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SEBASTIANO BOSCARINO, FRANCIS FILBET, AND GIOVANNI RUSSO

Abstract. In this paper we consider a new formulation of implicit-explicit (IMEX) methods for the numerical discretization of time dependent partial differential equations. We construct several semi-implicit Runge-Kutta methods up to order three. This approach is particularly suited for problems where the stiff and non-stiff components cannot be well separated. We present different numerical simulations for reaction-diffusion, convection diffusion and nonlinear diffusion system of equations. Finally, we conclude by a stability analysis of the schemes for linear problems.

Contents

1. Introduction

A well-known approach in the numerical solution of evolutionary problems in partial differential equations is the method of lines. In this approach a partial differential equation is first discretized in space by finite difference or finite element techniques and converted into a system of ordinary differential equations (ODEs)

$$\begin{cases} \dfrac{du}{dt}(t) = \mathcal{F}(t,u(t)) + \dfrac{1}{\varepsilon}\mathcal{G}(t,u(t)), \quad \forall\, t \geq t_0, \\ \\ u(t_0) = u_0, \end{cases} \tag{1}$$

where ε is a small parameter, which generates some stiffness in the system.

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The development of numerical schemes for systems of stiff ODEs of the form (1) attracted a lot of attention in the last decades. Systems of such form often arise from the discretization of partial differential equations, such as convection-diffusion equations and hyperbolic systems with relaxation. In previous works we considered the latter case which in recent years has been a very active field of research, due to its great impact on applied sciences. In fact, relaxation is important in many physical situations, for example it arises in discrete kinetic theory of rarefied gases, hydrodynamical models for semiconductors, linear and non-linear waves, viscoelasticity, traffic flows, shallow water [12, 13, 17, 25, 26, 27, 23].

Hopefully, when a problem with easily separable stiff and non-stiff components is considered, a combination of implicit and explicit Runge-Kutta methods can be used. The implicit method is used to treat the stiff component $\mathcal{G}(t,u(t))/\varepsilon$ in a stable fashion while the non-stiff component $\mathcal{F}(t,u(t))$ of the system is treated using the explicit scheme. These combined implicit/explicit (IMEX) schemes are already used for several problems, including convection-diffusion-reaction systems, hyperbolic systems with relaxation, collisional kinetic equations, and so on.

However it is not always easy to separate stiff and non-stiff components, and therefore the use of standard IMEX schemes is not straightforward. In such cases one usually relies on fully implicit schemes or in some linearized version of them, such as Rosenbrock schemes, [21]. The latter are general purpose semi-implicit schemes, that do not make use of the particular structure of the system. In many cases of interest, it is possible to adopt different semi-implicit schemes, which exploit the structure of the system, resulting in a very effective tool, being a good compromise among accuracy, stability and robustness. For instance in [6], the authors consider nonlinear hyperbolic systems containing fully nonlinear and stiff relaxation terms in the limit of arbitrary late times. The dynamics is asymptotically governed by effective systems which are of parabolic type and may contain degenerate and/or fully nonlinear diffusion terms. Fully nonlinear relaxation terms can arise, for instance, in presence of *strong friction*, see for example in [2] and references therein. Furthermore, a general class of models of the same type were introduced by Kawashima and LeFloch (LeFloch and Kawashima, private communication) and proposed in [6]. For such problems in [6], the authors introduced a semi-implicit formulation based on implicit-explicit (IMEX) Runge-Kutta methods. Similarly in [29], the author introduced a semi-implicit method for computing the two models of motion by mean curvature and motion by surface diffusion which is stable for large time steps. In all such models a semi-implicit method is more effective than a fully implicit one.

In many cases the stiffness is associated to some variables. For example, if a system can be written in the *partitioned* form

$$\begin{cases} y(t)' = \mathcal{F}(t,y(t),z(t)), \\ \\ \varepsilon z(t)' = \mathcal{G}(t,y(t),z(t)), \end{cases} \tag{2}$$

then the stiffness is associated to variable z, and the corresponding equation will be treated implicitly, while the equation for y is treated explicitly. In other cases it is more convenient to associate the stiffness to a part of the right hand side, for example if a system has the *additive* form (1), in this case the term $\mathcal{F}(t,u(t))$ is treated explicitly while $\mathcal{G}(t,u(t))/\varepsilon$ is treated implicitly. It can be shown that the same system can be written in either form, however sometimes one of the two forms is more convenient.

Directly motivated by the above cases, in this paper we consider a more general problem of the form

$$\begin{cases} \dfrac{du}{dt}(t) = \mathcal{H}_\varepsilon(t,u(t),u(t)), \quad \forall\, t \geq t_0, \\ \\ u(t_0) = u_0, \end{cases} \tag{3}$$

where the function $\mathcal{H}$: $\mathbb{R}\times\mathbb{R}^m\times\mathbb{R}^m \to \mathbb{R}^m$ is sufficiently differentiable and the dependence on the second argument of $\mathcal{H}$ is non stiff, while the dependence on the third argument is stiff.

For example system (1) can be written as (3) by setting

$$\mathcal{H}_\varepsilon(t,u(t),v(t)) = \mathcal{F}(t,u(t)) + \frac{1}{\varepsilon}\mathcal{G}(t,v(t)).$$

The relation with partitioned system is obtained by observing that setting $y = z/\varepsilon$, system (3) implies

$$\begin{cases} \dfrac{dy}{dt}(t) \;=\; \mathcal{H}(t,y(t),z(t)/\varepsilon), \\ \\ \varepsilon\,\dfrac{dz}{dt}(t) \;=\; \mathcal{H}(t,y(t),z(t)/\varepsilon), \end{cases}$$

which is a particular case of partitioned system (2), in which $\mathcal{F} = \mathcal{G} = \mathcal{H}$. In this form it appears natural to use partitioned Runge-Kutta methods, which are explicit in y and implicit in z.

Thus, the formal equivalence among the various systems allows us to adopt techniques well know for additive or partitioned systems to more general cases.

A common way to construct semi-implicit schemes consists in adding and subtracting a stiff term which is easier to solve, and which is somehow "close" to the original right hand side of the equation. Given an equation of the form

$$u' = F(u),$$

this is replaced by an equation of the form

$$u' = F(u) - G(u) + G(u). \tag{4}$$

The term G is then treated implicitly, while the term $F - G$ is treated explictly. The idea is that the stabilization introduced by the implicit treatment of the second term allows for an explicit treatment of the first one, $F - G$, which, by itself, is not necessarily non-stiff. Such ideas have been adopted, for example, by Smereka [29] in the context of flow by mean curvature and surface diffusion, by Jin and Filbet [19] in the context of the Boltzmann equation of rarefied gas dynamics when the Knudsen number is very small, and in the context of hyperbolic systems with diffusive relaxation [6, 9, 11]. Notice that such penalization technique expressed by Eq.4 is a particular case of Eq.(3).

The aim of this paper is to propose a new class of semi-implicit schemes based on IMEX Runge-Kutta methods which are strongly inspired by partitioned Runge-Kutta methods, [20] and very much related to the additive Runge-Kutta methods of Zhong [32]. In the next section, we describe the general framework to construct this new class of semi-implicit Runge-Kutta schemes based on partitioned schemes. Several schemes are proposed with different stability properties and order of accuracy. We next compare the numerical solutions with exact ones available in the literature for reaction-diffusion problem and nonlinear convection-diffusion equation. After this validation step, we perform several numerical computations to show the robustness of our approach (nonlinear Fokker-Planck equation, Hele-Shaw flow and surface diffusion flow). The last section is devoted to a preliminary study of stability properties of our schemes and we introduce the notion of F-stability where the main point is to make use of the dissipative nature of the stiff term to increase the time step.

2. Numerical methods for ODEs

In this section we review the concept of partitioned Runge-Kutta methods and derive a new class of semi-implicit Runge-Kutta methods. Then we remind several definitions on the classification of Runge-Kutta schemes and then propose several schemes up to third order of accuracy.

2.1. From Partitioned to semi-implicit Runge-Kutta methods.

In the literature some interesting numerical methods do not belong to the classical class of implicit or explicit Runge-Kutta methods. They are called *partitioned* Runge-Kutta methods. In order to present these methods we consider differential equations in the partitioned form,

$$\left\{\begin{array}{l} \dfrac{dy}{dt}(t) \,=\, \mathcal{F}(t, y(t), z(t)), \\ \\ \dfrac{dz}{dt}(t) \,=\, \mathcal{G}(t, y(t), z(t)), \end{array}\right. \tag{5}$$

where $y(t)$ and $z(t)$ may be vectors of different dimensions and $y(t_0) = y_0$, $z(t_0) = z_0$ are the initial conditions.

The idea of the partitioned Runge-Kutta methods is to apply two different Runge-Kutta methods, *i.e.*

$$\begin{array}{c|c} \hat{c} & \hat{A} \\ \hline & \hat{b}^T \end{array} \qquad \begin{array}{c|c} c & A \\ \hline & b^T \end{array} \tag{6}$$

where we treat the first variable y with the first method, $\hat{A}$, $\hat{b}^T = (\hat{b}_1, \cdots, \hat{b}_s)$, $\hat{c} = (\hat{c}_1, \cdots, \hat{c}_s)$ and the second variable z with the second method, A, $b^T = (b_1, \cdots, b_s)$, $c = (c_1, \cdots, c_s)$ under the usual assumption

$$\sum_j \hat{a}_{i,j} \,=\, \hat{c}_i, \quad \text{and} \quad \sum_j a_{ij} \,=\, c_i, \quad \text{for} \quad 1 \le i \le s. \tag{7}$$

In other words, if we consider a numerical approximation (y^n, z^n) of (5) at time t^n, a partitioned Runge-Kutta method for the solution of (5) is given by

$$\left\{\begin{array}{l} k_i \,=\, \mathcal{F}\left(t^n + \hat{c}_i \Delta t, y^n + \Delta t \displaystyle\sum_{j=1}^{s} \hat{a}_{ij} k_j, z^n + \Delta t \sum_{j=1}^{s} a_{ij} \ell_j\right), \quad 1 \le i \le s, \\ \\ \ell_i \,=\, \mathcal{G}\left(t^n + c_i \Delta t, y^n + \Delta t \displaystyle\sum_{j=1}^{s} \hat{a}_{ij} k_j, z^n + \Delta t \sum_{j=1}^{s} a_{ij} \ell_j\right), \quad 1 \le i \le s \end{array}\right. \tag{8}$$

and the numerical solution at the next time step is given by

$$\left\{\begin{array}{l} y^{n+1} \,=\, y^n \,+\, \Delta t \displaystyle\sum_{i=1}^{s} \hat{b}_i k_i, \\ \\ z^{n+1} = z^n + \Delta t \displaystyle\sum_{i=1}^{s} b_i \ell_i. \end{array}\right. \tag{9}$$

Now to derive a general semi-implicit Runge-Kutta scheme, we only observe that we can rewrite system (3) as

$$\left\{\begin{array}{l} \dfrac{dy}{dt}(t) \,=\, \mathcal{H}(t, y(t), z(t)), \\ \\ \dfrac{dz}{dt}(t) \,=\, \mathcal{H}(t, y(t), z(t)), \end{array}\right. \tag{10}$$

with initial conditions $y(t_0) = y_0$, $z(t_0) = y_0$. In this way the system is a particular case of partitioned system in which $\mathcal{F} = \mathcal{G}$ but with an additional computational cost since we double the number of variables. Applying the partitioned Runge-Kutta method (8)-(9) we have

$$\left\{ \begin{array}{l} k_i \,=\, \mathcal{H}\left(t^n + \hat{c}_i \Delta t, Y_i, Z_i\right), \quad 1 \le i \le s, \\ \\ \ell_i \,=\, \mathcal{H}\left(t^n + c_i \Delta t, Y_i, Z_i\right), \quad 1 \le i \le s, \end{array} \right. \tag{11}$$

with

$$\left\{ \begin{array}{l} Y_i \,=\, y^n \,+\, \Delta t \displaystyle\sum_{j=1}^{s} \hat{a}_{i,j}\, k_j, \quad 1 \le i \le s, \\ \\ Z_i \,=\, y^n \,+\, \Delta t \displaystyle\sum_{j=1}^{s} a_{ij}\, \ell_j, \quad 1 \le i \le s, \end{array} \right. \tag{12}$$

and the numerical solutions at the next time step are

$$\left\{ \begin{array}{l} y^{n+1} \,=\, y^n \,+\, \Delta t \displaystyle\sum_{i=1}^{s} \hat{b}_i\, k_i, \\ \\ z^{n+1} \,=\, y^n \,+\, \Delta t \displaystyle\sum_{i=1}^{s} b_i\, \ell_i. \end{array} \right. \tag{13}$$

At this stage let us adress some comments on several issues : number of evaluations, storage, order of accuracy and embedded methods.

