

UNCONDITIONALLY ENERGY STABLE FULLY DISCRETE SCHEMES FOR A CHEMO-REPULSION MODEL

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ABSTRACT. This work is devoted to studying unconditionally energy stable and mass-conservative numerical schemes for the following repulsive-productive chemotaxis model: find $u \geq 0$, the cell density, and $v \geq 0$, the chemical concentration, such that

$$\begin{cases} \partial_t u - \Delta u - \nabla \cdot (u \nabla v) = 0 & \text{in } \Omega, \ t > 0, \\ \partial_t v - \Delta v + v = u & \text{in } \Omega, \ t > 0, \end{cases}$$

in a bounded domain $\Omega \subseteq \mathbb{R}^d$, $d = 2, 3$. By using a regularization technique, we propose three fully discrete Finite Element (FE) approximations. The first one is a nonlinear approximation in the variables (u, v) ; the second one is another nonlinear approximation obtained by introducing $\sigma = \nabla v$ as an auxiliary variable; and the third one is a linear approximation constructed by mixing the regularization procedure with the energy quadratization technique, in which other auxiliary variables are introduced. In addition, we study the well-posedness of the numerical schemes, proving unconditional existence of solution, but conditional uniqueness (for the nonlinear schemes). Finally, we compare the behavior of such schemes throughout several numerical simulations and provide some conclusions.

1. INTRODUCTION

Chemotaxis is a biological phenomenon in which the movement of living organisms is induced by a chemical stimulus. The chemotaxis is called attractive when the organisms move towards regions with higher chemical concentration, while if the motion is towards lower concentrations, the chemotaxis is called repulsive. In this paper, we study unconditionally energy stable fully discrete schemes for the following parabolic-parabolic repulsive-productive chemotaxis model (with linear production term):

$$(1) \quad \begin{cases} \partial_t u - \Delta u = \nabla \cdot (u \nabla v) & \text{in } \Omega, \ t > 0, \\ \partial_t v - \Delta v + v = u & \text{in } \Omega, \ t > 0, \\ \frac{\partial u}{\partial \mathbf{n}} = \frac{\partial v}{\partial \mathbf{n}} = 0 & \text{on } \partial\Omega, \ t > 0, \\ u(\mathbf{x}, 0) = u_0(\mathbf{x}) \geq 0, \ v(\mathbf{x}, 0) = v_0(\mathbf{x}) \geq 0 & \text{in } \Omega, \end{cases}$$

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in a bounded domain $\Omega \subseteq \mathbb{R}^d$, $d = 2, 3$, with boundary $\partial\Omega$. The unknowns for this model are $u(\mathbf{x}, t) \geq 0$, the cell density, and $v(\mathbf{x}, t) \geq 0$, the chemical concentration. Problem (1) is conservative in u , because the total mass $\int_{\Omega} u(\cdot, t)$ remains constant in time, as we can check by integrating equation (1)₁ in Ω :

$$(2) \quad \frac{d}{dt} \left(\int_{\Omega} u(\cdot, t) \right) = 0, \quad \text{i.e.,} \quad \int_{\Omega} u(\cdot, t) = \int_{\Omega} u_0 := m_0 \quad \forall t > 0.$$

Problem (1) is well-posed [7]: in 3D domains, there exist global in time nonnegative weak solutions of model (1) in the following sense:

$$\begin{aligned} u &\in C_w([0, T]; L^1(\Omega)) \cap L^{5/4}(0, T; W^{1,5/4}(\Omega)) \quad \forall T > 0, \\ v &\in L^\infty(0, T; H^1(\Omega)) \cap L^2(0, T; H^2(\Omega)) \cap C([0, T]; L^2(\Omega)) \quad \forall T > 0, \\ \partial_t u &\in L^{4/3}(0, T; W^{1,\infty}(\Omega)'), \quad \partial_t v \in L^{5/3}(0, T; L^{5/3}(\Omega)) \quad \forall T > 0, \end{aligned}$$

satisfying the variational formulation of the u -equation,

$$\int_0^T \langle \partial_t u, \bar{u} \rangle + \int_0^T (\nabla u, \nabla \bar{u}) + \int_0^T (u \nabla v, \nabla \bar{u}) = 0 \quad \forall \bar{u} \in L^4(0, T; W^{1,\infty}(\Omega)) \quad \forall T > 0,$$

and the v -equation pointwisely,

$$\partial_t v - \Delta v + v = u \quad \text{a.e. } (t, \mathbf{x}) \in (0, +\infty) \times \Omega.$$

Moreover, for 2D domains, there exists a unique classical and bounded in time solution. A key step of the existence proof in [7] is to establish an energy equality, which in a formal manner is obtained as follows: if we consider

$$F(s) := s(\ln s - 1) + 1 \geq 0 \Rightarrow F'(s) = \ln s \Rightarrow F''(s) = s^{-1} \quad \forall s > 0,$$

then multiplying (1)₁ by $F'(u)$, (1)₂ by $-\Delta v$, integrating over Ω , using (1)₃, and adding, the chemotactic and production terms cancel and we obtain

$$(3) \quad \frac{d}{dt} \int_{\Omega} \left(F(u) + \frac{1}{2} |\nabla v|^2 \right) d\mathbf{x} + \int_{\Omega} \left(4 |\nabla(\sqrt{u})|^2 + |\Delta v|^2 + |\nabla v|^2 \right) d\mathbf{x} = 0.$$

The aim of this work is to design numerical methods for model (1) conserving, at the discrete level, the mass-conservation and energy-stability properties of the continuous model (see (2)–(3), respectively). There are only a few works about numerical analysis for chemotaxis models. For instance, for the Keller-Segel system (i.e., with chemo-attraction and linear production), Filbet studied in [9] the existence of discrete solutions and the convergence of a finite volume scheme. Saito, in [16, 17], proved error estimates for a conservative Finite Element (FE) approximation. A mixed FE approximation is studied in [14]. In [8], some error estimates are proved for a fully discrete discontinuous FE method. In the case where the chemotaxis occurs in heterogeneous medium, in [6] the convergence of a combined finite volume-nonconforming finite element scheme is studied, and some discrete properties are proved.

Some previous energy stable numerical schemes have also been studied in the chemotaxis framework. A finite volume scheme for a Keller-Segel model with an additional cross-diffusion term satisfying the energy-stability property (that means, a discrete energy decreases in time) has been studied in [5]. Unconditionally energy stable time-discrete numerical schemes and fully discrete FE schemes for a chemo-repulsion model with quadratic production has been analyzed in [11, 12], respectively. However, as far as we know, for the chemo-repulsion model with linear

production (1) there are no works studying energy-stable schemes. We emphasize that the numerical analysis of energy stability in the chemo-repulsion model with linear production has greater difficulties than the case of quadratic production [11, 12]. In fact, in the continuous case of quadratic production, in order to obtain an energy equality, it is necessary to test the u -equation by u , and the v -equation by $-\Delta v$, which, if we want to move to the fully discrete approximation, is much easier than the case of linear production in which, as it was said before, the energy equality is obtained by multiplying the u -equation by the nonlinear function $F'(u) = \ln u$.

In this paper, we propose three unconditionally energy stable fully discrete schemes, in which, in order to obtain rigorously a discrete version of the energy law (3), we argue through a regularization technique. This regularization procedure has been used in previous works to deal with the test function $F'(u) = \ln u$ in fully discrete approximations, as, for example, for a cross-diffusion competitive population model [3] or a cross-diffusion segregation problem arising from a model of interacting particles [10]. The model that will be analyzed in this paper differs primarily from these previous works in the fact that, in our case, the term of self-diffusion in $(1)_1$ is $\nabla \cdot (\nabla u)$ and it is not in the form $\nabla \cdot (u \nabla u)$ as in [3, 10], which makes the analysis a bit more difficult. In fact, in the continuous problem, if we multiply equation $(1)_1$ by $F'(u) = \ln u$, in our case we obtain the dissipative term $\int_{\Omega} \frac{1}{u} |\nabla u|^2$ (which does not provide an estimate for ∇u), while in the cases of [3, 10], $\int_{\Omega} |\nabla u|^2$ is obtained, which gives directly an estimate for ∇u in $L^2(\Omega)$.

The outline of this paper is as follows. In Section 2, we give the notation and define the regularized functions that will be used in the fully discrete approximations. In Section 3, we study a nonlinear fully discrete FE approximation of (1) in the original variables (u, v) . We prove the well-posedness of the numerical approximation, and show the mass-conservation and energy-stability properties of this scheme by imposing the orthogonality condition on the mesh (see hypothesis **(H)** in Section 3). In Section 4, we analyze another nonlinear FE approximation obtained by introducing $\sigma = \nabla v$ as an auxiliary variable, and again, we prove the well-posedness of the scheme, as well as its mass-conservation and energy-stability properties, but without imposing the orthogonality condition **(H)**. In Section 5, we study a linear fully discrete FE approximation constructed by mixing the regularization procedure with the Energy Quadraticization (EQ) strategy, in which the energy of the system is transformed into a quadratic form by introducing new auxiliary variables. This EQ technique has been applied to different fields such as liquid crystals [2, 21], phase fields [20] (and references therein), and molecular beam epitaxial growth [18] models, among others. Finally, in Section 6, we compare the behavior of the schemes throughout several numerical simulations, and provide some conclusions in Section 7.

2. NOTATION AND PRELIMINARY RESULTS

First, we recall some functional spaces which will be used throughout this paper. We will consider the usual Sobolev spaces $H^m(\Omega)$ and Lebesgue spaces $L^p(\Omega)$, $1 \leq p \leq \infty$, with norms $\|\cdot\|_m$ and $\|\cdot\|_{L^p}$, respectively. In particular, the $L^2(\Omega)$ -norm will be denoted by $\|\cdot\|_0$. Throughout (\cdot, \cdot) denotes the standard L^2 -inner product over Ω . We denote $\mathbf{H}_{\sigma}^1(\Omega) := \{\sigma \in \mathbf{H}^1(\Omega) : \sigma \cdot \mathbf{n} = 0 \text{ on } \partial\Omega\}$ and we will use the following equivalent norms in $H^1(\Omega)$ and $\mathbf{H}_{\sigma}^1(\Omega)$, respectively (see [15] and

[1, Corollary 3.5], respectively):

$$\|u\|_1^2 = \|\nabla u\|_0^2 + \left(\int_{\Omega} u \right)^2 \quad \forall u \in H^1(\Omega),$$

$$\|\sigma\|_1^2 = \|\sigma\|_0^2 + \|\operatorname{rot} \sigma\|_0^2 + \|\nabla \cdot \sigma\|_0^2 \quad \forall \sigma \in \mathbf{H}_{\sigma}^1(\Omega),$$

where $\operatorname{rot} \sigma$ denotes the well-known rotational operator (also called curl) which is scalar for 2D domains and vectorial for 3D ones. If Z is a general Banach space, its topological dual space will be denoted by Z' . Moreover, the letters C, K will denote different positive constants which may change from line to line (or even within the same line). In order to construct energy-stable fully discrete schemes for problem (1), we are going to follow a regularization procedure. We will use the approach introduced by Barrett and Blowey [3]. Let $\varepsilon \in (0, 1)$ and consider the truncated function $\lambda_{\varepsilon} : \mathbb{R} \rightarrow [\varepsilon, \varepsilon^{-1}]$ given by

$$(4) \quad \lambda_{\varepsilon}(s) := \begin{cases} \varepsilon & \text{if } s \leq \varepsilon, \\ s & \text{if } \varepsilon \leq s \leq \varepsilon^{-1}, \\ \varepsilon^{-1} & \text{if } s \geq \varepsilon^{-1}. \end{cases}$$

If we define

$$(5) \quad F_{\varepsilon}''(s) := \frac{1}{\lambda_{\varepsilon}(s)},$$

then we can integrate twice in (5), imposing the conditions $F_{\varepsilon}'(1) = F_{\varepsilon}(1) = 0$, and we obtain a convex function $F_{\varepsilon} : \mathbb{R} \rightarrow [0, +\infty)$ such that $F_{\varepsilon} \in C^{2,1}(\mathbb{R})$ (see Figure 1). Even more, for $\varepsilon \in (0, e^{-2})$, it holds [3] that

$$(6) \quad F_{\varepsilon}(s) \geq \frac{\varepsilon}{2}s^2 - 2 \quad \forall s \geq 0 \quad \text{and} \quad F_{\varepsilon}(s) \geq \frac{s^2}{2\varepsilon} \quad \forall s \leq 0.$$

Finally, we will use the following result to get large time estimates [13].

