CONVERGENCE OF FINITE DIFFERENCE SCHEMES FOR NONLINEAR COMPLEX REACTION-DIFFUSION PROCESSES

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Abstract. This paper is devoted to the proof of the convergence properties of a class of finite difference schemes applied to nonlinear complex reaction-diffusion equations. We investigate the accuracy of the numerical solution considering implicit and semi-implicit discretizations. To illustrate the theoretical results we present some numerical examples computed with a semi-implicit scheme applied to a nonlinear equation.

Key words. finite differences, complex reaction-diffusion, convergence

AMS subject classifications. 65M12, 65M06

1. Introduction. Let Ω be a bounded open set in $\mathbb{R}^d$, $d \in \{1, 2\}$, with boundary $\Gamma = \partial\Omega$. Here we consider $\bar{\Omega} = \Omega \cup \partial\Omega$ an interval for $d = 1$ and a union of rectangles for $d = 2$. Let $Q = \Omega \times (0, T]$, with $T > 0$, and $v : \bar{Q} = \bar{\Omega} \times [0, T] \longrightarrow \mathbb{C}$. We consider a reaction-diffusion process with a nonconstant complex coefficient $D(x, t, v) = D_R(x, t, v) + iD_I(x, t, v)$ and nonconstant complex reaction term $F(x, t, v) = F_R(x, t, v) + iF_I(x, t, v)$, where $D_R(x, t, v)$, $D_I(x, t, v)$, $F_R(x, t, v)$, $F_I(x, t, v)$ are real functions dependent on v. We need to assume that

$$D_R(x, t, v) \geq \xi > 0, \qquad (x, t) \in \bar{Q}, \tag{1.1}$$

and that there exists a constant $L > 0$ such that

$$|D(x, t, v)| \leq L, \qquad (x, t) \in \bar{Q}. \tag{1.2}$$

Inequalities (1.1) and (1.2) can easily be shown to hold for the diffusion coefficient in [2, 6, 20].

We define the initial boundary value problem for the unknown complex function $u = u_R + iu_I$,

$$\frac{\partial u}{\partial t}(x, t) = \nabla \cdot (D(x, t, u)\nabla u(x, t)) + F(x, t, u), \quad (x, t) \in Q, \tag{1.3}$$

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under the initial condition

$$u(x,0) = u^0(x), \quad x \in \overline{\Omega}, \tag{1.4}$$

with either the Dirichlet boundary condition

$$u(x,t) = 0, \quad x \in \Gamma, \quad t \in [0,T], \tag{1.5}$$

or the Neumann boundary condition

$$\frac{\partial u}{\partial \nu}(x,t) = 0, \quad x \in \Gamma, \quad t \in [0,T], \tag{1.6}$$

where $\frac{\partial u}{\partial \nu}$ denotes the derivative in the direction of the exterior normal to Γ. For the reaction term we will consider the decomposition

$$F(x,t,v) = F_L(x,t,v) + F_{NL}(x,t,v), \tag{1.7}$$

where F_L is a linear operator with respect to v,

$$F_L(x,t,v) = f(x,t) + A(x,t)v(x,t).$$

We assume that the problem is well posed, in the sense that it admits a unique solution (in the classical or the weak sense) and it depends continuously on the data.

The present paper focuses on deriving convergence results for a class of finite difference schemes for (1.3)–(1.4), with (1.5) or (1.6), in one and two dimensions. We first note that expression (1.3) involves both Schrödinger type equations and parabolic equations and includes the possibility of having a source term, a linear reaction term, a nonlinear reaction term, or none of them (see (1.7)).

In the theory of heat conduction and chemical diffusion processes, if the thermal conductivity depends on the unknown function, the temperature distribution in a bounded medium is governed by this initial-boundary value problem, where F represents the reaction mechanisms [28]. Diffusion processes are also commonly used in image processing as, for example, in noise removal, inpainting, stereo vision, or optical flow (see, e.g., [6, 9, 20, 21, 25, 27, 30, 31, 34]). In particular, nonlinear complex diffusion proved to be successfully applied in medical imaging despeckling and denoising [17, 27]. Although diverse numerical schemes have been implemented to approximately solve the resulting mathematical model, no formal mathematical analysis has been yet carried out in order to gather the properties of approximate solutions such as error estimates and rates of convergence.

In [2] the authors studied the stability of a one parameter class of finite difference schemes for the nonlinear complex diffusion equation. Both explicit and implicit schemes were considered. In [3] the authors analyzed the stability of implicit and semi-implicit finite difference schemes for nonlinear complex reaction-diffusion processes. In image denoising, the stability proof in [2] is important for the cases where the resolution of the used image is fixed. However, in the cases where it is possible to increase the resolution of the image from previously acquired ones, it is also important to establish convergence results for the filtering process.

The numerical analysis of finite difference schemes for nonlinear diffusion and reaction-diffusion equations has been investigated extensively and is widely documented in the literature (see, e.g., [23, 28]). The convergence of finite difference methods for systems of nonlinear reaction-diffusion equations with real variables was studied in [22]. For the complex case, we mention [29], where the authors consider the analysis of conservative schemes for a coupled nonlinear Schrödinger system. To the best of our knowledge there is no rigorous proof of the convergence of finite difference schemes for (1.3). Writing this equation as a system in the variables u_R and u_I, we obtain a particular reaction-diffusion system of real variables. We did not find in the literature convergence estimates for similar systems. This paper fills this gap in the theory of finite difference schemes applied to the considered problem.

For the sake of clarity, we restrict the approach to the case of domains which in two dimensions are a union of rectangles. It is well known that numerical schemes applied to boundary value problems on domains with re-entrance corners may suffer from a global loss of accuracy caused by the influence of corner singularities. In order to regain the full order of convergence, one common strategy is to use a systematic mesh refinement near the corner points [10, 11]. Alternative strategies can be found in, e.g., [7, 13, 19, 33]. In this paper we assume that the exact solution is smooth enough, and so this pollution effect is not an issue.

The paper is organized as follows. In section 2 we describe the implicit and semi-implicit numerical methods simultaneously by embedding them into a one-parameter family of finite difference schemes. The core section of this paper is section 3, where the rigorous proof of convergence is presented, taking into account the influence of the regularity of the solution on the error estimate. In the last section some numerical experiments are shown to illustrate the theoretical analysis. The paper ends with an appendix with the proof of some technical lemmata.

2. Numerical method.

Let us construct a nonequidistant rectangular grid, $\mathcal{R}_h$, on $\overline{Q}$. Let $\mathcal{R} = \prod_{k=1}^{d}(x_{k,0}, x_{k,N_k})$ such that $\Omega \subseteq \mathcal{R}$. We define the space grid by

$$\mathcal{R}_h = \prod_{k=1}^{d} \mathcal{R}_{h_k},$$

where $\mathcal{R}_{h_k} = \{x_{k,0} < x_{k,1} < \cdots < x_{k,N_k}\}$. We associate each grid point x_j with the coordinate $j = (j_1, \ldots, j_d)$. Let $(h_{k,j_k})_{0 \le j_k \le N_k - 1}$ be a vector of mesh-sizes (i.e., positive numbers) in the kth spatial coordinate direction, $k = 1, \ldots, d$. We denote by h the maximal mesh-size. Points halfway between two adjacent grid points are denoted by $x_{j+(1/2)e_k} = x_j + (1/2)h_{k,j_k}e_k$ and $x_{j-(1/2)e_k} = x_j - (1/2)h_{k,j_k-1}e_k$, where e_k is the unit vector in the kth direction. We will also use the notation $h_{k,j_k-1/2} = (h_{k,j_k-1} + h_{k,j_k})/2$. We define $\Omega_h = \Omega \cap \mathcal{R}_h$, $\Gamma_h = \Gamma \cap \mathcal{R}_h$, and $\bar{\Omega}_h = \Omega_h \cup \Gamma_h$. The grid $\mathcal{R}_h$ is assumed to be such that the vertices of $\bar{\Omega}$ are in Γ_h.

For the temporal interval we consider the mesh

$$0 = t^0 < t^1 < \cdots < t^{M-1} < t^M = T,$$

where $M \ge 1$ is an integer and $\Delta t^m = t^{m+1} - t^m$, $m = 0, \ldots, M-1$. We denote by $\overline{Q}_h^{\Delta t}$ the mesh in $\overline{Q}$ defined by the Cartesian product of the space grid $\overline{\Omega}_h$ and a grid in the temporal domain. Let $Q_h^{\Delta t} = \overline{Q}_h^{\Delta t} \cap Q$ and $\Gamma_h^{\Delta t} = \overline{Q}_h^{\Delta t} \cap \Gamma \times [0, T]$. We associate the coordinate $(j, m) = (j_1, \ldots, j_d, m)$ to the point $(x_j, t^m) \in \overline{Q}_h^{\Delta t}$ and associate $(j + (1/2)e_k, m)$ and $(j - (1/2)e_k, m)$ to the midpoints $(x_{j+(1/2)e_k}, t^m)$ and $(x_{j-(1/2)e_k}, t^m)$, respectively.

We consider the notation $V_j^m = V(x_j, t^m)$, $V_{j+(1/2)e_k}^m = V(x_{j+(1/2)e_k}, t^m)$, and $V_{j-(1/2)e_k}^m = V(x_{j-(1/2)e_k}, t^m)$ for a function V defined on $\overline{Q}$. For the formulation of the finite difference approximations, we use the centered finite difference quotients in the kth spatial direction,

$$\delta_k V_j^m = \frac{V_{j+(1/2)e_k}^m - V_{j-(1/2)e_k}^m}{h_{k,j_k-1/2}}, \quad \delta_k V_{j-(1/2)e_k}^m = \frac{V_j^m - V_{j-e_k}^m}{h_{k,j_k-1}}, \quad k = 1, 2.$$

If $d = 1$, these definitions are simplified for the case of one spatial coordinate instead of two.

