 y(t)$ to the stiff part of the system (1.1). Applying (1.5) to (2.9) and putting $z_0 = h\lambda_0$, $z_1 = h\lambda_1$, we obtain

$$\begin{aligned} Y^{[n+1]} &= (z_0\mathbf{A} + z_1\mathbf{A}^*)Y^{[n+1]} + \mathbf{U}y^{[n]}, \\ y^{[n+1]} &= (z_0\mathbf{B} + z_1\mathbf{B}^*)Y^{n+1]} + \mathbf{V}y^{[n]}, \end{aligned}$$

$n = 0, 1, \dots$. Assuming that the matrix $\mathbf{I} - z_0\mathbf{A} - z_1\mathbf{A}^*$ is nonsingular, this is equivalent to the vector recurrence relation

$$y^{[n+1]} = \mathbf{M}(z_0, z_1)y^{[n]}, \tag{2.10}$$

$n = 0, 1, \dots$, with the stability matrix $\mathbf{M}(z_0, z_1)$ defined by

$$\mathbf{M}(z_0, z_1) = \mathbf{V} + (z_0\mathbf{B} + z_1\mathbf{B}^*)(\mathbf{I} - z_0\mathbf{A} - z_1\mathbf{A}^*)^{-1}\mathbf{U}. \tag{2.11}$$

We also define the stability function $p(w, z_0, z_1)$ of the IMEX scheme (1.5) as the stability polynomial of $\mathbf{M}(z_0, z_1)$, i.e.,

$$p(w, z_0, z_1) = \det\big(w\mathbf{I} - \mathbf{M}(z_0, z_1)\big). \tag{2.12}$$

To investigate stability properties of (1.5) is is usually more convenient to work with the polynomial $(1 - \lambda z_1)^s p(w, z_0, z_1)$, where λ is the diagonal element of the coefficient matrix $\mathbf{A}^*$. This polynomial will be denoted by the same symbol $p(w, z_0, z_1)$.

We say that the IMEX GLM (1.5) is stable for given $z_0, z_1 \in \mathbb{C}$ if all the roots $w_i(z_0, z_1)$, $i = 1, 2, \dots, r$, of the stability function $p(w, z_0, z_1)$ are inside of the unit circle. In this paper we will be mainly interested in IMEX schemes which are A-stable with respect to the implicit part $z_1 \in \mathbb{C}$. To investigate such methods we consider, similarly as in [7, 14, 28], the sets

$$\mathcal{S}_\alpha = \Big\{ z_0 \in \mathbb{C}: \text{ the IMEX GLM is stable for any } z_1 \in \mathcal{A}_\alpha \Big\},$$

where the set $\mathcal{A}_\alpha \subset \mathbb{C}$ is defined by

$$\mathcal{A}_\alpha = \Big\{ z \in \mathbb{C}: \ \mathrm{Re}(z) < 0 \quad \text{and} \quad |\mathrm{Im}(z)| \leq \tan(\alpha)|\mathrm{Re}(z)| \Big\}.$$

It follows from the maximum principle that $\mathcal{S}_\alpha$ has a simple representation given by

$$\mathcal{S}_\alpha = \left\{ \begin{array}{rl} z_0 \in \mathbb{C}: & \text{the IMEX GLM is stable for any} \\ & z_1 = -|y|/\tan(\alpha) + iy, \ y \in \mathbb{R} \end{array} \right\}. \tag{2.13}$$

For fixed values of $y \in \mathbb{R}$ we define also the sets

$$\mathcal{S}_{\alpha,y} = \left\{ \begin{array}{rl} z_0 \in \mathbb{C}: & \text{the IMEX GLM is stable for fixed} \\ & z_1 = -|y|/\tan(\alpha) + iy \end{array} \right\}. \tag{2.14}$$

Observe that

$$\mathcal{S}_\alpha = \bigcap_{y \in \mathbb{R}} \mathcal{S}_{\alpha,y}. \tag{2.15}$$

Observe also that the region $\mathcal{S}_{\alpha,0}$ is independent of α, and corresponds to the region of absolute stability of the explicit method with coefficients $\mathbf{c}$, $\mathbf{A}$, $\mathbf{U}$, $\mathbf{B}$, and $\mathbf{V}$. This region will be denoted by $\mathcal{S}_E$. We have

$$\mathcal{S}_\alpha \subset \mathcal{S}_E, \tag{2.16}$$

and we will look for IMEX DIMSIMs for which the stability region $\mathcal{S}_\alpha$ contains a large part of the stability region $\mathcal{S}_E$ of the explicit method.

All these regions $\mathcal{S}_E$, $\mathcal{S}_{\alpha,y}$, and $\mathcal{S}_\alpha$, for fixed $y \in \mathbb{R}$ and $\alpha \in (0, \pi/2]$, can be determined by the algorithms developed in a recent paper [7]. These algorithms are based on some variants of boundary locus method to compute the boundaries $\partial\mathcal{S}_E$, $\partial\mathcal{S}_{\alpha,y}$, and $\partial\mathcal{S}_\alpha$, of the regions $\mathcal{S}_E$, $\mathcal{S}_{\alpha,y}$, and $\mathcal{S}_\alpha$. We refer to the paper [7] for a detailed description of these algorithms. The areas of $\mathcal{S}_E$ and $\mathcal{S}_\alpha$ can be computed by numerical integration in polar coordinates. We refer again to [7] for a detailed description of this process.