Lemma 2.1. *Assume that $\delta, \beta, k > 0$ and $d^n \geq 0$ satisfy*

$$(1 + \delta k)d^{n+1} \leq d^n + k\beta \quad \forall n \geq 0.$$

Then, for any $n_0 \geq 0$,

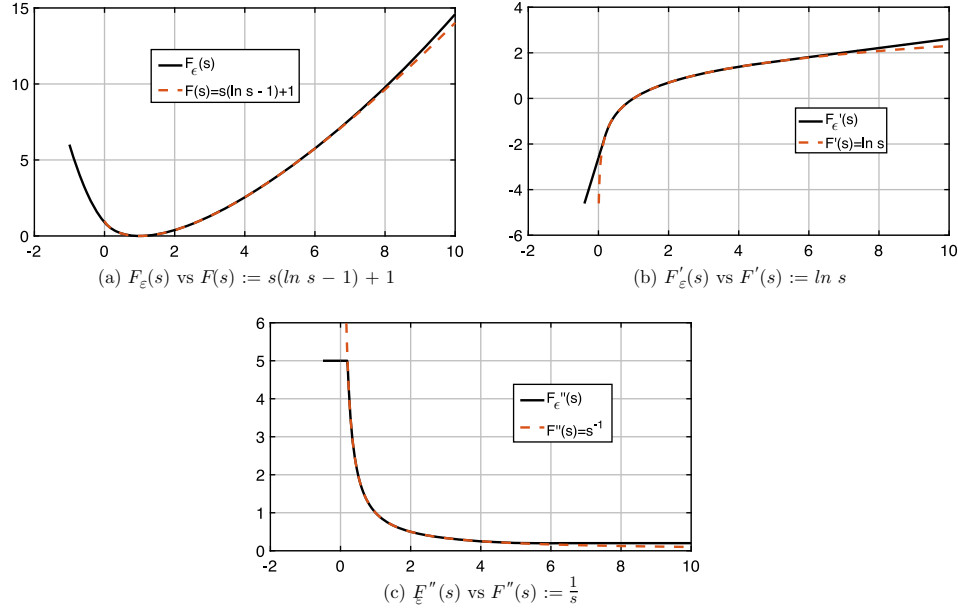
$$d^n \leq (1 + \delta k)^{-(n-n_0)} d^{n_0} + \delta^{-1} \beta \quad \forall n \geq n_0.$$

3. SCHEME UV

In this section, we propose an energy-stable nonlinear fully discrete scheme (in the variables (u, v)) associated to model (1). With this aim, taking into account the functions λ_{ε} and F_{ε} and their derivatives, we consider the following regularized version of problem (1): find $u_{\varepsilon}, v_{\varepsilon} : \Omega \times [0, T] \rightarrow \mathbb{R}$ such that

$$(7) \quad \begin{cases} \partial_t u_{\varepsilon} - \Delta u_{\varepsilon} - \nabla \cdot (\lambda_{\varepsilon}(u_{\varepsilon}) \nabla v_{\varepsilon}) = 0 & \text{in } \Omega, \ t > 0, \\ \partial_t v_{\varepsilon} - \Delta v_{\varepsilon} + v_{\varepsilon} = u_{\varepsilon} & \text{in } \Omega, \ t > 0, \\ \frac{\partial u_{\varepsilon}}{\partial \mathbf{n}} = \frac{\partial v_{\varepsilon}}{\partial \mathbf{n}} = 0 & \text{on } \partial\Omega, \ t > 0, \\ u_{\varepsilon}(\mathbf{x}, 0) = u_0(\mathbf{x}) \geq 0, \ v_{\varepsilon}(\mathbf{x}, 0) = v_0(\mathbf{x}) \geq 0 & \text{in } \Omega. \end{cases}$$

Remark 3.1. The idea is to define a fully discrete scheme associated to (7), taking in general $\varepsilon = \varepsilon(k, h)$, such that $\varepsilon(k, h) \rightarrow 0$ as $(k, h) \rightarrow 0$.

FIGURE 1. Function F_ϵ and its derivatives.

Observe that multiplying $(7)_1$ by $F'_\epsilon(u_\epsilon)$, $(7)_2$ by $-\Delta v_\epsilon$, integrating over Ω , and adding, again the chemotactic and production terms cancel, and we obtain the energy law

$$(8) \quad \frac{d}{dt} \int_{\Omega} \left(F_\epsilon(u_\epsilon) + \frac{1}{2} |\nabla v_\epsilon|^2 \right) d\mathbf{x} + \int_{\Omega} \left(F''_\epsilon(u_\epsilon) |\nabla u_\epsilon|^2 + |\Delta v_\epsilon|^2 + |\nabla v_\epsilon|^2 \right) d\mathbf{x} = 0.$$

In particular, the modified energy $\mathcal{E}_\epsilon(u, v) = \int_{\Omega} (F_\epsilon(u) + \frac{1}{2} |\nabla v|^2) d\mathbf{x}$ is decreasing in time.

Remark 3.2. The convergence of the regularized version (7) towards the starting continuous system (1) as the parameter ϵ tends to zero is not clear, since the ϵ -independent estimates for u_ϵ obtained from the energy law (8) are not sufficient to pass to the limit. In [3, 10], regularized problems have also been considered for two cross-diffusion models; and in these cases, thanks to the fact that the self-diffusion term for u possesses one term in the form $-\nabla \cdot (u \nabla u)$, it is possible to obtain better estimates independent of ϵ , concretely for ∇u_ϵ in a certain L^p -space, allowing the necessary compactness in order to pass to the limit as ϵ goes to zero.

Then, we consider a fully discrete approximation using FE in space and backward Euler in time (considered for simplicity on a uniform partition of $[0, T]$ with time step $k = T/N : (t_n = nk)_{n=0}^{n=N}$). Let Ω be a polygonal domain. We consider a shape-regular and quasi-uniform family of triangulations of Ω , denoted by $\{\mathcal{T}_h\}_{h>0}$, with simplices K , $h_K = \text{diam}(K)$ and $h := \max_{K \in \mathcal{T}_h} h_K$, so that $\overline{\Omega} = \bigcup_{K \in \mathcal{T}_h} \overline{K}$. Moreover, in this case we will assume the following hypothesis:

- (H) The triangulation is structured in the sense that all simplices have a right angle.

We choose the following continuous FE spaces for u and v :

$$(U_h, V_h) \subset H^1(\Omega)^2, \quad \text{generated by } \mathbb{P}_1, \mathbb{P}_m \text{ with } m \geq 1.$$

Remark 3.3. The right angle requirement and the choice of \mathbb{P}_1 -continuous FE for U_h are necessary in order to obtain the relation (11) below, which is essential in order to prove the energy-stability of the scheme \mathbf{UV} (see Theorem 3.8 below).

Let J be the set of vertices of \mathcal{T}_h and $\{\mathbf{a}_j\}_{j \in J}$ the coordinates of these vertices. We denote the Lagrange interpolation operator by $\Pi^h : C(\overline{\Omega}) \rightarrow U_h$, and we introduce the discrete semi-inner product on $C(\overline{\Omega})$ (which is an inner product in U_h) and its induced discrete seminorm (norm in U_h):

$$(9) \quad (u_1, u_2)^h := \int_{\Omega} \Pi^h(u_1 u_2), \quad |u|_h = \sqrt{(u, u)^h}.$$

Remark 3.4. In U_h , the norms $|\cdot|_h$ and $\|\cdot\|_0$ are equivalent uniformly with respect to h (see [4]).

We also consider the L^2 -projection $Q^h : L^2(\Omega) \rightarrow U_h$ given by

$$(10) \quad (Q^h u, \bar{u})^h = (u, \bar{u}) \quad \forall \bar{u} \in U_h,$$

and the standard H^1 -projection $R^h : H^1(\Omega) \rightarrow V_h$. Moreover, for each $\varepsilon \in (0, 1)$ we consider the construction of the operator $\Lambda_\varepsilon : U_h \rightarrow L^\infty(\Omega)^{d \times d}$ given in [3], satisfying that $\Lambda_\varepsilon u^h$ is a symmetric and positive definite matrix for all $u^h \in U_h$ and a.e. \mathbf{x} in Ω , and the following relation holds:

$$(11) \quad (\Lambda_\varepsilon u^h) \nabla \Pi^h(F'_\varepsilon(u^h)) = \nabla u^h \quad \text{in } \Omega.$$

Basically, $\Lambda_\varepsilon u^h$ is a constant by elements matrix such that (11) holds by elements. We highlight that (11) is satisfied due to the right angle constraint requirement **(H)** and the choice of \mathbb{P}_1 -continuous FE for U_h . Moreover, the following stability estimate holds [3, 10]:

$$(12) \quad \|\Lambda_\varepsilon(u^h)\|_{L^r}^r \leq C(1 + \|u^h\|_1^2) \quad \forall u^h \in U_h \quad (\text{for } r = 2(d+1)/d),$$

where the constant $C > 0$ is independent of ε and h . We recall the result below concerning $\Lambda_\varepsilon(\cdot)$ (see [3, Lemma 2.1]).

Lemma 3.5. *Let $\|\cdot\|$ denote the spectral norm on $\mathbb{R}^{d \times d}$. Then for any given $\varepsilon \in (0, 1)$ the function $\Lambda_\varepsilon : U_h \rightarrow [L^\infty(\Omega)]^{d \times d}$ is continuous and satisfies*

$$(13) \quad \varepsilon \xi^T \xi \leq \xi^T \Lambda_\varepsilon(u^h) \xi \leq \varepsilon^{-1} \xi^T \xi \quad \forall \xi \in \mathbb{R}^d, \quad \forall u^h \in U_h.$$

In particular, for all $u_1^h, u_2^h \in U_h$ and $K \in \mathcal{T}_h$ with vertices $\{\mathbf{a}_i^K\}_{i=0}^d$, it holds that

$$(14) \quad \|(\Lambda_\varepsilon(u_1^h) - \Lambda_\varepsilon(u_2^h))|_K\| \leq \varepsilon^{-2} \max_{l=1, \dots, d} \{|u_1^h(\mathbf{a}_l^K) - u_2^h(\mathbf{a}_l^K)| + |u_1^h(\mathbf{a}_0^K) - u_2^h(\mathbf{a}_0^K)|\},$$

where \mathbf{a}_0^K is a fixed acute-angled vertex.

Let $A_h : V_h \rightarrow V_h$ be the linear operator defined as

$$(A_h v^h, \bar{v}) = (\nabla v^h, \nabla \bar{v}) + (v^h, \bar{v}) \quad \forall \bar{v} \in V_h.$$

Then, the following estimate holds (see, for instance, [12, Theorem 3.2]):

$$(15) \quad \|v^h\|_{W^{1,6}} \leq C \|A_h v^h\|_0 \quad \forall v^h \in V_h.$$

Taking into account the regularized problem (7), we consider the following first-order in time, nonlinear, and coupled scheme:

• **Scheme UV:**

Initialization: Let $(u_h^0, v_h^0) = (Q^h u_0, R^h v_0) \in U_h \times V_h$.

Time step n : Given $(u_\varepsilon^{n-1}, v_\varepsilon^{n-1}) \in U_h \times V_h$, compute $(u_\varepsilon^n, v_\varepsilon^n) \in U_h \times V_h$ solving

$$(16) \quad \begin{cases} (\delta_t u_\varepsilon^n, \bar{u})^h + (\nabla u_\varepsilon^n, \nabla \bar{u}) + (\Lambda_\varepsilon(u_\varepsilon^n) \nabla v_\varepsilon^n, \nabla \bar{u}) = 0 & \forall \bar{u} \in U_h, \\ (\delta_t v_\varepsilon^n, \bar{v}) + (A_h v_\varepsilon^n, \bar{v}) - (u_\varepsilon^n, \bar{v}) = 0 & \forall \bar{v} \in V_h, \end{cases}$$

where, in general, we denote $\delta_t a^n := \frac{a^n - a^{n-1}}{k}$.

3.1. Mass conservation and energy-stability. Since $\bar{u} = 1 \in U_h$ and $\bar{v} = 1 \in V_h$, we deduce that the scheme **UV** is conservative in u_ε^n , that is,

$$(17) \quad \begin{aligned} (u_\varepsilon^n, 1) &= (u_\varepsilon^n, 1)^h = (u_\varepsilon^{n-1}, 1)^h = \dots = (u_h^0, 1)^h = (u_h^0, 1) \\ &= (Q^h u_0, 1) = (u_0, 1) := m_0, \end{aligned}$$

and we have the following behavior for $\int_\Omega v_\varepsilon^n$:

$$(18) \quad \delta_t \left(\int_\Omega v_\varepsilon^n \right) + \int_\Omega v_\varepsilon^n = \int_\Omega u_\varepsilon^n = m_0.$$

Lemma 3.6 (Estimate of $|\int_\Omega v_\varepsilon^n|$). *The following estimate holds:*

$$(19) \quad \left| \int_\Omega v_\varepsilon^n \right| \leq (1+k)^{-n} \left| \int_\Omega v_0 \right| + m_0 \quad \forall n \geq 0.$$

Proof. From (18) we have $(1+k) \left| \int_\Omega v_\varepsilon^n \right| - \left| \int_\Omega v_\varepsilon^{n-1} \right| \leq k m_0$, and therefore, applying Lemma 2.1 (for $\delta = 1$ and $\beta = m_0$), we arrive at

$$\left| \int_\Omega v_\varepsilon^n \right| \leq (1+k)^{-n} \left| \int_\Omega v_\varepsilon^0 \right| + m_0 = (1+k)^{-n} \left| \int_\Omega R^h v_0 \right| + m_0,$$

which implies (19). \square

Definition 3.7. A numerical scheme with solution $(u_\varepsilon^n, v_\varepsilon^n)$ is called energy-stable with respect to the energy

$$(20) \quad \mathcal{E}_\varepsilon^h(u, v) = (F_\varepsilon(u), 1)^h + \frac{1}{2} \|\nabla v\|_0^2$$

if this energy is time decreasing, that is, $\mathcal{E}_\varepsilon^h(u_\varepsilon^n, v_\varepsilon^n) \leq \mathcal{E}_\varepsilon^h(u_\varepsilon^{n-1}, v_\varepsilon^{n-1})$ for all $n \geq 1$.