We use the notation $\tilde{Q}_h^{\Delta t}$ for the set $Q_h^{\Delta t}$ or $\overline{Q}_h^{\Delta t}$, in the case of Dirichlet or Neumann boundary conditions. On $\overline{Q}_h^{\Delta t}$ we approximate (1.3)–(1.4) by the one-parameter family of finite difference schemes: find $U_j^m \approx u(x_j, t^m)$ such that

$$\frac{U_j^{m+1} - U_j^m}{\Delta t^m} = \sum_{k=1}^{d} \delta_k (D_j^{m,\mu} \delta_k U_j^{m+1}) + F_j^{m,\mu} \quad \text{in} \quad \tilde{Q}_h^{\Delta t}, \tag{2.1}$$

with

$$U_j^0 = u^0(x_j) \quad \text{in} \quad \overline{\Omega}_h, \tag{2.2}$$

and either

$$U_j^m = 0 \quad \text{in} \quad \Gamma_h^{\Delta t}, \tag{2.3}$$

in the case of homogeneous Dirichlet boundary conditions (1.5), or

$$\sum_{k=1}^{d} \left(h_{k,j_k-e_k} \delta_k U_{j+(1/2)e_k}^m + h_{k,j_k+e_k} \delta_k U_{j-(1/2)e_k}^m \right) \nu_k = 0 \quad \text{in} \quad \Gamma_h^{\Delta t}, \tag{2.4}$$

in the case of homogeneous Neumann boundary conditions (1.6), where ν_k represents the kth component of the normal vector ν. In (2.1) we consider

$$D_{j+(1/2)e_k}^{m,\mu} = \frac{D(x_j, t^{m+1}, U_j^{m+\mu}) + D(x_{j+e_k}, t^{m+1}, U_{j+e_k}^{m+\mu})}{2}, \quad \mu \in \{0, 1\},$$

where

$$U_j^{m+\mu} = \mu U_j^{m+1} + (1-\mu) U_j^m, \quad \mu \in \{0, 1\}, \tag{2.5}$$

and

$$F_j^{m,\mu} = F_{Lj}^{m+1} + F_{NLj}^{m,\mu} = f_{x_j}^{m+1} + A(x_j, t^{m+1}) U_j^{m+1} + F_{NLj}^{m,\mu},$$

where, as, e.g., in [24],

$$f_{x_j}^{m+1} = \frac{1}{|\omega_j|} \int_{\omega_j} f(x, t^{m+1})\, dx, \tag{2.6}$$

with $\omega_j = \prod_{k=1}^{d} (x_{j-(1/2)e_k}, x_{j+(1/2)e_k}) \subset \Omega$ and $|\omega_j|$ the measure of ω_j, and

$$F_{NLj}^{m,\mu} = F_{NL}(x_j, t^{m+1}, U_j^{m+\mu}), \quad \mu \in \{0, 1\}. \tag{2.7}$$

Note that the cases $\mu = 0$ and $\mu = 1$ correspond to a semi-implicit and an implicit discretization, respectively. In the semi-implicit case, the diffusion coefficient and the nonlinear part of the reaction term are treated explicitly.

3. Convergence. The main result of this paper is Theorem 3.1. Estimates for the difference between the pointwise restriction of the exact solution on the discretization nodes and the finite difference solution are proved. The key idea is to start by finding a variational system for the error. We obtain error estimates using the Bramble–Hilbert lemma (see Lemma A.1 in the appendix) in order to derive the highest possible accuracy assuming the minimum hypothesis on the smoothness of the exact solution.

To provide a proper functional setting, we need to define spaces involving time-dependent functions [16]. Let X denote a Banach space with norm $\|.\|_X$. In what follows, X is shorthand for any of the usual Sobolev spaces $W^{s,p}(\Omega)$ (which we also denote by $H^s(\Omega)$ in the case $p = 2$) or the Banach space $L^\infty(\Omega)$. The space $L^\infty(0,T;X)$ consists of all measurable functions $v : [0,T] \to X$ with

$$\|v\|_{L^\infty(0,T;X)} = \operatorname*{ess\,sup}_{0\le t\le T} \|v(t)\|_X < \infty,$$

and $C([0,T];X)$ is the space of continuous functions $v : [0,T] \to X$ with

$$\|v\|_{C([0,T];X)} = \max_{0\le t\le T} \|v(t)\|_X < \infty.$$

In what follows, $\|\cdot\|_h$ will denote the discrete L^2 norm, which will be specified later in this section. In the next theorem, $D(u)$ and $F_{NL}(u)$ denote the functions on the variables x and t, $D(x,t,u(x,t))$ and $F_{NL}(x,t,u(x,t))$.

THEOREM 3.1. *Let the weak solution u of (1.3)–(1.4), with (1.5) or (1.6), lie in $C([0,T];\, H^{1+r}(\Omega)\cap W^{1,\infty}(\Omega))$, $r \in \{1,2\}$, where Ω is an interval (in the case $d = 1$) or a union of rectangles (in the case $d = 2$). Let us assume that D and F_{NL} are Lipschitz continuous with respect to the third component, with Lipschitz constant C_D and C_F, respectively, in the sense that*

$$|D(x,t,v) - D(x,t,w)| \le C_D|v(x,t) - w(x,t)| \quad \forall (x,t) \in \bar{Q}, \tag{3.1}$$

$$|F_{NL}(x,t,v) - F_{NL}(x,t,w)| \le C_F|v(x,t) - w(x,t)| \quad \forall (x,t) \in \bar{Q}, \tag{3.2}$$

and $D(u) \in C([0,T];W^{2,\infty}(\Omega))$, $F_{NL}(u), Au \in C([0,T];H^2(\Omega))$, $f \in C([0,T];L^2(\Omega))$. If (1.1) and (1.2) hold, and $\frac{\partial u}{\partial t} \in C([0,T];H^2(\Omega))$, $\frac{\partial^2 u}{\partial t^2} \in L^\infty(0,T;\, H^1(\Omega))$, then the numerical solution U of (2.1)–(2.2), with (2.3) or (2.4), satisfies the error estimate

$$\max_{1\le m\le M} \|\mathrm{R}_h u(t^m) - U^m\|_h \le \mathcal{O}(h^r) + \mathcal{O}(\Delta t), \tag{3.3}$$

where $\mathrm{R}_h u$ denotes the pointwise restriction of the function u to the space grid $\overline{\Omega}_h$.

We will prove the convergence for the bidimensional case. For the proof we follow some arguments taken from [4, 5, 15, 18]. In what follows, C denotes a generic positive constant.

We first note that, as a result of Taylor expansion about t^{m+1},

$$\frac{u(x,t^{m+1}) - u(x,t^m)}{\Delta t^m} = \frac{\partial u}{\partial t}(x,t^{m+1}) + \Delta t^m \rho_u^m(x) \quad \forall x \in \Omega, \tag{3.4}$$

with

$$\|\rho_u^m\|_{L^2(\Omega)} \le C \left\| \frac{\partial^2 u}{\partial t^2} \right\|_{L^\infty(t^m,t^{m+1};L^2(\Omega))},$$

and, for any sufficiently smooth function $g(t)$,

$$g(t^{m+1}) = g(t^m) + \Delta t^m \rho_g^m, \quad \text{with} \quad |\rho_g^m| \leq \left\| \frac{dg}{dt} \right\|_{L^\infty(t^m, t^{m+1})}. \tag{3.5}$$

Let us consider the numerical method (2.1)–(2.2) assuming Neumann boundary conditions. For Dirichlet boundary conditions the proof follows the same steps.

We rewrite (2.1)–(2.2), (2.4) as a system by separating the real and imaginary parts, U_R and U_I, respectively, of the main variable $U = (U_0, \ldots, U_N)$. We shall then study the convergence of the family of finite difference schemes: find $U_j^m \approx u(x_j, t^m)$ such that

(3.6)

$$\begin{cases} \dfrac{U_{Rj}^{m+1} - U_{Rj}^m}{\Delta t^m} = \displaystyle\sum_{k=1}^{2} \left(\delta_k (D_{Rj}^{m,\mu} \delta_x U_{Rj}^{m+1}) - \delta_k (D_{Ij}^{m,\mu} \delta_x U_{Ij}^{m+1}) \right) + F_{Rj}^{m,\mu} \quad \text{in} \quad \tilde{Q}_h^{\Delta t}, \\ \dfrac{U_{Ij}^{m+1} - U_{Ij}^m}{\Delta t^m} = \displaystyle\sum_{k=1}^{2} \left(\delta_k (D_{Ij}^{m,\mu} \delta_x U_{Rj}^{m+1}) + \delta_k (D_{Rj}^{m,\mu} \delta_x U_{Ij}^{m+1}) \right) + F_{Ij}^{m,\mu} \quad \text{in} \quad \tilde{Q}_h^{\Delta t}, \end{cases}$$

with initial condition

$$U_{Rj}^0 = u_R^0(x_j), \quad U_{Ij}^0 = u_I^0(x_j) \quad \text{in} \quad \overline{\Omega}_h,$$

and homogeneous Neumann boundary conditions

$$\sum_{k=1}^{d} \left(h_{k,j_k - e_k} \delta_k U_{Rj+(1/2)e_k}^m + h_{k,j_k + e_k} \delta_k U_{Rj-(1/2)e_k}^m \right) \nu_k = 0 \quad \text{in} \quad \Gamma_h^{\Delta t},$$

$$\sum_{k=1}^{d} \left(h_{k,j_k - e_k} \delta_k U_{Ij+(1/2)e_k}^m + h_{k,j_k + e_k} \delta_k U_{Ij-(1/2)e_k}^m \right) \nu_k = 0 \quad \text{in} \quad \Gamma_h^{\Delta t}.$$

We start by introducing some notation related to the space domain. For each $x_j = (x_{j_1}, x_{j_2}) \in \bar{\Omega}_h$, we define the rectangle $\square_j = (x_{j_1}, x_{j_1+1}) \times (x_{j_2}, x_{j_2+1})$ and $|\square_j|$ the measure of $\square_j$. The discrete inner products, for the two-dimensional (2D) case, are

$$\begin{aligned} (U, V)_h = \sum_{\square_j \subset \Omega} \frac{|\square_j|}{4} \big(& U_{j_1,j_2} \overline{V}_{j_1,j_2} + U_{j_1+1,j_2} \overline{V}_{j_1+1,j_2} \\ & + U_{j_1,j_2+1} \overline{V}_{j_1,j_2+1} + U_{j_1+1,j_2+1} \overline{V}_{j_1+1,j_2+1} \big), \end{aligned}$$

$$(U, V)_{h_1^*} = \sum_{\square_j \subset \Omega} \frac{|\square_j|}{2} \left(U_{j_1+1/2,j_2} \overline{V}_{j_1+1/2,j_2} + U_{j_1+1/2,j_2+1} \overline{V}_{j_1+1/2,j_2+1} \right),$$

and

$$(U, V)_{h_2^*} = \sum_{\square_j \subset \Omega} \frac{|\square_j|}{2} \left(U_{j_1,j_2+1/2} \overline{V}_{j_1,j_2+1/2} + U_{j_1+1,j_2+1/2} \overline{V}_{j_1+1,j_2+1/2} \right).$$

Their correspondent norms are denoted by $\|.\|_h$, $\|.\|_{h_1^*}$, and $\|.\|_{h_2^*}$, respectively.

