Mathematical Models and Methods in Applied Sciences

FRACTIONAL STEP METHODS FOR SPECTRAL APPROXIMATION OF ADVECTION-DIFFUSION EQUATIONS

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Several classical fractional step schemes are proposed for the spectral approximation of advection-diffusion equation in two-dimensional geometries. Suitable boundary conditions are studied in order to preserve the accuracy of the schemes at each step. An example is given about the application of the fractional step schemes to solve problems with large Péclet number.

1. Introduction

The fractional step schemes are based on the idea of splitting a differential operator into the sum of terms of simpler form, in order to reduce the resolution of the original equation to a sequence of simpler subproblems.
These schemes are considered in order to either reduce two or three dimensional steady problems to a sequence of one-dimensional ones (as the Alternating Direction Iterative method -ADI- [8], [2]) or to split differential operators, reflecting complex situations, in terms of simpler model problems. The idea is to subdivide each time step in two or more substeps so that intermediate solutions are computed by the resolution of a single part of the original problem (see for example [10], [6], [5]). The splitting of the differential operator can be done either at differential or at algebraic level. In the first case the problem is reformulated as a sequence of well-definite differential subproblems with their boundary conditions, each of them will then be discretized in space. In the second case the splitting is done on the algebraic structure, obtained after a suitable spatial discretization.
In this work we will focus our attention on the differential approach, in particular we propose boundary conditions which can be imposed at the intermediate substeps without loss of accuracy.
The idea is to modify the bilinear forms associated to the suboperators by suitable terms on the Neumann boundary. These terms don't change the nature of the problem but, at a fractional time level, they balance the natural boundary condition of the complete operator. More precisely, among the boundary terms arising from

integration by parts we treat implicitely only those which garantee the well-posedeness of the problem at hand.
The advection-diffusion equation is considered and the splitting proposed separates the diffusive term from the advective one. The potential numerical instability, occuring for the cases when equations are dominated by first order transport terms, can be avoided by the successive resolution of pure diffusive and advective problems. The spectral methods are used for the spatial discretization and the generalized Galerkin formulation is used in order to solve the elliptic and first order advective problems. We observe that this splitting is relevant only for the stability analysis of the schemes and not for their accuracy.

In this paper we focus our attention on two topics: the accuracy and the stability of the examined fractional step schemes. The analysis of the accuracy can be carried out on a large area of test problems: with constant and variable coefficients and with different boundary condition types. The analysis of the stability gives clear conclusions if "simple" model problem are considered, such as homogenous Dirichlet boundary conditions and constant coefficients (in this particular case the absolute stability of the scheme is ensured). In the more general case of variable coefficients or non homogeneous Dirichlet boundary conditions, our numerical results don't allow any clear conclusion about stability condition on the time-step.

An outline of this paper is as follows.
In section 2 we recall the Peaceman-Rachford, Douglas-Rachford and θ-method (or Strang method) fractional step schems as they are known in literature when they are applied to an algebraic operator splitting. The basic concept related to the accuracy, consistency and stability are recalled. In section 3 the advection diffusion problem, its variational formulation and its differential splitting are presented. In section 4, after a brief recalling of the basic definitions of spectral methods, the spectral generalized Galerkin formulation is given for the model elliptic and pure advective problems. In section 5 the approaches, used to impose the boundary conditions at the substeps, are presented and they are applied to the Peaceman-Rachford scheme; a convergence analysis is carried out. In section 6 numerical results are presented. The first tables proove the theoretical accuracy results exposed in Section 5; the following ones show the spectral radius of the step-operator matrices versus the time-step Δt, the interpolant degree N and the other parameters of the problem. Finally a problem with large Péclet number is approximated and solved by fractional step schemes, showing that fractional step schemes on the splitting of the advection diffusion problem can give succesfull results.

2. Operator Splitting and Fractional Step Methods

Let us consider the following parabolic equation:
$\forall t \in (0, \overline{t})$ look for $u(t)$:

$$\frac{\partial u}{\partial t} + \mathcal{L}u = f \qquad\qquad \text{in } \Omega \times (0, \bar{t}) \tag{2.1}$$

with initial condition $u = u_0$ in $\Omega \times \{0\}$ and suitable boundary conditions on $\partial\Omega \times (0, \bar{t})$. f is a suitable given function and $\mathcal{L}$ is a linear elliptic differential operator.

Let us introduce a discretization of the interval $[0, \bar{t}]$, say $t_0 = 0$, $t_n = t_0 + n \cdot \Delta t$, with $n = 1, ..., n_{max}$ and $n_{max} = \left[\frac{\bar{t}}{\Delta t}\right] - 1$, and let us denote $u^n = u(t_n)$, $u^{n+\alpha} = u(t_n + \alpha \cdot \Delta t)$ with $\alpha \in (0, 1]$.

We denote by L the matrix that arises from a consistent space discretization of the differential operator $\mathcal{L}$ in (2.1); now we intentionally preserve general notations, and we refer to Section 4 for a detailed description of the space discretization used in this paper. Therefore we define an algebraic splitting for L so that $L = L_1 + L_2 + ... + L_M$ with $M \geq 2$.

In this Section we present the fractional step schemes on the algebraic operator splitting, as they are more known in literature.

After we have presented the spectral approximation (Section 4), we will deal with the fractional step schemes on the differential operator splitting. However we point out that, if homogeneous Dirichlet boundary conditions are imposed in (2.1), the algebraic splitting is equivalent to the differential one.

An example of fractional step scheme applied to problem (2.1) is the following one (see [7]):

for $n = 0, ..., n_{max}$ look for u^{n+1}:

$$\begin{cases} u^0 = u_0 \\ \frac{u^{n+1/M} - u^n}{\Delta t/M} + L_1 u^n = 0 \\ \quad\vdots \\ \frac{u^{n+1} - u^{n+(M-1)/M}}{\Delta t/M} + L_M u^{n+(M-1)/M} = f^n. \end{cases} \tag{2.2}$$

This fractional step scheme has M steps, and the intermediate solution at step $n + \frac{j}{M}$ is computed by solving an implicit problem on the matrix L_j.

In order to study the convergence of the solution of a fractional step scheme to the exact solution of the original problem we need to study the stability and the consistency of the scheme itself. We will deal with these topics in the following subsections.

2.1. *Stability and Convergence Analysis*

Let $\Delta t > 0$ be a time step, and $n = 0, .., n_{max}$ such that

$$u^n = u(t_n) = u(t_0 + n\Delta t). \tag{2.3}$$

We introduce the following discretization in time for the problem (2.1):

$$\begin{cases} u^{n+1} = Tu^n + \alpha\Delta t\ F^n & n = 0, .., n_{max} \\ u^0 = u_0, \end{cases} \tag{2.4}$$

where the linear operator T is said *step operator*, α is a real positive parameter and $F^n = Sf^n$ is the image of the source term f^n by the linear *source operator* S.

We observe that every fractional step scheme can be written as (2.4) by eliminating the fractional solutions. The choice of the operators T and S characterize completely the fractional step scheme, hence the study of the fractional step scheme can be reduced to the study of the scheme (2.4).

The scheme (2.4) is said *stable* if there exist two positive constants C_1 and C_2 such that

$$||u^n||_V \leq C_1||u_0||_V + C_2 \cdot \max_{n=0,..,n_{max}} ||F^n||_V. \tag{2.5}$$

The conditions

$$||T|| < 1 \qquad \text{and} \qquad ||S|| < C, \tag{2.6}$$

where $||\cdot||$ is a suitable norm for the discrete operators T and S and C is a positive constant, are sufficient conditions to ensure the bound (2.5).
In practice to check the condition (2.6) is reduced to check that the spectral radius $\rho(T)$ of the discrete operator T is less than 1. The scheme (2.4) is said *absolutely stable* if the condition (2.5) is satisfied for every $\Delta t > 0$, otherwise the scheme is *conditionally stable* and, in general, the stability region depends from the space discretization.
A fractional step scheme is said *consistent* if the corresponding scheme (2.4) is consistent in the classical meaning. Moreover the order of accuracy of (2.4) is also the order of accuracy of the corresponding fractional step scheme.

We introduce now the fractional step schemes that we will use in the following sections and we analyze their stability, consistency and accuracy.

2.2. *The Peaceman-Rachford scheme (PR)*

The Peaceman-Rachford scheme reads:

$$\begin{cases} \frac{u^{n+1/2}-u^n}{\Delta t/2} + L_1 u^{n+1/2} + L_2 u^n = f^{n+1/2} \\ \\ \frac{u^{n+1}-u^{n+1/2}}{\Delta t/2} + L_2 u^{n+1} + L_1 u^{n+1/2} = f^{n+1/2} \end{cases} \tag{2.7}$$

The step operator associated to the PR scheme is

$$T_{PR} = \left(\frac{2}{\Delta t}I + L_2\right)^{-1} \left(\frac{2}{\Delta t}I - L_1\right) \left(\frac{2}{\Delta t}I + L_1\right)^{-1} \left(\frac{2}{\Delta t}I - L_2\right). \tag{2.8}$$

If the eigenvalues of L_1 and L_2 are non-negative and L_1 and L_2 have a common system of eigenvectors, the PR scheme is absolutely stable ([7]).

