Linearly Implicit Domain Decomposition Methods for Nonlinear Time-Dependent Reaction-Diffusion Problems

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Summary. A new family of linearly implicit fractional step methods is proposed for the efficient numerical solution of a class of nonlinear time-dependent reaction-diffusion equations. By using the method of lines, the original problem is first discretized in space via a mimetic finite difference technique. The resulting differential system of stiff nonlinear equations is locally decomposed by suitable Taylor expansions and a domain decomposition splitting for the linear terms. This splitting is then combined with a linearly implicit one-step scheme belonging to the class of so-called fractional step Runge-Kutta methods. In this way, the original problem is reduced to the solution of several linear systems per time step which can be trivially decomposed into a set of uncoupled subsystems. As compared to classical domain decomposition techniques, our proposal does not require any Schwarz iterative procedure. The convergence of the designed method is illustrated by numerical experiments.

1 Introduction

In this paper, we consider nonlinear parabolic initial-boundary value problems of the following form: Find $\psi : \Omega \times [0,T] \to \mathbb{R}$ such that

$$\begin{cases} \frac{\partial \psi(\underline{x},t)}{\partial t} = \operatorname{div}(K(\psi)\operatorname{grad}\psi) + g(\underline{x},t,\psi) + f(\underline{x},t), & (\underline{x},t) \in \Omega \times (0,T], \\ \psi(\underline{x},0) = \psi_0(\underline{x}), & \underline{x} \in \Omega, \\ \psi(\underline{x},t) = \psi_D(\underline{x},t), & (\underline{x},t) \in \partial\Omega \times [0,T], \end{cases} \tag{1}$$

where $\Omega \subseteq \mathbb{R}^2$, $K(\psi)$ is a 2×2 nonlinear symmetric positive-definite tensor, $g(\underline{x},t,\psi)$ is a nonlinear reaction term and $f(\underline{x},t)$ denotes the source/sink term. Initial and boundary data are given by $\psi_0(\underline{x})$ and $\psi_D(\underline{x},t)$, respectively. For the sake of simplicity, only Dirichlet boundary conditions are considered.

The numerical solution of problem (1) is carried out via the method of lines, thus combining a spatial discretization stage with the subsequent time integration process. For the first stage, we use a mimetic finite difference (MFD) method formulated on

logically rectangular meshes. Our method extends the ideas discussed in [7] for linear parabolic problems to the nonlinear case (1) by introducing a quadratic bivariate interpolation approach in the discretization process. As for the time integration, the resulting system of nonlinear ordinary differential equations is locally decomposed by applying suitable Taylor expansions and a domain decomposition splitting for the linear terms. This kind of splitting was used in [2] for solving linear parabolic problems and has been recently surveyed by [5] in the context of regionally-additive schemes. Here, we combine such a technique with an extension of the class of linearly implicit fractional step methods designed and analyzed in [3, 4]. The totally discrete scheme is shown to be second-order convergent in both space and time under a mild stability restriction.

The remainder of the paper is divided into three sections. The first two briefly describe the spatial discretization and time integration processes. Also in Sec. 3, a linearly implicit splitting scheme due to Hundsdorfer and Verwer (cf. [1]) is introduced for comparison purposes. Finally, in the last section, some experiments illustrate the numerical behaviour of the proposed method.

2 Spatial Discretization

The spatial discretization of problem (1) is based on an MFD scheme derived from the support-operator method. This method, initially proposed in [6] and subsequently discussed in [7], provides a methodology for constructing discrete analogues of the invariant first-order differential operators appearing in the original problem (i.e., divergence and gradient).