Let $E = \mathrm{R}_h u - U$, $E_R = \mathrm{R}_h u_R - U_R$, and $E_I = \mathrm{R}_h u_I - U_I$. Multiplying both members of the first and second equations of (3.6) by E_R^{m+1} and E_I^{m+1}, respectively, according to the discrete inner product (3.7), using (3.4), and taking into account the boundary conditions, we obtain

$$\begin{aligned}
&\left(\frac{E_R^{m+1}-E_R^m}{\Delta t^m}, E_R^{m+1}\right)_h + \sum_{k=1}^{2} \|(D^{m,\mu}_{R+(1/2)e_k})^{1/2}\delta_k E_R^{m+1}\|^2_{h_k^*} \\
&\quad = \left(\mathrm{R}_h \frac{\partial u_R}{\partial t}(t^{m+1}), E_R^{m+1}\right)_h + \Delta t^m \left(\rho^m_{u_R}, E_R^{m+1}\right)_h \\
&\quad + \sum_{k=1}^{2}\left(D^{m,\mu}_{R+(1/2)e_k}\delta_k^+ \mathrm{R}_h u_R^{m+1}, \delta_k E_R^{m+1}\right)_{h_k^*} \\
&\quad - \sum_{k=1}^{2}\left(D^{m,\mu}_{I+(1/2)e_k}\delta_k \mathrm{R}_h u_I^{m+1}, \delta_k E_R^{m+1}\right)_{h_k^*} \\
&\quad + \sum_{k=1}^{2}\left(D^{m,\mu}_{I+(1/2)e_k}\delta_k E_I^{m+1}, \delta_k E_R^{m+1}\right)_{h_k^*} - \left(F_R^{m,\mu}, E_R^{m+1}\right)_h
\end{aligned} \tag{3.7}$$

and

$$\begin{aligned}
&\left(\frac{E_I^{m+1}-E_I^m}{\Delta t^m}, E_I^{m+1}\right)_h + \sum_{k=1}^{2} \|(D^{m,\mu}_{R+(1/2)e_k})^{1/2}\delta_k E_I^{m+1}\|^2_{h_k^*} \\
&\quad = \left(\mathrm{R}_h \frac{\partial u_I}{\partial t}(t^{m+1}), E_I^{m+1}\right)_h + \Delta t^m \left(\rho^m_{u_I}, E_I^{m+1}\right)_h \\
&\quad + \sum_{k=1}^{2}\left(D^{m,\mu}_{I+(1/2)e_k}\delta_k \mathrm{R}_h u_R^{m+1}, \delta_k E_I^{m+1}\right)_{h_k^*} \\
&\quad - \sum_{k=1}^{2}\left(D^{m,\mu}_{R+(1/2)e_k}\delta_k \mathrm{R}_h u_I^{m+1}, \delta_k E_I^{m+1}\right)_{h_k^*} \\
&\quad + \sum_{k=1}^{2}\left(D^{m,\mu}_{I+(1/2)e_k}\delta_k E_R^{m+1}, \delta_k E_I^{m+1}\right)_{h_k^*} - \left(F_I^{m,\mu}, E_I^{m+1}\right)_h .
\end{aligned} \tag{3.8}$$

In order to provide the desired bounds, we start by deducing that

$$\begin{aligned}
\left(\frac{E_R^{m+1}-E_R^m}{\Delta t^m}, E_R^{m+1}\right)_h &= \frac{1}{\Delta t^m}\left(E_R^{m+1}, E_R^{m+1}\right)_h - \frac{1}{\Delta t^m}\left(E_R^{m}, E_R^{m+1}\right)_h \\
&= \frac{1}{2\Delta t^m}\|E_R^{m+1}\|_h^2 - \frac{1}{2\Delta t^m}\|E_R^{m}\|_h^2 + \frac{1}{2\Delta t^m}\|E_R^{m+1}-E_R^m\|_h^2.
\end{aligned}$$

Then

$$\left(\frac{E_R^{m+1}-E_R^m}{\Delta t^m}, E_R^{m+1}\right)_h \geq \frac{1}{2\Delta t^m}\left(\|E_R^{m+1}\|_h^2 - \|E_R^m\|_h^2\right). \tag{3.9}$$

Likewise

$$\left(\frac{E_I^{m+1}-E_I^m}{\Delta t^m}, E_I^{m+1}\right)_h \geq \frac{1}{2\Delta t^m}\left(\|E_I^{m+1}\|_h^2 - \|E_I^m\|_h^2\right). \tag{3.10}$$

Let $x = (x_1, x_2)$ and $x_j = (x_{j_1}, x_{j_2})$. We will consider the contribution of each rectangle $\Box_j$, which we subdivide into four congruent subrectangles R_1, R_2, R_3, R_4 such that P_i is the common vertex of the region $\Box_j$ and R_i, $i = 1, \ldots, 4$, respectively, that is, $P_1 = (x_{j_1}, x_{j_2})$, $P_2 = (x_{j_1+1}, x_{j_2})$, $P_3 = (x_{j_1+1}, x_{j_2+1})$, $P_4 = (x_{j_1}, x_{j_2+1})$.

Integrating both sides of (1.3) over $|\Box_j|$, multiplying in both members the contribution of R_i by $\overline{E}(P_i, t^{m+1})$, and using integration and a summation by parts, we may conclude that

(3.11)
$$
\begin{aligned}
&\|E_R^M\|_h^2 + \|E_I^M\|_h^2 \\
&\quad + 2\sum_{m=0}^{M-1} \Delta t^m \sum_{k=1}^{2} \left(\|(D^{m,\mu}_{R+(1/2)e_k})^{1/2} \delta_k E_R^{m+1}\|_{h_k^*}^2 + \|(D^{m,\mu}_{R+(1/2)e_k})^{1/2} \delta_k E_I^{m+1}\|_{h_k^*}^2 \right) \\
&\le 2\sum_{m=0}^{M-1} \Delta t^m (|T_1| + |T_2| + |T_3| + |T_4| + |T_5| + |T_6| + |T_7| + |T_8| + |T_9|),
\end{aligned}
$$

where the expressions for $T_1, \ldots, T_9$ are defined in what follows. In the previous bound we took into account the boundary conditions, the fact that $\|E^0\|_h = 0$, and (3.9) and (3.10).

In (3.12)

$$
T_1 = \sum_{\Box_j \subset \Omega} T_1(\Box_j) \quad \text{and} \quad T_2 = \sum_{\Box_j \subset \Omega} T_2(\Box_j),
$$

which is the contribution of the region $\Box_j$ to T_1 and T_2, given, respectively, by

$$
T_1(\Box_j) = \frac{h_{1,j_1} h_{2,j_2}}{4} \sum_{i=1}^{4} \frac{\partial u_R}{\partial t}(P_i, t^{m+1}) \left(E_R^{m+1}\right)_{P_i} - \sum_{i=1}^{4} \int_{R_i} \frac{\partial u_R}{\partial t}(x, t^{m+1})\, dx (E_R^{m+1})_{P_i}
$$

and

$$
T_2(\Box_j) = \frac{h_{1,j_1} h_{2,j_2}}{4} \sum_{i=1}^{4} \frac{\partial u_I}{\partial t}(P_i, t^{m+1}) \left(E_I^{m+1}\right)_{P_i} - \sum_{i=1}^{4} \int_{R_i} \frac{\partial u_I}{\partial t}(x, t^{m+1})\, dx (E_I^{m+1})_{P_i},
$$

where $(E_R^{m+1})_{P_i}$ denotes $E_R(P_i, t^{m+1})$ and $(E_I^{m+1})_{P_i}$ denotes $E_I(P_i, t^{m+1})$.

We set

$$
T_3 = \Delta t^m \left(\rho^m_{u_R}, E_R^{m+1}\right)_h + \Delta t^m \left(\rho^m_{u_I}, E_I^{m+1}\right)_h .
$$

In order to introduce T_4, we start by defining the line segments $S^a_{j_1+1/2} = \{x_{j_1+1/2}\} \times (x_{j_2}, x_{j_2+1/2})$, $S^b_{j_1+1/2} = \{x_{j_1+1/2}\} \times (x_{j_2+1/2}, x_{j_2+1})$, $S^a_{j_2+1/2} =$

$(x_{j_1}, x_{j_1+1/2}) \times \{x_{j_2+1/2}\}$, and $S^b_{j_2+1/2} = (x_{j_1+1/2}, x_{j_1+1}) \times \{x_{j_2+1/2}\}$. Then we set

$$
\begin{aligned}
T_4 = \sum_{\square_j \subset \Omega} h_{1,j_1} \Bigg(\int_{S^a_{j_1+1/2}} D_R(x_{j_1+1/2}, x_2, t^{m+1}, u) \frac{\partial u_R}{\partial x_1}(x_{j_1+1/2}, x_2, t^{m+1})\, dx_2 \\
\times (\delta_1 E_R^{m+1})_{j_1+1/2, j_2} \Bigg) \\
+ \sum_{\square_j \subset \Omega} h_{1,j_1} \Bigg(\int_{S^b_{j_1+1/2}} D_R(x_{j_1+1/2}, x_2, t^{m+1}, u) \frac{\partial u_R}{\partial x_1}(x_{j_1+1/2}, x_2, t^{m+1})\, dx_2 \\
\times (\delta_1 E_R^{m+1})_{j_1+1/2, j_2+1} \Bigg) \\
+ \sum_{\square_j \subset \Omega} h_{2,j_2} \Bigg(\int_{S^a_{j_2+1/2}} D_R(x_1, x_{j_2+1/2}, t^{m+1}, u) \frac{\partial u_R}{\partial x_2}(x_1, x_{j_2+1/2}, t^{m+1})\, dx_1 \\
\times (\delta_2 E_R^{m+1})_{j_1, j_2+1/2} \Bigg) \\
+ \sum_{\square_j \subset \Omega} h_{2,j_2} \Bigg(\int_{S^b_{j_2+1/2}} D_R(x_1, x_{j_2+1/2}, t^{m+1}, u) \frac{\partial u_R}{\partial x_2}(x_1, x_{j_2+1/2}, t^{m+1})\, dx_1 \\
\times (\delta_2 E_R^{m+1})_{j_1+1, j_2+1/2} \Bigg) \\
- \left(D^{m,\mu}_{R+(1/2)e_1} \delta_1 \mathrm{R}_h u_R^{m+1}, \delta_1 E_R^{m+1} \right)_{h_1^*} - \left(D^{m,\mu}_{R+(1/2)e_2} \delta_2 \mathrm{R}_h u_R^{m+1}, \delta_2 E_R^{m+1} \right)_{h_2^*}.
\end{aligned}
$$

The terms T_5, T_6, and T_7 are analogous to T_4 replacing D_R, u_R, and E_R by D_I, u_I, and E_R for T_5; by D_I, u_R, and E_I for T_6; and by D_R, u_I, and E_I for T_7.