Remark 2.1 (Concerning the number of evaluations of $\mathcal{H}$)**.** *In general, k_i and ℓ_i given by (11) for all $1 \le i \le s$ are different. However, with the additional assumption $\hat{c}_i = c_i$ for $i = 1, \cdots, s$, we have $\ell_i = k_i$ for $i = 1, \cdots, s$, and only one evaluation of $\mathcal{H}$ is needed in (11). On the other hand, if the system (10) is autonomous, i.e. if $\mathcal{H}$ does not explicitly depend on time, then from (11) we have $\ell_i = k_i$ for $i = 1, \ldots, s$ independently on the assumption $\hat{c}_i = c_i$ for $i = 1, \cdots, s$. Therefore, only one set needs to be computed:*

$$k_i \,=\, \mathcal{H}\left(y^n \,+\, \Delta t \sum_{i=1}^{s} \hat{a}_{i,j}\, k_j,\; y^n \,+\, \Delta t \sum_{i=1}^{s} a_{ij}\, k_j\right), \quad 1 \le i \le s.$$

Remark 2.2 (Concerning the storage issues and order of accuracy)**.** *If $\ell_i = k_i$ for $i = 1, \ldots, s$, under the additional assumption $\hat{b}_i = b_i$ for $i = 1, \cdots, s$ then also the numerical solutions are the same, i.e. $z^{n+1} = y^{n+1}$ and no duplication of variables is needed. In fact, by keeping track of the Runge-Kutta fluxes k_i rather than of the stage values Y_i and Z_i, one avoids the duplication of the number of variables.*

Note, however, that even in the general case, i.e. if $b_i \neq \hat{b}_i$, $i = 1, \cdots, s$ or $c_i \neq \hat{c}_i$, $i = 1, \cdots, s$ and the system is not autonomous, for a method which is consistent to order p, one has:

$$y^{n+1} = y(t^{n+1}) + \mathcal{O}(\Delta t^{p+1}), \quad z^{n+1} = z(t^{n+1}) + \mathcal{O}(\Delta t^{p+1}).$$

Considering that $z(t^{n+1}) = y(t^{n+1})$, then on has $z^{n+1} = y^{n+1} + \mathcal{O}(\Delta t^{p+1})$ which means that if we neglect the difference between z^{n+1} and y^{n+1} and choose, for example, to advance y^{n+1} and to set, at the beginning of a new time step, $z^{n+1} = y^{n+1}$, then one obtains another scheme still of order p, with no duplication of variables.

Hereafter we assume that we follow the evolution of y^n, and we set $z^n := y^n$, at the beginning of each time step. We expect that in general it is more accurate to follows the non stiff variable y, but there may be exception, and for some scheme it may be more convenient to follow the evolution of the stiff variable z ant to set $y^n := z_n$ at the beginning of the time step.

Remark 2.3 (Embedded methods)**.** *From the above remarks, if we use y^{n+1} to advance the solution, and compute z^{n+1} by a lower order method, obtained with a different choice of b_i, then one can construct an embedded method, which can be used for an automatic time step control* [20].

Now we are ready to propose semi-implicit Runge-Kutta methods in order to solve problem (3) when the dependence from the second variable is stiff. We will treat the first variable explicitly, and the second one implicitly. A semi-implicit Runge-Kutta method is implemented as follows. First we set $z_n = y^n$ and compute the stage fluxes for $i = 1, \dots, s$, we set $Y_1 = \tilde{Z}_1 = y^n$ and

$$\left\{ \begin{array}{l} Y_i \;=\; y^n \;+\; \Delta t \displaystyle\sum_{j=1}^{i-1} \hat{a}_{ij}\, k_j, \quad 2 \le i \le s, \\ \\ \tilde{Z}_i \;=\; y^n \;+\; \Delta t \displaystyle\sum_{j=1}^{i-1} a_{ij}\, \ell_j, \quad 2 \le i \le s \\ \\ \ell_i \;=\; \mathcal{H}\left(t^n + c_i \Delta t, Y_i, \tilde{Z}_i \;+\; \Delta t\, a_{ii}\, \ell_i\right), \quad 1 \le i \le s, \\ \\ k_i \;=\; \mathcal{H}\left(t^n + \hat{c}_i \Delta t, Y_i, \tilde{Z}_i \;+\; \Delta t\, a_{ii}\, \ell_i\right), \quad 1 \le i \le s, \end{array} \right. \tag{14}$$

and, finally update the numerical solution

$$y^{n+1} \;=\; y^n \;+\; \Delta t \sum_{i=1}^{s} b_i\, k_i. \tag{15}$$

In most cases the system is autonomous, and duplication of variables is not necessary, in this case (14) reduces to

$$\left\{ \begin{array}{l} Y_i \;=\; y^n \;+\; \Delta t \displaystyle\sum_{j=1}^{i-1} \hat{a}_{ij}\, k_j, \quad 2 \le i \le s, \\ \\ \tilde{Z}_i \;=\; y^n \;+\; \Delta t \displaystyle\sum_{j=1}^{i-1} a_{ij}\, k_j, \quad 2 \le i \le s \\ \\ k_i \;=\; \mathcal{H}\left(Y_i, \tilde{Z}_i \;+\; \Delta t\, a_{ii}\, k_i\right), \quad 1 \le i \le s. \end{array} \right.$$

Remark 2.4. *We note that this new approach includes Zhong's method* [32]. *The theory developed in* [32] *for additive semi-implicit Runge-Kutta methods can be extended in a straightforward manner to the semi-implicit Runge-Kutta methods. In fact, by setting* $\mathcal{H}(y, y) = \mathcal{F}(y) + \mathcal{G}(y)$ *we obtain for the numerical method*

$$\begin{aligned} k_i \;&=\; \mathcal{H}\left(y^n + \sum_{j=1}^{j-1} \hat{a}_{ij} k_j, y^n + \sum_{j=1}^{j-1} a_{ij} k_j + a_{ii} k_i\right), \\ &=\; \mathcal{F}\left(y^n + \sum_{j=1}^{j-1} \hat{a}_{ij} k_j\right) \;+\; \mathcal{G}\left(y^n + \sum_{j=1}^{j-1} a_{ij} k_j + a_{ii} k_i\right), \end{aligned}$$

for $i = 1, \cdots s$ *and for the numerical solution*

$$y^{n+1} \;=\; y^n \;+\; \sum_{i=1}^{s} b_i\, k_i,$$

which are exactly those proposed by Zhong [32].

In the following we propose different types of semi-implicit Runge-Kutta methods and verify that the order conditions are the same as the ones satisfied by the explicit and implicit Runge-Kutta schemes.

2.2. **Classification of IMEX Runge-Kutta schemes.** IMEX Runge-Kutta schemes present in the literature can be classified in three different types characterized by the structure of the matrix $A = (a_{ij})_{i,j=1}^{s}$ of the implicit scheme. Following [7], we will rely on the following notions [1, 13, 27].

Definition 2.1. *An IMEX Runge-Kutta method is said to be* **of type A** [27] *if the matrix $A \in \mathbb{R}^{s\times s}$ is invertible. It is said to be* **of type CK** [13] *if the matrix $A \in \mathbb{R}^{s\times s}$ can be written in the form*

$$A = \begin{pmatrix} 0 & 0 \\ a & \mathcal{A} \end{pmatrix},$$

in which the matrix $\mathcal{A} \in \mathbb{R}^{(s-1)\times(s-1)}$ invertible. Finally, it is said to be **of type ARS** [1] *if it is a special case of the type CK with the vector $a = 0$.*

Schemes of type CK are very attractive since they allow some simplifying assumptions, that make order conditions easier to treat, therefore permitting the construction of higher order IMEX Runge-Kutta schemes. On the other hand, schemes of type A are more amenable to a theoretical analysis, since the matrix A of the implicit scheme is invertible.

2.3. **Order conditions and numerical schemes.** Runge-Kutta methods (14)-(15) are a special case of the semi-implicit ones (8)-(9). Thus, the order conditions for (14) and (15) are a direct consequence of the classical order conditions computed for partitioned Runge-Kutta methods. It is possible to give a representation of these order conditions by means of *bi-colored trees* [22].

We shall show here how to construct a family of second order semi-implicit Runge-Kutta methods of the type (14)-(15). We set $\hat{b}_i = b_i$ for $i = 1, \cdots, s$ and use the previous notation for the explicit and implicit part. Therefore we have

Proposition 2.1. *Assume (6) and (7). Then, the semi-implicit Runge-Kutta method is of order 2, if*

$$\sum_i b_i \,=\, 1, \quad \sum_i b_i\, c_i \,=\, 1/2, \quad \sum_i b_i\, \hat{c}_i \,=\, 1/2. \tag{16}$$

Proof. By the assumption $\hat{b}_i = b_i$ for $i = 1, \cdots, s$, the proof is a trivial consequence of results for order conditions from Chapter III in [22]. □

We first consider second order schemes with two stages and for practical reasons we consider *singly diagonally implicit Runge-Kutta* (SDIRK) schemes for the implicit part, *i.e.* $a_{ii} = \gamma$, for $i = 1, \cdots s$. The Butcher tableau takes then the following form

$$\begin{array}{c|cc} 0 & 0 & 0 \\ \hat{c} & \hat{c} & 0 \\ \hline & b_1 & b_2 \end{array} \qquad \begin{array}{c|cc} \gamma & \gamma & 0 \\ c & c-\gamma & \gamma \\ \hline & b_1 & b_2 \end{array} \tag{17}$$

We propose a family of second order methods with SDIRK implicit part satisfying order conditions in Proposition 2.1. These schemes have the following coefficients:

$$b_1 \,=\, 1 - b_2, \quad \hat{c} \,=\, 1/(2\, b_2), \quad c = (1/2 - \gamma(1 - b_2))/b_2, \tag{18}$$

where $b_2 \neq 0$ and $\gamma > 0$ are free parameters.