Let us consider a discretization of Ω by means of a logically rectangular grid Ω_h, where h denotes the spatial mesh size. The first step in the MFD technique consists of choosing suitable degrees of freedom for semidiscrete scalar and vector functions: in this work, the former are defined at the cell centers of the mesh, while the latter are considered to be at the mesh nodes. We shall denote by V_h and $\tilde{V}_h$ the vector spaces of semidiscrete scalar and vector functions defined on the cell centers and nodes of Ω_h, respectively. As a second step, we equip these spaces with suitable scalar products, namely $[\cdot,\cdot]_{V_h}$ and $[\cdot,\cdot]_{\tilde{V}_h}$ (see [7] for details). The third step is to derive a discrete approximation to the divergence operator, $\mathrm{div}_h : \tilde{V}_h \to V_h$, which we shall refer to as the *prime operator*. Such an approximation is provided by the Gauss divergence theorem. Finally, the fourth step lies in defining a discrete gradient operator, $\widetilde{\mathrm{grad}}_h : V_h \to \tilde{V}_h$, as the adjoint to the discrete divergence div_h with respect to the previous scalar products, i.e.:

$$[\mathrm{div}_h\, \underline{\tilde{u}}_h, \varphi_h]_{V_h} \equiv [\underline{\tilde{u}}_h, -\widetilde{\mathrm{grad}}_h\, \varphi_h]_{\tilde{V}_h} \quad \forall\, \varphi_h \equiv \varphi_h(t) \in V_h,\ \forall\, \underline{\tilde{u}}_h \equiv \underline{\tilde{u}}_h(t) \in \tilde{V}_h. \tag{2}$$

Since $\widetilde{\mathrm{grad}}_h$ is somehow deduced from the so-called prime operator, we call it the *derived operator*. Within this framework, we shall denote by $\psi_h(t)$ and $g_h(t,\psi_h)$ the semidiscrete approximations to the scalar functions $\psi(\underline{x},t)$ and $g(\underline{x},t,\psi)$ at the cell centers of the mesh. Analogously, $f_h(t) \equiv r_h f(\underline{x},t)$, where r_h denotes the restriction operator to the cell centers of Ω_h.

The standard MFD method formulated in [7] is defined for linear problems in which $K \equiv K(\underline{x})$ does not depend on ψ. However, the more general case considered here requires an extension of this method to deal with the nonlinearity arising from $K(\psi)$. Let us briefly present the main features of such an extension. Recalling problem (1) and once we have defined the discrete operators div_h and $\widetilde{\mathrm{grad}}_h$, we need to approximate the matrix-vector product $K(\psi)\,\mathrm{grad}\,\psi$. For this product to be well-posed, since the components of $\widetilde{\mathrm{grad}}_h\,\psi_h$ are given at the mesh nodes (as derived from (2)), the elements of $K(\psi)$ must also be evaluated at this location. Let us denote by $\tilde{\psi}_h$ the approximations to the unknown ψ at the nodes of Ω_h. Then, the discretization of tensor $K(\psi)$, given by $\tilde{K}_h(\tilde{\psi}_h)$, is obtained by suitably evaluating its elements at $\tilde{\psi}_h$. As a result, the second-order nonlinear term $\mathrm{div}_h(\tilde{K}_h(\tilde{\psi}_h)\,\widetilde{\mathrm{grad}}_h\,\psi_h)$ possess a local stencil involving nine cell-centered values ψ_h (as described in [7]) as well as four nodal values $\tilde{\psi}_h$ (due to the discrete tensor $\tilde{K}_h(\tilde{\psi}_h)$). In order to eliminate these values from the local stencil, we apply a quadratic bivariate interpolation method which permits to obtain $\tilde{\psi}_h$ as a linear combination of the corresponding nine values of ψ_h. Consequently, the discrete diffusion operator will be given by $A_h(\cdot) \equiv \mathrm{div}_h(\tilde{K}_h(\cdot)\,\widetilde{\mathrm{grad}}_h\,\cdot) : V_h \to V_h$ and the local stencil of $A_h(\psi_h)$ will thus have a compact nine-cell structure.