Finally,

$$
T_8 = \sum_{\square_j \subset \Omega} \left(\frac{h_{1,j_1} h_{2,j_2}}{4} \sum_{i=1}^{4} (F_R^{m,\mu})_{P_i} \left(E_R^{m+1}\right)_{P_i} - \sum_{i=1}^{4} \int_{R_i} F_R(x, t^{m+1}, u)\, dx (E_R^{m+1})_{P_i} \right)
$$

and

$$
T_9 = \sum_{\square_j \subset \Omega} \left(\frac{h_{1,j_1} h_{2,j_2}}{4} \sum_{i=1}^{4} (F_I^{m,\mu})_{P_i} \left(E_I^{m+1}\right)_{P_i} - \sum_{i=1}^{4} \int_{I_i} F_I(x, t^{m+1}, u)\, dx (E_I^{m+1})_{P_i} \right).
$$

Let us start by estimating T_1. First, note the equality

$$
\begin{aligned}
4 \sum_{i=1}^{4} c_i d_i = \sum_{i=1}^{4} c_i \sum_{i=1}^{4} d_i + (c_1 + c_2 - c_3 - c_4)(d_1 + d_2 - d_3 - d_4) \\
+ (c_1 - c_2 + c_3 - c_4)(d_1 - d_2 + d_3 - d_4) \\
+ (c_1 - c_2 - c_3 + c_4)(d_1 - d_2 - d_3 + d_4),
\end{aligned}
$$

with

$$
c_i = \frac{h_{1,j_1} h_{2,j_2}}{4} \frac{\partial u_R}{\partial t}(P_i, t^{m+1}) - \int_{R_i} \frac{\partial u_R}{\partial t}(x, t^{m+1})\, dx
$$

and $d_i = (E_R^{m+1})_{P_i}$. We apply this equality to $4T_1(\square_j)$ and study the behavior of the four resulting sums $T_{1a}(\square_j)$, $T_{1b}(\square_j)$, $T_{1c}(\square_j)$, and $T_{1d}(\square_j)$. Using the inequality (A.1) of Lemma A.2, we obtain

$$\left|\frac{h_{1,j_1}h_{2,j_2}}{4}\sum_{i=1}^{4}\frac{\partial u_R}{\partial t}(P_i,t^{m+1}) - \int_{\square_j}\frac{\partial u_R}{\partial t}(x,t^{m+1})\,dx\right| \\ \le C(h_{1,j_1}^2 + h_{2,j_2}^2)\max_{\substack{s_1+s_2=2\\ s_1,s_2\in\{0,1,2\}}}\left\|\frac{\partial^3 u_R}{\partial t\partial x_1^{s_1}\partial x_2^{s_2}}(t^{m+1})\right\|_{L^1(\square_j)},$$

and then

$$|T_{1a}(\square_j)| \le C(h_{1,j_1}^2 + h_{2,j_2}^2)\max_{s_1+s_2=2}\left\|\frac{\partial^3 u_R}{\partial t\partial x_1^{s_1}\partial x_2^{s_2}}(t^{m+1})\right\|_{L^1(\square_j)}\sum_{i=1}^{4}\left|(E_R^{m+1})_{P_i}\right|.$$

We can write $T_{1b}(\square_j)$ in the form

$$(c_1+c_2-c_3-c_4)(d_1+d_2-d_3-d_4) \\ = (c_1+c_2-c_3-c_4)h_{2,j_2}(-(\delta_2 E_R^{m+1})_{P_4-(1/2)e_2} - (\delta_2 E_R^{m+1})_{P_3-(1/2)e_2}),$$

and we obtain

$$|T_{1b}(\square_j)| \le |c_1+c_2-c_3-c_4|h_{2,j_2}\left(\left|(\delta_2 E_R^{m+1})_{P_4-(1/2)e_2}\right| + \left|(\delta_2 E_R^{m+1})_{P_3-(1/2)e_2}\right|\right).$$

Using inequality (A.2) of Lemma A.2, we get

$$|c_i| \le C(h_{1,j_1}+h_{2,j_2})\max_{s=1,2}\left\|\frac{\partial^2 u_R}{\partial t\partial x_s}(t^{m+1})\right\|_{L^1(\square_j)}, \quad i=1,2,3,4,$$

and then

$$|T_{1b}(\square_j)| \le C(h_{1,j_1}^2 + h_{2,j_2}^2)\max_{s=1,2}\left\|\frac{\partial^2 u_R}{\partial t\partial x_s}(t^{m+1})\right\|_{L^1(\square_j)} \\ \times\left(\left|(\delta_2 E_R^{m+1})_{P_4-(1/2)e_2}\right| + \left|(\delta_2 E_R^{m+1})_{P_3-(1/2)e_2}\right|\right).$$

The other sums, $T_{1c}(\square_j)$ and $T_{1d}(\square_j)$, can be bounded in the same way as $T_{1b}(\square_j)$. Summing the contribution of all the rectangles in the domain, we obtain

$$|T_1| \le C\left(\sum_{\square_j\subset\bar\Omega}(h_{1,j_1}^2+h_{2,j_2}^2)^2\left\|\frac{\partial u_R}{\partial t}(t^{m+1})\right\|_{H^2(\square_j)}^2\right)^{1/2} \\ \times\left(\|E_R^{m+1}\|_h + \|\delta_1 E_R^{m+1}\|_{h_1^*} + \|\delta_2 E_R^{m+1}\|_{h_2^*}\right),$$

and then using the inequality $ab \le \varepsilon a^2 + \frac{1}{4\varepsilon}b^2$ for all $a,b\in\mathbb{R}$ and $\varepsilon>0$, we get

$$|T_1| \le Ch^4\left(1+\frac{1}{\epsilon}\right)\left\|\frac{\partial u_R}{\partial t}(t^{m+1})\right\|_{H^2(\Omega)}^2 + \|E_R^{m+1}\|_h^2 + \epsilon\left(\|\delta_1 E_R^{m+1}\|_{h_1^*}^2 + \|\delta_2 E_R^{m+1}\|_{h_2^*}^2\right),$$

where ϵ is an arbitrary positive constant. Likewise we obtain an analogous estimate for T_2.

For T_3 we have

$$
\begin{aligned}
|T_3| &\le C\Delta t^m \left(\|\rho^m_{u_R}\|_{H^1(\Omega)}\|E_R^{m+1}\|_h + \|\rho^m_{u_I}\|_{H^1(\Omega)}\|E_I^{m+1}\|_h\right), \\
&\le C\frac{(\Delta t^m)^2}{4}\left\|\frac{\partial^2 u_R}{\partial t^2}\right\|^2_{L^\infty(t^m,t^{m+1};H^1(\Omega))} + \|E_R^{m+1}\|_h^2 \\
&\quad + C\frac{(\Delta t^m)^2}{4}\left\|\frac{\partial^2 u_I}{\partial t^2}\right\|^2_{L^\infty(t^m,t^{m+1};H^1(\Omega))} + \|E_I^{m+1}\|_h^2. \qquad (3.12)
\end{aligned}
$$

Let us now obtain an estimate for T_4. We split T_4 into several terms, $|T_4| = |T_{4a_1} + T_{4a_2} + T_{4b_1} + T_{4b_2}|$, where

$$
\begin{aligned}
T_{4a_1} = &\sum_{\square_j\subset\Omega} h_{1,j_1}\Bigg(\int_{S^a_{j_1+1/2}} (D_R(x_{j_1+1/2},x_2,t^{m+1},u) - D_R(x_{j_1+1/2},x_2,t^{m+1},u^{m+\mu})) \\
&\qquad\qquad \times\frac{\partial u_R}{\partial x_1}(x_{j_1+1/2},x_2,t^{m+1})\,dx_2(\delta_1 E_R^{m+1})_{j_1+1/2,j_2}\Bigg) \\
&+\sum_{\square_j\subset\Omega} h_{1,j_1}\Bigg(\int_{S^b_{j_1+1/2}} (D_R(x_{j_1+1/2},x_2,t^{m+1},u) - D_R(x_{j_1+1/2},x_2,t^{m+1},u^{m+\mu})) \\
&\qquad\qquad \times\frac{\partial u_R}{\partial x_1}(x_{j_1+1/2},x_2,t^{m+1})\,dx_2(\delta_1 E_R^{m+1})_{j_1+1/2,j_2+1}\Bigg),
\end{aligned}
$$

$$
\begin{aligned}
T_{4b_1} = &\sum_{\square_j\subset\Omega} h_{1,j_1}\Bigg(\int_{S^a_{j_1+1/2}} D_R(x_{j_1+1/2},x_2,t^{m+1},u^{m+\mu})\frac{\partial u_R}{\partial x_1}(x_{j_1+1/2},x_2,t^{m+1})\,dx_2 \\
&\qquad\qquad \times(\delta_1 E_R^{m+1})_{j_1+1/2,j_2}\Bigg) \\
&+\sum_{\square_j\subset\Omega} h_{1,j_1}\Bigg(\int_{S^b_{j_1+1/2}} D_R(x_{j_1+1/2},x_2,t^{m+1},u^{m+\mu})\frac{\partial u_R}{\partial x_1}(x_{j_1+1/2},x_2,t^{m+1})\,dx_2 \\
&\qquad\qquad \times(\delta_1 E_R^{m+1})_{j_1+1/2,j_2+1}\Bigg) \\
&- \left(D^{m,\mu}_{R+(1/2)e_1}\delta_1 \mathrm{R}_h u_R^{m+1}, \delta_1 E_R^{m+1}\right)_{h_1^*},
\end{aligned}
$$

where we used the notation

$$
u^{m+\mu}(x,t^{m+1}) = u(x,t^{m+\mu}).
$$

Analogously, we define T_{4a_2} and T_{4b_2} which have the natural correspondence to T_{4a_1} and T_{4b_1} with respect to the space variable x_2.