One drawback of the present approach (14)-(15) for non autonomous ODE may come from the fact that it would require twice evaluations of the right hand side $\mathcal{H}$ for the computation of $(k_i)_{1\leq i\leq s}$ and $(\ell_i)_{1\leq i\leq s}$. However for second order schemes with two stages, it is easy to verify that the evaluation of $(\ell_i)_{1\leq i\leq 2}$ is enough and the choice $k_1 = \ell_1$, (which is equivalent to set $\hat{c}_1 = c_1 \neq 0$) does not modify the order of the scheme even if condition (7) is not satisfied. In fact, for low orders, condition (7) is not necessary, see [24] for details.

We list below the second and third order schemes that we are used in the paper.

2.3.1. **The second order semi-implicit Runge-Kutta scheme.** A first example of scheme satisfying the second order conditions given in Proposition 2.1 is $b_2 = \gamma = 1/2$, which yields the following table

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & 1/2 & 1/2 \end{array} \qquad \begin{array}{c|cc} 1/2 & 1/2 & 0 \\ 1/2 & 0 & 1/2 \\ \hline & 1/2 & 1/2 \end{array} \tag{19}$$

This scheme is of type A and its stability region will be studied later.

2.3.2. **The stiffly accurate semi-implicit Runge-Kutta scheme.** Another chocie is $b_2 = \gamma$, $c = 1$, where γ is chosen as the smallest root of the polynomial $\gamma^2 - 2\gamma + 1/2 = 0$, *i.e.* $\gamma = 1 - 1/\sqrt{2}$ and $\hat{c} = 1/(2\gamma)$, it gives

$$\begin{array}{c|cc} 0 & 0 & 0 \\ \hat{c} & \hat{c} & 0 \\ \hline & 1-\gamma & \gamma \end{array} \qquad \begin{array}{c|cc} \gamma & \gamma & 0 \\ 1 & 1-\gamma & \gamma \\ \hline & 1-\gamma & \gamma \end{array} \tag{20}$$

2.3.3. **The IMEX-SSP2(2,2,2) L-stable scheme.** We choose $b_2 = 1/2$, $\hat{c} = 1$ and $\gamma = 1 - 1/\sqrt{2}$, *i.e.* the corresponding Butcher tableau is given by

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & 1/2 & 1/2 \end{array} \qquad \begin{array}{c|cc} \gamma & \gamma & 0 \\ 1-\gamma & 1-2\gamma & \gamma \\ \hline & 1/2 & 1/2 \end{array} \tag{21}$$

2.3.4. **The stiffly accurate IMEX-SSP2(3,3,2) L-stable scheme.** Finally, another second order scheme with three stages will be studied. The IMEX-SSP2(3,3,2) L-stable scheme is given by

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 \\ 1 & 1/2 & 1/2 & 0 \\ \hline & 1/3 & 1/3 & 1/3 \end{array} \qquad \begin{array}{c|ccc} 1/4 & 1/4 & 0 & 0 \\ 1/4 & 0 & 1/4 & 0 \\ 1 & 1/3 & 1/3 & 1/3 \\ \hline & 1/3 & 1/3 & 1/3 \end{array} \tag{22}$$

Now, we shall show how to construct a family of third order semi-implicit Runge-Kutta methods of the type (14)-(15). We set $\hat{b}_i = b_i$ for $i = 1, \cdots, s$ and use the previous notation for the explicit and implicit part. Thus we prove that

Proposition 2.2. *Assume (6) and (7). Then, the semi-implicit Runge-Kutta method is of order three, if it satisfies the conditions (16) and the implicit part satisfies the classical third order conditions*

$$\sum_i b_i c_i^2 \, = \, 1/3, \quad \sum_{i,j} b_i \, a_{ij} \, c_j \, = \, 1/6, \tag{23}$$

the explicit part satisfies the classical third order conditions

$$\sum_i b_i \, \hat{c}_i^2 \, = \, 1/3, \quad \sum_{i,j} b_i \, \hat{a}_{ij} \, \hat{c}_j \, = \, 1/6, \tag{24}$$

and moreover the additional coupling conditions

$$\sum_i b_i \, \hat{c}_i \, c_i \, = \, 1/3, \quad \sum_{i,j} b_i \, a_{ij} \, \hat{c}_j \, = \, 1/6, \quad \sum_{i,j} b_i \, \hat{a}_{ij} \, c_j \, = \, 1/6. \tag{25}$$

are satisfied.

Proof. By the assumption $\hat{b}_i = b_i$ for $i = 1, \cdots, s$, the proof is a trivial consequence of results for order conditions from Chapter III in [22]. □

2.3.5. **the IMEX-SSP3(4,3,3) L-stable scheme.** A possible choice satisfying the properties of Proposition 2.2 is given by the IMEX-SSP3(4,3,3) L-stable scheme, *i.e.*

$$
\begin{array}{c|cccc}
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
1 & 0 & 1 & 0 & 0 \\
1/2 & 0 & 1/4 & 1/4 & 0 \\
\hline
 & 0 & 1/6 & 1/6 & 2/3
\end{array}
\qquad
\begin{array}{c|cccc}
\alpha & \alpha & 0 & 0 & 0 \\
0 & -\alpha & \alpha & 0 & 0 \\
1 & 0 & 1-\alpha & \alpha & 0 \\
1/2 & \beta & \eta & 1/2-\beta-\eta-\alpha & \alpha \\
\hline
 & 0 & 1/6 & 1/6 & 2/3
\end{array}
\tag{26}
$$

with $\alpha = 0.24169426078821$, $\beta = \alpha/4$ and $\eta = 0.12915286960590$.

For this particular choice, let us observe that the number of evaluations of the right hand side $\mathcal{H}$ is still reasonable since the coefficients $c_i = \hat{c}_i$ for $2 \leq i \leq 4$ and only c_1 differs from $\hat{c}_1$.

3. Applications

In this section we present several numerical tests for nonlinear PDEs for reaction-diffusion systems and nonlinear convection-diffusion equation for which we verify the order of accuracy and stability issues with respect to the CFL condition. Then, we treat a nonlinear Fokker-Planck equation to investigate the long time behavior of the numerical solution obtained from (14)-(15). Finally we complete this section with numerical tests on Hele-Shaw flow and surface diffusion flow.

We monitor L_1 and L_∞ norms of the error, defined as:

$$
\begin{cases}
\varepsilon_\infty = \max\limits_{0\leq n\leq N_T} \max\limits_{i,j} \|\omega_{i,j}^n - \omega(t^n, x_i, y_j)\|, \\[2ex]
\varepsilon_1 = \max\limits_{0\leq n\leq N_T} \sum\limits_{i,j} \Delta x\, \Delta y\, \|\omega_{i,j}^n - \omega(t^n, x_i, y_j)\|.
\end{cases}
$$

For space discretization we will apply basic fourth order discretization with central finite difference for first derivative

$$
\nabla_h \omega_i = \frac{-\omega_{i+2} \,+\, 8\,\omega_{i+1} \,-\, 8\,\omega_{i-1} \,+\, \omega_{i-2}}{12\,h}
$$

where h is the space step, and for the second derivative is discretized using a fourth order central finite difference scheme as well

$$
\nabla_h^2 \omega_i = \frac{-\omega_{i+2} \,+\, 16\,\omega_{i+1} \,-\, 30\,\omega_i \,+\, 16\,\omega_{i-1} \,-\, \omega_{i-2}}{12\,h^2}.
$$

3.1. **Test 1 - Reaction-diffusion problem.** We first consider a very simple reaction-diffusion system with nonlinear source for which there are explicit solutions.

To demonstrate the optimal accuracy of the semi-implicit method in various norms, we consider the reaction-diffusion system problem [31] together with periodic boundary conditions: $\omega = (\omega_1, \omega_2) : \mathbb{R}^+ \times (0, 2\pi)^2 \mapsto \mathbb{R}^2$

$$
\begin{cases}
\dfrac{\partial \omega_1}{\partial t} \;=\; \Delta\omega_1 \;-\; \alpha_1(t)\,\omega_1^2 \;+\; \dfrac{9}{2}\,\omega_1 \;+\; \omega_2 \;+\; f(t), \qquad t \geq 0, \quad (x,y) \in (0,2\pi)^2, \\[2ex]
\dfrac{\partial \omega_2}{\partial t} \;=\; \Delta\omega_2 \;+\; \dfrac{7}{2}\,\omega_2\,, \qquad t \geq 0, \quad (x,y) \in (0,2\pi)^2,
\end{cases}
$$

with $\alpha(t) = 2\,e^{t/2}$ and $f(t) = -2e^{-t/2}$. The initial conditions are extracted from the exact solutions

$$
\begin{cases}
\omega_1(t,x,y) \;=\; \exp(-0.5t)\,(1 \,+\, \cos(x)), \\[2ex]
\omega_2(t,x,y) \;=\; \exp(-0.5t)\,\cos(2\,x).
\end{cases}
$$

To apply our semi-implicit scheme (14)-(15) we rewrite this PDE in the form (3) with $u = (u_1, u_2)$ the component treated explicitly, $v = (v_1, v_2)$ the component treated implicitly and

$$\mathcal{H}(t,u,v) = \begin{pmatrix} \Delta v_1 \; - \; \alpha(t) u_1 \, v_1 \; + \; \dfrac{9u_1}{2} \; + \; v_2 \; + \; f(t) \\ \\ \Delta v_2 \; + \; \dfrac{7\, v_2}{2} \end{pmatrix}.$$

Since the Δ operator induces some stiffness it is treated implicitly whereas reaction terms are treated according to the sign of the reaction term and are linearized in order to avoid the numerical solution of a fully nonlinear problem. Concerning the spatial discretization, we simply apply a fourth order central finite differente method to the Δ operator. A fourth order accurate scheme for spatial derivatives is applied in order to bring out the order of accuracy of the second and third order time discretization.

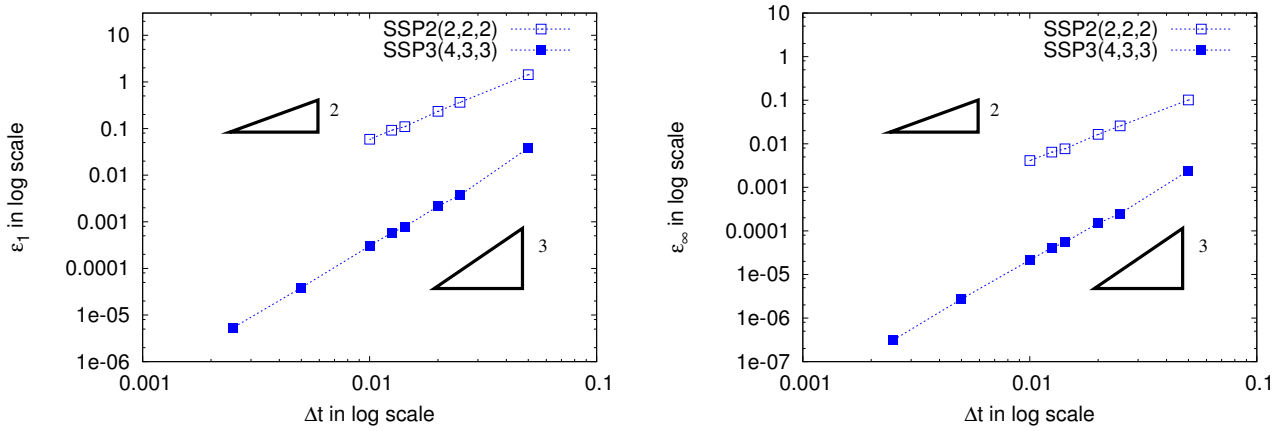
To estimate the order of accuracy of the schemes we compute a numerical approximation and refine the time step Δt according to the space step $\Delta x = \Delta y$ in such a way the CFL condition associated to the diffusion operator is violated, that is, we apply an hyperbolic CFL condition where we refine the time step and the space step simultaneously

$$\lambda \; = \; \frac{2\Delta t}{\Delta x},$$

with $\lambda = 1$.