Theorem 3.8 (Unconditional stability). *The scheme **UV** is unconditionally energy stable with respect to $\mathcal{E}_\varepsilon^h(u, v)$. In fact, if $(u_\varepsilon^n, v_\varepsilon^n)$ is a solution of **UV**, then the following discrete energy law holds:*

$$(21) \quad \delta_t \mathcal{E}_\varepsilon^h(u_\varepsilon^n, v_\varepsilon^n) + \varepsilon \frac{k}{2} \|\delta_t u_\varepsilon^n\|_0^2 + \frac{k}{2} \|\delta_t \nabla v_\varepsilon^n\|_0^2 + \varepsilon \|\nabla u_\varepsilon^n\|_0^2 + \|(A_h - I)v_\varepsilon^n\|_0^2 + \|\nabla v_\varepsilon^n\|_0^2 \leq 0.$$

Proof. Testing (16)₁ by $\bar{u} = \Pi^h(F'_\varepsilon(u_\varepsilon^n))$ and (16)₂ by $\bar{v} = (A_h - I)v_\varepsilon^n$, adding and taking into account that $\Lambda_\varepsilon(u_\varepsilon^n)$ is symmetric as well as (11) (which implies that $\nabla \Pi^h(F'_\varepsilon(u_\varepsilon^n)) = \Lambda_\varepsilon^{-1}(u_\varepsilon^n) \nabla u_\varepsilon^n$), the terms $-(\Lambda_\varepsilon(u_\varepsilon^n) \nabla v_\varepsilon^n, \nabla \Pi^h(F'_\varepsilon(u_\varepsilon^n))) = -(\nabla v_\varepsilon^n, \Lambda_\varepsilon(u_\varepsilon^n) \nabla \Pi^h(F'_\varepsilon(u_\varepsilon^n))) = -(\nabla v_\varepsilon^n, \nabla u_\varepsilon^n)$ and $(u_\varepsilon^n, (A_h - I)v_\varepsilon^n) = (\nabla u_\varepsilon^n, \nabla v_\varepsilon^n)$ cancel, and we obtain

$$(22) \quad \begin{aligned} &(\delta_t u_\varepsilon^n, F'_\varepsilon(u_\varepsilon^n))^h + \int_\Omega (\nabla u_\varepsilon^n)^T \cdot \Lambda_\varepsilon^{-1}(u_\varepsilon^n) \cdot \nabla u_\varepsilon^n d\mathbf{x} \\ &+ \delta_t \left(\frac{1}{2} \|\nabla v_\varepsilon^n\|_0^2 \right) + \frac{k}{2} \|\delta_t \nabla v_\varepsilon^n\|_0^2 + \|(A_h - I)v_\varepsilon^n\|_0^2 + \|\nabla v_\varepsilon^n\|_0^2 = 0. \end{aligned}$$

Moreover, observe that from the Taylor formula we have

$$F_\varepsilon(u_\varepsilon^{n-1}) = F_\varepsilon(u_\varepsilon^n) + F'_\varepsilon(u_\varepsilon^n)(u_\varepsilon^{n-1} - u_\varepsilon^n) + \frac{1}{2}F''_\varepsilon(\theta u_\varepsilon^n + (1-\theta)u_\varepsilon^{n-1})(u_\varepsilon^{n-1} - u_\varepsilon^n)^2,$$

with $\theta \in (0, 1)$, and therefore,

$$(23) \quad F'_\varepsilon(u_\varepsilon^n)\delta_t u_\varepsilon^n = \delta_t(F_\varepsilon(u_\varepsilon^n)) + \frac{k}{2}F''_\varepsilon(\theta u_\varepsilon^n + (1-\theta)u_\varepsilon^{n-1})(\delta_t u_\varepsilon^n)^2.$$

Then, using (23) and taking into account that Π^h is linear and $F''_\varepsilon(s) \geq \varepsilon$ for all $s \in \mathbb{R}$, we have

$$\begin{aligned} (\delta_t u_\varepsilon^n, F'_\varepsilon(u_\varepsilon^n))^h &= \int_\Omega \Pi^h(\delta_t u_\varepsilon^n \cdot F'_\varepsilon(u_\varepsilon^n)) \\ &= \delta_t \left(\int_\Omega \Pi^h(F_\varepsilon(u_\varepsilon^n)) \right) + \frac{k}{2} \int_\Omega \Pi^h(F''_\varepsilon(\theta u_\varepsilon^n + (1-\theta)u_\varepsilon^{n-1})(\delta_t u_\varepsilon^n)^2) \\ (24) \quad &\geq \delta_t(F_\varepsilon(u_\varepsilon^n), 1)^h + \varepsilon \frac{k}{2} |\delta_t u_\varepsilon^n|^2_h. \end{aligned}$$

Thus, from (13), (22), (24), and Remark 3.4, we arrive at (21). \square

Corollary 3.9 (Uniform estimates). *Assume that $(u_0, v_0) \in L^2(\Omega) \times H^1(\Omega)$. Let $(u_\varepsilon^n, v_\varepsilon^n)$ be a solution of scheme **UV**. Then, it holds that*

$$\begin{aligned} (25) \quad &(F_\varepsilon(u_\varepsilon^n), 1)^h + \frac{1}{2} \|v_\varepsilon^n\|_1^2 \\ &+ k \sum_{m=1}^n (\varepsilon \|\nabla u_\varepsilon^m\|_0^2 + \|(A_h - I)v_\varepsilon^m\|_0^2 + \|\nabla v_\varepsilon^m\|_0^2) \leq C_0 \quad \forall n \geq 1, \end{aligned}$$

$$(26) \quad k \sum_{m=n_0+1}^{n+n_0} \|v_\varepsilon^m\|_{W^{1,6}}^2 \leq C_1(1 + kn) \quad \forall n \geq 1,$$

where the integer $n_0 \geq 0$ is arbitrary and with the constants $C_0, C_1 > 0$ depending on the data (Ω, u_0, v_0) , but independent of k, h, n , and ε . Moreover, if $\varepsilon \in (0, e^{-2})$, the following estimates hold:

$$(27) \quad \int_\Omega (\Pi^h(u_{\varepsilon-}^n))^2 \leq C_0 \varepsilon \quad \text{and} \quad \int_\Omega |u_\varepsilon^n| \leq m_0 + C\sqrt{\varepsilon} \quad \forall n \geq 1,$$

where $u_{\varepsilon-}^n := \min\{u_\varepsilon^n, 0\} \leq 0$ and the constant $C > 0$ depends on the data (Ω, u_0, v_0) , but is independent of k, h, n , and ε .

Proof. First, using the inequality $s(\ln s - 1) \leq s^2$ for all $s > 0$ (which implies $F_\varepsilon(s) \leq C(s^2 + 1)$ for all $s \geq 0$) and taking into account that $(u_h^0, v_h^0) = (Q^h u_0, R^h v_0)$, $u_0 \geq 0$ (and therefore, $u_h^0 \geq 0$), as well as the definition of F_ε , we have

$$\begin{aligned} \mathcal{E}_\varepsilon^h(u_h^0, v_h^0) &= \int_\Omega \Pi^h(F_\varepsilon(u_h^0)) + \frac{1}{2} \|\nabla v_h^0\|_0^2 \leq C \int_\Omega \Pi^h((u_h^0)^2 + 1) + \frac{1}{2} \|\nabla v_h^0\|_0^2 \\ (28) \quad &\leq C(\|u_h^0\|_0^2 + \|\nabla v_h^0\|_0^2 + 1) \leq C(\|u_0\|_0^2 + \|v_0\|_1^2 + 1) \leq C_0, \end{aligned}$$

with the constant $C_0 > 0$ depending on the data (Ω, u_0, v_0) , but independent of k, h, n , and ε . Therefore, from the discrete energy law (21) and (28), we have

$$(29) \quad \mathcal{E}_\varepsilon^h(u_\varepsilon^n, v_\varepsilon^n) + k \sum_{m=1}^n (\varepsilon \|\nabla u_\varepsilon^m\|_0^2 + \|(A_h - I)v_\varepsilon^m\|_0^2 + \|\nabla v_\varepsilon^m\|_0^2) \leq \mathcal{E}_\varepsilon^h(u_h^0, v_h^0) \leq C_0.$$

Thus, from (19) and (29) we conclude (25). Moreover, adding (21) from $m = n_0 + 1$ to $m = n + n_0$, and using (15) and (25), we deduce (26). On the other hand, if $\varepsilon \in (0, e^{-2})$, from (6)₂ and taking into account that $F_\varepsilon(s) \geq 0$ for all $s \in \mathbb{R}$, we have $\frac{1}{2\varepsilon}(u_{\varepsilon-}^n(\mathbf{x}))^2 \leq F_\varepsilon(u_\varepsilon^n(\mathbf{x}))$ for all $u_\varepsilon^n \in U_h$; and therefore, using that $(\Pi^h(u))^2 \leq \Pi^h(u^2)$ for all $u \in C(\bar{\Omega})$, we have

$$\frac{1}{2\varepsilon} \int_{\Omega} (\Pi^h(u_{\varepsilon-}^n))^2 \leq \frac{1}{2\varepsilon} \int_{\Omega} \Pi^h((u_{\varepsilon-}^n)^2) \leq \int_{\Omega} \Pi^h(F_\varepsilon(u_\varepsilon^n)) \leq C_0,$$

where in the last inequality (25) was used. Thus, we obtain (27)₁. Finally, considering $u_{\varepsilon+}^n := \max\{u_\varepsilon^n, 0\} \geq 0$, taking into account that $u_\varepsilon^n = u_{\varepsilon+}^n + u_{\varepsilon-}^n$ and $|u_\varepsilon^n| = u_{\varepsilon+}^n - u_{\varepsilon-}^n = u_\varepsilon^n - 2u_{\varepsilon-}^n$, and using the Hölder and Young inequalities as well as (17) and (27)₁, we have

$$\begin{aligned} \int_{\Omega} |u_\varepsilon^n| &\leq \int_{\Omega} \Pi^h |u_\varepsilon^n| = \int_{\Omega} u_\varepsilon^n - 2 \int_{\Omega} \Pi^h(u_{\varepsilon-}^n) \\ &\leq m_0 + C \left(\int_{\Omega} (\Pi^h(u_{\varepsilon-}^n))^2 \right)^{1/2} \leq m_0 + C\sqrt{\varepsilon}, \end{aligned}$$

which implies (27)₂. \square

Remark 3.10. The $l^\infty(L^1)$ -norm is the only norm in which u_ε^n is bounded independently of (k, h) and ε (see (27)₂); and this bound is not enough to prove the convergence towards weak solutions of model (1) when the parameters (k, h) and ε tend to zero.

Remark 3.11. We can also obtain ε -dependent bounds for u_ε^n . In fact, from (6) and taking into account that $\varepsilon \in (0, e^{-2})$, we can deduce that $\frac{\varepsilon}{2}s^2 \leq F_\varepsilon(s) + 2$ for all $s \in \mathbb{R}$, which together with (25) implies that $(\sqrt{\varepsilon} u_\varepsilon^n)$ is bounded in $l^\infty(L^2) \cap l^2(H^1)$.

Remark 3.12 (Approximated positivity).