Next, we will derive in detail the bounds for T_{4a_1} and T_{4b_1}. Provided the assumption $u(t) \in H^3(\Omega)$ holds, we can use the Sobolev embedding theorem [1] to conclude that the norm $\|u(t)\|_{W^{1,\infty}(\Omega)}$ is bounded and that the embedding $H^3(\Omega) \hookrightarrow C^1(\overline{\Omega})$ is continuous. If we only assume the regularity $u(t) \in H^2(\Omega)$, this argument does not hold in two dimensions. In this case we use L^2-embedding theorems for traces [1].

In the case $\mu = 1$, $T_{4a_1} = 0$. In the case $\mu = 0$, by (3.1) and (3.5), we get

$$|T_{4a_1}| \le C_D \Delta t^m \left\| \frac{\partial u}{\partial t} \right\|_{L^\infty(t^m, t^{m+1}; L^\infty(\Omega))} \sum_{\square_j \subset \Omega} h_{1,j_1} \left(\int_{S^a_{j_1+1/2}} \left| \frac{\partial u_R}{\partial x_1}(x_{j_1+1/2}, x_2, t^{m+1}) \right| dx_2 \times \left| (\delta_1 E_R^{m+1})_{j_1+1/2, j_2} \right| \right)$$
$$+ C_D \Delta t^m \left\| \frac{\partial u}{\partial t} \right\|_{L^\infty(t^m, t^{m+1}; L^\infty(\Omega))} \sum_{\square_j \subset \Omega} h_{1,j_1} \left(\int_{S^b_{j_1+1/2}} \left| \frac{\partial u_R}{\partial x_1}(x_{j_1+1/2}, x_2, t^{m+1}) dx_2 \right| \times \left| (\delta_1 E_R^{m+1})_{j_1+1/2, j_2+1} \right| \right).$$

The trace theorems (see, e.g., section 2.1.3 of [26]) provide the bound

$$\left(\int_{S^a_{j_1+1/2}} \left| \frac{\partial u_R}{\partial x_1}(x_{j_1+1/2}, x_2, t^{m+1}) \right|^2 dx_2 \right)^{1/2}$$
$$\le C h_{2,j_2}^{1/2} |\square_j|^{-1/2} \left(\left\| \frac{\partial u_R}{\partial x_1}(t^{m+1}) \right\|_{L^2(\square_j)} + \mathrm{diam}(\square_j) \left\| \frac{\partial u_R}{\partial x_1}(t^{m+1}) \right\|_{H^1(\square_j)} \right). \tag{3.13}$$

By the Cauchy–Schwarz inequality, it follows that

$$|T_{4a_1}| \le C \Delta t^m \left\| \frac{\partial u}{\partial t} \right\|_{L^\infty(t^m, t^{m+1}; L^\infty(\Omega))} \|u_R(t^{m+1})\|_{H^2(\Omega)} \|\delta_1 E_R^{m+1}\|_{h_1^*}$$
$$\le C \frac{(\Delta t^m)^2}{4\epsilon} \left\| \frac{\partial u}{\partial t} \right\|^2_{L^\infty(t^m, t^{m+1}; L^\infty(\Omega))} \|u_R(t^{m+1})\|^2_{H^2(\Omega)} + \epsilon \|\delta_1 E_R^{m+1}\|^2_{h_1^*}.$$

In order to estimate T_{4b_1}, we first consider that $u(t) \in H^2(\Omega) \cap W^{1,\infty}(\Omega)$. Using the inequality (A.3) of Lemma A.2, we deduce that

$$\left| D_R(x_{j_1+1/2}, x_2, t^{m+1}, u^{m+\mu}) - \frac{D_R(x_{j_1+1}, x_{j_2}, t^{m+1}, u^{m+\mu}) + D_R(x_{j_1}, x_{j_2}, t^{m+1}, u^{m+\mu})}{2} \right|$$
$$\le C |\square_j|^{-1/2} (h_{1,j_1} + h_{2,j_2}) \|D_R(t^{m+1}, u^{m+\mu})\|_{H^1(\square_j)}, \tag{3.14}$$

and, since D_R is Lipschitz continuous with respect to the third component, from (3.1) we obtain

$$\left| \frac{D_R(x_{j_1+1}, x_{j_2}, t^{m+1}, u^{m+\mu}) + D_R(x_{j_1}, x_{j_2}, t^{m+1}, u^{m+\mu})}{2} - D^{m,\mu}_{Rj+(1/2)e_1} \right|$$
$$\le C_D \frac{|(E_R^{m+1})_{j_1, j_2}| + |(E_R^{m+1})_{j_1+1, j_2}|}{2}. \tag{3.15}$$

From the inequality (A.4) of Lemma A.2 and (1.2) we get

$$\sum_{\square_j\subset\Omega} h_{1,j_1}\left(\int_{S^a_{j_1+1/2}} D^{m,\mu}_{Rj+(1/2)e_1}\frac{\partial u_R}{\partial x_1}(x_{j_1+1/2},x_2,t^{m+1})\,dx_2(\delta_1 E_R^{m+1})_{j_1+1/2,j_2}\right)$$
$$-\sum_{\square_j\subset\Omega}\frac{|\square_j|}{2}\left(D^{m,\mu}_{Rj+(1/2)e_1}\delta_1 u_R^{m+1}(x_{j_1+1/2},x_{j_2})(\delta_1 E_R^{m+1})_{j_1+1/2,j_2}\right)$$
$$\leq C\sum_{\square_j\subset\Omega}\left((h_{1,j_1}+h_{2,j_2})|\square_j|^{1/2}\left\|\frac{\partial u_R}{\partial x_1}(t^{m+1})\right\|_{H^1(\square_j)}(\delta_1 E_R^{m+1})_{j_1+1/2,j_2}\right). \tag{3.16}$$

Collecting the estimates (3.14), (3.15), and (3.16) and applying the Cauchy–Schwarz inequality, we get

$$\begin{aligned}|T_{4b_1}| &\leq Ch\left\|D_R(t^{m+1},u^{m+\mu})\right\|_{H^1(\Omega)}\|u_R(t^{m+1})\|_{W^{1,\infty}(\Omega)}\|\delta_1 E_R^{m+1}\|_{h_1^*}\\
&\quad + C\|u_R(t^{m+1})\|_{W^{1,\infty}(\Omega)}\|E_R^{m+1}\|_h\|\delta_1 E_R^{m+1}\|_{h_1^*}\\
&\quad + Ch\left\|\frac{\partial u_R}{\partial x_1}(t^{m+1})\right\|_{H^1(\Omega)}\|\delta_1 E_R^{m+1}\|_{h_1^*}\\
&\leq C\frac{h^2}{4\epsilon}\left\|D_R(t^{m+1},u^{m+\mu})\right\|^2_{H^1(\Omega)}\|u_R(t^{m+1})\|^2_{W^{1,\infty}(\Omega)}+\epsilon\|\delta_1 E_R^{m+1}\|^2_{h_1^*}\\
&\quad + \frac{C}{4\epsilon}\|u_R(t^{m+1})\|^2_{W^{1,\infty}(\Omega)}\|E_R^{m+1}\|^2_h+\epsilon\|\delta_1 E_R^{m+1}\|^2_{h_1^*}\\
&\quad + C\frac{h^2}{\epsilon}\|u_R(t^{m+1})\|^2_{H^2(\Omega)}+\epsilon\|\delta_1 E_R^{m+1}\|^2_{h_1^*}.\end{aligned}$$

Let us now assume that $u(t)\in H^3(\Omega)$. The estimates (3.14) and (3.16) do not recover the desired order of convergence. Hence we have to exploit the alternating behavior in the x_2-direction using the approach from [15, Lemma 5.2]. With the aid of inequality (A.5) of Lemma A.2, we get

$$\begin{aligned}|T_{4b_1}| &\leq C\frac{h^2}{4\epsilon}\left\|D_R(t^{m+1},u^{m+\mu})\right\|^2_{W^{2,\infty}(\Omega)}\|u_R(t^{m+1})\|^2_{H^3(\Omega)}+\epsilon\|\delta_1 E_R^{m+1}\|^2_{h_1^*}\\
&\quad +\frac{C}{4\epsilon}\|u_R(t^{m+1})\|^2_{W^{1,\infty}(\Omega)}\|E_R^{m+1}\|^2_h+\epsilon\|\delta_1 E_R^{m+1}\|^2_{h_1^*}.\end{aligned}$$

The estimates for T_5, T_6, and T_7 are obtained in an analogous way.