Obviously, for a fully explicit scheme like the Runge-Kutta method, this condition would lead to some instabilities of the numerical solution since a parabolic CFL is necessary.

The semi-implicit schemes are expected to be stable even for large time step when the parabolic CFL condition is not satisfied. Absolute error in L^1 and L^∞ norms at time $T = 2$ are shown in Figure 1 for the IMEX-SSP2(2,2,2) L-stable scheme (21) but also for the IMEX-SSP3(4,3,3) L-stable scheme (26). As expected the order of accuracy is satisfied for all second and third order schemes.



(a) L^1 error norm (b) L^∞ error norm

FIGURE 1. Test 1 - Reaction-diffusion problem: (a) L^1 error norm and (b) L^∞ error norm for the IMEX-SSP2(2,2,2) L-stable scheme (21) and for the IMEX-SSP3(4,3,3) L-stable scheme (26).

3.2. **Test 2 - Nonlinear convection-diffusion equation.** We consider the following nonlinear convection diffusion equation on the whole space $\mathbb{R}^2$ and apply a fourth order central finite difference

scheme for the first and second spatial derivatives

$$\begin{cases} \dfrac{\partial \omega}{\partial t} + [V + \mu \nabla \log(\omega)] \cdot \nabla \omega - \mu \Delta \omega = 0, \quad (t,x) \in \mathbb{R}^+ \times \mathbb{R}^2, \\ \omega_0(t=0) = e^{-\|x\|^2/2}, \end{cases}$$

where $V = {}^t(1,1)$, $\mu = 0.5$. The exact solution is given by

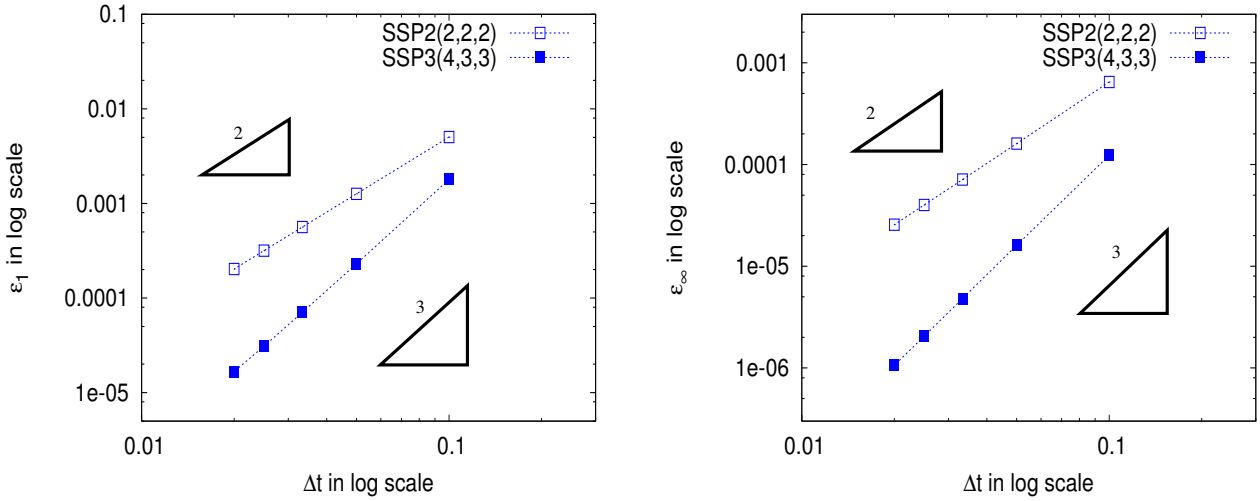
$$\omega(t,x) = \frac{1}{\sqrt{4\,\mu\,t+1}}\, e^{-\frac{\|x - V\,t\|^2}{8\,\mu\,t+2}}, \quad t \geq 0, \quad x \in \mathbb{R}^2.$$

After the space discretization, we apply our semi-implicit scheme (14)-(15) by writing the system of ODEs in the form (3) with u the component treated explicitly, v the component treated implicitly and

$$\mathcal{H}(t,u,v) = -(V + \mu \nabla \log(u)) \cdot \nabla v + \mu \Delta v.$$

We treat both the convection and diffusion implicitly but we only deal with a linear system at each time step. The computational domain in space is $(-10,10)^2$ and the final time is $T = 0.5$. As in the previous case, the space step is chosen sufficiently small to neglect the influence of the space discretization and the time step Δt is taken proportional to Δx such that $\Delta t = \lambda \Delta x$, with $\lambda = 1$. Therefore, the classical CFL condition for convection diffusion problem $\Delta t = O(\Delta x^2)$ is not verified.

In Figure 2 we present the numerical error both for L^1 and L^∞ norms for the IMEX-SSP2(2,2,2) L-stable scheme (21) and the IMEX-SSP3(4,3,3) L-stable scheme (26) and still verify the correct order of accuracy.



(a) L^1 error norm (b) L^∞ error norm

FIGURE 2. Test 2 - Nonlinear convection-diffusion problem: (a) L^1 error norm and (b) L^∞ error norm for the second order IMEX-SSP2(2,2,2) L-stable scheme (21) and the third order IMEX-SSP3(4,3,3) L-stable scheme (26).

3.3. **Test 3 - Nonlinear Fokker-Planck equations for fermions and bosons.** In [15, 14], a nonlinear Fokker-Planck type equation modelling the relaxation of fermion and boson gases is studied.

This equation has a linear diffusion and a nonlinear convection term:

$$\left\{ \begin{array}{l} \dfrac{\partial \omega}{\partial t} \;=\; \mathrm{div}\left(x\,(1\,+\,k\,\omega)\,\omega \;+\; \nabla\omega\right), \quad x \in \mathbb{R}^d, \quad t>0, \\ \\ \omega(x,0)=\omega_0(x), \end{array} \right. \tag{27}$$

with $k=1$ in the boson case and $k=-1$ in the fermion case. For this equation, the explicit solution is not known except steady states, but there are several works devoted to the long time behavior based on the knowledge of the qualitative bahavior of the entropy functional. The long time behavior of this model has been rigorously investigated quite recently in [14] via an entropy-dissipation approach. More precisely, the stationary solution of (27) is given by the Fermi-Dirac ($k=-1$) and Bose-Einstein ($k=1$) distributions:

$$\omega^{eq}(x) = \frac{1}{\beta e^{\frac{|x|^2}{2}} - k}, \tag{28}$$

where $\beta \geq 0$ is such that ω^{eq} has the same mass as the initial data ω_0. For this equation, there exists an entropy functional given by

$$\mathcal{E}(\omega) := \int_{\mathbb{R}^d} \left(\frac{|x|^2}{2}\omega \;+\; \omega\log(\omega) - k(1+k\omega)\log(1+k\omega) \right) dx,$$

such that

$$\frac{d}{dt}\mathcal{E}(\omega) \;=\; -\mathcal{I}(t),$$

where the entropy dissipation $\mathcal{I}(t)$ is defined by

$$\mathcal{I}(t) \;:=\; \int_{\mathbb{R}^d} \omega\,(1+k\omega) \left| \nabla \left(\frac{|x|^2}{2} + \log\left(\frac{\omega}{1+k\omega} \right) \right) \right|^2 dx.$$

Then decay rates towards equilibrium are given in [15, 14] for fermion case in any dimension and for 1D boson case by relating the entropy and its dissipation. Here we want to approximate this nonlinear equation and study the long time behavior of the numerical solution [5].

To apply our semi-implicit scheme we rewrite this PDE in the form (3) with u the component treated explicitly, v the component treated implicitly and

$$\mathcal{H}(t,u,v) \;=\; \mathrm{div}\left(x\,(1\,+\,k\,u)\,v \;+\; \nabla v\right) = \;\mathrm{div}\left(x\,(1\,+\,k\,u)\,v\right) \;+\; \Delta v$$

and we apply a fourth order spatial discretization for the convective and diffusive components.

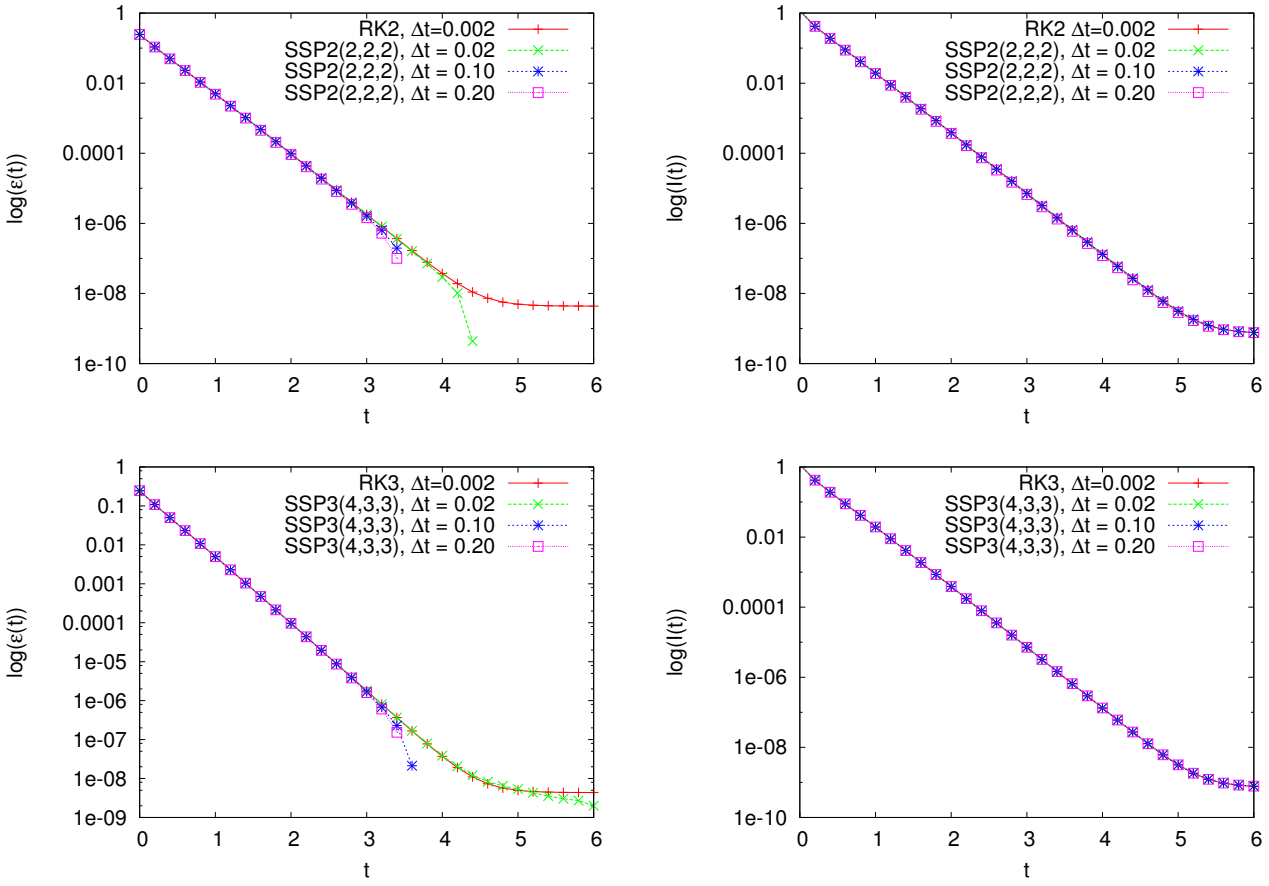
We consider the nonlinear Fokker-Planck equation (27) for fermions ($k=-1$) in 2D. The initial condition is chosen as

$$\omega_0(x) = \frac{1}{2\pi}|x|^2 \exp\left(-\frac{|x|^2}{2}\right), \quad x \in \mathbb{R}^2,$$

and the computational domain is $(-10,10)^2$ with the space step $\Delta x = 0.1$.