Under these assumptions, denoting by $\lambda_k^{(j)} = \alpha_k^{(j)} + i\beta_k^{(j)}$ the eigenvalues of the matrix L_j, $j = 1, 2$, the eigenvalues of T_{PR} are:

$$\lambda_{PR_k} = \left(\frac{2}{\Delta t} + \lambda_k^{(2)}\right)^{-1}\left(\frac{2}{\Delta t} - \lambda_k^{(1)}\right)\left(\frac{2}{\Delta t} + \lambda_k^{(1)}\right)^{-1}\left(\frac{2}{\Delta t} - \lambda_k^{(2)}\right) \tag{2.9}$$

and

$$|\lambda_{PR_k}| = \frac{\sqrt{\left(\frac{2}{\Delta t} - \alpha_k^{(1)}\right)^2 + (\beta_k^{(1)})^2}\sqrt{\left(\frac{2}{\Delta t} - \alpha_k^{(2)}\right)^2 + (\beta_k^{(2)})^2}}{\sqrt{\left(\frac{2}{\Delta t} + \alpha_k^{(1)}\right)^2 + (\beta_k^{(1)})^2}\sqrt{\left(\frac{2}{\Delta t} + \alpha_k^{(2)}\right)^2 + (\beta_k^{(2)})^2}}. \tag{2.10}$$

The condition $\alpha_k^{(j)} > 0$ for $j = 1, 2$ is sufficient in order to have $|\lambda_{PR_k}| < 1$ for each k, and $\rho(T_{PR}) < 1$.

About the accuracy, by eliminating $u^{n+1/2}$ from the two steps of the scheme we obtain:

$$\frac{u^{n+1} - u^n}{\Delta t} + \frac{1}{2}L(u^{n+1} + u^n) = f^{n+1/2} - \frac{\Delta t^2}{4}L_1L_2\left(\frac{u^{n+1} - u^n}{\Delta t}\right) \tag{2.11}$$

which is equivalent to the Crank-Nicolson scheme up to a term of second order in Δt.

2.3. *The Douglas-Rachford scheme (DR)*

The Douglas-Rachford scheme reads:

$$\begin{cases} \frac{u^{n+1/2} - u^n}{\Delta t} + L_1 u^{n+1/2} + L_2 u^n = f^{n+1/2} \\ \frac{u^{n+1} - u^{n+1/2}}{\Delta t} + L_2 u^{n+1} = L_2 u^n \end{cases} \tag{2.12}$$

The step operator associated to the DR scheme is

$$T_{DR} = \left(\frac{1}{\Delta t}I + L_2\right)^{-1}\left[\frac{1}{\Delta t}I\left(\frac{1}{\Delta t}I + L_1\right)^{-1}\left(\frac{1}{\Delta t}I - L_2\right) + L_2\right]. \tag{2.13}$$

If the eigenvalues of L_1 and L_2 are non-negative and L_1 and L_2 have a common system of eigenfunctions, the DR scheme is absolutely stable ([7]).
Again, denoting by $\lambda_k^{(j)} = \alpha_k^{(j)} + i\beta_k^{(j)}$ the eigenvalues of the matrix L_j, $j = 1, 2$, the eigenvalues of T_{DR} are:

$$\lambda_{DR_k} = \left(\frac{1}{\Delta t} + \lambda_k^{(2)}\right)^{-1}\left[\frac{1}{\Delta t}\left(\frac{1}{\Delta t} + \lambda_k^{(1)}\right)^{-1}\left(\frac{1}{\Delta t} - \lambda_k^{(2)}\right) + \lambda_k^{(2)}\right] \tag{2.14}$$

and

$$|\lambda_{DR_k}| = \left[\Delta t\sqrt{\left(\frac{2}{\Delta t}+\alpha_k^{(1)}\right)^2+(\beta_k^{(1)})^2}\sqrt{\left(\frac{2}{\Delta t}+\alpha_k^{(2)}\right)^2+(\beta_k^{(2)})^2}\right]^{-1} \cdot$$
$$\cdot\left[\Delta t\sqrt{\left(\frac{2}{\Delta t}+\alpha_k^{(1)}\right)^2+(\beta_k^{(1)})^2}\sqrt{(\alpha_k^{(2)})^2+(\beta_k^{(2)})^2}+\right. \tag{2.15}$$
$$\left.+\sqrt{\left(\frac{2}{\Delta t}-\alpha_k^{(2)}\right)^2+(\beta_k^{(2)})^2}\right]$$

The condition $\alpha_k^{(j)} > 0$ for $j = 1, 2$ is sufficient in order to have $|\lambda_{DR_k}| < 1$ for each k.

By eliminating $u^{n+1/2}$ from the two steps of the scheme one obtains:

$$\frac{u^{n+1}-u^n}{\Delta t} + Lu^{n+1} = f^{n+1/2} - \Delta t^2 L_1 L_2\left(\frac{u^{n+1}-u^n}{\Delta t}\right) \tag{2.16}$$

which is equivalent to the implicit first order Euler scheme up to a term of second order in Δt.

2.4. *The θ-method*

The θ-method, with $\theta \in \left(0, \frac{1}{2}\right)$, reads:

$$\begin{cases} \frac{u^{n+\theta}-u^n}{\theta\Delta t} + L_1 u^{n+\theta} + L_2 u^n = f^{n+\theta} \\ \frac{u^{n+1-\theta}-u^{n+\theta}}{(1-2\theta)\Delta t} + L_2 u^{n+1-\theta} + L_1 u^{n+\theta} = f^{n+\theta} \\ \frac{u^{n+1}-u^{n+1-\theta}}{\theta\Delta t} + L_1 u^{n+1} + L_2 u^{n+1-\theta} = f^{n+1} \end{cases} \tag{2.17}$$

with $\theta \in \left(0, \frac{1}{2}\right)$.

The step operator associated to the θ-method is the following one:

$$\begin{aligned} T_\theta = &\left(\frac{1}{\theta\Delta t}I + L_1\right)^{-1}\left(\frac{1}{\theta\Delta t}I - L_2\right)\left(\frac{1}{(1-2\theta)\Delta t}I + L_2\right)^{-1} \\ &\left(\frac{1}{(1-2\theta)\Delta t}I - L_1\right)\left(\frac{1}{\theta\Delta t}I + L_1\right)^{-1}\left(\frac{1}{\theta\Delta t}I - L_2\right). \end{aligned} \tag{2.18}$$

The absolute stability is ensured if the real part of the eigenvalues of L_1 and L_2 are non negative and if L_1 and L_2 have a common system of eigenfunctions. We have:

$$\lambda_{\theta_k} = \frac{\left(\frac{1}{\theta\Delta t} - \lambda_k^{(2)}\right)^2\left(\frac{1}{(1-2\theta)\Delta t} - \lambda_k^{(1)}\right)}{\left(\frac{1}{\theta\Delta t} + \lambda_k^{(1)}\right)^2\left(\frac{1}{(1-2\theta)\Delta t} + \lambda_k^{(2)}\right)} \tag{2.19}$$

and

$$|\lambda_{\theta_k}| = \frac{\left[\left(\frac{1}{\theta\Delta t} - \alpha_k^{(1)}\right)^2 + (\beta_k^{(1)})^2\right]\sqrt{\left(\frac{1}{(1-2\theta)\Delta t} - \alpha_k^{(2)}\right)^2 + (\beta_k^{(2)})^2}}{\left[\left(\frac{1}{\theta\Delta t} + \alpha_k^{(1)}\right)^2 + (\beta_k^{(1)})^2\right]\sqrt{\left(\frac{1}{(1-2\theta)\Delta t} + \alpha_k^{(2)}\right)^2 + (\beta_k^{(2)})^2}} \tag{2.20}$$

are less than one for each value of Δt if $\alpha_k^{(j)} > 0$ for $j = 1, 2$.

If $\theta = 1 - \frac{\sqrt{2}}{2}$ the scheme is second order accurate in Δt, otherwise it is only a first order scheme in Δt ([3]).

3. The Advection-Diffusion Problem

3.1. *Problem statement*

In this Section we present the non-stationary advection-diffusion problem:

$$\begin{cases} \dfrac{\partial u}{\partial t} + \mathcal{L}u = f & \text{in } \Omega \times (0, \bar{t}) \\ u = g & \text{on } \partial\Omega_D \times (0, \bar{t}) \\ \dfrac{\partial u}{\partial \mathbf{n}_{\mathcal{L}}} = h & \text{on } \partial\Omega_N \times (0, \bar{t}) \\ u = u_0 & \text{in } \Omega \times \{0\} \end{cases} \tag{3.21}$$

where $\bar{t} > 0$, Ω is an open subset of $\mathbb{R}^2$, $\partial\Omega$ is the boundary of Ω, $\partial\Omega_D$ and $\partial\Omega_N$ provide a partition of $\partial\Omega$ such that $\partial\Omega_D \cap \partial\Omega_N = \emptyset$ and $\overline{\partial\Omega_D} \cup \overline{\partial\Omega_N} = \overline{\partial\Omega}$. The functions g, h, u_0 are prescribed from data, and $\mathcal{L}$ is the following differential operator:

$$\mathcal{L}u = -\operatorname{div}(\nu\nabla u) + \operatorname{div}(\mathbf{b}u) + b_0 u \tag{3.22}$$

where $\nu|_\Omega > 0$ is the kinematic viscosity, $\mathbf{b} = (b_1, b_2)^T$ is a given vector field and b_0 is a non-negative absorbing coefficient. We take ν, b_1, b_2 and b_0 in $L^\infty(\Omega)$ and we assume that they are constant in time. The term

$$\frac{\partial u}{\partial \mathbf{n}_{\mathcal{L}}} = \nu\nabla u \cdot \mathbf{n} - \mathbf{b}\cdot\mathbf{n}u \qquad \text{on } \partial\Omega \tag{3.23}$$

is the conormal derivative associated to the operator $\mathcal{L}$, and $\mathbf{n}$ represents the unit outward vector to $\partial\Omega$.