We write T_8 in the form $|T_8| = |T_{8a}+T_{8b}|$, with

$$T_{8a}=\sum_{\square_j\subset\Omega}\left(\frac{|\square_j|}{4}\sum_{i=1}^4 (F^{m,\mu}_{LR})_{P_i}\left(E_R^{m+1}\right)_{P_i}-\sum_{i=1}^4\int_{R_i}F_{LR}(x,t^{m+1},u)\,dx(E_R^{m+1})_{P_i}\right)$$

and

$$T_{8b}=\sum_{\square_j\subset\Omega}\left(\frac{|\square_j|}{4}\sum_{i=1}^4 (F^{m,\mu}_{NLR})_{P_i}\left(E_R^{m+1}\right)_{P_i}-\sum_{i=1}^4\int_{R_i}F_{NLR}(x,t^{m+1},u)\,dx(E_R^{m+1})_{P_i}\right).$$

According to (2.6),

$$\sum_{\square_j\subset\Omega}\left(\frac{|\square_j|}{4}\sum_{i=1}^4 f^{m+1}_{P_i}\left(E_R^{m+1}\right)_{P_i}-\sum_{i=1}^4\int_{R_i}f(x,t^{m+1})\,dx(E_R^{m+1})_{P_i}\right)=0.$$

To estimate T_{8a} note that

$$\begin{aligned}&\left|\left(\mathrm{R}_h A_R(t^{m+1})E_R^{m+1} - \mathrm{R}_h A_I(t^{m+1})E_I^{m+1}, E_R^{m+1}\right)_h\right|\\ &\quad\le \frac{1}{4}\|A(t^{m+1})\|^2_{L^\infty(\Omega)}\|E^{m+1}\|_h^2 + \|E_R^{m+1}\|_h^2,\end{aligned}$$

and, using the same type of analysis as for T_1,

$$\begin{aligned}&\Bigg|\sum_{\square_j\subset\Omega}\left(\frac{|\square_j|}{4}\sum_{i=1}^4\left(A_R(P_i,t^{m+1})u_R(P_i,t^{m+1}) + A_I(P_i,t^{m+1})u_I(P_i,t^{m+1})\right)(E_R^{m+1})_{P_i}\right.\\ &\qquad\left. -\sum_{i=1}^4\int_{R_i} A_R(x,t^{m+1})u_R(x,t^{m+1}) + A_I(x,t^{m+1})u_I(x,t^{m+1})\,dx(E_R^{m+1})_{P_i}\right)\Bigg|\\ &\le Ch^4\left(1+\frac{1}{\epsilon}\right)\left\|A(t^{m+1})u(t^{m+1})\right\|^2_{H^2(\Omega)} + \|E_R^{m+1}\|_h^2 + \epsilon\left(\|\delta_1 E_R^{m+1}\|^2_{h_1^*} + \|\delta_2 E_R^{m+1}\|^2_{h_2^*}\right).\end{aligned}$$

From the previous inequalities we conclude that

$$\begin{aligned}|T_{8a}| &\le \frac{1}{4}\|A(t^{m+1})\|^2_{L^\infty(\Omega)}\|E^{m+1}\|_h^2 + 2\|E_R^{m+1}\|_h^2\\ &\quad + Ch^4\left(1+\frac{1}{\epsilon}\right)\left\|A(t^{m+1})u(t^{m+1})\right\|^2_{H^2(\Omega)} + \epsilon\left(\|\delta_1 E_R^{m+1}\|^2_{h_1^*} + \|\delta_2 E_R^{m+1}\|^2_{h_2^*}\right).\end{aligned}$$

We write T_{8b} in the form

$$\begin{aligned}T_{8b} &= \left(F_{NLR}^{m,\mu}, E_R^{m+1}\right)_h - \left(\mathrm{R}_h F_{NLR}(t^{m+1}, u^{m+\mu}), E_R^{m+1}\right)_h\\ &\quad + \left(\mathrm{R}_h F_{NLR}(t^{m+1}, u^{m+\mu}), E_R^{m+1}\right)_h - \sum_{\square_j\subset\Omega}\left(\sum_{i=1}^4\int_{R_i} F_{NLR}(x,t^{m+1},u)\,dx(E_R^{m+1})_{P_i}\right).\end{aligned}$$

Using (3.2), we have

$$\begin{aligned}\left|\left(F_{NLR}^{m,\mu}, E_R^{m+1}\right)_h - \left(\mathrm{R}_h F_{NLR}(t^{m+1}, u^{m+\mu}), E_R^{m+1}\right)_h\right| &\le C_F\|E^{m+\mu}\|_h\|E_R^{m+1}\|_h\\ &\le \frac{C_F^2}{2}\|E^{m+\mu}\|_h^2 + \frac{1}{2}\|E_R^{m+1}\|_h^2.\end{aligned}\tag{3.17}$$

In the case $\mu = 1$,

$$\sum_{j=0}^N\int_{x_{j-1/2}}^{x_{j+1/2}}\left(F_{NLR}(x,t^{m+1},u^{m+\mu}) - F_{NLR}(x,t^{m+1},u)\right)dx(E_R^{m+1})_j = 0,$$

and, in the case $\mu = 0$, by (3.2) and (3.5),

$$\begin{aligned}&\sum_{\square_j\subset\Omega}\left(\sum_{i=1}^4\int_{R_i} F_{NLR}(x,t^{m+1},u^{m+\mu}) - F_{NLR}(x,t^{m+1},u)\,dx(E_R^{m+1})_{P_i}\right)\\ &\qquad\le C_F\Delta t^m\left\|\frac{\partial u}{\partial t}\right\|_{L^\infty(t^m,t^{m+1};L^\infty(\Omega))}\|E_R^{m+1}\|_h\\ &\qquad\le \frac{C_F^2}{2}(\Delta t^m)^2\left\|\frac{\partial u}{\partial t}\right\|^2_{L^\infty(t^m,t^{m+1};L^\infty(\Omega))} + \frac{1}{2}\|E_R^{m+1}\|_h^2.\end{aligned}\tag{3.18}$$

From (3.17) and (3.18) and using the same type of analysis as for T_1, we get

$$|T_{8b}| \leq \frac{C_F^2}{2}\|E^{m+\mu}\|_h^2 + 2\|E_R^{m+1}\|_h^2 + Ch^4\left(1+\frac{1}{\epsilon}\right)\left\|F_{NLR}(t^{m+1}, u^{m+\mu})\right\|_{H^2(\Omega)}^2$$
$$+\epsilon\left(\|\delta_1 E_R^{m+1}\|_{h_1^*}^2 + \|\delta_2 E_R^{m+1}\|_{h_2^*}^2\right) + \frac{C_F^2}{2}(\Delta t^m)^2\left\|\frac{\partial u}{\partial t}\right\|_{L^\infty(t^m,t^{m+1};L^\infty(\Omega))}^2.$$

For T_9 we use the same type of analysis as for T_8.

Considering all the contributions, we apply the discrete version of Gronwall's lemma (see, e.g., [14, 32]) to obtain the convergence estimate (3.3) for the 2D case.

Remark 1. If we consider, in the numerical method, (2.6) replaced by

$$f_{x_j}^{m+1} = f(x_j, t^{m+1}), \tag{3.19}$$

we must assume that the source f has the same regularity restrictions as the linear part of the reactive term A to obtain the order of convergence established in Theorem 3.1.

4. Numerical results. In this section, we will illustrate the theoretical results for convergence for the semi-implicit method (that is, $m = 1$ and $\mu = 0$) for both Dirichlet and Neumann boundary conditions and also considering reactive and non-reactive source terms. We will discritize the reactive term using (3.19) instead of (2.6).

4.1. Dirichlet case without reactive term. Let us consider the equation

$$\frac{\partial u}{\partial t} = \nabla\cdot(D\nabla u) + f, \quad x_1, x_2 \in (0,\pi)\times(0,\pi),\ t\in(0,1],$$

with initial condition given by

$$u(x_1, x_2, 0) = \sin(x_1)\sin(x_2)$$

and homogeneous Dirichlet boundary conditions. Given two constants $\alpha, \beta \in \mathbb{C}$, for

$$f(x_1,x_2,t) = (\alpha+2\beta)\sin(x_1)\sin(x_2)e^{\alpha t}$$
$$+\left(2\sin^2(x_1)\sin^2(x_2) - \cos^2(x_1)\sin^2(x_2) - \sin^2(x_1)\cos^2(x_2)\right)e^{2\alpha t}$$

and $D(x_1,x_2,t,u) = \beta + u$, the exact solution is $u(x_1,x_2,t) = \sin(x_1)\sin(x_2)e^{\alpha t}$. For the following, we will consider $\alpha = -2-2i$, $\beta = 1+1i$. We also note that in this case f does not depend on u. In the following examples we will consider reactive terms, that is, source terms f that depend on the solution u.

To illustrate the linear numerical order of convergence in time, we will consider constant spatial step sizes $h_1 = h_2$ and step in time Δt. Moreover, we will successively halve the spatial step sizes h_1, h_2 and step in time Δt. One gets the approximations $U^M_{\frac{N_1+1}{2},\frac{N_2+1}{2}}$ for $u(\pi/2,\pi/2,T) = -0.05632 - 0.12306i$ on the central point $(\pi/2,\pi/2)$ of the spatial domain at the final time $T = 1$, given in Table 1. We note that

$$E^M_{\frac{N_1+1}{2},\frac{N_2+1}{2}} = u(\pi/2,\pi/2,T) - U^M_{\frac{N_1+1}{2},\frac{N_2+1}{2}}.$$

Moreover, the order of convergence p can be approximated by

$$p \approx \log_2(|E_n|/|E_{n+1}|), \tag{4.1}$$

TABLE 1

Approximation, error, and numerical estimate on the order of convergence p for the Dirichlet case, obtained by halving the step in time and the spatial step sizes.

$h_1 = h_2$	Δt	$U^M_{\frac{N_1+1}{2},\frac{N_2+1}{2}}$	$E^M_{\frac{N_1+1}{2},\frac{N_2+1}{2}}$	$\lvert E^M_{\frac{N_1+1}{2},\frac{N_2+1}{2}} \rvert$	p
$\pi/2$	1	0.23565-0.10324i	0.29197+0.01982i	0.29264	0.79414
$\pi/4$	1/2	0.11239-0.11884i	0.16871+0.00422i	0.16876	0.76446
$\pi/8$	1/4	0.04300-0.12548i	0.09932–0.00242i	0.09935	0.83094
$\pi/16$	1/8	–0.00056-0.12628i	0.05576–0.00322i	0.05585	0.89736
$\pi/32$	1/16	–0.02642-0.12535i	0.02990–0.00229i	0.02998	0.94333
$\pi/64$	1/32	–0.04078-0.12440i	0.01553–0.00134i	0.01559	0.97023
$\pi/128$	1/64	–0.04839-0.12378i	0.00793–0.00072i	0.00796	0.98474
$\pi/256$	1/128	–0.05232-0.12343i	0.00400–0.00037i	0.00402	-

TABLE 2

Discrete L^2 norm of the error and numerical estimate on the order of convergence p for the Dirichlet case, obtained by halving the step in time and the spatial step sizes.