The discretization process described in this section gives rise to a stiff nonlinear differential system of the form:

$$\psi_h'(t) = F_h(t,\psi_h) \equiv A_h(\psi_h) + g_h(t,\psi_h) + f_h(t), \quad t \in (0,T], \tag{3}$$

with initial condition $\psi_h(0) = \psi_{h,0} \equiv r_h\psi_0(\underline{x})$. The MFD method has been theoretically proved to be second-order convergent when applied to linear elliptic problems with either Dirichlet or Neumann conditions discretized on smooth grids. Also if linear parabolic problems are considered, the numerical behaviour of this spatial discretization technique shows convergence of order 2 (cf. [7]).

3 Time Integration

In this section, we introduce a family of linearly implicit time integrators based on a splitting of the semidiscrete problem derived in (3). For that purpose, let us first consider a decomposition of the spatial domain Ω into s overlapping subdomains, i.e. $\Omega = \bigcup_{j=1}^{s} \Omega_j$, where $\Omega_j = \bigcup_{k=1}^{s_j} \Omega_{jk}$ such that $\Omega_{jk} \cap \Omega_{j\ell} = \emptyset$ if $k \neq \ell$. Associated to such a decomposition, we construct a sufficiently smooth partition of unity consisting of s functions $\rho_j : \Omega \to [0,1]$, for $j = 1,2,\ldots,s$, which satisfy the following properties:

$$\rho_j(\underline{x}) = \begin{cases} 0 & \text{if } \underline{x} \in \Omega \setminus \Omega_j, \\ h_j(\underline{x}) & \text{if } \underline{x} \in \bigcup_{\substack{k=1 \\ k\neq j}}^{s} (\Omega_j \cap \Omega_k), \\ 1 & \text{if } \underline{x} \in \Omega_j \setminus \bigcup_{\substack{k=1 \\ k\neq j}}^{s} (\Omega_j \cap \Omega_k), \end{cases} \tag{4}$$

where $0 \le h_j(\underline{x}) \le 1$ and $\sum_{j=1}^{s} h_j(\underline{x}) = 1$ for any $\underline{x}$ located in the overlapping regions. From these restrictions, it is obvious that $\Omega_j \equiv supp\,(\rho_j(\underline{x}))$, for $j = 1,2,\ldots,s$.

In order to introduce the time integration in a simple way, we divide the time interval $[0,T]$ into subintervals $[t_n,t_{n+1}]$ of the same length, where $t_n = n\tau$, for $n = 0,1,\ldots,N_T \equiv [T/\tau]$, and $\tau > 0$ is the constant time step. In the following, we shall denote by $\psi_{h,n}$ the numerical approximations to the semidiscrete solution values $\psi_h(t_n)$. Now, recalling the differential system (3), we consider the Taylor expansion of $A_h(\psi_h)$ around $\psi_{h,n}$:

$$A_h(\psi_h) = A_h(\psi_{h,n}) + J_h(\psi_{h,n})(\psi_h - \psi_{h,n}) + B_h(\psi_h,\psi_{h,n}), \tag{5}$$

where J_h denotes the Jacobian matrix $dA_h/d\psi_h$. If we consider $\breve{f}_h(\psi_{h,n}) \equiv A_h(\psi_{h,n}) - J_h(\psi_{h,n})\,\psi_{h,n}$ as an additional source/sink term, we can rewrite (5) as $A_h(\psi_h) = \breve{f}_h(\psi_{h,n}) + J_h(\psi_{h,n})\,\psi_h + B_h(\psi_h,\psi_{h,n})$. Note that the last term in this expression is nonlinear. Furthermore, using the partition of unity introduced in (4), we split the linear terms $J_h(\psi_{h,n})$, $\breve{f}_h(\psi_{h,n})$ and $f_h(t)$ as follows:

$$\begin{aligned}
2J_h(\psi_{h,n}) &= \sum_{j=1}^{s} J_h^j(\psi_{h,n}), \qquad && \text{where } J_h^j(\psi_{h,n}) = R_h(\rho_j(\underline{x}))J_h(\psi_{h,n}),\\
\breve{f}_h(\psi_{h,n}) &= \sum_{j=1}^{s} \breve{f}_h^j(\psi_{h,n}), \qquad && \text{where } \breve{f}_h^j(\psi_{h,n}) = R_h(\rho_j(\underline{x}))\breve{f}_h(\psi_{h,n}),\\
f_h(t) &= \sum_{j=1}^{s} f_h^j(t), \qquad && \text{where } f_h^j(t) = R_h(\rho_j(\underline{x}))f_h(t),
\end{aligned} \tag{6}$$

with $R_h(\rho_j(\underline{x}))$ being a diagonal matrix whose main diagonal is given by $r_h\rho_j(\underline{x})$. Finally, the right-hand side from (3) can be rewritten in the following form:

$$F_h(t,\psi_h) \equiv F_h^0(t,\psi_h) + F_h^1(t,\psi_h) + \cdots + F_h^s(t,\psi_h), \tag{7}$$

where $F_h^0(t,\psi_h) \equiv g_h(t,\psi_h) + B_h(\psi_h,\psi_{h,n})$ comprises the nonlinear part of $F_h(t,\psi_h)$, whereas $F_h^j(t,\psi_h) \equiv J_h^j(\psi_{h,n})\,\psi_h + \breve{f}_h^j(\psi_{h,n}) + f_h^j(t)$, for $j = 1,2,\ldots,s$, are linear non-homogeneous terms.

According to the ideas proposed in [3] for linear parabolic problems and subsequently adapted in [4] to the semilinear case, we can integrate (3) by using the splitting (7), together with the following fractional step method:

$$\begin{cases}
\psi_{h,n}^1 = \psi_{h,n},\\
\psi_{h,n}^2 = \psi_{h,n}^1 + \tau\sum_{k=1}^{2}\alpha_k F_h^{i_k}(t_n^k,\psi_{h,n}^k) + \frac{\tau}{2}F_h^0(t_n^1,\psi_{h,n}^1),\\
\psi_{h,n}^j = \psi_{h,n}^{j-1} + \tau\sum_{k=j-1}^{j}\alpha_k F_h^{i_k}(t_n^k,\psi_{h,n}^k), \quad j = 3,4,\ldots,2s-2,\\
\psi_{h,n}^{2s-1} = \psi_{h,n}^{2s-2} + \tau\sum_{k=2s-2}^{2s-1}\alpha_k F_h^{i_k}(t_n^k,\psi_{h,n}^k)\\
\qquad\qquad - \frac{\tau}{2}F_h^0(t_n^1,\psi_{h,n}^1) + \tau F_h^0(t_n^s,\psi_{h,n}^s),\\
\psi_{h,n+1} = \psi_{h,n}^{2s-1}, \qquad\qquad n = 0,1,\ldots,N_T-1,
\end{cases} \tag{8}$$

where $i_k = k$, for $k = 1,2,\ldots,s$, and $i_k = 2s-k$, for $k = s+1,s+2,\ldots,2s-1$. The intermediate times are $t_{n,1} = t_n$, $t_{n,k} = t_n + \tau/2$, for $k = 2,3,\ldots,2s-2$, and $t_{n,2s-1} =$

$t_n + \tau = t_{n+1}$, whereas the method coefficients are given by $\alpha_1 = \alpha_s = \alpha_{2s-1} = 1/2$ and $\alpha_k = 1/4\ \forall k \in \{2,3,\ldots,s-1\} \cup \{s+1, s+2, \ldots, 2s-2\}$. Note that (8) is a linearly implicit one-step method with $(2s-1)$ internal stages belonging to the class of so-called fractional step Runge-Kutta (FSRK) methods (cf. [4]). It considers implicit contributions of the linear terms $\{F_h^j\}_{j=1}^s$, while explicitly handling the nonlinear term F_h^0. Recall that this term involves both the non-stiff reaction term $g_h(t, \psi_h)$ and the stiff remainder $B_h(\psi_h, \psi_{h,n})$. The former will not affect the stability of the scheme, provided it satisfies a Lipschitz condition (cf. [4]); by contrast, a mild stability restriction will arise due to the latter. A deeper insight on the stability properties of (8) will be provided in the last section.