Given an open and not empty subset Σ of $\partial\Omega$, we denote by γ_Σ the trace operator from $H^1(\Omega)$ to $H^{1/2}(\Sigma)$ and by E_Σ the extension operator from $H^{1/2}(\Sigma)$ to $H^1(\Omega)$ (see [9]).
We define:

$$V_g := \{u \in H^1(\Omega) : \gamma_{\partial\Omega_D} u = g\}, \tag{3.24}$$

$$L^2(0,\bar{t};X) := \{u : (0,\bar{t}) \to X \ : \ \int_0^{\bar{t}} ||u(t)||_X^2 < \infty\}, \qquad (3.25)$$

and by $C^0((0,\bar{t});X)$ the space of the functions $u:(0,T)\to X$ such that the map $t :\longrightarrow u(t)$ is continuous.

Then we assume that: $f \in L^2(\Omega\times(0,\bar{t}))$, $g \in L^2(\partial\Omega_D \times (0,\bar{t}))$, $h \in L^2(\partial\Omega_N \times (0,\bar{t}))$ and $u_0 \in L^2(\Omega)$. Following [9] (pag. 364), the weak formulation of problem (3.21) formally reads

find $u \in C^0([0,\bar{t}];L^2(\Omega)) \cap L^2(0,\bar{t};V_g)$ such that
$\forall t \in (0,T], \quad (u(t) - E_{\partial\Omega_D} g(t)) \in V_0$ and

$$\begin{cases} \dfrac{d}{dt}\displaystyle\int_\Omega u(t)v\mathrm{d}\Omega + a(u(t),v) = \int_\Omega f(t)v\mathrm{d}\Omega + \int_{\partial\Omega_N} h(t)v\mathrm{d}\partial\Omega \quad \forall v \in V_0 \\ \\ u(0) = u_0, \end{cases} \qquad (3.26)$$

where

$$a(u,v) = \int_\Omega \nu\nabla u\cdot\nabla v\mathrm{d}\Omega - \int_\Omega (\mathbf{b}u)\cdot\nabla v\mathrm{d}\Omega + \int_\Omega b_0 uv\mathrm{d}\Omega \qquad \forall u,v \in H^1(\Omega) \quad (3.27)$$

is the bilinear form associated to the differential operator $\mathcal{L}$. The term (3.23) is the natural Neumann boundary condition associated to the formulation (3.26).

Remark. Instead of (3.21) we can consider the problem

$$\begin{cases} \dfrac{\partial u}{\partial t} + \mathcal{L}u = f & \text{in } \Omega\times(0,\bar{t}) \\ u = g & \text{on } \partial\Omega_D \times (0,\bar{t}) \\ \nu\dfrac{\partial u}{\partial \mathbf{n}} = h_e & \text{on } \partial\Omega_N \times (0,\bar{t}) \\ u = u_0 & \text{in } \Omega\times\{0\}, \end{cases} \qquad (3.28)$$

which differs from (3.21) for the Neumann boundary condition. The bilinear form associated to the operator $\mathcal{L}$ formally reads

$$\tilde{a}(u,v) = \int_\Omega \nu\nabla u\cdot\nabla v \ \mathrm{d}\Omega + \int_\Omega (\mathrm{div}(\mathbf{b}u) + b_0 u)v \ \mathrm{d}\Omega \qquad \forall u,v \in H^1(\Omega). \quad (3.29)$$

3.2. *Operator splitting*

The advection-diffusion operator $\mathcal{L}$ is split as $\mathcal{L} = \mathcal{L}_1 + \mathcal{L}_2$ with

$$\mathcal{L}_1 u = -\operatorname{div}(\nu\nabla u) \qquad (3.30)$$

and

$$\mathcal{L}_2 u = \operatorname{div}(\mathbf{b}u) + b_0 u. \qquad (3.31)$$

The operator $\mathcal{L}_1$ is a pure diffusive operator, while the operator $\mathcal{L}_2$ is an advective operator. The splitting we have choosen is quite simple and natural; the advection-diffusion problem is seen as the sum of its two basic components.

Inside the problem (3.21) the bilinear form associated to the operator $\mathcal{L}_1$ and $\mathcal{L}_2$ are:

$$a_1(u,v) = \int_\Omega \nu \nabla u \cdot \nabla v \mathrm{d}\Omega \tag{3.32}$$

and

$$a_2(u,v) = -\int_\Omega \mathbf{b}u \cdot \nabla v \ \mathrm{d}\Omega + \int_\Omega b_0 uv \ \mathrm{d}\Omega \qquad \forall u, v \in H^1(\Omega), \tag{3.33}$$

while inside the problem (3.28) we have:

$$\tilde{a}_1(u,v) = a_1(u,v) \tag{3.34}$$

and

$$\tilde{a}_2(u,v) = \int_\Omega (\mathrm{div}(\mathbf{b}u) + b_0 u) v \ \mathrm{d}\Omega \qquad \forall u, v \in H^1(\Omega). \tag{3.35}$$

We observe that, when in the fractional step scheme we advance with the operator $\mathcal{L}_1$, we have to solve an elliptic problem, otherwise when we advance with the operator $\mathcal{L}_2$ we have to solve a hyperbolic problem.
For the advective problem we define the *inflow boundary* $\partial\Omega_{in}$ as

$$\partial\Omega_{in} := \{\mathbf{x} \in \partial\Omega : \mathbf{b}(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) < 0\} \tag{3.36}$$

and the outflow boundary $\partial\Omega_{out} := \partial\Omega \backslash \partial\Omega_{in}$. On $\partial\Omega_{in}$ an inflow boundary condition is enforced, while on $\partial\Omega_{out}$ no boundary conditions are considered.

Remark. We observe that a priori there are no relations between $\partial\Omega_D$ and $\partial\Omega_{in}$, since the original problem is an advection-diffusion problem with Dirichlet and/or Neumann boundary conditions. Nevertheless, in the context of the operator splitting, the hyperbolic problem must be well defined, in particular it must have well definite inflow conditions on $\partial\Omega_{in}$. To this aim two ways can be followed. The first way consists of assigning on $\partial\Omega_{in}$ the solution of the previous step, that is possible even if $\partial\Omega_{in}$ is not a subset of $\partial\Omega_D$, but the temporal discretization scheme becomes a first order scheme, even if its theoretical accuracy is grater than one.
The second alternative consists of requiring that $\partial\Omega_{in} \subset \partial\Omega_D$ and, in this way, the formal accuracy order of the scheme is not degraded.

4. Spectral Approximation

We introduce now the basic notations of spectral methods in order to discretize the spatial differential operator $\mathcal{L}$. On the reference domain $\Omega^* = (-1,1)^2$ we define the LGL nodes $\{(\xi_i, \eta_j)\}_{i,j=1}^{(N+1)}$ as the $(N+1)^2$ zeros of the polynomial $(1-\xi^2)(1-$

$\eta^2)L'_N(\xi)L'_N(\eta)$, where $L'_N(\xi)$ is the derivative of the Legendre polynomial of degree N defined on $(-1,1)$ ([1]). The weights associated to the LGL nodes (ξ_i, η_j) are

$$w_{ij} = \gamma_i\gamma_j = \left(\frac{2}{N(N+1)}\frac{1}{L'_N(\xi_i)}\right)\left(\frac{2}{N(N+1)}\frac{1}{L'_N(\eta_j)}\right) \tag{4.37}$$

for $i,j = 1,..,N+1$, where γ_i , γ_j are the weights associated to the one-dimensional Legendre-Gauss-Lobatto quadrature formulas ([2]). The $L^2(\Omega^*)$ inner product is approximated by the Gaussian quadrature formulas and, given two integrable functions u, v on Ω^*, it reads:

$$(u,v)_{N,\Omega^*} := \sum_{i,j=1}^{N+1} u(\xi_i,\eta_j)v(\xi_i,\eta_j)w_{ij} \simeq \int_{\Omega^*} u(\xi,\eta)v(\xi,\eta)\ \mathrm{d}\Omega. \tag{4.38}$$

It is well known that the Legendre-Gauss-Lobatto formulas, on $N+1$ nodes, are exact for polynomials up to degree $2N-1$ (see [2]).