(1) From (27)₁, the following estimate holds:

$$\max_{n \geq 0} \|\Pi^h(u_{\varepsilon-}^n)\|_0^2 \leq C_0\varepsilon.$$

(2) Assume V_h is furnished by \mathbb{P}_1 -continuous FE and consider the following approximation for the v -equation:

$$(30) \quad (\delta_t v_\varepsilon^n, \bar{v})^h + (\tilde{A}_h v_\varepsilon^n, \bar{v})^h - (u_\varepsilon^n, \bar{v})^h = 0 \quad \forall \bar{v} \in V_h,$$

where $\tilde{A}_h : V_h \rightarrow V_h$ is the operator defined by $(\tilde{A}_h v_h, \bar{v})^h = (\nabla v_h, \nabla \bar{v}) + (v_h, \bar{v})^h$ for all $\bar{v} \in V_h$. Then the unconditional energy-stability also holds and the following estimates are satisfied:

$$(31) \quad \max_{n \geq 0} \|\Pi^h(v_{\varepsilon-}^n)\|_0^2 \leq C\varepsilon \quad \text{and} \quad k \sum_{m=1}^n \|\Pi^h(v_{\varepsilon-}^m)\|_1^2 \leq C\varepsilon(kn),$$

where the constant C is independent of k, h, n , and ε . In fact, testing by $\bar{v} = \Pi^h(v_{\varepsilon-}^n) \in V_h$ in (30), taking into account that $(\nabla \Pi^h(v_{\varepsilon+}^n), \nabla \Pi^h(v_{\varepsilon-}^n)) \geq 0$ (owing to the interior angles of the triangles or tetrahedra are less than or equal to $\pi/2$), and using again that $(\Pi^h(v))^2 \leq \Pi^h(v^2)$ for all $v \in C(\bar{\Omega})$,

we have

$$\begin{aligned} \left(\frac{1}{k} + 1\right) \|\Pi^h(v_{\varepsilon-}^n)\|_0^2 + \|\nabla \Pi^h(v_{\varepsilon-}^n)\|_0^2 &\leq \int_{\Omega} \Pi^h \left[\left(u_{\varepsilon-}^n + \frac{1}{k} v_{\varepsilon-}^{n-1}\right) v_{\varepsilon-}^n \right] \\ &\leq \int_{\Omega} \Pi^h \left[\left(u_{\varepsilon-}^n + \frac{1}{k} v_{\varepsilon-}^{n-1}\right) v_{\varepsilon-}^n \right] \\ &\leq \frac{1}{2} \left(\frac{1}{k} + 1\right) \|\Pi^h(v_{\varepsilon-}^n)\|_0^2 + \frac{1}{2} \|\Pi^h(u_{\varepsilon-}^n)\|_0^2 + \frac{1}{2k} \|\Pi^h(v_{\varepsilon-}^{n-1})\|_0^2, \end{aligned}$$

from which, using (27)₁, we arrive at

$$(32) \quad \frac{1}{2} \left(\frac{1}{k} + 1\right) \|\Pi^h(v_{\varepsilon-}^n)\|_0^2 + \|\nabla \Pi^h(v_{\varepsilon-}^n)\|_0^2 \leq \frac{1}{2} C_0 \varepsilon + \frac{1}{2k} \|\Pi^h(v_{\varepsilon-}^{n-1})\|_0^2.$$

Therefore, if $v_h^0 \geq 0$ (which holds for instance by considering $v_h^0 = \tilde{R}^h v_0$, where \tilde{R}^h is an average interpolator of Clement or Scott-Zhang type, and using that $v_0 \geq 0$), using Lemma 2.1 in (32), we conclude (31)₁. Finally, multiplying (32) by k and adding from $m = 1$ to $m = n$, and using again that $v_h^0 \geq 0$, we arrive at (31)₂.

3.2. Well-posedness. In this subsection, we will prove the well-posedness of the scheme **UV**. We recall that, taking into account that we remain in finite dimension, all norms are equivalents.

Theorem 3.13 (Unconditional existence). *There exists at least one solution $(u_{\varepsilon}^n, v_{\varepsilon}^n)$ of the scheme **UV**.*

Proof. We will use the Leray-Schauder fixed point theorem. With this aim, given $(u_{\varepsilon}^{n-1}, v_{\varepsilon}^{n-1}) \in U_h \times V_h$, we define the operator $R : U_h \times V_h \rightarrow U_h \times V_h$ by $R(\tilde{u}, \tilde{v}) = (u, v)$, such that $(u, v) \in U_h \times V_h$ solves the following linear decoupled problem:

$$(33) \quad u \in U_h \quad \text{s.t.} \quad \frac{1}{k} (u, \bar{u})^h + (\nabla u, \nabla \bar{u}) = \frac{1}{k} (u_{\varepsilon}^{n-1}, \bar{u})^h - (\Lambda_{\varepsilon}(\tilde{u}) \nabla \tilde{v}, \nabla \bar{u}) \quad \forall \bar{u} \in U_h,$$

$$(34) \quad v \in V_h \quad \text{s.t.} \quad \frac{1}{k} (v, \bar{v}) + (A_h v, \bar{v}) = \frac{1}{k} (v_{\varepsilon}^{n-1}, \bar{v}) + (\tilde{u}, \bar{v}) \quad \forall \bar{v} \in V_h.$$

- (1) R is well defined. Applying the Lax-Milgram theorem to (33) and (34), we can deduce that, for each $(\tilde{u}, \tilde{v}) \in U_h \times V_h$, there exists a unique $(u, v) \in U_h \times V_h$ solution of (33)–(34).
- (2) Let us now prove that all possible fixed points of αR (with $\alpha \in (0, 1]$) are bounded. In fact, observe that if (u, v) is a fixed point of αR , then $R(u, v) = (\frac{1}{\alpha} u, \frac{1}{\alpha} v)$, and therefore (u, v) satisfies the coupled system

$$(35) \quad \begin{cases} \frac{1}{k} (u, \bar{u})^h + (\nabla u, \nabla \bar{u}) + \alpha (\Lambda_{\varepsilon}(u) \nabla v, \nabla \bar{u}) = \frac{\alpha}{k} (u_{\varepsilon}^{n-1}, \bar{u})^h \quad \forall \bar{u} \in U_h, \\ \frac{1}{k} (v, \bar{v}) + (A_h v, \bar{v}) - \alpha (u, \bar{v}) = \frac{\alpha}{k} (v_{\varepsilon}^{n-1}, \bar{v}) \quad \forall \bar{v} \in V_h. \end{cases}$$

Then, testing (35)₁ and (35)₂ by $\bar{u} = \Pi^h(F'_{\varepsilon}(u))$ and $\bar{v} = (A_h - I)v$, respectively, proceeding as in Theorem 3.8, and taking into account that $\alpha \in (0, 1]$, we obtain

$$(36) \quad \begin{aligned} (F_{\varepsilon}(u), 1)^h + \frac{1}{2} \|\nabla v\|_0^2 + k (\varepsilon \|\nabla u\|_0^2 + \|(A_h - I)v\|_0^2 + \|\nabla v\|_0^2) \\ \leq (F_{\varepsilon}(\alpha u_{\varepsilon}^{n-1}), 1)^h + \frac{\alpha^2}{2} \|\nabla v_{\varepsilon}^{n-1}\|_0^2 \leq C(u_{\varepsilon}^{n-1}, v_{\varepsilon}^{n-1}), \end{aligned}$$

where the last estimate is α -independent (arguing as in (28)). Moreover, proceeding as in Lemma 3.6 and Corollary 3.9 (taking into account (36)), we deduce $\|(u, v)\|_{L^1 \times H^1} \leq C$, where the constant C depends on data $(\Omega, u_\varepsilon^{n-1}, v_\varepsilon^{n-1}, \varepsilon)$, but it is independent of α and h .

- (3) We prove that R is continuous. Let $\{(\tilde{u}^l, \tilde{v}^l)\}_{l \in \mathbb{N}} \subset U_h \times V_h \hookrightarrow W^{1,\infty}(\Omega)^2$ be a sequence such that

$$(37) \quad (\tilde{u}^l, \tilde{v}^l) \rightarrow (\tilde{u}, \tilde{v}) \text{ in } U_h \times V_h \text{ as } l \rightarrow +\infty.$$

In particular, since we remain in finite dimension, $\{(\tilde{u}^l, \tilde{v}^l)\}_{l \in \mathbb{N}}$ is bounded in $W^{1,\infty}(\Omega)^2$. Then, if we denote $(u^l, v^l) = R(\tilde{u}^l, \tilde{v}^l)$, we can deduce

$$\begin{aligned} \frac{1}{2k} \|(u^l, v^l)\|_0^2 + \frac{1}{2} \|\nabla u^l\|_0^2 + \frac{1}{2} \|v^l\|_1^2 \\ \leq \frac{1}{2k} \|(u_\varepsilon^{n-1}, v_\varepsilon^{n-1})\|_0^2 + (1 + \|\tilde{u}^l\|_1^2)^{2/r} \|\nabla \tilde{v}^l\|_{L^\infty}^2 + C \|\tilde{u}^l\|_0^2 \leq C, \end{aligned}$$

where in the first inequality (12) was used and C is a constant independent of $l \in \mathbb{N}$. Therefore, $\{(u^l, v^l) = R(\tilde{u}^l, \tilde{v}^l)\}_{l \in \mathbb{N}}$ is bounded in $U_h \times V_h \hookrightarrow W^{1,\infty}(\Omega)^2$. Then, there exists a subsequence of $\{R(\tilde{u}^l, \tilde{v}^l)\}_{l \in \mathbb{N}}$, still denoted by $\{R(\tilde{u}^l, \tilde{v}^l)\}_{l \in \mathbb{N}}$, such that

$$(38) \quad R(\tilde{u}^l, \tilde{v}^l) \rightarrow (u', v') \text{ in } W^{1,\infty}(\Omega)^2, \text{ as } l \rightarrow +\infty.$$

Then, from (37)–(38) and using Lemma 3.5, a standard procedure allows us to pass to the limit, as l goes to $+\infty$, in (33)–(34) (with $(\tilde{u}^l, \tilde{v}^l)$ and (u^l, v^l) instead of (\tilde{u}, \tilde{v}) and (u, v) , respectively), and we deduce that $R(\tilde{u}, \tilde{v}) = (u', v')$. Therefore, we have proved that any convergent subsequence of $\{R(\tilde{u}^l, \tilde{v}^l)\}_{l \in \mathbb{N}}$ converges to $R(\tilde{u}, \tilde{v})$ in $U_h \times V_h$, and from uniqueness of $R(\tilde{u}, \tilde{v})$, we conclude that the whole sequence $R(\tilde{u}^l, \tilde{v}^l) \rightarrow R(\tilde{u}, \tilde{v})$ in $U_h \times V_h$. Thus, R is continuous.

Therefore, the hypotheses of the Leray-Schauder fixed point theorem (in finite dimension) are satisfied and we conclude that the map R has a fixed point (u, v) , that is, $R(u, v) = (u, v)$, which is a solution of the scheme **UV**. \square

Lemma 3.14 (Conditional uniqueness). *If $k g(h, \varepsilon) < 1$ (where $g(h, \varepsilon) \uparrow +\infty$ as $h \downarrow 0$ or $\varepsilon \downarrow 0$), then the solution $(u_\varepsilon^n, v_\varepsilon^n)$ of the scheme **UV** is unique.*

Proof. Suppose that there exist $(u_\varepsilon^{n,1}, v_\varepsilon^{n,1}), (u_\varepsilon^{n,2}, v_\varepsilon^{n,2}) \in U_h \times V_h$, two possible solutions of the scheme **UV**. Then, defining $u = u_\varepsilon^{n,1} - u_\varepsilon^{n,2}$ and $v = v_\varepsilon^{n,1} - v_\varepsilon^{n,2}$, we have that $(u, v) \in U_h \times V_h$ satisfies, for all $(\bar{u}, \bar{v}) \in U_h \times V_h$,

$$(39) \quad \frac{1}{k} (u, \bar{u})^h + (\nabla u, \nabla \bar{u}) + (\Lambda_\varepsilon(u_\varepsilon^{n,1}) \nabla v, \nabla \bar{u}) + ((\Lambda_\varepsilon(u_\varepsilon^{n,1}) - \Lambda_\varepsilon(u_\varepsilon^{n,2})) \nabla v_\varepsilon^{n,2}, \nabla \bar{u}) = 0,$$

$$(40) \quad \frac{1}{k} (v, \bar{v}) + (A_h v, \bar{v}) = (u, \bar{v}).$$

Taking $\bar{u} = u$, $\bar{v} = A_h v$ in (39)–(40), adding the resulting expressions, and using the fact that $\int_\Omega u = 0$ and the equivalence of the norms $\|\cdot\|_0$ and $|\cdot|_h$ in U_h given

in Remark 3.4, we obtain

$$\begin{aligned}
\frac{1}{k} \|(u, \nabla v)\|_0^2 + \|(u, A_h v)\|_{H^1 \times L^2}^2 &\leq \|u\|_0 \|A_h v\|_0 \\
&+ \|\Lambda_\varepsilon(u_\varepsilon^{n,1})\|_{L^6} \|\nabla v\|_{L^3} \|\nabla u\|_0 + \|\Lambda_\varepsilon(u_\varepsilon^{n,1}) - \Lambda_\varepsilon(u_\varepsilon^{n,2})\|_{L^\infty} \|\nabla v_\varepsilon^{n,2}\|_0 \|\nabla u\|_0 \\
&\leq \frac{1}{4} \|A_h v\|_0^2 + \|u\|_0^2 + \frac{1}{4} \|\nabla u\|_0^2 + \frac{1}{4} \|A_h v\|_0^2 + C \|\Lambda_\varepsilon(u_\varepsilon^{n,1})\|_{L^6}^4 \|\nabla v\|_0^2 \\
&+ \frac{1}{4} \|\nabla u\|_0^2 + \|\Lambda_\varepsilon(u_\varepsilon^{n,1}) - \Lambda_\varepsilon(u_\varepsilon^{n,2})\|_{L^\infty}^2 \|\nabla v_\varepsilon^{n,2}\|_0^2.
\end{aligned}$$

Then, taking into account (12), (14), (25), (27)₂ and using the inverse inequalities $\|u^h\|_{L^6}^2 \leq C_1(h) \|u^h\|_{L^r}^2$, $\|u^h\|_1^2 \leq C_2(h) \|u^h\|_{L^1}^2$, and $\|u^h\|_{L^\infty}^2 \leq C_3(h) \|u^h\|_0^2$ for all $u^h \in U_h$, we have

$$\begin{aligned}
\|(u, \nabla v)\|_0^2 + \frac{k}{2} \|(u, A_h v)\|_{H^1 \times L^2}^2 \\
\leq k (1 + C \|\Lambda_\varepsilon(u_\varepsilon^{n,1})\|_{L^6}^4) \|(u, \nabla v)\|_0^2 + k C_0 C \varepsilon^{-2} \|u\|_{L^\infty}^2 \\
\leq k \left(1 + C_1(h)^2 (1 + C_2(h))^{4/r} + k C_0 C_3(h) \varepsilon^{-2} \right) \|(u, \nabla v)\|_0^2 := k g(h, \varepsilon) \|(u, \nabla v)\|_0^2.
\end{aligned}$$