3 Transformed IMEX DIMSIMs

Similarly as in [6, 17], to increase our chances of finding SSP explicit GLMs with large SSP coefficients $\mathcal{C}$ we consider a very general class of transformed IMEX methods. These schemes are defined by multiplying the relation for $y^{[n+1]}$ in (1.5) by $\mathbf{T}\otimes\mathbf{I}$, where $\mathbf{T}\in\mathbb{R}^{r\times r}$, and $\det(\mathbf{T})\neq 0$. This leads to

$$\begin{aligned}
Y^{[n+1]} &= h(\mathbf{A}\otimes\mathbf{I})f\big(Y^{[n+1]}\big) + h(\mathbf{A}^*\otimes\mathbf{I})g\big(Y^{[n+1]}\big)\\
&\quad + (\mathbf{U}\otimes\mathbf{I})(\mathbf{T}^{-1}\otimes\mathbf{I})(\mathbf{T}\otimes\mathbf{I})y^{[n]},\\
(\mathbf{T}\otimes\mathbf{I})y^{[n+1]} &= h(\mathbf{T}\otimes\mathbf{I})(\mathbf{B}\otimes\mathbf{I})f\big(Y^{[n+1]}\big) + h(\mathbf{T}\otimes\mathbf{I})(\mathbf{B}^*\otimes\mathbf{I})g\big(Y^{[n+1]}\big)\\
&\quad + (\mathbf{T}\otimes\mathbf{I})(\mathbf{V}\otimes\mathbf{I})(\mathbf{T}^{-1}\otimes\mathbf{I})(\mathbf{T}\otimes\mathbf{I})y^{[n]},
\end{aligned} \tag{3.1}$$

$n=0,1,\ldots,N-1$. Putting

$$\overline{y}^{[n+1]} = (\mathbf{T}\otimes\mathbf{I})y^{[n+1]}, \quad \overline{y}^{[n]} = (\mathbf{T}\otimes\mathbf{I})y^{[n]},$$

the equation (3.10 can be written in the form

$$\begin{aligned}
Y^{[n+1]} &= h(\overline{\mathbf{A}}\otimes\mathbf{I})f(Y^{[n+1]}) + h(\overline{\mathbf{A}^*}\otimes\mathbf{I})g(Y^{[n+1]}) + (\overline{\mathbf{U}}\otimes\mathbf{I})\overline{y}^{[n]},\\
\overline{y}^{[n+1]} &= h(\overline{\mathbf{B}}\otimes\mathbf{I})f(Y^{[n+1]}) + h(\overline{\mathbf{B}^*}\otimes\mathbf{I})g(Y^{[n+1]}) + (\overline{\mathbf{V}}\otimes\mathbf{I})\overline{y}^{[n]},
\end{aligned} \tag{3.2}$$

where the transformed coefficient matrices $\overline{\mathbf{A}}$, $\overline{\mathbf{A}^*}$, $\overline{\mathbf{U}}$, $\overline{\mathbf{B}}$, $\overline{\mathbf{B}^*}$, and $\overline{\mathbf{V}}$, are defined by

$$\begin{aligned}
\overline{\mathbf{A}} = \mathbf{A}, \quad \overline{\mathbf{A}^*} = \mathbf{A}^*, \quad \overline{\mathbf{U}} = \mathbf{U}\mathbf{T}^{-1},\\
\overline{\mathbf{B}} = \mathbf{T}\mathbf{B}, \quad \overline{\mathbf{B}^*} = \mathbf{T}\mathbf{B}^*, \quad \overline{\mathbf{V}} = \mathbf{T}\mathbf{V}\mathbf{T}^{-1}.
\end{aligned} \tag{3.3}$$

It was demonstrated in [6] that transformed explicit and implicit methods preserve the order p and stage order $q=p$ of the original schemes. As a result, it follows from [28], that the transformed IMEX method (3.2) preserve the order p and stage order $q=p$ of the original IMEX method (1.5).

Transformed IMEX GLMs (3.2) preserve also absolute stability properties of the original IMEX schemes (1.5). This follows from

$$\begin{aligned}
\overline{\mathbf{M}}(z_0,z_1) &= \overline{\mathbf{V}} + (z_0\overline{\mathbf{B}} + z_1\overline{\mathbf{B}^*})(\mathbf{I} - z_0\overline{\mathbf{A}} + z_1\overline{\mathbf{A}^*})^{-1}\overline{\mathbf{U}}\\
&= \mathbf{T}\mathbf{V}\mathbf{T}^{-1} + (z_0\mathbf{T}\mathbf{B} + z_1\mathbf{T}\mathbf{B}^*)(\mathbf{I} - z_0\mathbf{A} + z_1\mathbf{A}^*)^{-1}\mathbf{U}\mathbf{T}^{-1}\\
&= \mathbf{T}\big(\mathbf{V} + (z_0\mathbf{B} + z_1\mathbf{B}^*)(\mathbf{I} - z_0\mathbf{A} + z_1\mathbf{A}^*)^{-1}\mathbf{U}\big)\mathbf{T}^{-1}\\
&= \mathbf{M}(z_0,z_1),
\end{aligned}$$

which shows that the stability matrix $\overline{\mathbf{M}}(z_0, z_1)$ of the transformed method is similar to the stability matrix $\mathbf{M}(z_0, z_1)$ of the original method. Hence, it follows that

$$\overline{p}(z_0, z_1) = \det\big(w\mathbf{I} - \overline{\mathbf{M}}(z_0, z_1)\big) = \det\big(w\mathbf{I} - \mathbf{M}(z_0, z_1)\big) = p(z_0, z_1),$$

and we can conclude that the transformed explicit, implicit, and IMEX methods have identical absolute stability properties as the original explicit, implicit, and the IMEX methods. However, SSP properties of the transformed explicit GLMs are, in general, different from SSP properties of the original explicit methods, and we will search for transformed explicit DIMSIMs with maximal SSP coefficients. In addition, we will monitor the size of the region of absolute stability $\mathcal{S}_\alpha$ for $\alpha \in (0, \pi/2)$, preferably for $\alpha = \pi/2$, of the IMEX schemes, assuming that the implicit part of the method is A-, or L-stable.

4 Construction of SSP transformed IMEX DIMSIMs

In this section we investigate transformed SSP IMEX DIMSIMs of order $p = 1, 2, 3$, and 4, with $q = r = s = p$. Our aim is to construct IMEX methods whose explicit part has large SSP coefficient, the implicit part is A- or L-stable, and the overall IMEX scheme has large region of absolute stability. These methods will be compared with transformed SSP DIMSIMs investigated recently in [17].