Since (8) is an FSRK method, its internal stages consist of linear systems with the coefficient matrices $(I_h - \tau\alpha_j J_h^{i_j}(\psi_{h,n}))$, for $j = 2,3,\ldots,2s-1$. Owing to the domain decomposition splitting (6), each one of these linear systems involves the unknowns lying just in one of the subdomains $\{\Omega_j\}_{j=1}^s$. Moreover, since each subdomain Ω_j comprises s_j disjoint connected components, such a system can be easily decomposed into s_j uncoupled subsystems which allow a straightforward parallelization. As a difference with respect to classical domain decomposition methods, artificial boundary conditions are not required on each subdomain and, hence, no Schwarz iterative procedures are involved in the computations.

Following [4], the previous method can be proved to be of classical order 2. In fact, if we consider the case in which the number of levels $s = 2$ and apply the method to a linear parabolic problem, we recover the time integration process involved in the classical Peaceman-Rachford alternating direction implicit scheme. Therefore, (8) may be considered as a generalization of the Peaceman-Rachford scheme (cf. [3]).

As mentioned above, the conditional stability of (8) involves a mild stability restriction which makes it competitive with other existing linearly implicit splitting methods of order 2. For illustration, we shall compare our proposal with the so-called Hundsdorfer and Verwer scheme analyzed in [1]. This scheme is based on the technique of stabilizing corrections and, when applied to problem (3) with splitting (7), it leads to:

$$\begin{cases} \psi_{h,n}^0 = \psi_{h,n} + \tau F_h(t_n, \psi_{h,n}), & \\ \psi_{h,n}^j = \psi_{h,n}^{j-1} + \theta\tau\big(F_h^j(t_{n+1}, \psi_{h,n}^j) - F_h^j(t_n, \psi_{h,n})\big), & j = 1,2,\ldots,s, \\ \widehat{\psi}_{h,n}^0 = \psi_{h,n}^0 + \sigma\tau\big(F_h(t_{n+1}, \psi_{h,n}^s) - F_h(t_n, \psi_{h,n})\big), & \\ \widehat{\psi}_{h,n}^j = \widehat{\psi}_{h,n}^{j-1} + \theta\tau\big(F_h^j(t_{n+1}, \widehat{\psi}_{h,n}^j) - F_h^j(t_{n+1}, \psi_{h,n}^s)\big), & j = 1,2,\ldots,s, \\ \psi_{h,n+1} = \widehat{\psi}_{h,n}^s, & n = 0,1,\ldots,N_T - 1. \end{cases} \tag{9}$$

For any given θ, the scheme (9) is conditionally convergent of classical order 2, whenever $\sigma = \frac{1}{2}$, and of order 1 otherwise. Although the stability restriction of this method is similar to that of (8), it requires two more implicit stages in order to achieve the same accuracy.

4 Numerical Results

This section shows the numerical behaviour of methods (8) and (9) in the solution of nonlinear parabolic problems of type (1). In particular, let us consider (1) posed on the unit square $\Omega \equiv \{\underline{x} = (x,y) \in \mathbb{R}^2 : 0 < x < 1,\ 0 < y < 1\}$. Tensor $K(\psi)$ is a symmetric positive-definite nonlinear matrix defined as $K(\psi) = Q(\theta)\, D(\psi)\, Q(\theta)^T$, where $Q(\theta)$ is a 2×2 rotation matrix with angle $\theta = \pi/4$ and $D(\psi)$ is a 2×2 diagonal matrix whose diagonal entries are $1+\psi^2$ and $1+8\psi^2$. The nonlinear reaction term is chosen to be $g(\psi) = -(1+\psi^2)\, e^{-\psi}$, whereas the source/sink term $f(\underline{x},t)$ and both initial and Dirichlet boundary conditions are defined in such a way that $\psi(x,y,t) = e^{11-4t} x^4 (1-x)^4 y^4 (1-y)^4$ is the exact solution of the problem.