Therefore, if $k g(h, \varepsilon) < 1$, we conclude that $u = 0$, and therefore (from (40)) $v = 0$. \square

4. SCHEME US

In this section, we propose another energy-stable nonlinear fully discrete scheme associated to model (1), which is obtained by introducing the auxiliary variable $\sigma = \nabla v$. In fact, taking into account the functions λ_ε and F_ε and their derivatives (given in (4)–(5)), another regularized version of problem (1) reads: find $u_\varepsilon : \Omega \times [0, T] \rightarrow \mathbb{R}$ and $\sigma_\varepsilon : \Omega \times [0, T] \rightarrow \mathbb{R}^d$ such that

$$(41) \quad \begin{cases} \partial_t u_\varepsilon - \nabla \cdot (\lambda_\varepsilon(u_\varepsilon) \nabla (F'_\varepsilon(u_\varepsilon))) - \nabla \cdot (\lambda_\varepsilon(u_\varepsilon) \sigma_\varepsilon) = 0 & \text{in } \Omega, \ t > 0, \\ \partial_t \sigma_\varepsilon + \text{rot}(\text{rot } \sigma_\varepsilon) - \nabla(\nabla \cdot \sigma_\varepsilon) + \sigma_\varepsilon = \lambda_\varepsilon(u_\varepsilon) \nabla (F'_\varepsilon(u_\varepsilon)) & \text{in } \Omega, \ t > 0, \\ \frac{\partial u_\varepsilon}{\partial \mathbf{n}} = 0 & \text{on } \partial\Omega, \ t > 0, \\ \frac{\partial \mathbf{n}}{\partial \mathbf{n}} \cdot \mathbf{n} = 0, \ [\text{rot } \sigma_\varepsilon \times \mathbf{n}]_{\text{tang}} = 0 & \text{on } \partial\Omega, \ t > 0, \\ u_\varepsilon(\mathbf{x}, 0) = u_0(\mathbf{x}) \geq 0, \ \sigma_\varepsilon(\mathbf{x}, 0) = \nabla v_0(\mathbf{x}) & \text{in } \Omega. \end{cases}$$

This kind of formulation considering $\sigma = \nabla v$ as an auxiliary variable has been used in the construction of numerical schemes for other chemotaxis models (see for instance [12, 19]). Once problem (41) is solved, we can recover v_ε from u_ε solving

$$(42) \quad \begin{cases} \partial_t v_\varepsilon - \Delta v_\varepsilon + v_\varepsilon = u_\varepsilon & \text{in } \Omega, \ t > 0, \\ \frac{\partial v_\varepsilon}{\partial \mathbf{n}} = 0 & \text{on } \partial\Omega, \ t > 0, \\ v_\varepsilon(\mathbf{x}, 0) = v_0(\mathbf{x}) \geq 0 & \text{in } \Omega. \end{cases}$$

Observe that multiplying (41)₁ by $F'_\varepsilon(u_\varepsilon)$, (41)₂ by σ_ε , and integrating over Ω , we obtain the energy law

$$(43) \quad \frac{d}{dt} \int_\Omega \left(F_\varepsilon(u_\varepsilon) + \frac{1}{2} |\sigma_\varepsilon|^2 \right) d\mathbf{x} + \int_\Omega \lambda_\varepsilon(u_\varepsilon) |\nabla (F'_\varepsilon(u_\varepsilon))|^2 d\mathbf{x} + \|\sigma_\varepsilon\|_1^2 = 0.$$

In particular, the modified energy $\mathcal{E}_\varepsilon(u, \sigma) = \int_\Omega (F_\varepsilon(u) + \frac{1}{2} |\sigma|^2) d\mathbf{x}$ is decreasing in time.

Remark 4.1. As in Section 3, in this case again it is not clear how to prove the convergence of the regularized version (41) towards the starting continuous system (1) as ε goes to zero.

Then, we consider a fully discrete approximation of the regularized problem (41) using an FE discretization in space and the backward Euler discretization in time (again considered for simplicity on a uniform partition of $[0, T]$ with time step $k = T/N : (t_n = nk)_{n=0}^{n=N}$). Concerning the space discretization, we consider the triangulation as in the scheme **UV**, but in this case without imposing the constraint **(H)** related with the right-angle simplices. We choose the following continuous FE spaces for u_ε , σ_ε , and v_ε :

$$(U_h, \Sigma_h, V_h) \subset H^1(\Omega) \times \mathbf{H}_\sigma^1(\Omega) \times H^1(\Omega), \quad \text{generated by } \mathbb{P}_1, \mathbb{P}_m, \mathbb{P}_r \text{ with } m, r \geq 1.$$

Then, we consider the following first-order in time, nonlinear, and coupled scheme:

• **Scheme US:**

Initialization: Let $(u_h^0, \sigma_h^0) = (Q^h u_0, \tilde{Q}^h(\nabla v_0)) \in U_h \times \Sigma_h$.

Time step n : Given $(u_\varepsilon^{n-1}, \sigma_\varepsilon^{n-1}) \in U_h \times \Sigma_h$, compute $(u_\varepsilon^n, \sigma_\varepsilon^n) \in U_h \times \Sigma_h$ solving

$$(44) \quad \begin{cases} (\delta_t u_\varepsilon^n, \bar{u})^h + (\lambda_\varepsilon(u_\varepsilon^n) \nabla \Pi^h(F'_\varepsilon(u_\varepsilon^n)), \nabla \bar{u}) = -(\lambda_\varepsilon(u_\varepsilon^n) \sigma_\varepsilon^n, \nabla \bar{u}) \quad \forall \bar{u} \in U_h, \\ (\delta_t \sigma_\varepsilon^n, \bar{\sigma}) + (B_h \sigma_\varepsilon^n, \bar{\sigma}) = (\lambda_\varepsilon(u_\varepsilon^n) \nabla \Pi^h(F'_\varepsilon(u_\varepsilon^n)), \bar{\sigma}) \quad \forall \bar{\sigma} \in \Sigma_h, \end{cases}$$

where Q^h is the L^2 -projection on U_h defined in (10), \tilde{Q}^h is the standard L^2 -projection on Σ_h , and the operator B_h is defined as

$$(B_h \sigma_\varepsilon^n, \bar{\sigma}) = (\text{rot } \sigma_\varepsilon^n, \text{rot } \bar{\sigma}) + (\nabla \cdot \sigma_\varepsilon^n, \nabla \cdot \bar{\sigma}) + (\sigma_\varepsilon^n, \bar{\sigma}).$$

We recall that $\Pi^h : C(\bar{\Omega}) \rightarrow U_h$ is the Lagrange interpolation operator, and the discrete semi-inner product $(\cdot, \cdot)^h$ was defined in (9). Once the scheme **US** is solved, given $v_\varepsilon^{n-1} \in V_h$, we can recover $v_\varepsilon^n = v_\varepsilon^n(u_\varepsilon^n) \in V_h$ solving:

$$(45) \quad (\delta_t v_\varepsilon^n, \bar{v}) + (\nabla v_\varepsilon^n, \nabla \bar{v}) + (v_\varepsilon^n, \bar{v}) = (u_\varepsilon^n, \bar{v}) \quad \forall \bar{v} \in V_h.$$

Given $u_\varepsilon^n \in U_h$ and $v_\varepsilon^{n-1} \in V_h$, the Lax-Milgram theorem implies that there exists a unique $v_\varepsilon^n \in V_h$ solution of (45). The solvability of (44) will be proved in Subsection 4.2.

4.1. Mass conservation and energy-stability. Observe that the scheme **US** is also conservative in u (satisfying (17)) and also has the behavior for $\int_\Omega v_n$ given in (18).

Definition 4.2. A numerical scheme with solution $(u_\varepsilon^n, \sigma_\varepsilon^n)$ is called energy-stable with respect to the energy

$$(46) \quad \mathcal{E}_\varepsilon^h(u, \sigma) = (F_\varepsilon(u), 1)^h + \frac{1}{2} \|\sigma\|_0^2$$

if this energy is time decreasing, that is, $\mathcal{E}_\varepsilon^h(u_\varepsilon^n, \sigma_\varepsilon^n) \leq \mathcal{E}_\varepsilon^h(u_\varepsilon^{n-1}, \sigma_\varepsilon^{n-1})$ for all $n \geq 1$.

Theorem 4.3 (Unconditional stability). *The scheme **US** is unconditionally energy stable with respect to $\mathcal{E}_\varepsilon^h(u, \sigma)$. In fact, if $(u_\varepsilon^n, \sigma_\varepsilon^n)$ is a solution of **US**, then the following discrete energy law holds:*

$$(47) \quad \delta_t \mathcal{E}_\varepsilon^h(u_\varepsilon^n, \sigma_\varepsilon^n) + \varepsilon \frac{k}{2} \|\delta_t u_\varepsilon^n\|_0^2 + \frac{k}{2} \|\delta_t \sigma_\varepsilon^n\|_0^2 + \int_\Omega \lambda_\varepsilon(u_\varepsilon^n) |\nabla \Pi^h(F'_\varepsilon(u_\varepsilon^n))|^2 d\mathbf{x} + \|\sigma_\varepsilon^n\|_1^2 \leq 0.$$

Proof. Testing (44)₁ by $\bar{u} = \Pi^h(F'_\varepsilon(u_\varepsilon^n))$, (44)₂ by $\bar{\sigma} = \sigma_\varepsilon^n$, and adding, the terms $(\lambda_\varepsilon(u_\varepsilon^n)\nabla\Pi^h(F'_\varepsilon(u_\varepsilon^n)), \sigma_\varepsilon^n)$ cancel, and we obtain

$$\begin{aligned} (\delta_t u_\varepsilon^n, \Pi^h(F'_\varepsilon(u_\varepsilon^n)))^h + \int_\Omega \lambda_\varepsilon(u_\varepsilon^n) |\nabla\Pi^h(F'_\varepsilon(u_\varepsilon^n))|^2 dx \\ + \delta_t \left(\frac{1}{2} \|\sigma_\varepsilon^n\|_0^2 \right) + \frac{k}{2} \|\delta_t \sigma_\varepsilon^n\|_0^2 + \|\sigma_\varepsilon^n\|_1^2 = 0, \end{aligned}$$

which, proceeding as in (23)–(24) and using Remark 3.4, implies (47). \square

Corollary 4.4 (Uniform estimates). *Assume that $(u_0, v_0) \in L^2(\Omega) \times H^1(\Omega)$. Let $(u_\varepsilon^n, \sigma_\varepsilon^n)$ be a solution of scheme **US**. Then, it holds that*

$$(F_\varepsilon(u_\varepsilon^n), 1)^h + \|\sigma_\varepsilon^n\|_0^2 + k \sum_{m=1}^n (\varepsilon \|\nabla\Pi^h(F'_\varepsilon(u_\varepsilon^m))\|_0^2 + \|\sigma_\varepsilon^m\|_1^2) \leq C_0 \quad \forall n \geq 1,$$

with the constant $C_0 > 0$ depending on the data (Ω, u_0, v_0) , but independent of k, h, n , and ε . Moreover, if $\varepsilon \in (0, e^{-2})$, estimates (27) hold.

Proof. Proceeding as in (28) (using the fact that $(u_h^0, \sigma_h^0) = (Q^h u_0, \tilde{Q}^h(\nabla v_0))$), we can deduce that

$$(48) \quad (F_\varepsilon(u_h^0), 1)^h + \|\sigma_h^0\|_0^2 \leq C_0,$$

where $C_0 > 0$ is a constant depending on the data (Ω, u_0, v_0) , but independent of k, h, n , and ε . Therefore, from the discrete energy law (47) and estimate (48), we have

$$\begin{aligned} (F_\varepsilon(u_\varepsilon^n), 1)^h + \|\sigma_\varepsilon^n\|_0^2 + k \sum_{m=1}^n (\varepsilon \|\nabla\Pi^h(F'_\varepsilon(u_\varepsilon^m))\|_0^2 + \|\sigma_\varepsilon^m\|_1^2) \\ \leq (F_\varepsilon(u_h^0), 1)^h + \|\sigma_h^0\|_0^2 \leq C_0. \end{aligned}$$

Finally, the estimates given in (27) are proved as in Corollary 3.9. \square

Remark 4.5. The conclusions obtained in Remarks 3.10–3.11 and the approximated positivity results established in Remark 3.12 remain true for the scheme **US**.