For many examples of DIMSIMs constructed in the literature on the subject, the abscissa vector $\mathbf{c}$ has components uniformly distributed in the interval $[0, 1]$, i.e.,

$$\mathbf{c} = \begin{bmatrix} 0 & \frac{1}{s-1} & \cdots & \frac{s-2}{s-1} & 1 \end{bmatrix}^T \in \mathbb{R}^s.$$

In our search for IMEX schemes with good stability properties we relax this condition and consider methods with abscissa vector $\mathbf{c}$ of the more general form with abscissas satisfying the condition

$$0 < c_1 < c_2 < \cdots < c_{s-1} < c_s = 1.$$

Then the last stage $Y_s^{[n]}$ of the method (1.5) approximates the solution y to (1.1) at the point t_n. This simplifies the implementation of these methods since no special finishing procedure is needed. This is discussed in more detail in [17]. However, these methods still need starting procedures to compute sufficiently accurate starting vector $y^{[0]}$. Starting procedures for GLMs are discussed in [5, 6, 16, 17] and for IMEX methods in [1].

The case $p = 1$ is not very interesting and it is not properly allowed for this class of methods because it is not possible to construct an IMEX DIMSIMs with $p = q = r = s = 1$ where the implicit and the explicit parts share the same abscissa vector. However, if this last condition is relaxed (that is the implicit and the explicit part are allowed to have different abscissa vectors), then the explicit part is the forward Euler method, while the implicit part is A-stable for $\lambda \geq 1/2$ and L-stable for $\lambda = 1$. This last choice corresponds to the backward Euler method. In this case, the stability function $R(z_0, z_1)$ is the product of the stability function of the explicit method and the stability function of the implicit one. For this reason, the stability region $\mathcal{S}_{\frac{\pi}{2}}$ is equal to the stability region $\mathcal{S}_E$ of the explicit method, which corresponds to the forward Euler method for any λ. The IMEX scheme corresponding to $\lambda = 1/2$ will be denoted by IMEX DIMSIM1A, and to $\lambda = 1$ by IMEX DIMSIM1L.

For order $p = 2$ and $p = 3$ we succeeded in obtaining methods with SSP explicit part and SSP coefficients close to that obtained in [17], and with A- or L-stable implicit part. Unfortunately, in some cases these IMEX methods have quite small stability region $\mathcal{S}_{\frac{\pi}{2}}$ with respect to the stability region $\mathcal{S}_E$ of the explicit part. However, larger $\mathcal{S}_{\frac{\pi}{2}}$ stability regions can be obtained if one is willing to accept smaller SSP coefficients.

We have searched for IMEX schemes with large SSP coefficients of the explicit part and A- or L-stability of the implicit part by solving the minimization problem (2.6) subject to the nonlinear constrains (2.4), and the constrains (2.8) required for A-stability, or the requirement that the polynomials $p_1(z), p_2(z), \ldots, p_s(z)$ appearing in (2.7) have degree less than s, which is required for L-stability. These minimization problems were solved using the MATLAB function `fmincon` with randomly generated initial guesses.

The results of our numerical searches are summarized in Tables 4.1 and 4.2, where we have listed SSP coefficients $\mathcal{C}$, efficient SSP coefficients $\mathcal{C}_{eff}$, area($\mathcal{S}_E$), area($\mathcal{S}_{\pi/2}$), and intervals of absolute stability int($\mathcal{S}_E$), and int($\mathcal{S}_{\pi/2}$). These tables correspond to methods which have a good balance between area of the stability region $\mathcal{S}_{\frac{\pi}{2}}$ and magnitude of SSP coefficient. Table 4.1 corresponds to IMEX schemes for which the implicit part is A-stable, and Table 4.2 corresponds to IMEX schemes for which the implicit part is L-stable. The corresponding methods of order $p = 2$ $p = 3$, and $p = 4$ are denoted

Method	$\mathcal{C}$	$\mathcal{C}_{eff}$	area($\mathcal{S}_E$)	area($\mathcal{S}_{\pi/2}$)	int($\mathcal{S}_E$)	int($\mathcal{S}_{\pi/2}$)	area($\mathcal{S}_{RK}$)
IMEX DIMSIM1A	1	1	3.14	3.14	$(-2, 0)$	$(-2, 0)$	3.14
IMEX DIMSIM2A	1.38	0.69	7.14	4.66	$(-2.87, 0)$	$(-2.87, 0)$	5.87
IMEX DIMSIM3A	0.99	0.33	9.68	2.18	$(-3.57, 0)$	$(-1.32, 0)$	9.12
IMEX DIMSIM4A	0.51	0.13	9.68	0.15	$(-3.01, 0)$	$(-0.30, 0)$	12.70

Table 4.1: SSP coefficient $\mathcal{C}$, effective SSP coefficients $\mathcal{C}_{eff}$, area($\mathcal{S}_{\mathcal{E}}$) area($\mathcal{S}_{\pi/2}$), int($\mathcal{S}_E$), int($\mathcal{S}_{\pi/2}$), and area($\mathcal{S}_{RK}$), for transformed IMEX SSP DIMSIMs with $p = q = r = s = 1$, $p = q = r = s = 2$, $p = q = r = s = 3$, and $p = q = r = s = 4$, with A-stable implicit part.