If we consider a generic quadrilateral domain $\Omega \subset \mathbb{R}^2$ the LGL nodes $(\xi_i,\eta_j) \in \Omega^*$ are mapped in Ω by a one-to-one affine map $\mathbf{F}$ (whose jacobian is denoted J_F) and such that $\mathbf{F}(\xi_i,\eta_j) = (x_i, y_j) \in \Omega$ (see [4]). The quadrature formula on Ω reads :

$$(u,v)_{N,\Omega} := \sum_{i,j=1}^{N+1} u(x_i,y_j)v(x_i,y_j)w_{ij}|det J_F(\xi_i,\eta_j)|. \tag{4.39}$$

Therefore, for $u_N,\ v_N \in \mathbb{Q}_N$ we define the discrete bilinear form a_N, approximation of a, as:

$$a_N(u_N,v_N) = (\nu\nabla u_N - \mathbf{b}u_N, \nabla v_N)_{N,\Omega} + (b_0 u_N, v_N)_{N,\Omega} \qquad \forall u_N,\ v_N \in \mathbb{Q}_N. \tag{4.40}$$

If we set

$$\begin{aligned} a_{1N}(u_N,v_N) &= (\nu\nabla u_N, \nabla v_N)_{N,\Omega}, \\ a_{2N}(u_N,v_N) &= -(\mathbf{b}u_N, \nabla v_N)_{N,\Omega} + (b_0 u_N, v_N)_{N,\Omega}, \end{aligned} \tag{4.41}$$

then a_{1N} and a_{2N} are the discrete approximation of the bilinear forms a_1 and a_2, respectively.

The forms $\tilde{a}_1$ and $\tilde{a}_2$, defined in (3.33) and (3.35) are approximated by $\tilde{a}_{1N}$ and $\tilde{a}_{2N}$, respectively, where

$$\begin{aligned} \tilde{a}_{1N}(u_N,v_N) &= a_{1N}(u_N,v_N) = (\nu\nabla u_N, \nabla v_N)_{N,\Omega} \\ \tilde{a}_{2N}(u_N,v_N) &= (\mathrm{div}\, I_N(\mathbf{b}u_N) + b_0 u_N, v_N)_{N,\Omega}. \end{aligned} \tag{4.42}$$

Here, for all $v \in C^0(\overline{\Omega})$, $I_N v \in \mathbb{Q}_N(\Omega)$ denotes the interpolant of degree less than or equal to N in each variable of the function v at the Legendre Gauss-Lobatto nodes $(x_i,y_j) = \mathbf{F}(\xi_i,\eta_j)$ on Ω.

We set $V_N^g = V_g \cap \mathbb{Q}_N(\Omega)$ and $V_N = V_N^0$; the spectral approximation to problem (3.21) reads:

$\forall t \in (0,\bar{t}]$ find $u_N(t) \in V_N^g$: $(u_N(t) - I_N(E_{\partial\Omega_D} g(t))) \in V_N$:

$$\begin{cases} \dfrac{d}{dt}(u_N(t), v_N)_{N,\Omega} + a_N(u_N(t), v_N) = (f(t), v_N)_{N,\Omega} \quad \forall v_N \in V_N \\ u_N(0) = I_N u_0 . \end{cases} \tag{4.43}$$

Remark. At each step of a fractional step scheme we have to approximate time-independent elliptic adjoint problems and hyperbolic problems. To this aim we briefly present the approximation of these problems by the generalized Galerkin spectral methods.

4.1. *Spectral approximation of the elliptic problem*

Let us consider the following elliptic self-adjoint problem on a quadrilateral domain $\Omega \subset \mathbb{R}^2$:

$$\begin{cases} -\operatorname{div}(\nu\nabla u) + \alpha u = f & \text{in } \Omega \\ u = g & \text{on } \partial\Omega_D \\ \nu \dfrac{\partial u}{\partial \mathbf{n}} = h & \text{on } \partial\Omega_N , \end{cases} \tag{4.44}$$

whose variational formulation reads:
find $u \in V_g$ (see definition (3.24)) such that

$$\int_\Omega \nu\nabla u \cdot \nabla v \mathrm{d}\Omega + \int_\Omega \alpha u v \mathrm{d}\Omega = \int_\Omega f v \mathrm{d}\Omega + \int_{\partial\Omega_N} h v \mathrm{d}(\partial\Omega) \qquad \forall v \in V_0 . \tag{4.45}$$

Using the notation introduced at the beginning of this section the problem (4.45) is approximated by the generalized Galerkin spectral method as follows
find $u_N \in V_N^g$ such that

$$(\nu\nabla u_N, \nabla v_N)_{N,\Omega} + (\alpha u_N, v_N)_{N,\Omega} = (f, v_N)_{N,\Omega} + (h, v_N)_{N,\partial\Omega_N} \qquad \forall v_N \in V_N . \tag{4.46}$$

4.2. *Spectral approximation of the first-order advection problem*

The model problem we consider reads:
find $u \in H^1(\Omega)$ such that

$$\begin{cases} \operatorname{div}(\mathbf{b}u) + b_0 u = f & \text{in } \Omega \cup \partial\Omega_{out} \\ u = g & \text{on } \partial\Omega_{in} \end{cases} \tag{4.47}$$

where $\partial\Omega_{in}$ is the inflow boundary introduced in the previous section.

A possible variational formulation of this problem reads:

find $u \in L_2(\Omega)$ such that

$$-\int_\Omega \mathbf{b}u \cdot \nabla v \mathrm{d}\Omega + \int_\Omega b_0 u v \mathrm{d}\Omega = \int_\Omega f v \mathrm{d}\Omega - \int_{\partial\Omega_{in}} \mathbf{b}\cdot\mathbf{n} g \; v \mathrm{d}\partial\Omega \qquad \forall v \in H^1(\Omega), \tag{4.48}$$

Its generalized Galerkin spectral approximation is:
find $u_N \in \mathbb{Q}_N(\Omega)$ such that

$$-(\mathbf{b}u_N, \nabla v_N)_{N,\Omega} + (b_0 u_N, v_N)_{N,\Omega} = (f, v_N)_{N,\Omega} - (\mathbf{b}\cdot\mathbf{n}g, v_N)_{N,\partial\Omega_{in}} \qquad \forall v_N \in \mathbb{Q}_N(\Omega). \tag{4.49}$$

If we consider the bilinear form $\tilde{a}_2$ instead of a_2 the variational formulation of (4.47) reads: find $u \in H^1(\Omega)$ such that $\gamma_{\partial\Omega_{in}} u = g$ and

$$\int_\Omega (\mathrm{div}(\mathbf{b}u) + b_0)v\mathrm{d}\Omega = \int_\Omega fv\mathrm{d}\Omega \qquad \forall v \in L_2(\Omega). \tag{4.50}$$

The associated spectral approximation is:
find $u_N \in \mathbb{Q}_N(\Omega)$ such that

$$\begin{cases} (\mathrm{div}\, I_N(\mathbf{b}u_N) + b_0 u_N, v_N)_{N,\Omega} = (f, v_N)_{N,\Omega} & \forall v_N \in \mathbb{Q}_N(\Omega) \\ u_N = g & \text{at the LGL nodes on } \partial\Omega_{in}. \end{cases} \tag{4.51}$$

Remark. In the space $\mathbb{Q}_N(\Omega)$ we can consider the basis of Lagrange functions $\{\varphi_i(x,y)\}_{i=1}^{(N+1)^2}$ defined on the LGL nodes $\{\mathbf{x}_i = (x_{i_1}, y_{i_2})\}_{i_1,i_2=1}^{N+1}$ and we set $N_t = (N+1)^2$. This basis is orthogonal with respect to the discrete inner product (4.39) and every function $v_N \in \mathbb{Q}_N(\Omega)$ can be expanded as:

$$v_N(x,y) = \sum_{i=1}^{N_t} v_{N,i}\varphi_i(x,y) \tag{4.52}$$

where $v_{N,i} = v_N(x_{i_1}, y_{i_2})$.

Therefore we can denote by M the diagonal mass matrix

$$M_{ij} = (\varphi_j, \varphi_i)_{N,\Omega} \qquad i,j = 1,..,N_t, \tag{4.53}$$

and we set:

$$\begin{aligned} (A_1)_{ij} &= a_{1_N}(\varphi_j,\varphi_i), \quad (A_2)_{ij} = a_{2_N}(\varphi_j,\varphi_i), \quad i,j = 1,..,N_t \\ (\tilde{A}_1)_{ij} &= \tilde{a}_{1_N}(\varphi_j,\varphi_i), \quad (\tilde{A}_2)_{ij} = \tilde{a}_{2_N}(\varphi_j,\varphi_i), \quad i,j = 1,..,N_t. \end{aligned} \tag{4.54}$$

5. Spectral Fractional Step Schemes

In this paragraph the differential splitting on the advection diffusion problem is considered. Some approaches for the imposition of the boundary conditions are proposed and the accuracy of the resulting schemes are studied. The generalized Galerkin spectral discretization is considered. In view of the last remark of section 3 we suppose that $\partial\Omega_{in} \subset \partial\Omega_D$.

First of all we consider the elliptic steps (we name "elliptic" the steps which are implicit on the matrix L_1 and "hyperbolic" the steps which are implicit on the matrix L_2).

We denote by k_1, k_2 and k_3 three subsequent fractional time levels and we set $\tau_1 = (k_2 - k_1)\Delta t$ and $\tau_2 = (k_3 - k_2)\Delta t$. For example at the first step of the scheme PR we have $k_1 = n$, $k_2 = n + \dfrac{1}{2}$ and $k_3 = n + 1$ with $\tau_1 = \tau_2 = \dfrac{\Delta t}{2}$; while for the first and second steps of the θ-method we have $k_1 = n$, $k_2 = n + \theta$, $k_3 = n + 1 - \theta$, $\tau_1 = \theta\Delta t$ and $\tau_2 = (1 - 2\theta)\Delta t$.