Evolution of the discrete relative entropy $\mathcal{E}_\Delta(t^n)$, its dissipation $\mathcal{I}_\Delta(t^n)$ and $\|\omega^n - \omega^{eq}\|_{L^1}$ is presented in Figure 3. This is obtained by second order schemes, i.e. classical second order explicit Runge-Kutta scheme and IMEX-SSP2(2,2,2) (21) (Top), and by third order schemes, i.e. classical third order explicit Runge-Kutta scheme and IMEX-SSP3(4,3,3) (26) (Botton).

We observe exponential decay rate of these quantities, which is in agreement with the result proved by J. A. Carrillo, Ph. Laurençto and J. Rosado in [14] and the numerical results proposed in [5]. Classical Runge-Kutta schemes are subject to a parabolic condition whereas semi-implicit schemes can be used with a large time step without affecting the accuracy even for large time asymptotics.



(a) relative entropy functional $\mathcal{E}(t)$ (b) entropy dissipation $\mathcal{I}(t)$

FIGURE 3. Test 3 - Fokker-Planck equation. (a) Evolution of the relative entropy $\mathcal{E}_\Delta(t^n)$ and (b) the dissipation $\mathcal{I}_\Delta(t^n)$ for the second order explicit Runge-Kutta scheme and for the IMEX R-K SSP(2,2,2) scheme (21) (Top) and for the third order explicit third order Runge-Kutta scheme and IMEX-SSP(4,3,3) scheme (26) (Bottom).

3.4. **Test 4 - Hele-Shaw flow.** In this section we consider a fourth order nonlinear degenerate diffusion equation in one space dimension called the Hele-Shaw cell [3, 28]

$$\frac{\partial \omega}{\partial t} + \frac{\partial}{\partial x}\left(\omega \frac{\partial^3 \omega}{\partial x^3}\right) = 0, \quad x \in \mathbb{R}, \quad t \geq 0, \tag{29}$$

with $\omega(x, t = 0) = \omega_0(x) \geq 0$.

One of the remarkable features of equation (29) is that its nonlinearity guarantees the nonnegativity preserving property of the solution [4] and the conservation of mass

$$\int_{\mathbb{R}} \omega(t, x)dx = \int_{\mathbb{R}} \omega_0(x)dx.$$

Moreover there is dissipation of surface-tension energy, that is,

$$\frac{d}{dt}\int_{\mathbb{R}} \left|\frac{\partial \omega}{\partial x}\right|^2 dx = -\int_{\mathbb{R}} \omega \left|\frac{\partial^3 \omega}{\partial x^3}\right|^2 dx,$$

and dissipation of an entropy which highlights similarities with the Boltzmann equation

$$\frac{d}{dt}\int_{\mathbb{R}} \omega \, \log(\omega) dx = -\int_{\mathbb{R}} \left|\frac{\partial^2 \omega}{\partial x^2}\right|^2 \, dx.$$

On the one hand, we compare the numerical results obtained with our numerical approximation with the similarity property of monotonicity in time of solution

$$\omega(t,x) = \frac{1}{120(t+\tau)^{1/5}} \left[r^2 - \frac{x^2}{(t+\tau)^{2/5}}\right]_+^2,$$

where $[\cdot]_+$ denotes the positive part. We have chosen $r = 2$, $\tau = 4^{-5}$ and $x \in (-2, 2)$. This solution is only $\omega \in C^1(\mathbb{R}\times\mathbb{R})$ but the second derivative in space is discountinuous, therefore we cannot expect high order accuracy. Exact and numerical solutions at various times are reported in Fig. 5.

On the other hand, we consider the same problem with a given source term

$$f(\tau,x) = \frac{1}{8\tau^4} \exp\left(-\frac{x^2}{4\tau}\right) \left(2\,x^2\,\tau^2 + \left(x^4 + 6\tau^2 - 9x^2\tau\right) \exp\left(-\frac{x^2}{4\tau}\right)\right),$$

with $\tau = t + 1$ such that the exact solution is smooth and given by $\omega_{exact}(t,x) = \exp\left(-x^2/4(t+1)\right)$.

For the time discretization we apply the scheme (26) by writing the system of ODEs in the form (3) with u the component treated explicitly and the v component treated implicitly:

$$\mathcal{H}(t,u,v) \;=\; -\frac{\partial}{\partial x}\left(u\frac{\partial^3 v}{\partial x^3}\right) + f(t+1,x).$$

Concerning the space discretization, we apply a second order centred finite difference scheme for the space discretization

$$\mathcal{H}_\Delta(t,u_i,v_i) \;=\; -\frac{\mathcal{F}_{i+1/2} - \mathcal{F}_{i-1/2}}{\Delta x} + f(t+1,x_i),$$

with

$$\mathcal{F}_{i+1/2} = u_{i+1/2}\frac{v_{i+2} - 3v_i + 3v_{i-1} - v_{i-2}}{\Delta x^3},$$

with $u_{i+1/2} = (u_i + u_{i+1})/2$. The time step is chosen as previously such that Δt is proportional to the space step Δx. In this way the stability condition associated to an explicit time discretisation for this problem, i.e. $\Delta t \le C\Delta x^4$, is strongly violated.

The numerical error in L^1 and L^∞ for both test cases are reported in Fig. 4 at the final time $t = 0.35$. We observe a rate of convergence about 1.6 for both L^1 and L^∞ norms for the non smooth solution and second order accuracy for the smooth solution.

Of course for these large time steps, the numerical scheme does not preserve positivity, but only some small spurious oscillations occur for short times and then they are damped after several time iteration thanks to the diffusion process (see Fig. 5).

3.5. **Test 5 - Surface diffusion flow.** In this section, we consider the surface diffusion of graphs [18]

$$\frac{\partial \omega}{\partial t} + \mathrm{div} S(\omega) \;=\; 0, \quad x \in \mathbb{R}^2, \quad t \ge 0,$$

where the nonlinear differential operator S is given by

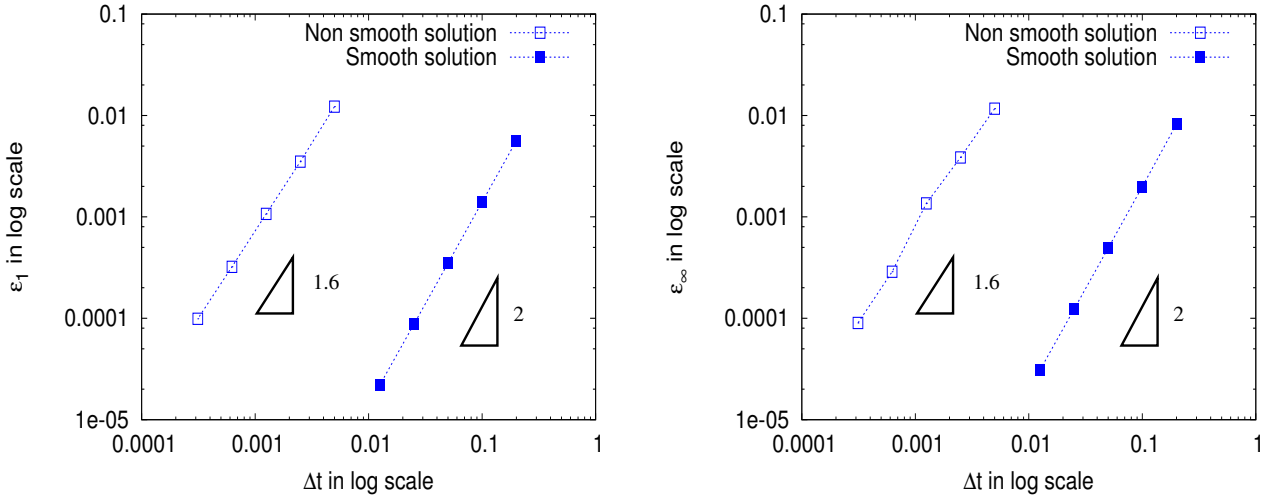
$$S(\omega) := \left(Q(\omega)\left(I - \frac{\nabla\omega\otimes\nabla\omega}{Q^2(\omega)}\right)\nabla N(\omega)\right),$$

where Q is the area element

$$Q(\omega) = \sqrt{1 + |\nabla\omega|^2}$$

and N is the mean curvature of the domain boundary Γ

$$N(\omega) := \left(\frac{\nabla\omega}{Q(\omega)}\right).$$



(a) L^1 error norm (b) L^∞ error norm

FIGURE 4. Test 4 - Hele-Shaw flow : (a) L^1 error norm and (b) L^∞ error norm for the IMEX-SSP2(2,2,2) L-stable scheme (21).