Method	$\mathcal{C}$	$\mathcal{C}_{eff}$	area($\mathcal{S}_E$)	area($\mathcal{S}_{\pi/2}$)	int($\mathcal{S}_E$)	int($\mathcal{S}_{\pi/2}$)	area($\mathcal{S}_{RK}$)
IMEX DIMSIM1L	1	1	3.14	3.14	$(-2, 0)$	$(-2, 0)$	3.14
IMEX DIMSIM2L	1.17	0.59	7.46	7.34	$(-3.01, 0)$	$(-3.01, 0)$	5.87
IMEX DIMSIM3L	0.85	0.28	9.52	3.84	$(-4.10, 0)$	$(-1.85, 0)$	9.12

Table 4.2: SSP coefficient $\mathcal{C}$, effective SSP coefficients $\mathcal{C}_{eff}$, area($\mathcal{S}_{\mathcal{E}}$) area($\mathcal{S}_{\pi/2}$), int($\mathcal{S}_E$), int($\mathcal{S}_{\pi/2}$), and area($\mathcal{S}_{RK}$), for transformed IMEX SSP DIMSIMs with $p = q = r = s = 1$, $p = q = r = s = 2$, $p = q = r = s = 3$, and $p = q = r = s = 4$, with L-stable implicit part.

by IMEX DIMSIM2A, IMEX DIMSIM2L, IMEX DIMSIM3A, IMEX DIMSIM3L, and IMEX DIMSIM4A. The coefficients of these methods are listed in the Appendix.

The stability regions of these methods for order $p = 2$, 3, and 4 are reported in Figures 4.1-4.3.

5 Numerical experiments

It has been shown in [13] (but also [15]) that IMEX RK can suffer from order reduction when applied to stiff problem. In order to confirm the good perfor-

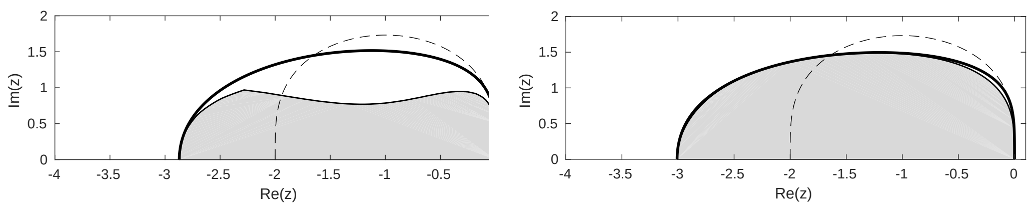

Figure 4.1: **Left:** Stability region $\mathcal{S}_E$ (thick line), stability region $\mathcal{S}_{\pi/2}$ (shaded region), of IMEX DIMSIM2A, and stability region of RK method of order $p = 2$ (dashed line). **Right:** Stability region $\mathcal{S}_E$ (thick line), stability region $\mathcal{S}_{\pi/2}$ (shaded region), of IMEX DIMSIM2L, and stability region of RK method of order $p = 2$ (dashed line).

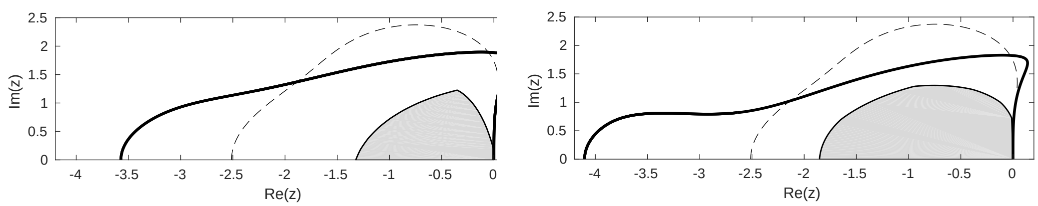

Figure 4.2: **Left:** Stability region $\mathcal{S}_E$ (thick line), stability region $\mathcal{S}_{\pi/2}$ (shaded region), of IMEX DIMSIM3A, and stability region of RK method of order $p = 3$ (dashed line). **Right:** Stability region $\mathcal{S}_E$ (thick line), stability region $\mathcal{S}_{\pi/2}$ (shaded region), of IMEX DIMSIM3L, and stability region of RK method of order $p = 3$ (dashed line).

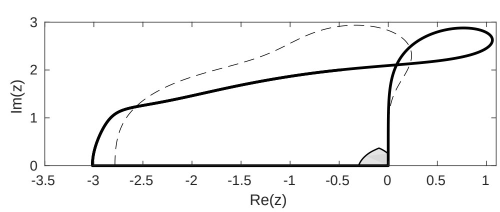

Figure 4.3: Stability region $\mathcal{S}_E$ (thick line), stability region $\mathcal{S}_{\pi/2}$ (shaded region), of IMEX DIMSIM4A, and stability region of RK method of order $p = 4$ (dashed line).

mances of the proposed methods when applied to stiff problems, we solved several problems from literature, such as shallow water equation [15, 21] with $\varepsilon = 10^{-8}$, Schnakenberg reaction-diffusion [2, 14, 23], Van der Pol oscillator [2, 15] with $\varepsilon = 10^{-6}$. In each considered case it has been confirmed that DIMSIM2A, DIMSIM2L, DIMSIM3A and DIMSIM3L converge and achieve the expected order of convergence, while order reduction can occur for IMEX RK of order $p = 2, 3$ and 4. We also noticed that the performances of the method DIMSIM4A were good too, but in some case, the behavior of the method was somehow erratic. This was probably motivated by the fact that the performances of this last method were sensitive to perturbation in the starting procedure, were IMEX RK methods sometimes were not enough to get good starting values.

For the sake of brevity, we report here detailed results for numerical resolution of an advection-reaction problem, an adsorption-desorption problem, and a shallow water problem.

5.1 Problem 1: advection-reaction

Consider next the linear advection-reaction equation [2, 7, 14]

$$\begin{cases} \dfrac{\partial u}{\partial t} + \alpha_1 \dfrac{\partial u}{\partial x} = -k_1 u + k_2 v + s_1, \\ \dfrac{\partial v}{\partial t} + \alpha_2 \dfrac{\partial v}{\partial x} = k_1 u - k_2 v + s_2, \end{cases} \tag{5.1}$$

$0 \le x \le 1$, $0 \le t \le 1$, with parameters

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

and with initial and boundary values

$$u(x,0) = 1 + s_2 x, \quad v(x,0) = \frac{k_1}{k_2} u(x,0) + \frac{s_2}{k_2}, \quad 0 \le x \le 1,$$

$$u(0,t) = \gamma_1(t), \quad v(0,t) = \gamma_2(t), \quad 0 \le t \le 1.$$

(Observe that the condition $v(0,t) = \gamma_2(t)$ does not have to be specified since $\alpha_2 = 0$). Discretization of (5.1) in space variable x on the uniform grid $x_i = i\Delta x$, $i = 0, 1, \ldots, N$, $N\Delta x = 1$, leads to the initial value problem for the system of ODEs of dimension $2N$, with non-stiff part corresponding to the advection terms, and stiff part corresponding to the reaction terms.