Two approaches (R1 and R2) are proposed for the approximation of the problem (3.21), which are based on the bilinear forms a_{1_N} e a_{2_N}. Two other (DN and D) are proposed for the problem (3.28), this time based on the bilinear forms $\tilde{a}_{1_N}$ and $\tilde{a}_{2_N}$.

Inside the Peaceman-Rachford and the Douglas-Rachford schemes there is one elliptic step and one hyperbolic step, while inside the $\theta-$method there are two elliptic steps and one hyperbolic. In the following approaches we propose the boundary conditions for the two basic problems. Both the elliptic steps of the $\theta-$method have to be solved by the same scheme.

We impose the boundary conditions at the final time level for the elliptic steps, and at the initial time level for the hyperbolic ones. It can be shown that equivalent accurate schemes can be obtained by imposing the boundary conditions at the initial time level for the elliptic steps, and at the final time level for the hyperbolic ones.

Approach R1

$$\begin{cases} \textit{Elliptic step} \\ \dfrac{1}{\tau}(u_N^{k_2} - u_N^{k_1}, v_N)_{N,\Omega} + a_{1N}(u_N^{k_2}, v_N) = \\ (f^{k_2}, v_N)_{N,\Omega} - a_{2N}(u_N^{k_1}, v_N) + (h^{k_2}, v_N)_{N,\partial\Omega_N} \\ u_N^{k_2} = g \text{ on } \partial\Omega_D \\ \\ \textit{Hyperbolic step} \\ \dfrac{1}{\tau}(u_N^{k_3} - u_N^{k_2}, v_N)_{N,\Omega} + a_{2N}(u_N^{k_3}, v_N) + (\mathbf{b}\cdot\mathbf{n}u_N^{k_3}, v_N)_{N,\partial\Omega_{out}} = \\ = (f^{k_2}, v_N)_{N,\Omega} - (\mathbf{b}\cdot\mathbf{n}g^{k_3}, v_N)_{N,\partial\Omega_{in}} - a_{1N}(u_N^{k_2}, v_N) + \left(\nu\dfrac{\partial u_N^{k_2}}{\partial \mathbf{n}}, v_N\right)_{N,\partial\Omega} \end{cases} \tag{5.55}$$

The approaches $R1$ and $R2$ differ for the treatment of the boundary conditions on the elliptic step. In the approach $R1$ the boundary condition on $\partial\Omega_N$ at the elliptic step is a natural condition for the complet bilinear form a_N evaluated at the final time level (k_2). As we will see in the next paragraph, this approach is first order accurate in Δt and, when applied to second order schemes like PR or θ-method, it drops the accuracy of these schemes to the first order in Δt.

In the approach $R2$ the terms $(\mathbf{b}\cdot\mathbf{n}u_N^{k_2}, v_N)_{N,\partial\Omega_N}$ and $(\mathbf{b}\cdot\mathbf{n}u_N^{k_1}, v_N)_{N,\partial\Omega_N}$, evaluated at the elliptic step, have been subtracted respectively from the left and the right hand sides of the equation in order to obtain both the natural condition for the problem (3.21) at the time level t_{k_2} and the natural boundary condition for the bilinear form a_{2_N} at the time level t_{k_1}. This technique is introduced in order to preserve the theoretical accuracy of the fractional step scheme used. In both the approaches, at the hyperbolic step, the natural boundary condition for the bilinear form a_{2_N} is enforced at the time level t_{k_3}.

Approach R2

$$\begin{cases} \textit{Elliptic step} \\ \dfrac{1}{\tau}(u_N^{k_2} - u_N^{k_1}, v_N)_{N,\Omega} + a_{1N}(u_N^{k_2}, v_N) - (\mathbf{b}\cdot\mathbf{n}u_N^{k_2}, v_N)_{N,\partial\Omega_N} = \\ (f^{k_2}, v_N) - a_{2N}(u_N^{k_1}, v_N) + (h^{k_2}, v_N)_{N,\partial\Omega_N} - (\mathbf{b}\cdot\mathbf{n}u_N^{k_1}, v_N)_{N,\partial\Omega_N} \\ u_N^{k_2} = g \text{ on } \partial\Omega_D \\ \\ \textit{Hyperbolic step} \\ \dfrac{1}{\tau}(u_N^{k_3} - u_N^{k_2}, v_N)_{N,\Omega} + a_{2N}(u_N^{k_3}, v_N) + (\mathbf{b}\cdot\mathbf{n}u_N^{k_3}, v_N)_{N,\partial\Omega_{out}} = \\ = (f^{k_1}, v_N)_{N,\Omega} - (\mathbf{b}\cdot\mathbf{n}g^{k_3}, u_N)_{N,\partial\Omega_{in}} - a_{1N}(u_N^{k_2}, v_N) + \left(\nu\dfrac{\partial u_N^{k_2}}{\partial\mathbf{n}}, v_N\right)_{N,\partial\Omega} \end{cases} \tag{5.56}$$

The two following approaches are proposed for the approximation in time of the problem (3.28). In this case the boundary treatment at the elliptic step is the same for both approaches; the difference is about the hyperbolic step.
In the DN approach the inflow condition is imposed weakly, while in the D approach the inflow condition is imposed strongly, following the formulations (4.49) and (4.51) respectively.

Approach DN

$$\begin{cases} \textit{Elliptic step} \\ \dfrac{1}{\tau}(u_N^{k_2} - u_N^{k_1}, v_N)_{N,\Omega} + \tilde{a}_{1N}(u_N^{k_2}, v_N) = \\ = (f^{k_2}, v_N)_{N,\Omega} - \tilde{a}_{2N}(u_N^{k_1}, v_N) + (h_e^{k_2}, v_N)_{N,\partial\Omega_N} \\ u_N^{k_2} = g \text{ on } \partial\Omega_D \\ \\ \textit{Hyperbolic step} \\ \dfrac{1}{\tau}(u_N^{k_3} - u_N^{k_2}, v_N)_{N,\Omega} + \tilde{a}_{2N}(u_N^{k_3}, v_N) - (\mathbf{b}\cdot\mathbf{n}u_N^{k_3}, v_N)_{N,\partial\Omega_{in}} = \\ = (f^{k_2}, v_N)_{N,\Omega} - (\mathbf{b}\cdot\mathbf{n}g^{k_3}, v_N)_{N,\partial\Omega_{in}} - \tilde{a}_{1N}(u_N^{k_2}, v_N) + \left(\nu\dfrac{\partial u_N^{k_2}}{\partial\mathbf{n}}, v_N\right)_{N,\partial\Omega} \end{cases} \tag{5.57}$$

Approach D

$$
\begin{cases}
\textit{Elliptic step} \\
\frac{1}{\tau}(u_N^{k_2} - u_N^{k_1}, v_N)_{N,\Omega} + \tilde{a}_{1N}(u_N^{k_2}, v_N) = \\
= (f^{k_2}, v_N)_{N,\Omega} - \tilde{a}_{2N}(u_N^{k_1}, v_N) + (h_e^{k_2}, v_N)_{N,\partial\Omega_N} \\
u_N^{k_2} = g \text{ on } \partial\Omega_D \\
\textit{Hyperbolic step} \\
\frac{1}{\tau}(u_N^{k_3} - u_N^{k_2}, v_N)_{N,\Omega} + \tilde{a}_{2N}(u_N^{k_3}, v_N) + (u_N^{k_3}, v_N)_{N,\partial\Omega_{in}} = \\
= (f^{k_3}, v_N)_{N,\Omega} + (g^{k_3}, u_N)_{N,\partial\Omega_{in}} - \tilde{a}_{1N}(u_N^{k_2}, v_N) + \left(\nu\frac{\partial u_N^{k_2}}{\partial \mathbf{n}}, v_N\right)_{N,\partial\Omega}
\end{cases}
\quad . \tag{5.58}
$$

5.1. *Application to the PR scheme: accuracy analysis*

In this paragraph we analyze the consistency and the accuracy of the PR scheme when the approaches $R1$, $R2$, DN or D are considered in order to impose the boundary conditions on the subproblems. We refer to the next section for the stability analysis of the schemes.
The approaches $R1$, $R2$, DN and D, exposed in the previous paragraph are used here inside the Peaceman-Rachford scheme, but the same analysis can be carried out on the other fractional step schemes as the Douglas-Rachford scheme or θ-method.