4.2. Well-posedness.

Theorem 4.6 (Unconditional existence). *There exists at least one solution $(u_\varepsilon^n, \sigma_\varepsilon^n)$ of scheme **US**.*

Proof. We will use the Leray-Schauder fixed point theorem. With this aim, given $(u_\varepsilon^{n-1}, \sigma_\varepsilon^{n-1}) \in U_h \times \Sigma_h$, we define the operator $R : U_h \times \Sigma_h \rightarrow U_h \times \Sigma_h$ by $R(\tilde{u}, \tilde{\sigma}) = (u, \sigma)$, such that $(u, \sigma) \in U_h \times \Sigma_h$ solves the following linear decoupled problem:

$$(49) \quad u \in U_h \quad \text{s.t.} \quad \frac{1}{k}(u, \bar{u})^h = \frac{1}{k}(u_\varepsilon^{n-1}, \bar{u})^h - (\lambda_\varepsilon(\tilde{u})\nabla\Pi^h(F'_\varepsilon(\tilde{u})), \nabla\bar{u}) \\ - (\lambda_\varepsilon(\tilde{u})\tilde{\sigma}, \nabla\bar{u}) \quad \forall \bar{u} \in U_h,$$

$$(50) \quad \sigma \in \Sigma_h \quad \text{s.t.} \quad \frac{1}{k}(\sigma, \bar{\sigma}) + (B_h \sigma, \bar{\sigma}) = \frac{1}{k}(\sigma_\varepsilon^{n-1}, \bar{\sigma}) + (\lambda_\varepsilon(\tilde{u})\nabla\Pi^h(F'_\varepsilon(\tilde{u})), \bar{\sigma}) \quad \forall \bar{\sigma} \in \Sigma_h.$$

- (1) R is well defined. Applying the Lax-Milgram theorem to (49) and (50), we can deduce that, for each $(\tilde{u}, \tilde{\sigma}) \in U_h \times \Sigma_h$, there exists a unique $(u, \sigma) \in U_h \times \Sigma_h$ solution of (49)–(50).

- (2) Let us now prove that all possible fixed points of αR (with $\alpha \in (0, 1]$) are bounded. In fact, observe that if (u, σ) is a fixed point of αR , then (u, σ) satisfies the coupled system

$$(51) \quad \begin{cases} \frac{1}{k}(u, \bar{u})^h + \alpha(\lambda_\varepsilon(u) \nabla \Pi^h(F'_\varepsilon(u)), \nabla \bar{u}) + \alpha(\lambda_\varepsilon(u) \sigma, \nabla \bar{u}) \\ = \frac{\alpha}{k}(u_\varepsilon^{n-1}, \bar{u})^h \quad \forall \bar{u} \in U_h, \\ \frac{1}{k}(\sigma, \bar{\sigma}) + (B_h \sigma, \bar{\sigma}) - \alpha(\lambda_\varepsilon(u) \nabla \Pi^h(F'_\varepsilon(u)), \bar{\sigma}) = \frac{\alpha}{k}(\sigma_\varepsilon^{n-1}, \bar{\sigma}) \quad \forall \bar{\sigma} \in \Sigma_h. \end{cases}$$

Then, testing (51)₁ and (51)₂ by $\bar{u} = \Pi^h(F'_\varepsilon(u)) \in U_h$ and $\bar{\sigma} = \sigma \in \Sigma_h$, respectively, proceeding as in Theorem 4.3, and taking into account that $\alpha \in (0, 1]$, we obtain

$$(52) \quad \begin{aligned} (F'_\varepsilon(u), 1)^h + \frac{1}{2} \|\sigma\|_0^2 + k(\varepsilon \lambda \|\nabla \Pi^h(F'_\varepsilon(u))\|_0^2 + \|\sigma\|_1^2) \\ \leq (F'_\varepsilon(\alpha u_\varepsilon^{n-1}), 1)^h + \frac{\alpha^2}{2} \|\sigma_\varepsilon^{n-1}\|_0^2 \leq C(u_\varepsilon^{n-1}, \sigma_\varepsilon^{n-1}), \end{aligned}$$

which implies $\|\sigma\|_1 \leq C$ (with the constant $C > 0$ independent of α). Moreover, proceeding as in the proof of (27) (using (52)) we deduce $\|u\|_{L^1} \leq C$, where the constant C depends on data $(\Omega, u_\varepsilon^{n-1}, \sigma_\varepsilon^{n-1}, \varepsilon)$.

- (3) We prove that R is continuous. Let $\{(\tilde{u}^l, \tilde{\sigma}^l)\}_{l \in \mathbb{N}} \subset U_h \times \Sigma_h \hookrightarrow W^{1,\infty}(\Omega) \times \mathbf{W}^{1,\infty}(\Omega)$ be a sequence such that

$$(53) \quad (\tilde{u}^l, \tilde{\sigma}^l) \rightarrow (\tilde{u}, \tilde{\sigma}) \quad \text{in } U_h \times \Sigma_h \quad \text{as } l \rightarrow +\infty.$$

In particular, $\{(\tilde{u}^l, \tilde{\sigma}^l)\}_{l \in \mathbb{N}}$ is bounded in $W^{1,\infty}(\Omega) \times \mathbf{W}^{1,\infty}(\Omega)$. Observe that from (53), we have that for h fixed, $\tilde{u}^l \rightarrow \tilde{u}$ in $C(\bar{\Omega})$; and thus, $F'_\varepsilon(\tilde{u}^l) \rightarrow F'_\varepsilon(\tilde{u})$ in $C(\bar{\Omega})$ since F'_ε is a Lipschitz continuous function. Then, the linearity and continuity of Π^h with respect to the $C^0(\bar{\Omega})$ -norm imply that $\Pi^h(F'_\varepsilon(\tilde{u}^l)) \rightarrow \Pi^h(F'_\varepsilon(\tilde{u}))$ in $C(\bar{\Omega})$. Moreover, if we denote $(u^l, \sigma^l) = R(\tilde{u}^l, \tilde{\sigma}^l)$, we can deduce (recall that $\varepsilon \leq \lambda_\varepsilon(s) \leq \varepsilon^{-1}$ for all $s \in \mathbb{R}$)

$$\begin{aligned} \frac{1}{2k} \|(u^l, \sigma^l)\|_0^2 + \frac{1}{2} \|\sigma^l\|_1^2 &\leq \frac{1}{2k} \|(u_\varepsilon^{n-1}, \sigma_\varepsilon^{n-1})\|_0^2 + C(h, k) \varepsilon^{-2} \|\tilde{\sigma}^l\|_{L^6}^2 \\ &\quad + C \varepsilon^{-2} \|\nabla \Pi^h(F'_\varepsilon(\tilde{u}^l))\|_0^2 + C(h, k) \varepsilon^{-2} \|\nabla \Pi^h(F'_\varepsilon(\tilde{u}^l))\|_0^2 \leq C, \end{aligned}$$

where C is a constant independent of $l \in \mathbb{N}$. Therefore, $\{(u^l, \sigma^l) = R(\tilde{u}^l, \tilde{\sigma}^l)\}_{l \in \mathbb{N}}$ is bounded in $U_h \times \Sigma_h \hookrightarrow W^{1,\infty}(\Omega) \times \mathbf{W}^{1,\infty}(\Omega)$. Then, since we remain in finite dimension, there exists a subsequence of $\{R(\tilde{u}^l, \tilde{\sigma}^l)\}_{l \in \mathbb{N}}$, still denoted by $\{R(\tilde{u}^l, \tilde{\sigma}^l)\}_{l \in \mathbb{N}}$, such that

$$(54) \quad R(\tilde{u}^l, \tilde{\sigma}^l) \rightarrow (u', \sigma') \quad \text{in } W^{1,\infty}(\Omega) \times \mathbf{W}^{1,\infty}(\Omega).$$

Then, from (53)–(54), a standard procedure allows us to pass to the limit, as l goes to $+\infty$, in (49)–(50) (with $(\tilde{u}^l, \tilde{\sigma}^l)$ and (u^l, σ^l) instead of $(\tilde{u}, \tilde{\sigma})$ and (u, σ) , respectively), and we deduce that $R(\tilde{u}, \tilde{\sigma}) = (u', \sigma')$. Therefore, we have proved that any convergent subsequence of $\{R(\tilde{u}^l, \tilde{\sigma}^l)\}_{l \in \mathbb{N}}$ converges to $R(\tilde{u}, \tilde{\sigma})$ in $U_h \times \Sigma_h$, and from uniqueness of $R(\tilde{u}, \tilde{\sigma})$, we conclude that the whole sequence $R(\tilde{u}^l, \tilde{\sigma}^l) \rightarrow R(\tilde{u}, \tilde{\sigma})$ in $U_h \times \Sigma_h$. Thus, R is continuous.

Therefore, the hypotheses of the Leray-Schauder fixed point theorem (in finite dimension) are satisfied and we conclude that the map R has a fixed point (u, σ) , that is, $R(u, \sigma) = (u, \sigma)$, which is a solution of nonlinear scheme **US**. \square

Lemma 4.7 (Conditional uniqueness). *If $k f(h, \varepsilon) < 1$ (where $f(h, \varepsilon) \uparrow +\infty$ when $h \downarrow 0$ or $\varepsilon \downarrow 0$), then the solution $(u_\varepsilon^n, \sigma_\varepsilon^n)$ of the scheme **US** is unique.*

Proof. Suppose that there exist $(u_\varepsilon^{n,1}, \sigma_\varepsilon^{n,1}), (u_\varepsilon^{n,2}, \sigma_\varepsilon^{n,2}) \in U_h \times \Sigma_h$, two possible solutions of the scheme **US**. Then, defining $u = u_\varepsilon^{n,1} - u_\varepsilon^{n,2}$ and $\sigma = \sigma_\varepsilon^{n,1} - \sigma_\varepsilon^{n,2}$, we have that $(u, \sigma) \in U_h \times \Sigma_h$ satisfies

$$(55) \quad \begin{aligned} & \frac{1}{k}(u, \bar{u})^h + (\lambda_\varepsilon(u_\varepsilon^{n,1}) \nabla \Pi^h (F'_\varepsilon(u_\varepsilon^{n,1}) - F'_\varepsilon(u_\varepsilon^{n,2})), \nabla \bar{u}) \\ & + ((\lambda_\varepsilon(u_\varepsilon^{n,1}) - \lambda_\varepsilon(u_\varepsilon^{n,2})) \nabla \Pi^h F'_\varepsilon(u_\varepsilon^{n,2}), \nabla \bar{u}) \\ & + (\lambda_\varepsilon(u_\varepsilon^{n,1}) \sigma, \nabla \bar{u}) + ((\lambda_\varepsilon(u_\varepsilon^{n,1}) - \lambda_\varepsilon(u_\varepsilon^{n,2})) \sigma_\varepsilon^{n,2}, \nabla \bar{u}) = 0 \quad \forall \bar{u} \in U_h, \end{aligned}$$

$$(56) \quad \begin{aligned} & \frac{1}{k}(\sigma, \bar{\sigma}) + (B_h \sigma, \bar{\sigma}) = (\lambda_\varepsilon(u_\varepsilon^{n,1}) \nabla \Pi^h (F'_\varepsilon(u_\varepsilon^{n,1}) - F'_\varepsilon(u_\varepsilon^{n,2})), \bar{\sigma}) \\ & + ((\lambda_\varepsilon(u_\varepsilon^{n,1}) - \lambda_\varepsilon(u_\varepsilon^{n,2})) \nabla \Pi^h F'_\varepsilon(u_\varepsilon^{n,2}), \bar{\sigma}) \quad \forall \bar{\sigma} \in \Sigma_h. \end{aligned}$$

Taking $\bar{u} = u$, $\bar{\sigma} = \sigma$ in (55)–(56), adding the resulting expressions, and using the fact that $\int_\Omega u = 0$ as well as Remark 3.4, estimates in Corollary 4.4, and some inverse inequalities, we obtain

$$\begin{aligned} & \frac{1}{k} \|(u, \sigma)\|_0^2 + \|\sigma\|_1^2 \leq \|\lambda_\varepsilon(u_\varepsilon^{n,1})\|_{L^\infty} \|\nabla \Pi^h (F'_\varepsilon(u_\varepsilon^{n,1}) - F'_\varepsilon(u_\varepsilon^{n,2}))\|_0 \|\nabla u\|_0 \\ & + \|\lambda_\varepsilon(u_\varepsilon^{n,1}) - \lambda_\varepsilon(u_\varepsilon^{n,2})\|_{L^\infty} \|\nabla \Pi^h F'_\varepsilon(u_\varepsilon^{n,2})\|_0 \|\nabla u\|_0 \\ & + \|\lambda_\varepsilon(u_\varepsilon^{n,1})\|_{L^\infty} \|\sigma\|_0 \|\nabla u\|_0 + \|\lambda_\varepsilon(u_\varepsilon^{n,1}) - \lambda_\varepsilon(u_\varepsilon^{n,2})\|_{L^\infty} \|\sigma_\varepsilon^{n,2}\|_0 \|\nabla u\|_0 \\ & + \|\lambda_\varepsilon(u_\varepsilon^{n,1})\|_{L^\infty} \|\nabla \Pi^h (F'_\varepsilon(u_\varepsilon^{n,1}) - F'_\varepsilon(u_\varepsilon^{n,2}))\|_0 \|\sigma\|_0 \\ & + \|\lambda_\varepsilon(u_\varepsilon^{n,1}) - \lambda_\varepsilon(u_\varepsilon^{n,2})\|_{L^3} \|\nabla \Pi^h F'_\varepsilon(u_\varepsilon^{n,2})\|_0 \|\sigma\|_{L^6} \\ & \leq \varepsilon^{-2} C(h) \|u\|_0^2 + \varepsilon^{-1} C(h) \|u\|_0^2 + \frac{1}{6} \|\sigma\|_0 + \varepsilon^{-2} C(h) \|u\|_0^2 + C_0 C(h) \|u\|_0^2 \\ & + \frac{1}{6} \|\sigma\|_0 + \varepsilon^{-4} C(h) \|u\|_0^2 + \frac{1}{6} \|\sigma\|_1 + \varepsilon^{-2} C(h) \|u\|_0^2, \end{aligned}$$

and therefore,

$$\|(u, \sigma)\|_0^2 + \frac{k}{2} \|\sigma\|_1^2 \leq k f(h, \varepsilon) \|u\|_0^2,$$

where $f(h, \varepsilon) \uparrow +\infty$ when $h \downarrow 0$ or $\varepsilon \downarrow 0$. Thus, if $k f(h, \varepsilon) < 1$, we conclude that $(u, \sigma) = (0, 0)$. \square

5. SCHEME **UZSW**

In this section, we design an energy-stable linear fully discrete scheme associated to model (1). With this aim, we consider the (u, σ) reformulation (41) used in Section 4, and we will use two additional techniques. In the first one, we introduce the test function for the u -equation as an auxiliary variable, that is, we consider the auxiliary variable $z_\varepsilon = F'_\varepsilon(u_\varepsilon)$; and in the second one we adapt the so-called “Energy Quadratzation (EQ) strategy” [2, 18, 20, 21], rewriting the energy of the system as a quadratic form via the auxiliary variable $w_\varepsilon = \sqrt{F_\varepsilon(u_\varepsilon) + C}$ with $C > 0$.