We consider the spatial discretization of (5.1) which corresponds to the time dependent Dirichlet data $\gamma_1(t) = 1 - \sin(12t)^4$ at the left boundary, where u_x is approximated by fourth-order central differences in the interior domain and third-order finite differences at the boundary, as in [2, 14].

The numerical results for the discretization of (5.1) with $N = 400$ spatial points are presented in Figure 5.1, where for the sake of comparison we also report the results obtained by IMEX RK methods constructed in [15]. For these tests, the reference solution was computed by `ODEPACK` routine `DLSODAR` ([12]) with absolute tolerance and relative tolerance equal to 10^{-14} and 10^{-12}, respectively.

To start the integration, we used the starting procedure described in Section 2 of [5], where the required starting values have been computed, for methods of order $p = 2$ and $p = 3$, by IMEX RK of the same order p, applied with a suitable stepsize, for the method of order $p = 4$, by `DLSODAR` with absolute tolerance and relative tolerance equal to 10^{-14} and 10^{-12}, respectively.

Figure 5.1 shows that all the presented IMEX DIMSIMs achieve the expected order of convergence for this stiff system of ODEs while order reduction to $p = 1$ occurs for IMEX RK of the same order.

5.2 Problem 2: adsorption-desorption model

Following Hundsdorfer and Ruuth [13] (see also [14]) we consider next the adsorption-desorption problem given by the equations

$$\begin{cases} u_t + a(t)u_x = \kappa\big(v - \phi(u)\big), \\ v_t = -\kappa\big(v - \phi(u)\big), \end{cases} \tag{5.2}$$

$0 \leq x \leq 1$, $t \in [0, t_{end}]$, $t_{end} = 1.25$, where $\phi(u) = k_1 u/(1 + k_2 u)$. The initial values are $u(x, 0) = v(x, 0) = 0$, $0 \leq x \leq 1$, and the boundary values are

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

As in [13] we choose the parameters $\kappa = 10^6$, $k_1 = 50$, $k_2 = 100$, and the velocity $a = a(t) = -\arctan\big(100(t-1)\big)/\pi$. Then $a(t) > 0$ for $0 \leq t \leq 1$, which corresponds to the adsorption phase, and $a(t) < 0$ for $t > 1$, which corresponds to the desorption phase.

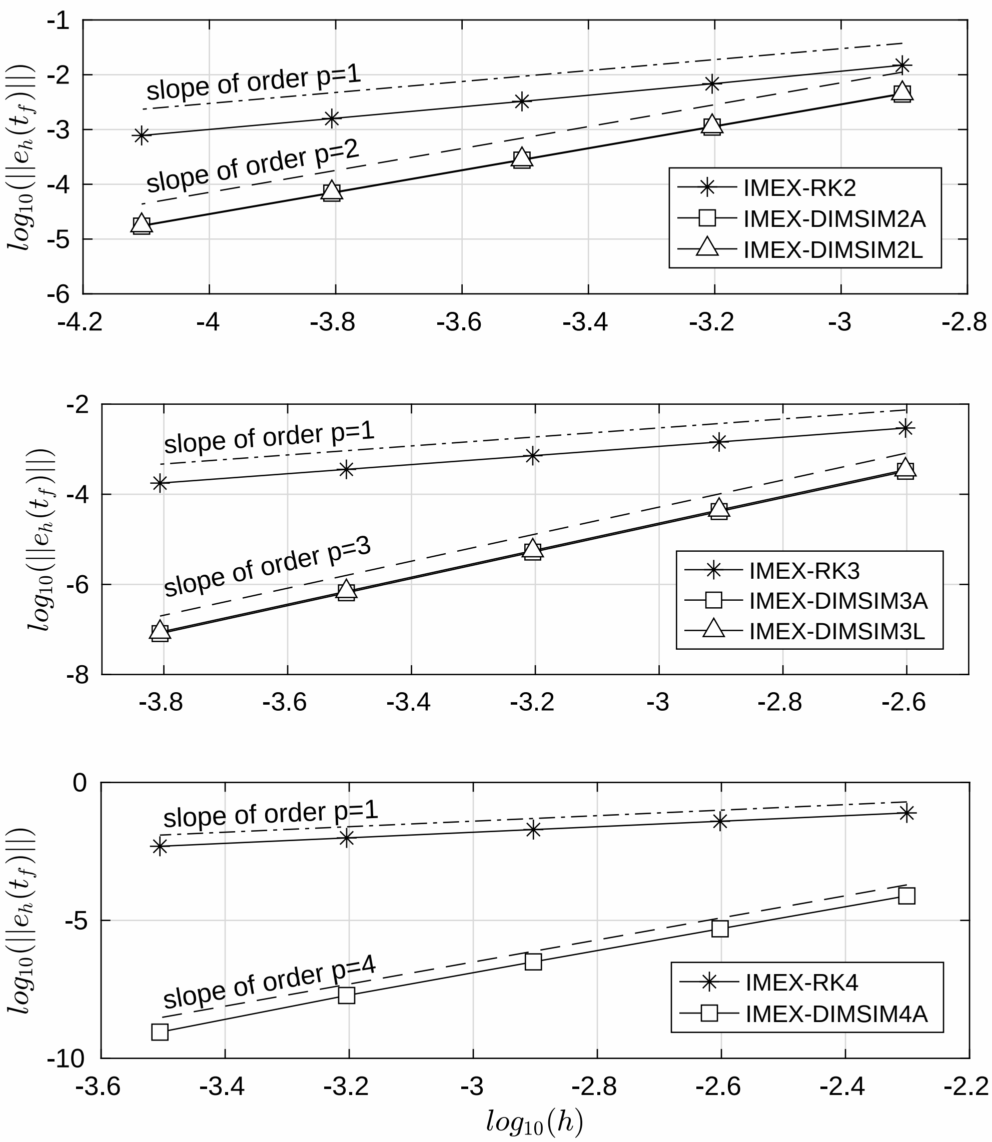

Figure 5.1: Error versus stepsize (double logarithmic scale plot) for SSP transformed IMEX DIMSIMs and IMEX RK, applied to the discretization of the Advection-Reaction problem (5.1), with $N = 401$, by fourth-order central differences in the interior domain and by third-order finite differences at the boundaries.