Scheme PR - approach R1
for $n = 0, .., n_{max}$ find $u_N^{n+1} \in V_N$:

$$
\begin{cases}
\frac{2}{\Delta t}(u_N^{n+1/2} - u_N^n, v_N)_{N,\Omega} + a_{1N}(u_N^{n+1/2}, v_N) = \\
= (f^{n+1/2}, v_N)_{N,\Omega} - a_{2N}(u_N^n, v_N) + (h^{n+1/2}, v_N)_{N,\partial\Omega_N} \\
u_N^{n+1/2} = g(t_{n+1/2}) \qquad\qquad \text{on } \partial\Omega_D \\
\frac{2}{\Delta t}(u_N^{n+1} - u_N^{n+1/2}, v_N)_{N,\Omega} + a_{2N}(u_N^{n+1}, v_N) + (\mathbf{b}\cdot\mathbf{n}u_N^{n+1}, v_N)_{N,\partial\Omega_{out}} = \\
= (f^{n+1/2} v_N)_{N,\Omega} - (\mathbf{b}\cdot\mathbf{n}g^{n+1}, v_N)_{N,\partial\Omega_{in}} - a_{1N}(u_N^{n+1/2}, v_N) + \\
+ \left(\nu\frac{\partial u_N^{n+1/2}}{\partial \mathbf{n}}, v_N\right)_{N,\partial\Omega}
\end{cases}
\tag{5.59}
$$

The scheme PR-R1 (5.59) is consistent and it is first order accurate in Δt. In fact, we first observe that the Dirichlet boundary condition, imposed at the first step, doesn't drop the accuracy of the scheme; therefore we sum the two steps of the scheme (5.59) and, since $h = \nu \dfrac{\partial u}{\partial \mathbf{n}} - \mathbf{b} \cdot \mathbf{n} u$, we have:

$$
\begin{aligned}
&\frac{2}{\Delta t}(u_{_N}^{n+1} - u_{_N}^{n}, v_{_N})_{N,\Omega} + 2a_{1N}(u_{_N}^{n+1/2}, v_{_N}) + a_{2N}(u_{_N}^{n+1} + u_{_N}^{n}, v_{_N}) = \\
&= 2(f^{n+1/2}, v_{_N})_{N,\Omega} + 2\left(\nu \frac{\partial u_{_N}^{n+1/2}}{\partial n}, v_{_N}\right)_{N,\partial\Omega_N} \\
&-(\mathbf{b} \cdot \mathbf{n} u_{_N}^{n+1}, v_{_N})_{N,\partial\Omega} - (\mathbf{b} \cdot \mathbf{n} u_{_N}^{n+1/2}, v_{_N})_{N,\partial\Omega_N}.
\end{aligned}
\tag{5.60}
$$

By defining

$$
f_{_N}^{n} = (f^{n}, v_{_N})_{N,\Omega}, \tag{5.61}
$$

$$
D_{ij} = \begin{cases} \left(\nu \dfrac{\partial \varphi_j}{\partial \mathbf{n}}, \varphi_i\right)_{N,\partial\Omega_N} & \text{if } \mathbf{x}_i \in \partial\Omega_{_N} \\ 0 & \text{otherwise,} \end{cases} \tag{5.62}
$$

$$
B_{ij}^{\Sigma} = \begin{cases} (\mathbf{b} \cdot \mathbf{n}\varphi_j, \varphi_i)_{N,\Sigma} & \text{if } \mathbf{x}_i \in \Sigma \qquad \text{with } \Sigma \subset \partial\Omega \\ 0 & \text{otherwise;} \end{cases} \tag{5.63}
$$

and

$$
L_1 = A_1 + D \qquad\qquad L_2 = A_2 + B^{\partial\Omega}, \tag{5.64}
$$

the matrix form of the scheme (5.60) reads:

$$
\begin{aligned}
&\frac{2}{\Delta t} M(u_{_N}^{n+1/2} - u_{_N}^{n}) + 2L_1 u_{_N}^{n+1/2} + L_2(u_{_N}^{n+1} + u_{_N}^{n}) = \\
&2f_{_N}^{n+1/2} - B^{\partial\Omega_N} u_{_N}^{n+1/2} - B^{\partial\Omega_N} u_{_N}^{n}.
\end{aligned}
\tag{5.65}
$$

By eliminating the intermediate solution, we obtain the following one-step scheme:

$$
\begin{aligned}
&M\left(\frac{u_{_N}^{n+1} - u_{_N}^{n}}{\Delta t}\right) + \frac{1}{2}\left[L_1(u_{_N}^{n+1} + u_{_N}^{n}) + L_2(u_{_N}^{n+1} + u_{_N}^{n})\right] = \\
&f_{_N}^{n+1/2} - \tfrac{\Delta t^2}{4} L_1 M^{-1} L_2 \left(\frac{u_{_N}^{n+1} - u_{_N}^{n}}{\Delta t}\right) + \\
&-\frac{\Delta t}{4}\left(\frac{2I}{\Delta t} - M^{-1}L_1\right) B^{\partial\Omega_N} \cdot \left[u_{_N}^{n} - \left(\frac{2I}{\Delta t} - M^{-1}L_1\right)^{-1}\right. \\
&\left.\left(\frac{2u_{_N}^{n+1}}{\Delta t} + M^{-1}L_2 u_{_N}^{n+1} - M^{-1} f_{_N}^{n+1/2}\right)\right]
\end{aligned}
\tag{5.66}
$$

that is first order accurate in Δt.

By applying the approach R2 to the PR scheme we have:

Scheme PR - approach R2
for $n = 0, .., n_{max}$ find $u_N^{n+1} \in V_N$:

$$\begin{cases} \dfrac{2}{\Delta t}(u_N^{n+1/2} - u_N^n, v_N)_{N,\Omega} + a_{1N}(u_N^{n+1/2}, v_N) - (\mathbf{b}\cdot\mathbf{n}u_N^{n+1/2}, v_N)_{N,\partial\Omega_N} = \\ = (f^{n+1/2}, v_N)_{N,\Omega} - a_{2N}(u_N^n, v_N) + (h^{n+1/2} - \mathbf{b}\cdot\mathbf{n}u_N^n, v_N)_{N,\partial\Omega_N} \\ u_N^{n+1/2} = g(t_{n+1/2}) \qquad\qquad \text{on } \partial\Omega_D \\ \dfrac{2}{\Delta t}(u_N^{n+1} - u_N^{n+1/2}, v_N)_{N,\Omega} + a_{2N}(u_N^{n+1}, v_N) + (\mathbf{b}\cdot\mathbf{n}u_N^{n+1}, v_N)_{N,\partial\Omega_{out}} = \\ = (f^{n+1/2}, v_N)_{N,\Omega} - (\mathbf{b}\cdot\mathbf{n}g^{n+1}, v_N)_{N,\partial\Omega_{in}} - a_{1N}(u_N^{n+1/2}, v_N) + \\ + \left(\nu\dfrac{\partial u_N^{n+1/2}}{\partial\mathbf{n}}, v_N\right)_{N,\partial\Omega} . \end{cases} \tag{5.67}$$

The scheme PR-R2 (5.67) is consistent and it is second order accurate in Δt.

As below we sum the two steps of the scheme (5.67) and by using the matrices L_1, L_2, D and $B^{\partial\Omega}$ we obtain

$$M\frac{u_N^{n+1} - u_N^n}{\Delta t} + L_1 u_N^{n+1} + \frac{1}{2}L_2(u_N^{n+1/2} + u_N^n) = f_N^{n+1/2}. \tag{5.68}$$

From the elliptic step we deduce:

$$L_1 u_N^{n+1/2} = f_N^{n+1/2} + \left(\frac{2}{\Delta t}M - L_2\right)u_N^n - \frac{2}{\Delta t}M u_N^{n+1/2}, \tag{5.69}$$

we substitute it in (5.68) and then we substitute $u_N^{n+1/2}$ by

$$\left(\frac{2}{\Delta t}M + L_1\right)^{-1}\left[f_N^{n+1/2} + \left(\frac{2}{\Delta t}M - L_2\right)u_N^n\right]. \tag{5.70}$$

We have the following scheme:

$$\begin{aligned} &M\frac{u_N^{n+1} - u_N^n}{\Delta t} + \frac{1}{2}\left[L_1(u_N^{n+1} + u_N^n) + L_2(u_N^{n+1} + u_N^n)\right] = \\ &= f_N^{n+1/2} - \frac{\Delta t^2}{4}L_1 M^{-1} L_2\left(\frac{u_N^{n+1} - u_N^n}{\Delta t}\right), \end{aligned} \tag{5.71}$$

which is the Crank-Nicolson scheme up to a second order term in Δt.

We consider now the PR scheme jointly with the approaches DN and D.

Scheme PR - approach DN
for $n = 0, .., n_{max} - 1$ find $u_N^{n+1} \in V_N$:

$$\left\{ \begin{array}{l} \dfrac{2}{\Delta t}(u_N^{n+1/2} - u_N^n, v_N)_{N,\Omega} + \tilde{a}_{1N}(u_N^{n+1/2}, v_N) = \\ = (f^{n+1/2}, v_N)_{N,\Omega} - \tilde{a}_{2N}(u_N^n, v_N) + (h_e^{n+1/2}, v_N)_{N,\partial\Omega_N} \\ u_N^{n+1/2} = g(t_{n+1/2}) \qquad\qquad \text{on } \partial\Omega_D \\ \\ \dfrac{2}{\Delta t}(u_N^{n+1} - u_N^{n+1/2}, v_N)_{N,\Omega} + \tilde{a}_{2N}(u_N^{n+1}, v_N) - (\mathbf{b}\cdot\mathbf{n}u_N^{n+1}, v_N)_{N,\partial\Omega_{in}} = \\ = (f^{n+1/2}, v_N)_{N,\Omega} - (\mathbf{b}\cdot\mathbf{n}g^{n+1}, v_N)_{N,\partial\Omega_{in}} - \tilde{a}_{2N}(u_N^{n+1/2}, v_N) + \\ + \left(\nu\dfrac{\partial u_N^{n+1/2}}{\partial \mathbf{n}}, v_N\right)_{N,\partial\Omega} . \end{array} \right. \tag{5.72}$$

The scheme PR-DN (5.72) is consistent and second order accurate in Δt. In fact if we sum the two steps of the scheme, we eliminate the intermediate solution and we use the matrices L_1, $L_2 = \tilde{A}_2$ and D we have:

$$\begin{array}{l} M\dfrac{u_N^{n+1} - u_N^n}{\Delta t} + \dfrac{1}{2}\left[L_1(u_N^{n+1} + u_N^n) + L_2(u_N^{n+1} + u_N^n)\right] = \\ = f_N^{n+1/2} - \dfrac{\Delta t^2}{4}L_1 M^{-1} L_2\left(\dfrac{u_N^{n+1} - u_N^n}{\Delta t}\right). \end{array} \tag{5.73}$$

It follows that the scheme PR-DN is second order accurate in Δt.