Then, a regularized version of problem (1) in the variables $(u_\varepsilon, z_\varepsilon, \sigma_\varepsilon, w_\varepsilon)$ is the following:

$$(57) \quad \begin{cases} \partial_t u_\varepsilon - \nabla \cdot (\lambda_\varepsilon(u_\varepsilon) \nabla z_\varepsilon) - \nabla \cdot (\lambda_\varepsilon(u_\varepsilon) \sigma_\varepsilon) = 0 & \text{in } \Omega, \ t > 0, \\ \partial_t \sigma_\varepsilon + \text{rot}(\text{rot } \sigma_\varepsilon) - \nabla(\nabla \cdot \sigma_\varepsilon) + \sigma_\varepsilon = \lambda_\varepsilon(u_\varepsilon) \nabla z_\varepsilon & \text{in } \Omega, \ t > 0, \\ \partial_t w_\varepsilon = \frac{1}{2\sqrt{F_\varepsilon(u_\varepsilon)} + C} F'_\varepsilon(u_\varepsilon) \partial_t u_\varepsilon & \text{in } \Omega, \ t > 0, \\ z_\varepsilon = \frac{1}{\sqrt{F_\varepsilon(u_\varepsilon)} + C} F'_\varepsilon(u_\varepsilon) w_\varepsilon & \text{in } \Omega, \ t > 0, \\ \frac{\partial z_\varepsilon}{\partial \mathbf{n}} = 0 & \text{on } \partial\Omega, \ t > 0, \\ \sigma_\varepsilon \cdot \mathbf{n} = 0, \ [\text{rot } \sigma_\varepsilon \times \mathbf{n}]_{\text{tang}} = 0 & \text{on } \partial\Omega, \ t > 0, \\ u_\varepsilon(\mathbf{x}, 0) = u_0(\mathbf{x}) \geq 0, \ \sigma_\varepsilon(\mathbf{x}, 0) = \nabla v_0(\mathbf{x}), \ w_\varepsilon(\mathbf{x}, 0) = \sqrt{F_\varepsilon(u_0(\mathbf{x})) + C} & \text{in } \Omega, \end{cases}$$

for all constant $C > 0$.

Remark 5.1. Notice that problems (41) and (57) are equivalent for all $C > 0$. In fact, if $(u_\varepsilon, \sigma_\varepsilon)$ is a solution of the scheme **US**, then defining $z_\varepsilon = F'_\varepsilon(u_\varepsilon)$ and $w_\varepsilon = \sqrt{F_\varepsilon(u_\varepsilon) + C}$, we deduce that $(u_\varepsilon, z_\varepsilon, \sigma_\varepsilon, w_\varepsilon)$ is a solution of the scheme **UZSW**. Reciprocally, if $(u_\varepsilon, z_\varepsilon, \sigma_\varepsilon, w_\varepsilon)$ is a solution of the scheme **UZSW**, then from the equivalence

$$\begin{cases} \partial_t w_\varepsilon = \frac{1}{2\sqrt{F_\varepsilon(u_\varepsilon)} + C} F'_\varepsilon(u_\varepsilon) \partial_t u_\varepsilon, \\ w_\varepsilon|_{t=0} = \sqrt{F_\varepsilon(u_0) + C}, \end{cases} \iff w_\varepsilon = \sqrt{F_\varepsilon(u_\varepsilon) + C}$$

and (57)₄, we deduce that $z_\varepsilon = F'_\varepsilon(u_\varepsilon)$, and therefore, $(u_\varepsilon, \sigma_\varepsilon)$ is a solution of (41).

As in the previous section, once (57) is solved, we can recover v_ε from u_ε solving (42). Observe that multiplying (57)₁ by z_ε , (57)₂ by σ_ε , (57)₃ by $2w_\varepsilon$, (57)₄ by $\partial_t u_\varepsilon$, integrating over Ω , and using the boundary conditions of (57), we obtain the energy law

$$\frac{d}{dt} \int_{\Omega} \left(|w_\varepsilon|^2 + \frac{1}{2} |\sigma_\varepsilon|^2 \right) d\mathbf{x} + \int_{\Omega} \lambda_\varepsilon(u_\varepsilon) |\nabla z_\varepsilon|^2 d\mathbf{x} + \|\sigma_\varepsilon\|_1^2 = 0.$$

In particular, the modified energy $\mathcal{E}(w, \sigma) = \int_{\Omega} (|w|^2 + \frac{1}{2} |\sigma|^2) d\mathbf{x}$ is decreasing in time. Then, we consider a fully discrete approximation of the regularized problem (57) using an FE discretization in space and a first-order semi-implicit discretization in time (again considered for simplicity on a uniform partition of $[0, T]$ with time step $k = T/N : (t_n = nk)_{n=0}^{n=N}$). Concerning the space discretization, we consider the triangulation as in the scheme **US** (hence, the constraint **(H)** related with the right-angle simplices is not imposed), and we choose the following continuous FE spaces for $u_\varepsilon, z_\varepsilon, \sigma_\varepsilon, w_\varepsilon$, and v_ε :

$$(U_h, Z_h, \Sigma_h, W_h, V_h) \subset H^1(\Omega)^5, \\ \text{generated by } \mathbb{P}_k, \mathbb{P}_l, \mathbb{P}_m, \mathbb{P}_r, \mathbb{P}_s \text{ with } k, l, m, r, s \geq 1 \text{ and } k \leq l.$$

Remark 5.2. The constraint $k \leq l$ implies $U_h \subseteq Z_h$ which will be used to prove the well-posedness of the scheme **UZSW** (see Theorem 5.6 below).

Then, we consider the following first-order in time, linear, and coupled scheme:

• **Scheme UZSW:**

Initialization: Let $(u_h^0, \sigma_h^0, w_{h,\varepsilon}^0) = (Q^h u_0, \tilde{Q}^h(\nabla v_0), \hat{Q}^h(\sqrt{F_\varepsilon(u_0)} + C)) \in U_h \times \Sigma_h \times W_h$.

Time step n : Given $(u_\varepsilon^{n-1}, \sigma_\varepsilon^{n-1}, w_\varepsilon^{n-1}) \in U_h \times \Sigma_h \times W_h$, compute $(u_\varepsilon^n, z_\varepsilon^n, \sigma_\varepsilon^n, w_\varepsilon^n) \in U_h \times Z_h \times \Sigma_h \times W_h$ solving

$$(58) \quad \begin{cases} (\delta_t u_\varepsilon^n, \bar{z}) + (\lambda_\varepsilon(u_\varepsilon^{n-1}) \nabla z_\varepsilon^n, \nabla \bar{z}) = -(\lambda_\varepsilon(u_\varepsilon^{n-1}) \sigma_\varepsilon^n, \nabla \bar{z}) \quad \forall \bar{z} \in Z_h, \\ (\delta_t \sigma_\varepsilon^n, \bar{\sigma}) + (B_h \sigma_\varepsilon^n, \bar{\sigma}) = (\lambda_\varepsilon(u_\varepsilon^{n-1}) \nabla z_\varepsilon^n, \bar{\sigma}) \quad \forall \bar{\sigma} \in \Sigma_h, \\ (\delta_t w_\varepsilon^n, \bar{w}) = \left(\frac{1}{2\sqrt{F_\varepsilon(u_\varepsilon^{n-1})} + C} F'_\varepsilon(u_\varepsilon^{n-1}) \delta_t u_\varepsilon^n, \bar{w} \right) \quad \forall \bar{w} \in W_h, \\ (z_\varepsilon^n, \bar{u}) = \left(\frac{1}{\sqrt{F_\varepsilon(u_\varepsilon^{n-1})} + C} F'_\varepsilon(u_\varepsilon^{n-1}) w_\varepsilon^n, \bar{u} \right) \quad \forall \bar{u} \in U_h. \end{cases}$$

Recall that $(B_h \sigma_\varepsilon^n, \bar{\sigma}) := (\text{rot } \sigma_\varepsilon^n, \text{rot } \bar{\sigma}) + (\nabla \cdot \sigma_\varepsilon^n, \nabla \cdot \bar{\sigma}) + (\sigma_\varepsilon^n, \bar{\sigma})$ for all $\bar{\sigma} \in \Sigma_h$, Q^h is the L^2 -projection on U_h defined in (10), and \tilde{Q}^h and \hat{Q}^h are the standard L^2 -projections on Σ_h and W_h , respectively. As in the scheme **US**, once the scheme **UZSW** is solved, given $v_\varepsilon^{n-1} \in V_h$, we can recover $v_\varepsilon^n = v_\varepsilon^n(u_\varepsilon^n) \in V_h$ solving (45).

5.1. Mass conservation and energy-stability. Observe that scheme **UZSW** is also conservative in u (satisfying (17)) and also has the behavior for $\int_\Omega v_n$ given in (18).

Definition 5.3. A numerical scheme with solution $(u_\varepsilon^n, z_\varepsilon^n, \sigma_\varepsilon^n, w_\varepsilon^n)$ is called energy-stable with respect to the energy

$$(59) \quad \mathcal{E}(w, \sigma) = \|w\|_0^2 + \frac{1}{2} \|\sigma\|_0^2$$

if this energy is time decreasing, that is, $\mathcal{E}(w_\varepsilon^n, \sigma_\varepsilon^n) \leq \mathcal{E}(w_\varepsilon^{n-1}, \sigma_\varepsilon^{n-1})$ for all $n \geq 1$.

Theorem 5.4 (Unconditional stability). *The scheme **UZSW** is unconditional energy stable with respect to $\mathcal{E}(w, \sigma)$. In fact, if $(u_\varepsilon^n, z_\varepsilon^n, \sigma_\varepsilon^n, w_\varepsilon^n)$ is a solution of **UZSW**, then the following discrete energy law holds:*

$$(60) \quad \delta_t \mathcal{E}(w_\varepsilon^n, \sigma_\varepsilon^n) + k \|\delta_t w_\varepsilon^n\|_0^2 + \frac{k}{2} \|\delta_t \sigma_\varepsilon^n\|_0^2 + \int_\Omega \lambda_\varepsilon(u_\varepsilon^{n-1}) |\nabla z_\varepsilon^n|^2 + \|\sigma_\varepsilon^n\|_1^2 = 0.$$

Proof. The proof follows from testing (58) by $(\bar{z}, \bar{\sigma}, \bar{w}, \bar{u}) = (z_\varepsilon^n, \sigma_\varepsilon^n, 2w_\varepsilon^n, \delta_t u_\varepsilon^n)$. \square

From the (local in time) discrete energy law (60), we deduce the following global in time estimates for the $(u_\varepsilon^n, z_\varepsilon^n, \sigma_\varepsilon^n, w_\varepsilon^n)$ solution of the scheme **UZSW**.

Corollary 5.5 (Uniform weak estimates). *Assume that $(u_0, v_0) \in L^2(\Omega) \times H^1(\Omega)$. Let $(u_\varepsilon^n, z_\varepsilon^n, \sigma_\varepsilon^n, w_\varepsilon^n)$ be a solution of scheme **UZSW**. Then, the following estimate holds:*

$$(61) \quad \|w_\varepsilon^n\|_0^2 + \|\sigma_\varepsilon^n\|_0^2 + k \sum_{m=1}^n \left(\int_\Omega \lambda_\varepsilon(u_\varepsilon^{m-1}) |\nabla z_\varepsilon^m|^2 + \|\sigma_\varepsilon^m\|_1^2 \right) \leq C_0 \quad \forall n \geq 1,$$

with the constant $C_0 > 0$ depending on the data (Ω, u_0, v_0) , but independent of k, h, n , and ε .