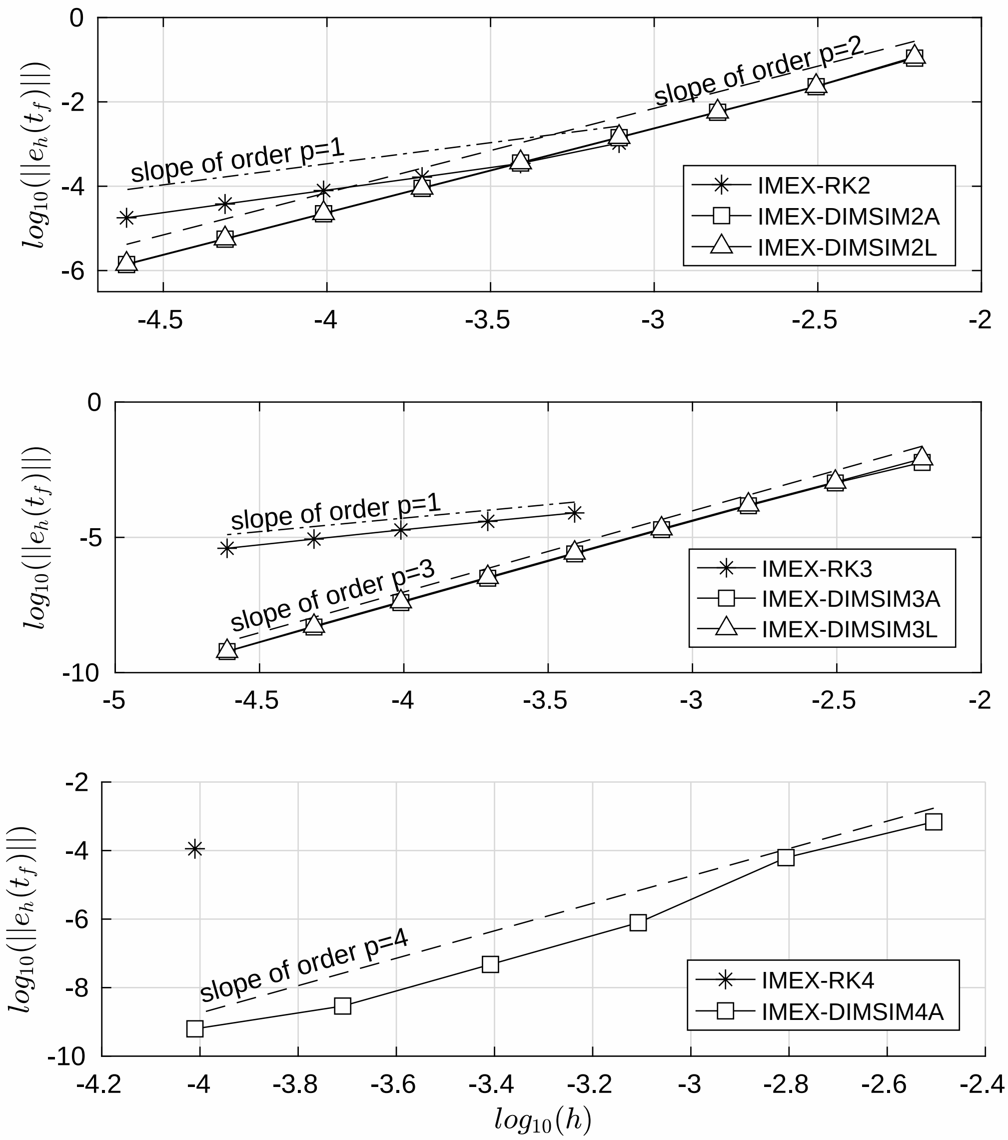

Figure 5.2: Error versus stepsize (double logarithmic scale plot) for SSP transformed IMEX DIMSIMs and IMEX RK, applied to the discretization of the Adsorption-desorption problem (5.2), with $N = 101$, by a WENO5 space discretization scheme.