The discretization of the spatial domain Ω is based on the construction of a smooth curvilinear grid $\Omega_h \equiv \{(\tilde{x}_{i,j}, \tilde{y}_{i,j})\}_{i,j=1}^N$ with coordinates:

$$\tilde{x}_{i,j} = \xi_{i,j} + 10\, \xi_{i,j} (1-\xi_{i,j}) (\tfrac{1}{2} - \xi_{i,j})\, \eta_{i,j} (1-\eta_{i,j}),$$
$$\tilde{y}_{i,j} = \eta_{i,j} + 10\, \eta_{i,j} (1-\eta_{i,j}) (\tfrac{1}{2} - \eta_{i,j})\, \xi_{i,j} (1-\xi_{i,j}),$$

where $\xi_{i,j} = (i-1)\, h$, $\eta_{i,j} = (j-1)\, h$ and $h = 1/(N-1)$. This grid is obtained from a uniform grid, by using an analytical transformation. Fig. 1 shows an example of such a grid for $N = 17$.

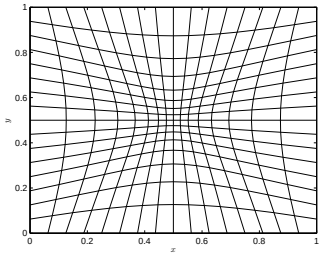
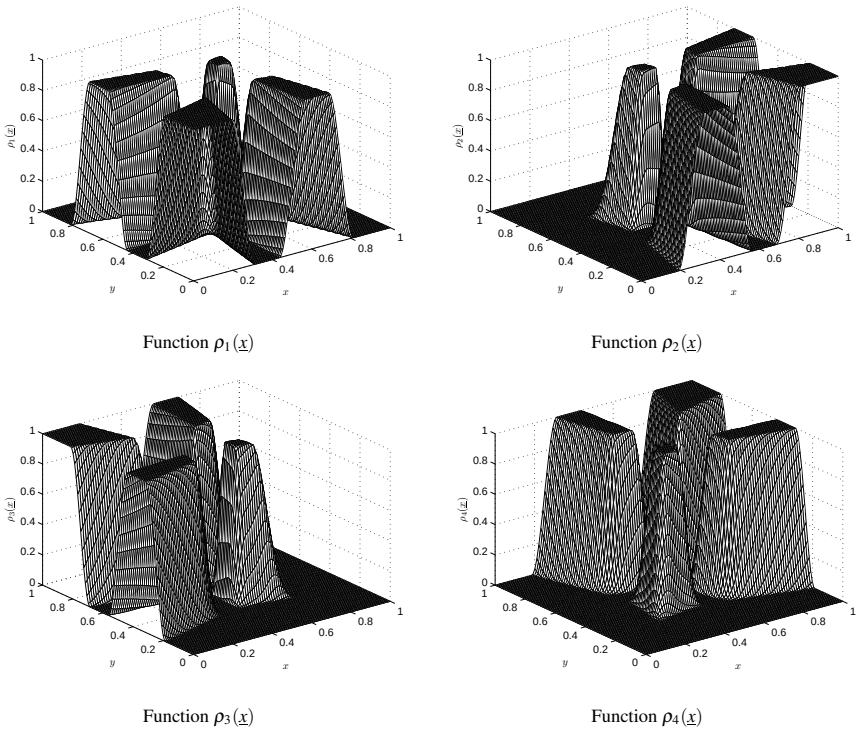


Fig. 1. Logically rectangular grid for $N = 17$.