$h_1 = h_2$	Δt	$\lVert u(.,.,T) - U^M \rVert_h$	p
$\pi/2$	1	0.45968	0.78001
$\pi/4$	1/2	0.26770	0.81094
$\pi/8$	1/4	0.15259	0.85691
$\pi/16$	1/8	0.08425	0.90866
$\pi/32$	1/16	0.04488	0.94786
$\pi/64$	1/32	0.02327	0.97208
$\pi/128$	1/64	0.01186	0.98554
$\pi/256$	1/128	0.00599	-

where E_n and E_{n+1} are the errors considering $\Delta t = 1/2^n$, $h_1 = h_2 = \pi/2^{n+1}$, $n = 0, 1, \ldots$. Similar results are obtained for the numerical convergence using the discrete L^2 norm of the error $\lVert u(.,.,T) - U^M\rVert_h$, as presented in Table 2. As expected, the numerical orders of convergence tend to 1.

To illustrate the quadratic numerical order of convergence in space, we will again consider constant spatial step sizes $h_1 = h_2$ and step in time Δt. Moreover, we will successively halve the spatial step sizes h_1, h_2, while we will successively divide by 4 the step in time Δt. The results are shown in Table 3 for pointwise convergence and in Table 4 for the error measured with the discrete L^2 norm. As expected, the numerical order of convergence tends to 2.

4.2. Neumann case with reactive term in L-shaped domain. Let us consider the equation

$$\frac{\partial u}{\partial t} = \nabla \cdot (D \nabla u) + f, \quad x_1, x_2 \in (-\pi, \pi) \times (0, \pi) \cup (0, \pi) \times (-\pi, 0], \ t \in (0, 1],$$

with initial condition given by

$$u(x_1, x_2, 0) = \cos(x_1)\cos(x_2)$$

and homogeneous Neumann boundary conditions. Again, given two constants $\alpha, \beta \in \mathbb{C}$, for

$$\begin{aligned} f(x_1, x_2, t, u) = {} & (\alpha + 2\beta)\cos(x_1)\cos(x_2)e^{\alpha t} + 2u^2 \\ & - \left(\sin^2(x_1)\cos^2(x_2) + \cos^2(x_1)\sin^2(x_2)\right) e^{2\alpha t} \end{aligned}$$

TABLE 3

Approximation, error, and numerical estimate on the order of convergence p for the Dirichlet case, obtained by halving the spatial step sizes and dividing by 4 the step in time.

$h_1 = h_2$	Δt	$U^M_{\frac{N_1+1}{2},\frac{N_2+1}{2}}$	$E^M_{\frac{N_1+1}{2},\frac{N_2+1}{2}}$	$\lvert E^M_{\frac{N_1+1}{2},\frac{N_2+1}{2}}\rvert$	p
$\pi/2$	1	0.05703–0.16807i	0.11335–0.04501i	0.12196	1.62845
$\pi/4$	1/4	−0.02090–0.14042i	0.03542–0.01736i	0.03945	1.89815
$\pi/8$	1/16	−0.04714–0.12833i	0.00918–0.00527i	0.01058	1.97857
$\pi/16$	1/64	−0.05402–0.12444i	0.00230–0.00138i	0.00269	1.99486
$\pi/32$	1/256	−0.05574–0.12341i	0.00058–0.00035i	0.00067	1.99873
$\pi/64$	1/1024	−0.05618–0.12315i	0.00014–0.00009i	0.00017	-

TABLE 4

Discrete L^2 norm of the error and numerical estimate on the order of convergence p for the Dirichlet case, obtained by halving the spatial step sizes and dividing by 4 the step in time.

$h_1 = h_2$	Δt	$\lVert u(.,.,T) - U^M \rVert_h$	p
$\pi/2$	1	0.19157	1.65693
$\pi/4$	1/4	0.06075	1.92837
$\pi/8$	1/16	0.01596	1.98124
$\pi/16$	1/64	0.00404	1.99522
$\pi/32$	1/256	0.00101	1.99880
$\pi/64$	1/1024	0.00025	-

and $D(x_1, x_2, t, u) = \beta + u$, the exact solution is $u(x_1, x_2, t) = \cos(x_1)\cos(x_2)e^{\alpha t}$. Again, we will consider $\alpha = -2 - 2i$, $\beta = 1 + 1i$.

To illustrate the linear numerical order of convergence in time, we will consider constant spatial step sizes $h_1 = h_2$ and step in time Δt. Moreover, we will halve the spatial step sizes h_1, h_2 and step in time Δt. The results are shown in Table 5 for pointwise convergence. Similar results are obtained for the numerical convergence using the discrete norm, as presented in Table 6. The numerical orders of convergence tend to 1.

To illustrate the quadratic numerical order of convergence in space, we will consider constant spatial step sizes $h_1 = h_2$ and step in time Δt. Moreover, we will halve the spatial step sizes h_1, h_2, while we will divide by 4 the step in time Δt. The results are shown in Table 7 for pointwise convergence and in Table 8 for the discrete norm. The numerical order of convergence is approximately 2, as expected. In Figure 1 we show the approximation and its errors at $T = 1$, with the last considered set of step sizes $h_1 = h_2 = \pi/64$ and step in time $\Delta t = 1/4096$.

4.3. Neumann case with reactive Lipschitz term and nonuniform mesh. Let us consider the equation

$$\frac{\partial u}{\partial t} = \nabla \cdot (D\nabla u) + f, \quad x_1, x_2 \in (0,\pi)\times(0,\pi),\ t \in (0,1],$$

with initial condition given by

$$u(x_1, x_2, 0) = \cos^2(x_1)\cos^2(x_2)$$

and homogeneous Neumann boundary conditions. Given two constants $\alpha, \beta \in \mathbb{C}$ for

$$\begin{aligned} f(x_1,x_2,t,u) =& (\alpha+4\beta)|u| - 2|u|\left(\cos^2(x_1)\left(3\sin^2(x_2)-\cos^2(x_2)\right)\right. \\ &\left.+\cos^2(x_2)\left(3\sin^2(x_1)-\cos^2(x_1)\right)\right)e^{\alpha t} \\ &-2B\left(\sin^2(x_1)\cos^2(x_2)+\cos^2(x_1)\sin^2(x_2)\right)e^{2\alpha t} \end{aligned}$$

TABLE 5

Approximation, error, and numerical estimate on the order of convergence p for the Neumann case with reactive term, obtained by halving the step in time and the spatial step sizes.

$h_1 = h_2$	Δt	$E^M_{\frac{3N_1+1}{4},\frac{3N_2+1}{4}}$	$\left\|E^M_{\frac{3N_1+1}{4},\frac{3N_2+1}{4}}\right\|$	p
$\pi/2$	1/4	−0.15826−0.07603i	0.17557	0.78530
$\pi/4$	1/8	−0.10155−0.00809i	0.10187	1.07784
$\pi/8$	1/16	−0.04826+0.00047i	0.04826	1.05809
$\pi/16$	1/32	−0.02316+0.00089i	0.02318	1.03151
$\pi/32$	1/64	−0.01133+0.00056i	0.01134	1.01606
$\pi/64$	1/128	−0.00560+0.00030i	0.00561	1.00806
$\pi/128$	1/256	−0.00278+0.00016i	0.00279	1.00403
$\pi/256$	1/512	−0.00139+0.00008i	0.00139	-

TABLE 6

Discrete L^2 norm of the error and numerical estimate on the order of convergence p for the Neumann case with reactive term, obtained by halving the step in time and the spatial step sizes.

$h_1 = h_2$	Δt	$\|u(.,.,T) - U^M\|_h$	p
$\pi/2$	1/4	1.24288	1.14767
$\pi/4$	1/8	0.56098	1.09666
$\pi/8$	1/16	0.26231	1.05930
$\pi/16$	1/32	0.12587	1.03198
$\pi/32$	1/64	0.06156	1.01651
$\pi/64$	1/128	0.03043	1.00838
$\pi/128$	1/256	0.01513	1.00422
$\pi/256$	1/512	0.00754	-

and $D(x_1, x_2, t, u) = \beta + |u|$, the exact solution is $u(x_1, x_2, t) = \cos^2(x_1)\cos^2(x_2)e^{\alpha t}$. Again, we will consider $\alpha = -4 - 4i$, $\beta = 1 + 1i$.

In order to numerically illustrate the linear convergence order in time, we randomly choose M in the set $\{20,21,\dots,100\}$ with uniform distribution. We then define N_1 and N_2 randomly and independently, with normal distribution of mean M and standard deviation 2. N_1 and N_2 are then rounded to the closest integer greater than or equal to 2. In this way, N_1 and N_2 vary (almost) linearly with respect to M. Then, we randomly and independently define the points

$$0 = x_{k,0} < x_{k,1} < x_{k,2} < \cdots < x_{k,N_k} = \pi, \quad k = 1, 2,$$

by a uniform distribution in $[0, \pi]$. We proceed similarly with time, randomly defining the instants by a uniform distribution in $[0, 1]$. We then solve the problem with the defined mesh and calculate the error in the discrete L^2 norm. The plot of the logarithm of this error depending on the logarithm of the maximum step in time considered for 300 different meshes is given in Figure 2 (left). The numerical convergence rate is approximated by the slope of the linear regression line, which is 1.0047. As expected, it is close to 1.

In order to numerically illustrate the quadratic convergence order in space, we randomly choose N_1 in the set $\{15,16,\dots,60\}$ with uniform distribution. We then set N_2 randomly with a normal distribution with mean N_1 and standard deviation 2. We set N_2 to the closest integer greater than or equal to 2. In order to show the quadratic order, we force M to grow by a factor of 4 each time that the minimum of N_1 and N_2 doubles. In this way, we choose M randomly by a normal distribution with mean $\frac{\min\{N_1^2,N_2^2\}}{4}$ and standard variation 2. We then solve the problem with the defined mesh and calculate the error in the discrete L^2 norm. The plot of the

TABLE 7
Approximation, error, and numerical estimate on the order of convergence p for the Neumann case with reactive term, obtained by halving the spatial step sizes and dividing by 4 the step in time.