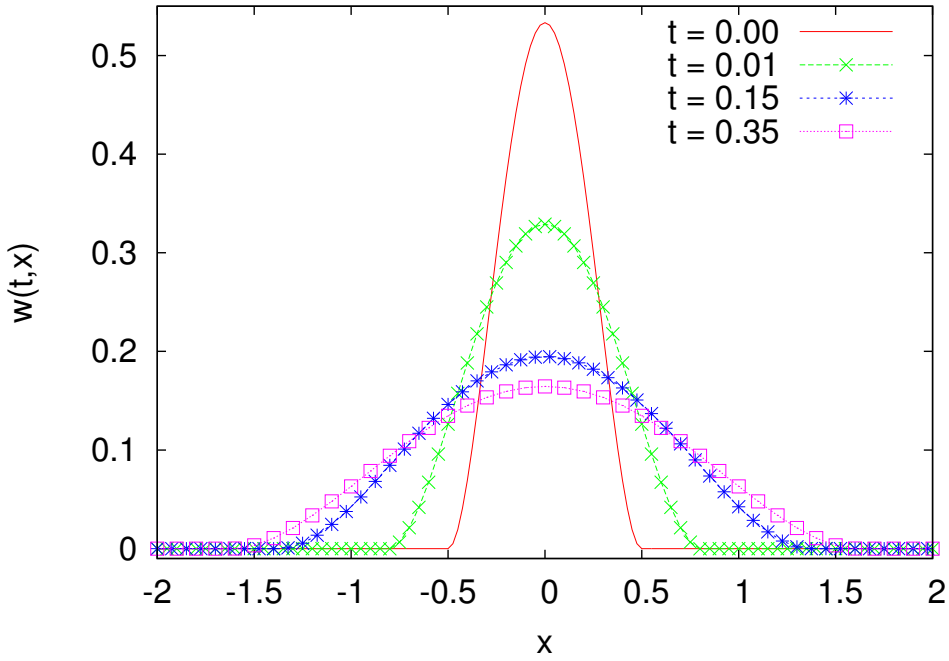


FIGURE 5. Test 4 - Hele-Shaw flow : time evolution of the numerical solution for the IMEX-SSP3(4,3,3) L-stable scheme (26) for $t = 0$, 0.01, 0.15 and 0.35.

The surface diffusion equation models the diffusion of mass within the bounding surface of a solid body, where $V = \Delta_\Gamma N(\omega)$ is the normal velocity of the evolving surface Γ,

$$V = -\frac{1}{Q(u)}\frac{\partial u}{\partial t},$$

and Δ_Γ denotes the Laplace-Beltrami operator [18].

There are many applications of these models, such as body shape dynamics, surface construction, computer data processing or image processing. This equation is a highly nonlinear fourth-order PDE. The higher order differential operators and additional nonlinearities for these kind of problems are difficult to analyze and to simulate numerically due to the stiffness of order Δx^4, where Δx is the space step [30]. We will apply our stable high order accurate methods based on semi-implicit time discretizations. Moreover, we will compare our time discretization with the one proposed by P. Smereka in [29] or in [19], where the operator S is split in two parts

$$S(\omega) = \underbrace{S(\omega) - \beta\,\Delta^2\omega}_{\text{less stiff part}} + \underbrace{\beta\,\Delta^2\omega}_{\text{stiff, dissipative part}},$$

where β is a free parameter to be determined and in [29] it is chosen as $\beta = 2$. The first part is then treated explicitly whereas the stiff and dissipative part is treated implicitly. This splitting technique is very effective to stabilize numerical schemes but it may affect the numerical accuracy.

With our approach there is no need to add and subtract terms, because the system is automatically stabilized by the proper choice of the variable that will be implicitly treated.

The solution of the surface diffusion of graphs verifies

$$\frac{1}{2}\frac{d}{dt}\int_\Omega \omega^2 dx + \int_\omega N^2(\omega) dx = 0,$$

giving L^2 stability.

We consider numerical solutions of the two-dimensional surface diffusion of graphs equation with the initial condition

$$\omega_0(x) = \frac{1}{2\pi T}\exp\left(-\frac{|x|^2}{2T}\right).$$

The computational domain is $(-10, 10)^2$ and we use a second order central finite difference scheme together with the second order SSP2(2,2,2) scheme (21) with

$$\mathcal{H}(u,v) := \left(Q(u)\left(I - \frac{\nabla u \otimes \nabla u}{Q^2(u)}\right)\nabla\mathcal{N}(u,v)\right),$$

and $\mathcal{N}$

$$\mathcal{N}(u,v) := \left(\frac{\nabla v}{Q(u)}\right).$$

We present in Figure 6 the time evolution of the L^2 norm of the numerical solution and its dissipation :

$$\frac{d}{dt}\mathcal{E}(\omega) \;=\; -\mathcal{I}(t),$$

where the functional $\mathcal{E}(\omega)$ and the dissipation $\mathcal{I}(t)$ are defined by

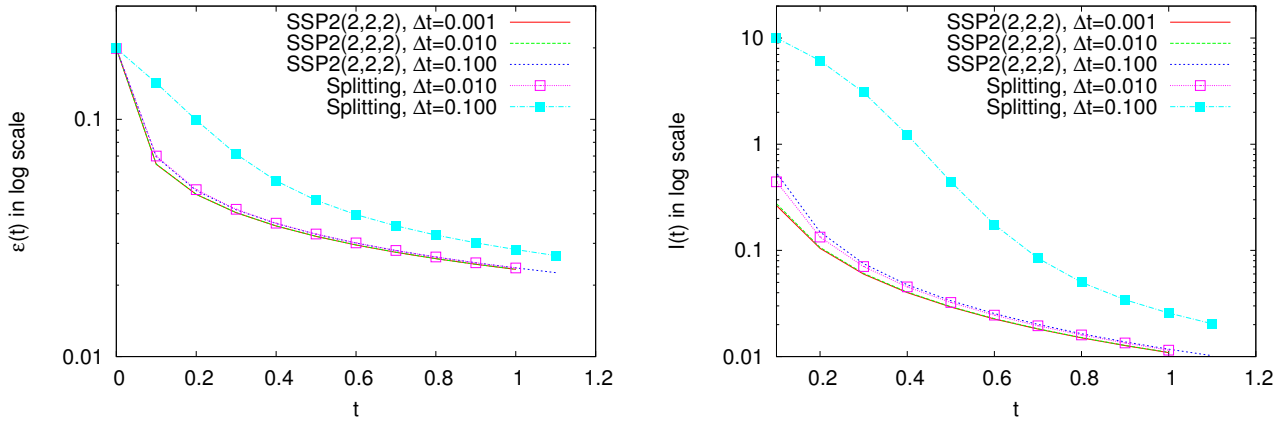
$$\mathcal{E}(\omega) = \int_\Omega \omega^2(t,x)dx, \qquad \mathcal{I}(t) = \int_\Omega N^2(\omega(t,x))dx.$$

The results show that our second order numerical scheme (21) is stable and accurate for large time steps whereas the one based on the splitting technique given in [29] is stable but less accurate for large time step $\Delta t = 0.1$. These numerical simulations illustrate the efficiency of our approach based on semi-implicit numerical schemes.

4. Stability analysis

In this section we perform a stability analysis of our schemes and introduce a new notion of stability taking into account that the implicit component is chosen accordingly to the stiffness of the initial problem.

We limit our analysis to the simpler linear case, while the fully non linear case requires further investigation. Since penalization method in the form 4 is a very common tool in several applications,



(a) functional $\mathcal{E}(t)$ (b) dissipation $\mathcal{I}(t)$

FIGURE 6. Test 5 - Surface diffusion flow. (a) Evolution of the L^2 norm and (b) the dissipation $\mathcal{I}_\Delta(t^n)$ for second order IMEX-SSP(2,2,2) L-stable scheme (21) and the one proposed in [29] based on a splitting technique in log scale.

we perform a general analysis of the IMEX Runge-Kutta schemes applied to the linear version of Eq.(4).

In order to introduce this, we consider the linear test equation

$$y' = \lambda y, \quad \lambda \in \mathbb{C}, \tag{30}$$

with $Re(\lambda) \leq 0$. A classical s-stage Runge-Kutta method with $b^T = (b_1, \cdots, b_s)$ and $A = (a_{ij})_{i,j=1,\cdots,s}$ applied to (30) yields

$$y^{n+1} \;=\; R(z)\, y^n, \tag{31}$$

with $z = \lambda\, h$ and $R(z) = 1 + z\, b^T (I, -z\, A)^{-1}\mathbf{1}$ and $\mathbf{1} = (1, 1, ..., 1)^T$. The function $R(z)$ is called the stability function of the Runge-Kutta method. Furthermore the stability function $R(z)$ of the method satisfies [21]

$$R(z) \;=\; \frac{\det(I \;-\; z\, A \;+\; z\mathbf{1}b^T)}{\det(I \;-\; z\, A)}.$$

From such relaxation one observes that the stability function $R(z)$ for s-stages explicit Runge-Kutta methods becomes a polynomial in the variable z, that is, if the method is of order p, then

$$R(z) \;=\; 1 + z + \frac{z^2}{2!} + \cdots + \frac{z^p}{p!} + \mathcal{O}(z^{p+1}).$$

Instead the stability function $R(z)$ for s-stages implicit Runge-Kutta methods becomes a rational function with numerator and denominator of degree less or equal s, *i.e.*

$$R(z) = \frac{P(z)}{Q(z)}, \quad \text{where } deg(P) = k, \quad \deg(Q) = j, \quad q = \max(k, j).$$

Now to analyse the stability properties of our semi-implicit methods (14)-(15), we write (30) as

$$y' \;=\; \underbrace{(\lambda + \mu)y}_{explicit} \;-\; \underbrace{\mu y}_{implicit}, \quad \lambda \in \mathbb{C}, \quad Re(\lambda) \leq 0, \quad \mu \in \mathbb{R}^+ \tag{32}$$

and applying the method (14)-(15) to the equation (32) with $y(t_0) = y_0 = 1$ and with $\mathcal{H}(t, y, y) = (\lambda + \mu)y - \mu y$, it yields

$$\begin{cases} k_i \;=\; (z+\eta)\left(1 \;+\; \displaystyle\sum_{j=1}^{i-1} \hat{a}_{ij} k_j\right) \;-\; \eta\left(1 + \displaystyle\sum_{j=1}^{i-1} a_{ij} k_j\right) \;-\; \eta\, a_{ii}\, k_i, \quad i = 1, \cdots, s, \\ \\ y^1 \;=\; 1 + \displaystyle\sum_{i=1}^{s} b_i k_i, \end{cases} \tag{33}$$

where $z = \lambda \Delta t$ and $\eta = \mu \Delta t$. Setting $a_{ii} = q_i$ for all i we get

$$k_i \;=\; \frac{1}{1+\eta q_i}\left[z\left(1 \;+\; \sum_{j=1}^{i-1} \hat{a}_{ij}\, k_j\right) \;+\; \eta \sum_{j=1}^{i-1} (\hat{a}_{ij} \;-\; a_{ij})\; k_j \right], \quad i = 1, \cdots, s.$$

Substituting the expression of k_i in the numerical solution we can write the stability function of method (14)-(15) as

$$R(z, \eta) \;=\; \frac{P(z, \eta)}{Q(\eta)}, \tag{34}$$

with numerator and denominator of degree less or equal s. Then as for a Runge-Kutta scheme, the function $R(z, \eta)$ is called the *stability function* of method (14)-(15). In classical A-stability analysis one considers the region S_A of the complex plane for which the stability function is less or equal one, *i.e.*

$$S_A = \{z \in \mathbb{C} : |R(z)| \leq 1\}.$$

However, when we add and subtract the term μy in (30), we observe that the stability function depends on the additional parameter $\eta = \mu \Delta t$, *i.e.*

$$R := R(z, \eta)$$

and we note that classical stability function of the explicit scheme is given by $R(z) = R(z, 0)$. When we increase the the parameter η, the stability region grows, and therefore the stability function depends on η:

$$S_A(\eta) = \{z \in \mathbb{C} : |R(z, \eta)| \leq 1\}.$$

As an example, let us consider the second order semi-implicit Runge-Kutta scheme (19). In Figure 7, we plot the region $S_A(\eta)$ for different values of the parameter η.