Afterwards, we consider a decomposition of Ω into $s = 4$ overlapping subdomains $\{\Omega_j\}_{j=1}^s$, each of which involves $s_j = 4$ disjoint connected components, for $j = 1,2,3,4$. Related to such a decomposition, we define a smooth partition of unity consisting of a sequence of functions $\{\rho_j(\underline{x})\}_{j=1}^s$ based on (4). This partition of unity is displayed on Fig. 2, where the overlapping subdomains are given by $\Omega_j \equiv supp\,(\rho_j(\underline{x}))$.

For the time integration of this test problem, we consider the linearly implicit FSRK method (8) as well as the Hundsdorfer and Verwer scheme (9), with $\theta = 1$ and $\sigma = 1/2$. Let us introduce the global error at time $t = t_n$ as $E_{h,\tau} = r_h \psi(\underline{x}, t_n) - \psi_{h,n}$, for $n = 1,2,\ldots,N_T$. Under certain discrete norm $\|\cdot\|_h$ and suitable stability restrictions between h and τ, it holds that $\|E_{h,\tau}\|_h \leq C(h^2 + \tau^2)$, being C a positive constant



Function $\rho_1(\underline{x})$ Function $\rho_2(\underline{x})$

Function $\rho_3(\underline{x})$ Function $\rho_4(\underline{x})$

Fig. 2. Smooth partition of unity $\{\rho_j(\underline{x})\}_{j=1}^{s}$ related to $\{\Omega_j\}_{j=1}^{s}$, for $s=4$.

independent of h and τ. In our convergence study, we shall measure these errors by using the discrete L^2-norm in space and the discrete maximum norm in time, denoted by $\|E_{h,\tau}\|_2$. Tables 1 and 2 present the asymptotic behaviour of the global errors when the scheme (8) is used for different values of h and τ. As expected, it is shown to be conditionally convergent of order 2 in both space (see Table 1) and time (see Table 2).

Table 1. Global errors obtained in method (8) for $\tau = 5 \cdot 10^{-8}$.

h	$h_0 = 2^{-4}$	$h_0/2$	$h_0/4$	$h_0/8$	$h_0/16$	$h_0/32$
$\|E_{h,\tau}\|_2$	4.530E-2	3.305E-3	5.028E-4	1.120E-4	2.639E-5	6.574E-6

Finally, Table 3 compares the stability restrictions arising between h and τ when both methods are applied to this example. Here, we compute the maximum time steps τ_h^{PR} and τ_h^{HV} which make (8) and (9) respectively stable for different mesh sizes h. In view of the numerical results, we can conclude that both schemes converge

Table 2. Global errors obtained in method (8) for $h = 2^{-7}$.

τ	$\tau_0 = 10^{-4}$	$\tau_0/2$	$\tau_0/4$	$\tau_0/8$	$\tau_0/16$	$\tau_0/32$
$\|E_{h,\tau}\|_2$	1.424E-5	3.562E-6	8.908E-7	2.227E-7	5.568E-8	1.392E-8

under a non-severe stability limitation which is revealed to be slightly milder for our proposal. We have performed additional experiments assuming different types of solutions on both smooth and non-smooth grids and the resulting stability restrictions preserve a similar behaviour. Therefore, the generalization of the Peaceman-Rachford method given by (8) may be considered as a remarkable alternative to other existing linearly implicit splitting methods of order 2.

Table 3. Maximum time steps τ_h^{PR} and τ_h^{HV} permitted for different mesh sizes h.

h	$h_0 = 2^{-4}$	$h_0/2$	$h_0/4$	$h_0/8$	$h_0/16$	$h_0/32$
τ_h^{PR}	2.30E-3	1.90E-3	7.30E-4	3.00E-4	1.25E-4	5.10E-5
τ_h^{HV}	2.20E-4	7.05E-5	2.12E-5	6.43E-6	1.90E-6	5.80E-7

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