Finally we have the scheme
Scheme PR - approach D
for $n = 0, .., n_{max} - 1$ find $u_N^{n+1} \in V_N$:

$$\left\{ \begin{array}{l} \dfrac{2}{\Delta t}(u_N^{n+1/2} - u_N^n, v_N)_{N,\Omega} + \tilde{a}_{1N}(u_N^{n+1/2}, v_N) = \\ = (f^{n+1/2}, v_N)_{N,\Omega} - \tilde{a}_{2N}(u_N^n, v_N) + (h_e^{n+1/2}, v_N)_{N,\partial\Omega_N} \\ u_N^{n+1/2} = g(t_{n+1/2}) \qquad\qquad \text{on } \partial\Omega_D \\ \\ \dfrac{2}{\Delta t}(u_N^{n+1} - u_N^{n+1/2}, v_N)_{N,\Omega} + \tilde{a}_{2N}(u_N^{n+1}, v_N) + (u_N^{n+1}, v_N)_{N,\partial\Omega_{in}} = \\ = (f^{n+1/2}, v_N)_{N,\Omega} + (g^{n+1}, v_N)_{N,\partial\Omega_{in}} - \tilde{a}_{1N}(u_N^{n+1/2}, v_N) + \\ + \left(\nu\dfrac{\partial u_N^{n+1/2}}{\partial \mathbf{n}}, v_N\right)_{N,\partial\Omega} . \end{array} \right. \tag{5.74}$$

The scheme PR-D (5.74) is consistent and second order accurate in Δt.

Once again, if we sum the two steps of the scheme, we eliminate the fractional solution and we consider the matrices L_1, L_2 and D we obtain:

$$
\begin{aligned}
& M\frac{u_{N}^{n+1}-u_{N}^{n}}{\Delta t}+\frac{1}{2}\left[L_1(u_{N}^{n+1}+u_{N}^{n})+L_2(u_{N}^{n+1}+u_{N}^{n})\right]= \\
& =f_{N}^{n+1/2}-\frac{\Delta t^2}{4}L_1M^{-1}L_2\left(\frac{u_{N}^{n+1}-u_{N}^{n}}{\Delta t}\right)
\end{aligned}
\tag{5.75}
$$

that is second order accurate in Δt.

The four approaches we have joint to the PR scheme can be applied also to the θ-method and the DR scheme. Since the DR scheme and the θ-method, with $\theta \neq 1-\frac{\sqrt{2}}{2}$, are first order accurate in Δt, all the four approaches will be equivalent from the accuracy view point.

The choice of one approach instead of another one could be suggested by the stability properties of each approaches.

5.2. *Stability analysis*

The splitting we have adopted on the advection-diffusion operator generates a matrix A_1 symmetric and positive definite and a not symmetric matrix A_2 whose eigenvalues have a priori not positive real part. Moreover, if the coefficients ν, $\mathbf{b}$ and b_0 are not constant and non homogeneous Dirichlet boundary conditions are considered, a common system of eigenvectors for A_1 and A_2 (and then for L_1 and L_2) is not ensured, so that the absolute stability for PR, DR and $\theta-$method is not ensured (see Section 2).

In general we can say that the schemes PR-DN, PR-R1, PR-R2 and PR-D are conditionally stable, and in some particular cases (for example if ν, $\mathbf{b}$ and b_0 are constant and the eigenvalues of A_2 have positive real parts) they can be absolutely stable.

We observe that the step operators of the scheme PR-DN and PR-R1 coincide, so that the same stability analysis can be done. A comparison between the stability of the four approaches can be done, by the analysis of the spectral radius of the step operator T_{PR}. In table 4 and in the following ones the spectral radius of the matrix T_{PR} is shown versus Δt, for the approaches R1, R2, DN e D and for different choices of the viscosity and of the vector filed $\mathbf{b}$.

First of all we observe that if homogeneous Dirichlet boundary conditions are considered the step operators of the approaches R1, R2 and DN coincide. In particular, if the real part of the eigenvalues of A_2 is not-negative (this property is ensured if $\left(\frac{1}{2}\operatorname{div}\mathbf{b}+b_0\right)\geq 0$), the numerical tests carry out that the schemes PR-R1, PR-DN and PR-D are absolutely stable, while the PR-R2 scheme is conditionally stable. On the contrary, if A_2 is a not-definite matrix, only the schemes PR-R1 and PR-DN seem to be absolutely stable.

Table 1. Accuracy for the PR scheme jointly with the four boundary conditions approaches.

Δt	e^n			
	PR-R1	PR-R2	PR-DN	PR-D
.001	.1932e-3	.2554e-6	.2580e-6	.2752e-6
.00316	.6191e-3	.2478e-5	.2504e-5	.2506e-5
.005	.9906e-3	.6254e-5	.6315e-5	.6393e-5
.01	.2042e-2	.2794e-4	.2813e-4	.2948e-4
.03162	.7160e-2	.4472e-3	.4480e-3	.4825e-3
.05	.1206e-1	.1358e-2	.1359e-2	.1450e-2
.1	.2759e-1	.6865e-2	.6870e-2	.7121e-1

Table 2. Accuracy for the DR scheme jointly with the four boundary conditions approaches.

Δt	e^n			
	DR-R1	DR-R2	DR-RDN	DR-D
.001	.6406e-3	.5266e-3	.5163e-3	.5162e-3
.00316	.2235e-2	.1789e-2	.1768e-2	.1839e-2
.005	.3927e-2	.3186e-2	.3165e-2	.3385e-2
.01	.9962e-2	.8486e-2	.8481e-2	.9261e-2
.03162	.4756e-1	.4344e-1	.4353e-1	.4629e-1
.05	.8432e-1	.7832e-1	.7849e-1	.8214e-1
.1	.1830e+0	.1736e+0	.1739e+0	.1783e+0

For the numerical results we refer to the next section.

6. Numerical Results

In this section we present the results about the accuracy and the stability of the fractional step schemes.

Let us define the error at time t_n as follows:

$$e^n := \frac{||u_N^n - u(t_n)||_{H^1(\Omega)}}{||u(t_n)||_{H^1(\Omega)}}. \tag{6.76}$$

In table 1 we can read the errors e^n at $t_n = 1$ with $t_0 = 0$, $N = 8$ for the schemes PR-R1, PR-R2, PR-DN and PR-D. The problem data are: $\Omega = (0,1)^2$, $\nu = 1.$, $\mathbf{b} = (\frac{y-x}{2}, xy)^T$, $b_0 = 0$, $\partial\Omega_D = \{(0,y),\ y \in [0,1]\} \cup \{(1,y),\ y \in [0,1]\}$. The test solution is $u(x,y,t) = e^{x+y+t}$. We read that the approcahes $R2$, DN and D preserve the second order of accuracy of the PR scheme, while $PR - R1$ becomes a first order accurate scheme. In table 2 the accuracy of the Douglas-Rachford scheme is shown. The test case is the same considered for the table 1 and all the approaches mantain the first order of the DR scheme. The θ-method is second order accurate for $\theta = 1 - \frac{\sqrt{2}}{2}$ and in table 3 we show the accuracy of the scheme for this particular value of θ. The test case is the same considered for the table 1. The considerations are the same as for the PR scheme.

Now we analyze the stability regions of the proposed fractional step schemes.

Table 3. Accuracy for the θ-method, with $\theta = 1 - \frac{\sqrt{2}}{2}$ jointly with the four boundary conditions approaches.

Δt	e^n			
	θ-R1	θ-R2	θ-DN	θ-D
.001	.1126e-3	.2031e-6	.2017e-6	.2017e-6
.00316	.3563e-3	.1915e-5	.1903e-5	.1902e-5
.005	.5634e-3	.4582e-5	.4553e-5	.4548e-5
.01	.1228e-2	.1654e-4	.1642e-4	.1691e-4
.03162	.3581e-2	.1242e-3	.1225e-3	.1217e-3
.05	.5676e-2	.2659e-3	.2608e-3	.2588e-3
.1	.1143e-1	.8013e-3	.7761e-3	.7713e-3

Table 4. The spectral radius of the step operator on the PR scheme. $N = 8$, $\nu = 10^{-3}$, $\mathbf{b}_i$ are choosen as in (6.77), while $b_0 = 0$.