The region corresponding to the limit $\eta \to 0$ will include the whole complex half plane $Re(z) \leq 0$. This motivates the following definition

Definition 4.1. *A semi-implicit scheme of the form (14)-(15) is said A_η-stable if*

$$\forall \quad z \in \mathring{\mathbb{C}}^- \quad \exists \quad \eta > 0 : z \in S_A(\eta). \tag{35}$$

4.1. **Analysis of F-stability.** Because in general the region $S_A(\eta)$ increases without bounds as $\eta \to \infty$, it may be more convenient to introduce the rescaled variable $\zeta = z/\eta$, and the corresponding stability region $S_F(\eta)$ in the new variable ζ is

$$S_F(\eta) = \{\zeta \in \mathbb{C} : |R(\zeta\eta, \eta)| \leq 1\}. \tag{36}$$

For example, the region $S_F(\eta)$ corresponding to (19) for increasing values of η is reported in Figure 8. On the one hand, we note that $z \in S_A(\eta)$ is equivalent to $\zeta \in S_F(\eta)$. On the other hand, we observe that, as $\eta \to \infty$, the region converges to a limit region $S_\infty = S_F(\infty)$. Such convergence appears to be monotonic in this case, at least for sufficiently large values of η. This behavior suggests us to adopt the following definition for the domain of F-stability, *i.e.* Forced-stability.

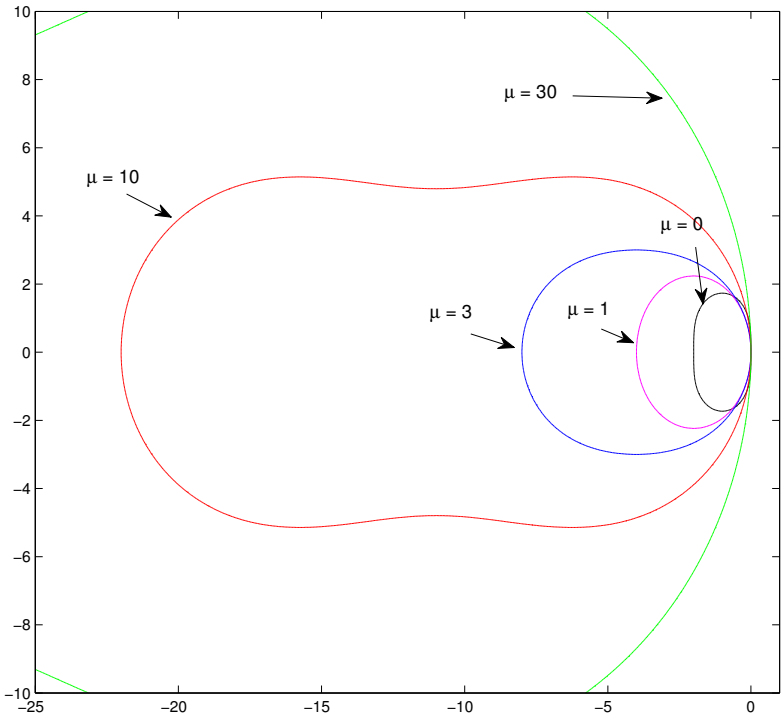


FIGURE 7. Stability Domains $S_A(\eta)$ for scheme (19) and values of $\eta = 0, 1, 3, 10, 30$.

Definition 4.2. *For a semi-implicit scheme of the form (14)-(15), we define the domain of F-stability as*

$$S_F = \{\zeta \in \mathbb{C} : sup_{\eta\in\mathbb{R}^+}|R(\zeta\eta, \eta)| \leq 1\}.$$

Then, we introduce the notion of F-stability as

Definition 4.3. *A semi-implicit scheme of the form (14)-(15) is said F-stable if*

$$\forall \quad z \in \mathring{\mathbb{C}}^- \quad \exists \quad \eta > 0 : z/\eta \in S_F.$$

This condition is more restrictive than (35), but is more convenient, because the region S_F does not depend on η. We conjecture that the two definitions are equivalent for all practical purposes.

It is clear from the definition that $S_F \subseteq S_\infty$. In all the schemes considered here we observe a monotonic convergence of $S_F(\eta) \to S_\infty$, and therefore that $S_F = S_\infty$. This suggests to formulate the following conjecture:

Conjecture 4.1. *Under general assumption it is: $S_F = S_\infty$.*

To prove such conjecture in general is technically difficult, and it will be investigated in a future work. Next we shall give some numerical evidence in order to validate this for some particular semi-implicit scheme.

Now we give an explicit representation of the stability function (34). By formula (34) the stability function $R(z, \eta)$ for a method (14)-(15) is of the form

$$R(z, \eta) = \frac{P(z, \eta)}{(1 + a_{11}\eta)(1 + a_{22}\eta)\cdots(1 + a_{ss}\eta)},$$

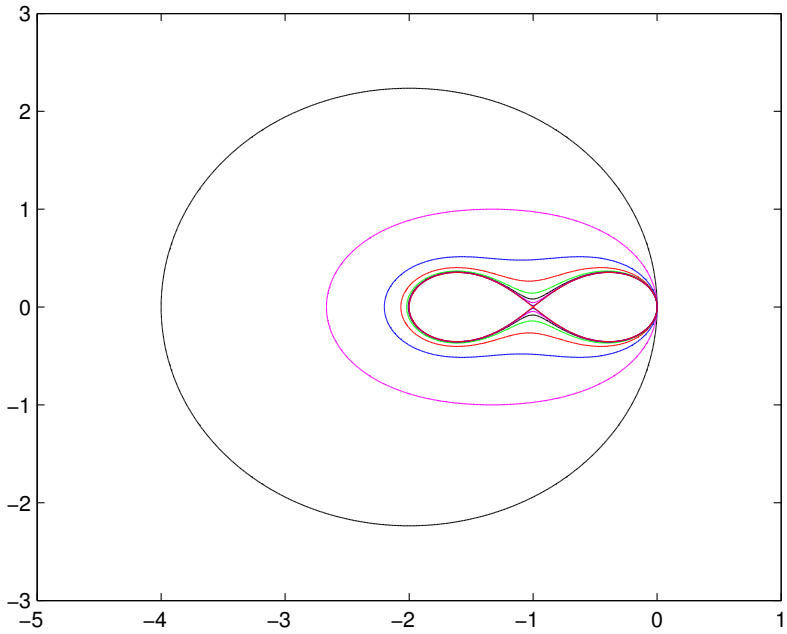


FIGURE 8. Stability Domains $S_F(\eta)$ for (19) and values of $\eta = 1, 3, 10, 30, 100, 300, 1000, 10000, 100000$.

because the determinant of the triangular matrix of the implicit method is the product of its diagonal entries. In particular if the implicit method is SDIRK with $a_{11} = a_{22} = \cdots = a_{ss} = \gamma$ we obtain

$$R(z,\eta) = \frac{P(z,\eta)}{(1+\gamma\eta)^s}.$$

An explicit form of the stability function is

$$R(z,\eta) = 1 + z\sum_{i=1}^{s} b_i \alpha_i(z,\eta),$$

with

$$\alpha_i(z,\eta) \;=\; \frac{1}{1+q_i\eta}\sum_{j=1}^{i} P_{i,j}(z,\eta),$$

and

$$\begin{cases} P_{i,i}(z,\eta) = 1, \quad 1 \le i \le s, \\ \\ P_{i,j}(z,\eta) = \displaystyle\sum_{m=j}^{i-1} \frac{1}{1+q_m\eta}\left(\hat{a}_{im}\,(z\,+\,\eta)\,-\,a_{im}\eta\right) P_{m,j}(z,\eta), \quad 1 \le j < i \le s, \end{cases}$$

where $q_i := a_{ii}$, for $i = 1, \cdots, s$. Then this leads to the following statement

Proposition 4.1. *The internal stage are given by:*

$$k_i = \frac{z}{1+q_i\eta}\sum_{j=1}^{i} P_{ij}(z,\eta), \quad 1 \le i \le s.$$

In the limit $\eta \to \infty$, with $\zeta = z/\eta$ we get

$$R^*(\zeta) = 1 + \zeta \sum_{i=1}^{s} b_i \alpha_i^*(\zeta),$$

with

$$\alpha_i^*(\zeta) = q_i^{-1} \sum_{j=1}^{i} P_{i,j}^*(\zeta),$$

and

$$\begin{cases} P_{i,i}^*(\zeta) = 1, \quad 1 \le i \le s, \\ \\ P_{i,j}^*(\zeta) = \displaystyle\sum_{m=j}^{i-1} q_m^{-1} \left(\hat{a}_{im}(1+\zeta) - a_{im}\right) P_{m,j}^*(\zeta), \quad 1 \le j < i \le s. \end{cases}$$

Finally we conclude this section considering schemes of type CK, *i.e.* $a_{11} = 0$ in the implicit part. Here we want to analyze the conditions under which the scheme is stable when $\eta \to \infty$. We consider system (33) and apply an IMEX Runge-Kutta scheme of type CK, obtaining, in vector notation

$$(I + \eta D)\boldsymbol{K} = z\boldsymbol{e} + ((z+\eta)\hat{\boldsymbol{a}} - \eta \boldsymbol{a})K_1 + ((z+\eta)\hat{\mathcal{A}}\boldsymbol{K} - \eta\mathcal{A})\hat{K}. \tag{37}$$

where $\boldsymbol{K} = (K_2, \cdots, K_s)^T \in \mathbb{R}^{s-1}$ and $\boldsymbol{K}_1 = z$, $\hat{\boldsymbol{a}} = (\hat{a}_{21}, \cdots, \hat{a}_{s1})^T$, $\boldsymbol{a} = (a_{21}, \cdots, a_{s1})^T$, $\mathcal{A} \in \mathbb{R}^{s-1 \times s-1}$ sub-metrix of A and $\hat{\mathcal{A}} \in \mathbb{R}^{s-1 \times s-1}$ sub-metrix of $\hat{A}$. We can rewrite (37) as

$$\left(\frac{1}{\eta} I + \mathcal{C}\right) \boldsymbol{K} = \zeta \left(\boldsymbol{e} + \eta\, \boldsymbol{c}\right), \tag{38}$$

where $\mathcal{C} := \mathcal{C}(\zeta) = (D - \zeta\hat{\mathcal{A}} - (\hat{\mathcal{A}} - \mathcal{A}))$, $\boldsymbol{c} := \boldsymbol{c}(\zeta) = \zeta\hat{\boldsymbol{a}} - (\hat{\boldsymbol{a}} - \boldsymbol{a})$ and $K_1 = \eta\zeta$. Then we obtain

$$\boldsymbol{K} = \left(\frac{1}{\eta} I + \mathcal{C}\right)^{-1} \zeta(\boldsymbol{e} + \eta\boldsymbol{c}). \tag{39}$$

The numerical solution y_1 can be written in the following form $y_1 = 1 + b_1 K_1 + \boldsymbol{b}^T \boldsymbol{K}$, with $\boldsymbol{b}^T = (b_2, \cdots, b_s)$, hence we get

$$y_1 = 1 + \zeta \left(b_1 \eta \boldsymbol{e} + \eta \boldsymbol{b}^T \left(\frac{1}{\eta} I + \mathcal{C}\right)^{-1} (\boldsymbol{e} + \eta \boldsymbol{c}) \right). \tag{40}$$