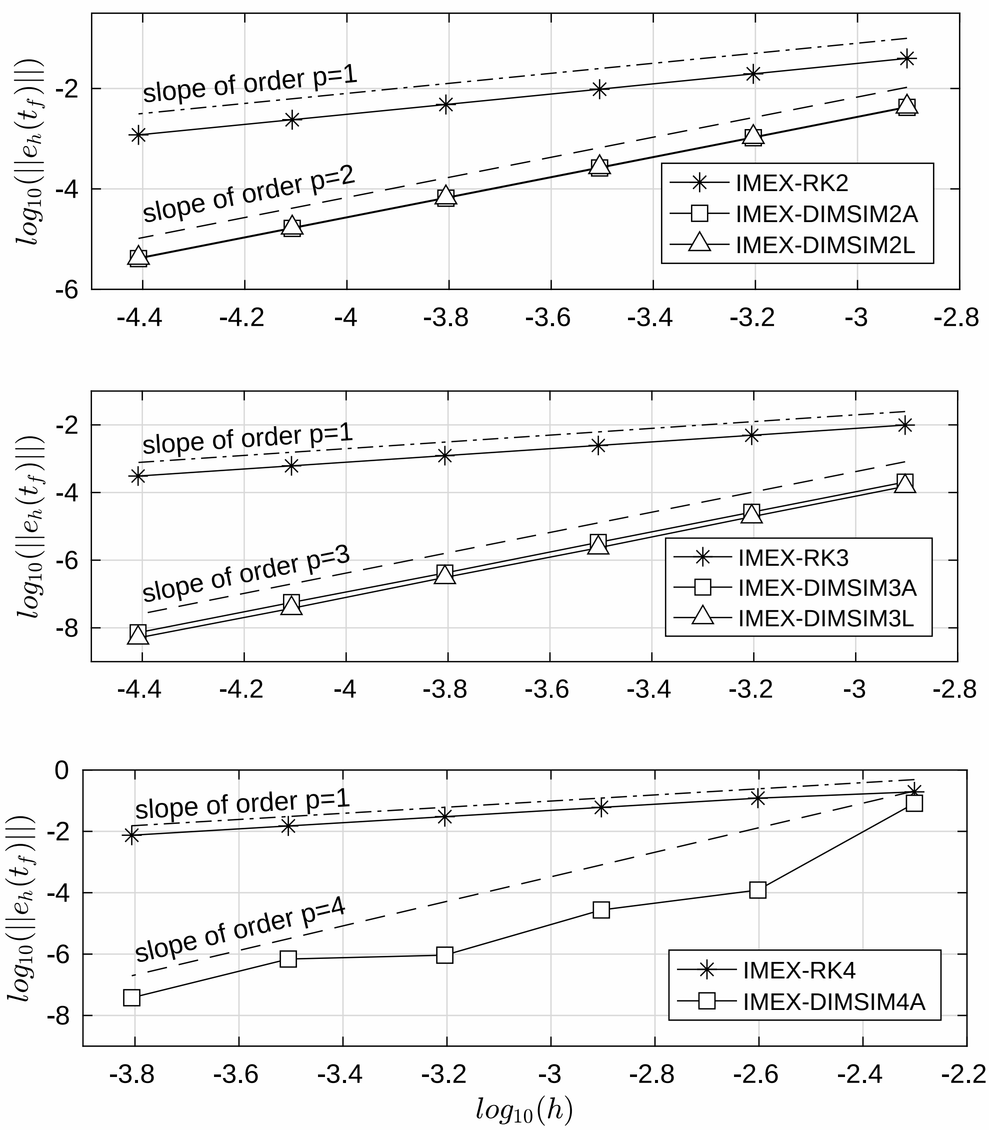

Figure 5.3: Error versus stepsize (double logarithmic scale plot) for SSP transformed IMEX DIMSIMs and IMEX RK, applied to the discretization of the shallow water problem (5.3), with $N = 201$, by a WENO5 space discretization scheme, and $\epsilon = 10^{-8}$.

As in [2], for the spatial discretization of u_x we have implemented the

WENO5 scheme [25] following the presentation in [27]. Further details can be found in [2].

The results of these tests are reported in Figure 5.2 where it is confirmed that all the presented IMEX DIMSIMs achieve the expected order of convergence for this stiff system of ODEs while order reduction to $p = 1$ occurs for IMEX RK of the same order. We also point out that several points on the line corresponding to IMEX RK of order $p = 4$ are missing because it did not converge for several values of the stepsize h.

5.3 Problem 3: shallow water model

We now consider a one-dimensional model of shallow water flow (compare [21, 19]):

$$\begin{cases} \frac{\partial}{\partial t}h + \frac{\partial}{\partial x}(hv) = 0, \\ \frac{\partial}{\partial t}(hv) + \frac{\partial}{\partial x}\left(h + \frac{1}{2}h^2\right) = \frac{1}{\varepsilon}\left(\frac{h^2}{2} - hv\right), \end{cases} \tag{5.3}$$

where h is the water height with respect to the bottom and hv is the flux of the velocity field. We use periodic boundary conditions and initial conditions at $t_0 = 0$

$$h(0,x) = 1 + \frac{1}{5}sin(8\pi x), \quad hv(0,x) = \frac{1}{2}h(0,x)^2, \tag{5.4}$$

with $x \in [0,1]$. For this problem the space derivative was discretized by a fifth order finite difference weighted essentially non-oscillatory (WENO) scheme following the implementation described in [25].

The numerical results for the discretization of (5.3) with $\epsilon = 10^{-8}$ and $N = 201$ spatial points are presented in Figure 5.3, where for the sake of comparison we also report the results obtained by IMEX Runge-Kutta methods constructed in [15]. For these tests, the reference solution was computed by `ODEPACK` routine `DLSODAR` ([12]) with absolute tolerance and relative tolerance equal to 10^{-14} and 10^{-12}, respectively.

To start the integration, we used the starting procedure described in Section 2 of [5], where the required starting values have been computed, for methods of order $p = 2$ and $p = 3$, by IMEX RK of the same order p, applied with a suitable stepsize, for the method of order $p = 4$, by `DLSODAR` with absolute tolerance and relative tolerance equal to 10^{-14} and 10^{-12}, respectively.

The results reported in Figure 5.3 confirm that the IMEX RK just has the asymptotic preserving property, while the methods proposed in this paper are also asymptotically accurate in the stiff limit for $\varepsilon \to 0$ (compare [21]). In other words, the IMEX RK methods converge, but the order drop to $p = 1$, while all the presented IMEX DIMSIMs achieve the expected order of convergence and no order reduction occurs.

A Appendix

In this Appendix we report the coefficients of the methods of order $p = 2, 3, 4$, described in Section 4.