	R1-DN			R2			D		
Δt	$\mathbf{b}_1$	$\mathbf{b}_2$	$\mathbf{b}_3$	$\mathbf{b}_1$	$\mathbf{b}_2$	$\mathbf{b}_3$	$\mathbf{b}_1$	$\mathbf{b}_2$	$\mathbf{b}_3$
.001	0.999	0.999	0.999	0.999	0.999	0.999	0.999	0.999	0.999
.01	0.999	0.998	0.999	0.999	0.999	0.999	0.999	0.998	0.999
.1	0.996	0.994	0.998	0.999	1.004	0.999	0.996	0.994	0.998
1.	0.976	0.960	0.987	1.034	1.115	1.020	0.990	0.957	0.987
10.	0.862	0.877	0.900	2.003	4.540	1.402	0.943	0.819	0.892
100.	0.960	0.818	0.960	4.348	1.150	8.672	0.960	0.915	0.924
1000.	0.995	0.973	0.995	31.075	1.014	1.053	0.995	0.989	0.954

We report the spectral radius of the step operator for the PR-R1, PR-R2, PR-DN and PR-D approaches versus Δt, for some values of the viscosity and for different choices of $\mathbf{b}$. All the eigenvalue problems are solved on the domain $\Omega = (0,1)^2$. In table 4 the spectral radius of the step operator T_{PR} is shown, for three different choices of the vector field $\mathbf{b}$, with $\frac{1}{2}\operatorname{div}\mathbf{b} + b_0 \geq 0$ in Ω. We have considered:

$$\mathbf{b}_1 = (x+y, xy)^T \qquad \mathbf{b}_2 = (e^x, e^y)^T \qquad \mathbf{b}_3 = (\log(x+1), \log(y+1))^T. \quad (6.77)$$

A Dirichlet condition is imposed on $\partial\Omega_{in}$ and a Neumann condition otherwise. We observe that the approaches R1, DN and D are absolutely stable, while this is not true for the R2 approach.

In table 5 we report the spectral radius of the step operator for the scheme PR-R2, versus N and Δt, with $\mathbf{b} = \mathbf{b}_2$ in order to have a stability condition on Δt versus the polynomial degree N. We empirically find this stability condition:

$$\Delta t \leq C\ N^{-p} \qquad \text{with } p \simeq 1.66. \quad (6.78)$$

In table 6 and in the following ones the spectral radius of the step operator T_{PR} with A_2 not-definite is reported. We consider three different choices for the vector field

$$\mathbf{b}_1 = (cos(\pi x), sin(\pi y))^T \qquad \mathbf{b}_2 = (x - e^x, y - e^y)^T \qquad \mathbf{b}_3 = (-(x+y)/2, xy)^T. \quad (6.79)$$

Table 5. The spectral radius of the step operator for the scheme PR-R2 versus Δt and the polynomial degree N. $\mathbf{b} = \mathbf{b}_2$ and $b_0 = 0$.

Δt	N					
	4	6	8	10	12	14
.001	0.993	0.997	0.999	0.999	0.999	0.999
.003	0.991	0.997	0.999	0.999	0.999	0.999
.01	0.991	0.998	0.999	0.999	0.999	0.999
.03	0.993	0.999	0.999	0.999	0.999	1.000
.1	0.998	0.999	1.004	1.004	1.003	1.003
.3	1.037	1.040	1.028	1.020	1.014	1.011
1.	1.383	1.194	1.115	1.078	1.063	1.052

Table 6. The spectral radius of the step operator on the PR scheme. $N = 8$, $\nu = 10^{-3}$ for $\mathbf{b}_i$ exposed in (6.79).

	R1-DN			R2			D		
Δt	$\mathbf{b}_1$	$\mathbf{b}_2$	$\mathbf{b}_3$	$\mathbf{b}_1$	$\mathbf{b}_2$	$\mathbf{b}_3$	$\mathbf{b}_1$	$\mathbf{b}_2$	$\mathbf{b}_3$
.001	0.999	0.999	0.999	0.999	0.999	0.999	0.999	0.999	0.999
.01	0.999	0.999	0.999	0.999	0.999	0.999	0.999	0.999	0.999
.1	0.998	0.997	0.999	0.999	0.999	0.999	0.998	0.998	0.999
1.	0.990	0.983	0.998	1.018	1.035	1.008	1.231	0.991	0.998
10.	0.957	0.862	0.994	1.742	2.456	1.271	21.091	2.142	1.620
100.	0.917	0.930	0.959	1.198	1.244	2.578	10.576	10.568	39.355
1000.	0.991	0.993	0.968	1.088	1.023	38.270	1.095	1.164	2.410

In table 6 the spectral radius is shown versus Δt and we find that the approaches $R1$ and DN are stable even if large values of Δt are considered.
In table 7 the spectral radius is shown versus Δt and N with $\mathbf{b} = \mathbf{b}_3$ of (6.79). We can see that the stability condition (6.78) is observed with a small perturbation due to the rounding errors.

Finally in table 8 we show the spectral radius versus Δt and the viscosity ν. Again we obtain good results for the R1 and DN approaches, while the R2 approach is conditionally stable with the following dependence on the viscosity ν: $\Delta t \leq C\,\nu$, for fix N.

6.1. *Application to stationary problems*

The fractional step schemes can also be applied to stationary problems. In this case the fractional step schems are considered as iterative methods in order to converge to the solution of the problem. The approximated problems has the following data: $\nu = 10^{-5}$, $\mathbf{b} = (-1, -1)^T$, $b_0 = 0$, $f = 0$ and $u = 0$ on $\partial\Omega$. The problem we have considered has been solved with the PR scheme with $N = 24$ and $\Delta t = 1$, the matrix A_2 has all the eigenvalues with not negative real parts, homogeneous Dirichlet boundary conditions are given and no stability problems arise from the resolution of this problem. In figure 1 we show the numerical solution of the stationary problem presenting a boundary layer; the numerical solution hasn't spurious oscillations and

Table 7. The spectral radius of the step operator for the scheme PR-R2 versus Δt and the polynomial degree N and $\mathbf{b} = \mathbf{b}_3$ of (6.79).

Δt	N					
	4	6	8	10	12	14
.001	0.994	0.997	0.999	0.999	0.999	0.999
.003	0.991	0.997	0.999	0.999	0.999	0.999
.01	0.990	0.997	0.999	0.999	0.999	0.999
.03	0.990	0.997	0.999	0.999	0.999	0.999
.1	0.991	0.998	0.999	0.999	0.999	0.999
.3	0.992	0.998	0.999	1.000	1.000	0.999
1.	0.996	1.010	1.008	1.006	1.003	1.000
10.	2.838	1.706	1.271	1.149	1.082	1.052

Table 8. The spectral radius versus Δt for different values of the viscosity. The vector field is $\mathbf{b} = (-(x+y)/2, xy)^T$, $b_0 = 0$ and $N = 10$. The approaches R1-DN and R2 are considered on the scheme PR.

	R1, DN			R2		
Δt	$\nu = 1.$	$\nu = 10.^{-2}$	$\nu = 10.^{-4}$	$\nu = 1.$	$\nu = 10.^{-2}$	$\nu = 10.^{-4}$
.001	0.999	0.999	0.999	0.999	0.999	0.999
.01	0.995	0.999	0.999	0.995	0.999	0.999
.1	0.983	0.999	0.999	0.983	0.999	0.999
1.	0.951	0.995	0.999	0.957	0.997	1.011
10.	0.953	0.981	0.999	0.953	0.990	1.232
100.	0.995	0.872	0.995	0.995	4.805	1.860
1000.	0.999	0.971	0.962	0.999	1.449	4.697

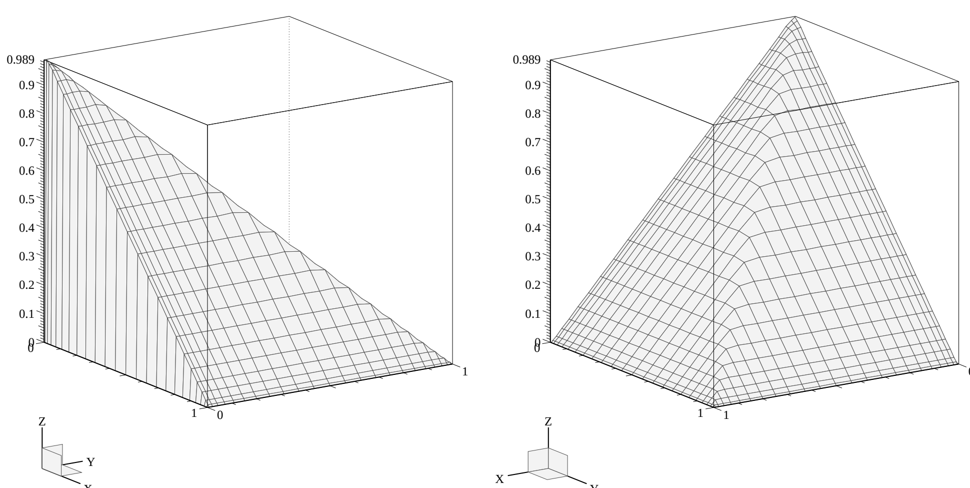

Fig. 1. A boundary layer problem approximated by the PR scheme

the layer is captured very well.

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