Therefore, by

$$\left(\frac{1}{\eta} I + \mathcal{C}\right)^{-1} = \left(I + \frac{1}{\eta}\mathcal{C}^{-1}\right)^{-1} \mathcal{C}^{-1} = \left(I - \frac{1}{\eta}\mathcal{C}^{-1} + \frac{1}{\eta^2}\mathcal{C}^{-2} + \cdots\right) \mathcal{C}^{-1}$$

and inserting the latter equality in (40), it yields

$$y_1 = 1 + \zeta \left(b_1\, \eta\, \boldsymbol{e} + \boldsymbol{b}^T \left(\frac{1}{\eta} I + \mathcal{C}\right)^{-1} \boldsymbol{e} + \boldsymbol{b}^T \mathcal{C}^{-1} \boldsymbol{c}\, \eta - \boldsymbol{b}^T \mathcal{C}^{-2} \boldsymbol{c} + \mathcal{O}\left(\frac{1}{\eta}\right) \right),$$

hence when $\eta \to \infty$ we require that

$$b_1 = 0, \quad \boldsymbol{b}^T \mathcal{C}^{-1}(\zeta) \boldsymbol{c}(\zeta) = 0 \quad \forall \zeta \tag{41}$$

otherwise the numerical solution does not converge and blows up. If conditions (41) are satisfied then we have

$$y^1 = 1 + \zeta \left(\boldsymbol{b}^T \mathcal{C}^{-1} \left(\boldsymbol{e} + \mathcal{C}^{-1} \boldsymbol{c}\right) \right).$$

We note that in general classical IMEX Runge-Kutta schemes of type CK presented in the literature do not satisfy conditions (41). As for IMEX Runge-Kutta schemes of type ARS, the condition $b_1 = 0$ is automatically satisfied in (41), the second one is not.

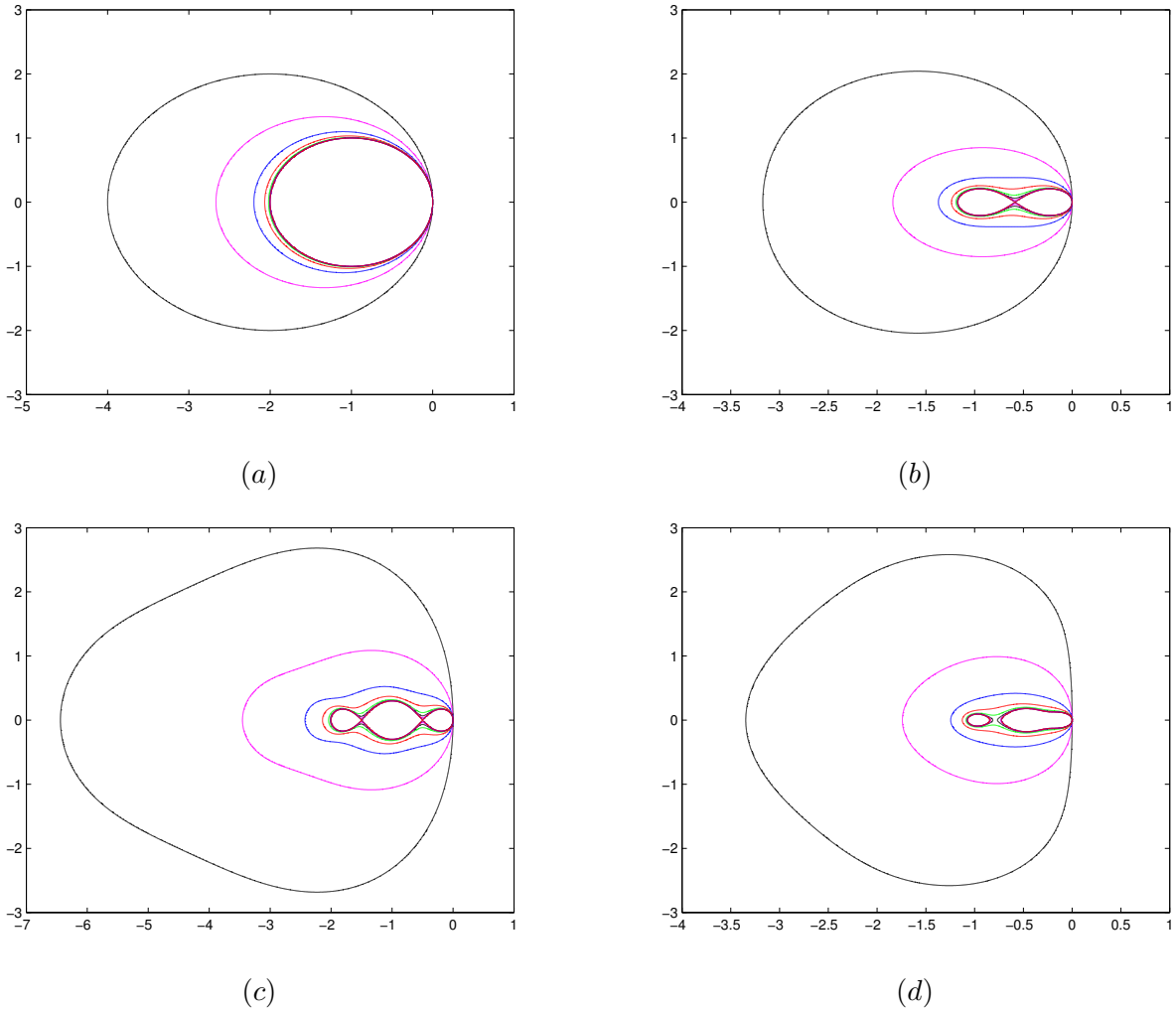


FIGURE 9. Stability Domains $R(\eta\,\zeta, \eta)$ for scheme (42) (a), scheme (21) (b), scheme (22) (c) and scheme (26) (d) for different increasing values of $\eta = 1, 3, 10, 30, 100, 300, 1000, 10000, 100000$

The possibility of finding new schemes of type CK satisfying these additional conditions is presently under investigation. In the present paper we shall limit ourselves to schemes of type A.

4.2. **F-stable schemes.** Now we list several F-stable schemes and we plot their stability domain $S_F(\eta)$ varying $\eta \in \mathbb{R}^+$. First we consider the classical forward-backward Euler scheme (FBE-IMEX), *i.e.*

$$\begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array} \qquad \begin{array}{c|c} 1 & 1 \\ \hline & 1 \end{array}, \tag{42}$$

it is F-stable and its stability domain is represented in Fig. 9. In section 2.3 we introduced several F-stable second order semi-implicit schemes of type A as (19), and (21)-(22) which are stiffly accurate schemes. Notice that several semi-implicit Runge-Kutta schemes of type A presented in section 2.3, as (21) and (22) and the third order scheme (26), were already proposed in [27]. Their stability regions $R(\zeta\eta, \eta)$ are represented in Fig. 8 and 9.

Now, as an example, in order to describe the pictures in Fig. 8 and 9, we investigate the general second order 2-stage semi-implicit scheme(17)-(18) . Then applying this method to the test equation

(32), calculations lead to the numerical solution $y_1 = R(\eta\zeta, \eta)y_0$ with

$$R(\eta\zeta, \eta) = \frac{\eta^2(\gamma^2 + 2\gamma\zeta + \frac{1}{2}\zeta^2) + \eta(2\gamma + \zeta) + 1}{(1 + \gamma\eta)^2}. \tag{43}$$

If $\eta \to 0$ this stability function converges to the following limit stability function:

$$R^*(\zeta) = 1 + 2\frac{\zeta}{\gamma} + \frac{\zeta^2}{2\gamma^2}. \tag{44}$$

In the Figure 8 the corresponding stability domains of (43) for different increasing values of $\eta \in \mathbb{R}^+$ are displayed for the scheme (42). We observe that the domains of $R(\eta\zeta, \eta)$ converges to the limit stability domain $R^*(\zeta)$ when $\eta \to \infty$. We note that the intersection of the limit stability domain $R^*(\zeta)$ with the negative real axis correspond to the values 0, -2γ and -4γ. This is trivial to prove by solving $R^*(\zeta) = \pm 1$ with $\zeta \in \mathbb{R}$. In particular, if we substitute these values to the stability function (43) we have $|R(\eta\zeta, \eta)| < 1$ and in the limit $\eta \to \infty$ it converges to ± 1.

Finally, in order to understand better the conjecture, its proof necessitates several preliminary results which are given by some analysis on semi-implicit Runge-Kutta schemes.

By the stability function $R(z, \eta)$,

$$R(z, \eta) = \frac{P(z, \eta)}{Q(\eta)}.$$

the stability region $S_F(\eta)$ (36) can be written as

$$S_F(\eta) = \{\zeta \in \mathbb{C} : F(\zeta, \eta) \geq 0\},$$

where $F(\zeta, \eta) = Q^2(\eta) - |P(\zeta, \eta)|^2$. A sufficient condition to prove that $S_\infty = S_F$ is that

$$\frac{\partial F}{\partial \eta} \leq 0, \quad \eta \geq 0, \quad \zeta \in S_\infty.$$

To prove such condition in general is technically difficult, then we just give a numerical evidence that this condition is indeed satisfied for the scheme (17)-(18), with stability function given by Eq. (43).

In Figure 10 we show the zero level sets of the function $\partial F/\partial\eta$ for various values of η, namely for $\eta = 1/5,\ 1/3,\ 1/2,\ 1,\ 2,\ 5,\ \infty$. The white region at the center is the intersection of the regions where $\partial F/\partial\eta \leq 0$, suggesting that such condition is satisfied for any $\eta \geq 0$, in a neighborhood of the limit region S_∞, which therefore coincides with S_F.

5. Acknowledgements

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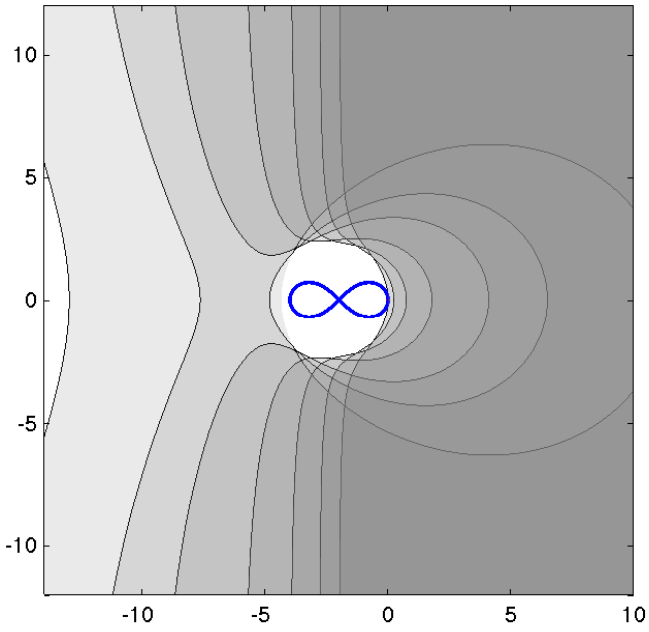

FIGURE 10. The regions in gray represent the sets in which $\partial F/\partial \eta \geq 0$, for various values of η. The white region at the center is the intersection of the regions for which $\partial F/\partial \eta \leq 0$

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