$h_1 = h_2$	Δt	$E^M_{\frac{3N_1+1}{4},\frac{3N_2+1}{4}}$	$\lvert E^M_{\frac{3N_1+1}{4},\frac{3N_2+1}{4}}\rvert$	p
$\pi/2$	1/4	−0.15826−0.07603i	0.17557	1.69909
$\pi/4$	1/16	−0.05407−0.00037i	0.05407	2.06101
$\pi/8$	1/64	−0.01286+0.00162i	0.01296	2.02298
$\pi/16$	1/256	−0.00315+0.00051i	0.00319	2.00339
$\pi/32$	1/1024	−0.00078+0.00014i	0.00080	1.99916
$\pi/64$	1/4096	−0.00020+0.00003i	0.00020	-

TABLE 8
Discrete L^2 norm of the error and numerical estimate on the order of convergence p for the Neumann case with reactive term, obtained by halving the spatial step sizes and dividing by 4 the step in time.

$h_1 = h_2$	Δt	$\lVert u(.,.,T) - U^M\rVert_h$	p
$\pi/2$	1/4	1.24288	2.11550
$\pi/4$	1/16	0.28681	2.03747
$\pi/8$	1/64	0.06987	2.00528
$\pi/16$	1/256	0.01740	1.99892
$\pi/32$	1/1024	0.00435	1.99850
$\pi/64$	1/4096	0.00109	-

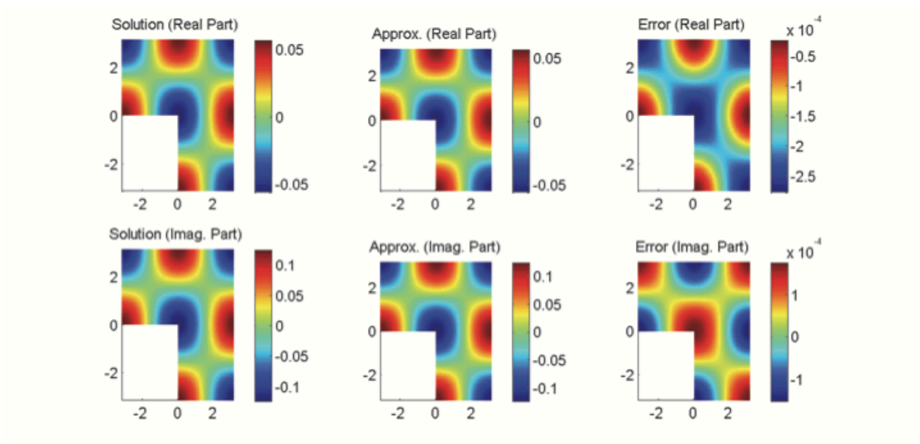

FIG. 1. *Real (top) and imaginary (bottom) parts of the exact solution (left), numerical solution (center), and error (right) for the example of section* 4.2 *at* $T = 1$.

logarithm of this error depending on the logarithm of the maximum spatial step sizes for 300 different meshes is given in Figure 2 (right). The numerical convergence rate is approximated by the slope of the linear regression line, which is 1.9540. As expected, it is close to 2. This example shows that the numerical orders of convergence are not affected by either a Lipschitz reactive term or nonuniform meshes, as already shown theoretically.

Appendix A. Technical lemmata. The following lemmata are technical tools needed to derive the convergence estimates. They are a consequence of the Bramble–

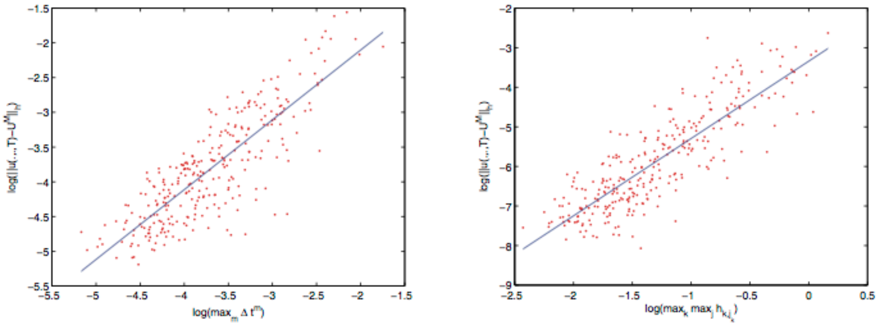

FIG. 2. *Left: Density plot and linear regression line (with slope 1.0047) of the logarithm of the discrete L^2 norm of the error depending on the logarithm of maximum of the steps in time Δt^m. Right: Density plot and linear regression line (with slope 1.9540) of the logarithm of the discrete L^2 norm of the error depending on the logarithm of maximum of the spatial step sizes h_{k,j_k}.*

Hilbert lemma (see, e.g., [8, 12]).

LEMMA A.1 (Bramble–Hilbert). *Suppose that Ω is a bounded open set in $\mathbb{R}^d$ with Lipschitz continuous boundary. Let λ be a bounded linear functional on the Sobolev space $W^{r,p}(\Omega)$, $r \geq 1$, $1 \leq p \leq \infty$, such that $\lambda(Q) = 0$ for any polynomial Q of degree less than or equal than $r-1$. Then there exists a positive constant $C = C(\Omega, r, p)$ such that*

$$|\lambda(v)| \leq C|v|_{W^{r,p}(\Omega)} \quad \forall v \in W^{r,p}(\Omega).$$

Let $\square_j = (x_{j_1}, x_{j_1+1}) \times (x_{j_2}, x_{j_2+1})$, $P_1 = (x_{j_1}, x_{j_2})$, $P_2 = (x_{j_1+1}, x_{j_2})$, $P_3 = (x_{j_1+1}, x_{j_2+1})$, $P_4 = (x_{j_1}, x_{j_2+1})$, and $S^a_{j_1+1/2} = \{x_{j_1+1/2}\} \times (x_{j_2}, x_{j_2+1/2})$.

LEMMA A.2. *For $v \in H^2(\square_j)$, the following estimate holds:*

(A.1)
$$\left| \frac{h_{1,j_1} h_{2,j_2}}{4} \sum_{i=1}^{4} v(P_i) - \int_{\square_j} v(x)\,dx \right| \leq C(h_{1,j_1}^2 + h_{2,j_2}^2) \max_{\substack{s_1+s_2=2 \\ s_1,s_2 \in \{0,1,2\}}} \left\| \frac{\partial^2 v}{\partial x_1^{s_1} \partial x_2^{s_2}} \right\|_{L^1(\square_j)},$$

(A.2)
$$\left| h_{1,j_1} h_{2,j_2}\, v(P_i) - \int_{\square_j} v(x)\,dx \right| \leq C(h_{1,j_1} + h_{2,j_2}) \max_{s=1,2} \left\| \frac{\partial v}{\partial x_s} \right\|_{L^1(\square_j)}, \quad i = 1,2,3,4,$$

$$\begin{aligned} &\left| v(x_{j_1+1/2}, x_2) - \frac{v(x_{j_1+1/2}, x_{j_2}) + v(x_{j_1+1/2}, x_{j_2+1})}{2} \right| \\ &\leq C(h_{1,j_1} + h_{2,j_2}) |\square_j|^{-1/2} \|v\|_{H^1(\square_j)}, \quad x_2 \in [x_{j_2}, x_{j_2+1}], \end{aligned} \tag{A.3}$$

$$\begin{aligned} &\left| \int_{S^a_{j_1+1/2}} \frac{\partial v}{\partial x_1}(x_{j_1+1/2}, x_2)\,dx_2 - \frac{h_{2,j_2}}{2} \delta_1 v(x_{j_1+1/2}, x_{j_2}) \right| \\ &\leq C(h_{1,j_1} + h_{2,j_2}) \left(\frac{h_{2,j_2}}{h_{1,j_1}} \right)^{1/2} \left\| \frac{\partial v}{\partial x_1} \right\|_{H^1(\square_j)}, \end{aligned} \tag{A.4}$$

and

$$\left| h_{1,j_1} \int_{x_{j_2}}^{x_{j_2+1}} v(x_{j_1+1/2}, x_2)\, dx_2 - \frac{h_{1,j_1} h_{2,j_2}}{2} \left(v(x_{j_1+1/2}, x_{j_2}) + v(x_{j_1+1/2}, x_{j_2+1}) \right) \right| \tag{A.5}$$
$$\leq C(h_{1,j_1} + h_{2,j_2}) |\square_j|^{1/2} \|v\|_{H^2(\square_j)}.$$

Proof. Let the function w be defined by

$$w(\xi, \eta) = v(x_{j_1} + \xi h_{1,j_1}, x_{j_2} + \eta h_{2,j_2}), \quad (\xi, \eta) \in [0,1] \times [0,1].$$

Then

$$\frac{h_{1,j_1} h_{2,j_2}}{4} \sum_{i=1}^{4} v(P_i) - \int_{\square_j} v(x)\, dx = h_{1,j_1} h_{2,j_2} \lambda(w)$$

with

$$\lambda(g) = \frac{g(0,0) + g(1,0) + g(0,1) + g(1,1)}{4} - \int_0^1 \int_0^1 g(\xi, \eta)\, d\xi\, d\eta,$$

$g \in W^{2,1}((0,1) \times (0,1))$. This functional is bounded in $W^{2,1}((0,1) \times (0,1))$ and vanishes for polynomials (in ξ and η) of degree 1. By the Bramble–Hilbert lemma the estimate $|\lambda(g)| \leq C|g|_{W^{2,1}((0,1)\times(0,1))}$ holds and we obtain the bound (A.1). To prove (A.2) we consider

$$h_{1,j_1} h_{2,j_2}\, v(P_1) - \int_{\square_j} v(x)\, dx = h_{1,j_1} h_{2,j_2} \lambda(w)$$

with

$$\lambda(g) = g(0,0) - \int_0^1 \int_0^1 g(\xi, \eta)\, d\xi\, d\eta,$$

$g \in W^{1,1}((0,1) \times (0,1))$. This functional is bounded and vanishes for polynomials of degree zero. By the Bramble–Hilbert lemma we obtain $|\lambda(g)| \leq C|g|_{W^{1,1}((0,1)\times(0,1))}$. The proof using the points P_2, P_3, and P_4 follows the same steps.

We obtain the estimates (A.3), (A.4), and (A.5) in a similar way, defining functionals λ that vanish for polynomials of degree 0, for (A.3) and (A.4), and polynomials of degree 1, for (A.5). We transform $\square_j$ into the unit square and apply the Bramble–Hilbert lemma. ◻

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