A.1 Coefficients of method DIMSIM2A

$$\mathbf{c} = \begin{bmatrix} 0.5207015987954746 & 1 \end{bmatrix}^T,$$

$$\overline{\mathbf{A}} = \begin{bmatrix} 0 & 0 \\ 0.6335780271090006 & 0 \end{bmatrix},$$

$$\overline{\mathbf{A}^*} = \begin{bmatrix} 0.9756662942012514 & 0 \\ 1.065344873186484 & 0.9756662942012514 \end{bmatrix},$$

$$\overline{\mathbf{U}} = \begin{bmatrix} 1 & 0 \\ 0.8760323181723925 & 1 \end{bmatrix}^T,$$

$$\overline{\mathbf{V}} = \begin{bmatrix} 0.8035259425918053 & 1.584881273180670 \\ 0.09961124839144930 & 0.1964740574081947 \end{bmatrix}.$$

A.2 Coefficients of method DIMSIM2L

$$\mathbf{c} = \begin{bmatrix} 0.5725000000000000 & 1 \end{bmatrix}^T,$$

$$\overline{\mathbf{A}} = \begin{bmatrix} 0 & 0 \\ 0.5507246376811594 & 0 \end{bmatrix},$$

$$\overline{\mathbf{A}^*} = \begin{bmatrix} 0.4025509997331064 & 0 \\ 0.3054637337141530 & 0.4025509997331064 \end{bmatrix},$$

$$\overline{\mathbf{U}} = \begin{bmatrix} 1 & 0 \\ 0.8970000000000000 & 1 \end{bmatrix}^T,$$

$$\overline{\mathbf{V}} = \begin{bmatrix} 0.7976747326679189 & 1.964322983806612 \\ 0.08216049746479565 & 0.2023252673320811 \end{bmatrix}.$$

A.3 Coefficients of method DIMSIM3A

$$\mathbf{c} = \begin{bmatrix} 0.3785922442536512 & 0.7369632894601272 & 1 \end{bmatrix}^T,$$

$$\overline{\mathbf{A}} = \begin{bmatrix} 0 & 0 & 0 \\ 0.6105030326964779 & 0 & 0 \\ 0.5054775907409634 & 0.3826213150653439 & 0 \end{bmatrix},$$

$$\overline{\mathbf{A}^*} = \begin{bmatrix} 0.5023463944444552 & 0 & 0 \\ -0.8899211224523407 & 0.5023463944444552 & 0 \\ -3.305290943287502 & 0.4193402392399124 & 0.5023463944444552 \end{bmatrix},$$

$$\overline{\mathbf{U}} = \begin{bmatrix} 1 & 0 & 0 \\ 0.6070215241878391 & 1 & 0 \\ 0.5361152778084712 & 1.091180739129647 & 1 \end{bmatrix}^T,$$

$$\overline{\mathbf{V}} = \begin{bmatrix} 0.5418838673478645 & 0.9017144383487438 & 2.958352027358458 \\ 0.2129486962575630 & 0.3543543656001081 & 1.162568670627143 \\ 0.01900613148571312 & 0.03162689316015439 & 0.1037617670520274 \end{bmatrix}.$$

A.4 Coefficients of method DIMSIM3L

$$\mathbf{c} = \begin{bmatrix} 0.4020684033460171 & 0.7554528159803609 & 1 \end{bmatrix}^T,$$

$$\overline{\mathbf{A}} = \begin{bmatrix} 0 & 0 & 0 \\ 0.5925366351567699 & 0 & 0 \\ 0.5582112117594124 & 0.3256969821842126 & 0 \end{bmatrix},$$

$$\overline{\mathbf{A}^*} = \begin{bmatrix} 0.5201730949739405 & 0 & 0 \\ -1.082981144838764 & 0.5201730949739405 & 0 \\ -2.860648399647160 & 0.2917933416909193 & 0.5201730949739405 \end{bmatrix},$$

$$\overline{\mathbf{U}} = \begin{bmatrix} 1 & 0 & 0 \\ 0.6343850217261301 & 1 & 0 \\ 0.5123644514467803 & 1.138668063964801 & 1 \end{bmatrix}^T,$$

$$\overline{\mathbf{V}} = \begin{bmatrix} 0.4816666646770200 & 0.7031253548332313 & 3.663136087971684 \\ 0.1761045471411361 & 0.2570731613311589 & 1.339297421217996 \\ 0.03435316450098294 & 0.05014791919551827 & 0.2612601739918211 \end{bmatrix}.$$

A.5 Coefficients of method DIMSIM4A

$$\mathbf{c} = \begin{bmatrix} 0.2561983471074380 & 0.4485981308411215 & 0.7622950819672131 & 1 \end{bmatrix}^T,$$

$$\overline{\mathbf{A}} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0.3245033112582781 & 0 & 0 & 0 \\ 0.1102941176470588 & 0.6486486486486486 & 0 & 0 \\ 0.3111111111111111 & 0.1603053435114504 & 0.4729729729729730 & 0 \end{bmatrix},$$

$$\overline{\mathbf{A}^*} = \begin{bmatrix} 1.228571428571429 & 0 & 0 & 0 \\ -2.659574468085106 & 1.228571428571429 & 0 & 0 \\ -6.431818181818182 & -0.4444444444444444 & 1.228571428571429 & 0 \\ -5.931034482758621 & -4.906250000000000 & 1.103448275862069 & 1.228571428571429 \end{bmatrix},$$

$$\overline{\mathbf{U}} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0.7011494252873563 & 1 & 0 & 0 \\ 0.2363213391750847 & 0.3563218390804598 & 1 & 0 \\ 0.3704826947154125 & 0.5083355703606088 & 0.6222222222222222 & 1 \end{bmatrix}^T,$$

$$\overline{\mathbf{V}} = \begin{bmatrix} 0.3181770223788457 & 1.319227410800732 & 0.2619374293792898 & 1.680623378297797 \\ 0.09508738599827574 & 0.3942518698944718 & 0.07828015130875329 & 0.5022552624798014 \\ 0.2091032901032768 & 0.8669852710621154 & 0.1721430978104653 & 1.104491692074865 \\ 0.02185292729383308 & 0.09060673356209266 & 0.01799029847272758 & 0.1154280099162172 \end{bmatrix}.$$

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