Proof. Proceeding as in (28) and taking into account that $u_0 \geq 0$ and $(u_h^0, \sigma_h^0, w_{h,\varepsilon}^0) = (Q^h u_0, \tilde{Q}^h(\nabla v_0), \hat{Q}^h(\sqrt{F_\varepsilon(u_0(\mathbf{x})) + C}))$, we have that

$$\begin{aligned}
 \|w_{h,\varepsilon}^0\|_0^2 + \frac{1}{2}\|\sigma_h^0\|_0^2 &= \|\hat{Q}^h(\sqrt{F_\varepsilon(u_0) + C})\|_0^2 + \frac{1}{2}\|\tilde{Q}^h(\nabla v_0)\|_0^2 \\
 &\leq \int_{\Omega} (F_\varepsilon(u_0) + C) + \frac{1}{2}\|\nabla v_0\|_0^2 \\
 &\leq C \int_{\Omega} ((u_0)^2 + 1) + \frac{1}{2}\|\nabla v_0\|_0^2 \\
 &\leq C(\|u_0\|_0^2 + \|v_0\|_1^2 + 1) \leq C_0,
 \end{aligned}
 \tag{62}$$

with the constant $C_0 > 0$ depending on the data (Ω, u_0, v_0) , but independent of k, h, n , and ε . Therefore, multiplying the discrete energy law (60) by k , adding from $m = 1$ to $m = n$, and using (62), we arrive at (61). \square

5.2. Well-posedness.

Theorem 5.6 (Unconditional unique solvability). *There exists a unique $(u_\varepsilon^n, z_\varepsilon^n, \sigma_\varepsilon^n, w_\varepsilon^n)$ solution of scheme **UZSW**.*

Proof. By linearity of the scheme **UZSW**, it suffices to prove uniqueness. Suppose that there exist $(u_{\varepsilon,1}^n, z_{\varepsilon,1}^n, \sigma_{\varepsilon,1}^n, w_{\varepsilon,1}^n), (u_{\varepsilon,2}^n, z_{\varepsilon,2}^n, \sigma_{\varepsilon,2}^n, w_{\varepsilon,2}^n) \in U_h \times Z_h \times \Sigma_h \times W_h$, two possible solutions of **UZSW**. Then defining $u = u_{\varepsilon,1}^n - u_{\varepsilon,2}^n$, $z = z_{\varepsilon,1}^n - z_{\varepsilon,2}^n$, $\sigma = \sigma_{\varepsilon,1}^n - \sigma_{\varepsilon,2}^n$, and $w = w_{\varepsilon,1}^n - w_{\varepsilon,2}^n$, we have that $(u, z, \sigma, w) \in U_h \times Z_h \times \Sigma_h \times W_h$ satisfies

$$(63) \quad \begin{cases} (u, \bar{z}) + k(\lambda_\varepsilon(u_\varepsilon^{n-1})\nabla z, \nabla \bar{z}) = -k(\lambda_\varepsilon(u_\varepsilon^{n-1})\sigma, \nabla \bar{z}) \quad \forall \bar{z} \in Z_h, \\ (\sigma, \bar{\sigma}) + k(B_h \sigma, \bar{\sigma}) = k(\lambda_\varepsilon(u_\varepsilon^{n-1})\nabla z, \bar{\sigma}) \quad \forall \bar{\sigma} \in \Sigma_h, \\ (w, \bar{w}) = \frac{1}{2} \left(\frac{1}{\sqrt{F_\varepsilon(u_\varepsilon^{n-1}) + C}} F'_\varepsilon(u_\varepsilon^{n-1}) u, \bar{w} \right) \quad \forall \bar{w} \in W_h, \\ (z, \bar{u}) = \left(\frac{1}{\sqrt{F_\varepsilon(u_\varepsilon^{n-1}) + C}} F'_\varepsilon(u_\varepsilon^{n-1}) w, \bar{u} \right) \quad \forall \bar{u} \in U_h. \end{cases}$$

Taking $(\bar{z}, \bar{\sigma}, \bar{w}, \bar{u}) = (z, \sigma, 2w, -u)$ in (63) and adding, we obtain

$$2\|w\|_0^2 + \|\sigma\|_0^2 + k \int_{\Omega} \lambda_\varepsilon(u_\varepsilon^{n-1}) |\nabla z|^2 + k \|\sigma\|_1^2 = 0.$$

Taking into account that $\lambda_\varepsilon(u_\varepsilon^{n-1}) \geq \varepsilon$, we deduce that $(\nabla z, \sigma, w) = (\mathbf{0}, \mathbf{0}, 0)$, hence $z = C := cte$. Moreover, using the fact that $w = 0$ and $z = C$, from (63)₄ we conclude that $z = 0$. Finally, taking $\bar{z} = u$ in (63)₁ (which is possible thanks to the choice $U_h \subseteq Z_h$), since $(\nabla z, \sigma) = (\mathbf{0}, \mathbf{0})$ we conclude $u = 0$. \square

6. NUMERICAL SIMULATIONS

The aim of this section is to compare the results of several numerical simulations using the schemes derived throughout the paper. We choose the spaces for (u, z, σ, w, v) generated by \mathbb{P}_1 -continuous FE. Moreover, we have chosen the 2D domain $[0, 2]^2$ with a structured mesh (then **(H)** holds and the scheme **UV** can be defined), and all the simulations are carried out using **FreeFem++** software. In the scheme **UZSW** we fix $C = 1$ (and thus, $F_\varepsilon(s) + C \geq 1$ for all $s \in \mathbb{R}$). Moreover, in the comparison we will also consider the classical Backward Euler scheme

for model (1), which is given for the following first-order in time, nonlinear, and coupled scheme:

• **Scheme BEUV:**

Initialization: Let $(u^0, v^0) = (Q^h u_0, R^h v_0) \in U_h \times V_h$.

Time step n : Given $(u^{n-1}, v^{n-1}) \in U_h \times V_h$, compute $(u^n, v^n) \in U_h \times V_h$ solving

$$\begin{cases} (\delta_t u^n, \bar{u}) + (\nabla u^n, \nabla \bar{u}) = -(u^n \nabla v^n, \nabla \bar{u}) \quad \forall \bar{u} \in U_h, \\ (\delta_t v^n, \bar{v}) + (A_h v^n, \bar{v}) = (u^n, \bar{v}) \quad \forall \bar{v} \in V_h. \end{cases}$$

Remark 6.1. The scheme **BEUV** has not been analyzed in the previous sections because it is not clear how to prove its energy-stability. In fact, observe that the scheme **UV** (which is the “closest” approximation to the scheme **BEUV** considered in this paper) differs from the scheme **BEUV** in the use of the truncated function λ_ε and the regularized function F_ε (see (4)–(5) and Figure 1) and in the approximation of cross-diffusion term $(u \nabla v, \nabla \bar{u})$, which are crucial for the proof of the energy-stability of the scheme **UV**.

The linear iterative methods used to approach the solutions of the nonlinear schemes **UV**, **US**, and **BEUV** are the following Picard methods, in which we denote $(u_\varepsilon^n, v_\varepsilon^n, \sigma_\varepsilon^n) := (u^n, v^n, \sigma^n)$.

- (i) Picard method to approach a solution (u^n, v^n) of the scheme **UV**:

Initialization ($l = 0$): Set $(u^0, v^0) = (u^{n-1}, v^{n-1}) \in U_h \times V_h$.

Algorithm: Given $(u^l, v^l) \in U_h \times V_h$, compute $(u^{l+1}, v^{l+1}) \in U_h \times V_h$ such that

$$\begin{cases} \frac{1}{k}(u^{l+1}, \bar{u})^h + (\nabla u^{l+1}, \nabla \bar{u}) = \frac{1}{k}(u^{n-1}, \bar{u})^h - (\Lambda_\varepsilon(u^l) \nabla v^{l+1}, \nabla \bar{u}) \quad \forall \bar{u} \in U_h, \\ \frac{1}{k}(v^{l+1}, \bar{v}) + (A_h v^{l+1}, \bar{v}) = \frac{1}{k}(v^{n-1}, \bar{v}) + (u^l, \bar{v}) \quad \forall \bar{v} \in V_h, \end{cases}$$

until the stopping criteria $\max \left\{ \frac{\|u^{l+1} - u^l\|_0}{\|u^l\|_0}, \frac{\|v^{l+1} - v^l\|_0}{\|v^l\|_0} \right\} \leq tol$.

- (ii) Picard method to approach a solution (u^n, σ^n) of the scheme **US**:

Initialization ($l = 0$): Set $(u^0, \sigma^0) = (u^{n-1}, \sigma^{n-1}) \in U_h \times \Sigma_h$.

Algorithm: Given $(u^l, \sigma^l) \in U_h \times \Sigma_h$, compute $(u^{l+1}, \sigma^{l+1}) \in U_h \times \Sigma_h$ such that

$$\begin{cases} \frac{1}{k}(u^{l+1}, \bar{u})^h + (\nabla u^{l+1}, \nabla \bar{u}) - (\nabla u^l, \nabla \bar{u}) \\ \quad = \frac{1}{k}(u^{n-1}, \bar{u})^h - (\lambda_\varepsilon(u^l) \nabla \Pi^h(F'_\varepsilon(u^l)), \nabla \bar{u}) - (\lambda_\varepsilon(u^l) \sigma^{l+1}, \nabla \bar{u}) \quad \forall \bar{u} \in U_h, \\ \frac{1}{k}(\sigma^{l+1}, \bar{\sigma}) + \langle B \sigma^{l+1}, \bar{\sigma} \rangle = \frac{1}{k}(\sigma^{n-1}, \bar{\sigma}) + (\lambda_\varepsilon(u^l) \nabla \Pi^h(F'_\varepsilon(u^l)), \bar{\sigma}) \quad \forall \bar{\sigma} \in \Sigma_h, \end{cases}$$

until the stopping criteria $\max \left\{ \frac{\|u^{l+1} - u^l\|_0}{\|u^l\|_0}, \frac{\|\sigma^{l+1} - \sigma^l\|_0}{\|\sigma^l\|_0} \right\} \leq tol$. Note that

a residual term $(\nabla(u^{l+1} - u^l), \nabla \bar{u})$ is considered. This term is required in order to improve the convergence of this iterative method. Indeed, since the self-diffusion term of the u -equation is rewritten in a nonlinear form, we have checked that this fact makes the convergence of the corresponding iterative method worse.

- (iii) Picard method to approach a solution (u^n, v^n) of the scheme **BEUV**:

Initialization ($l = 0$): Set $(u^0, v^0) = (u^{n-1}, v^{n-1}) \in U_h \times V_h$.

Algorithm: Given $(u^l, v^l) \in U_h \times V_h$, compute $(u^{l+1}, v^{l+1}) \in U_h \times V_h$ such that

$$\begin{cases} \frac{1}{k}(u^{l+1}, \bar{u}) + (\nabla u^{l+1}, \nabla \bar{u}) = \frac{1}{k}(u^{n-1}, \bar{u}) - (u^l \nabla v^{l+1}, \nabla \bar{u}) \quad \forall \bar{u} \in U_h, \\ \frac{1}{k}(v^{l+1}, \bar{v}) + (A_h v^{l+1}, \bar{v}) = \frac{1}{k}(v^{n-1}, \bar{v}) + (u^l, \bar{v}) \quad \forall \bar{v} \in V_h, \end{cases}$$

until the stopping criteria $\max \left\{ \frac{\|u^{l+1} - u^l\|_0}{\|u^l\|_0}, \frac{\|v^{l+1} - v^l\|_0}{\|v^l\|_0} \right\} \leq tol$.

In all numerical simulations, we fix $tol = 10^{-4}$. We take 10^{-4} as the tolerance parameter because in the very particular case of scheme **US** and very small ε , the error is stabilized at this tolerance. But, for the rest of the cases, the errors decrease more and the tolerance could be taken for instance at 10^{-6} .

Remark 6.2. In all cases, first we compute v^{l+1} (resp., σ^{l+1}) solving the v -equation (resp., σ -system) and then, inserting v^{l+1} (resp., σ^{l+1}) in the u -equation, we compute u^{l+1} .

6.1. Positivity of u^n . In this subsection, we compare the positivity of the variable $u^n \in U_h$ in the four schemes (**BEUV**, **UV**, **US**, and **UZSW**). The aim is to see numerically how the mesh size and the regularization parameter ε influence the values that the minimum of u^n takes. In all numerical simulations (in this subsection) we will consider a small time step $k = 10^{-5}$ in order to see the differences in the spatial approximations, and the initial conditions (see Figure 2)

$$u_0 = -10xy(2-x)(2-y) \exp(-10(y-1)^2 - 10(x-1)^2) + 10.0001,$$

$$v_0 = 100xy(2-x)(2-y) \exp(-30(y-1)^2 - 30(x-1)^2) + 0.0001.$$

Note that $u_0, v_0 > 0$ in Ω , $\min(u_0) = u_0(1, 1) = 0.0001$, and $\max(v_0) = v_0(1, 1) = 100.0001$.

6.1.1. Influence of the regularization parameter ε . Recall that for the three schemes studied in this paper, schemes **UV**, **UZSW**, and **US**, the positivity of the variable u^n is not clear. Moreover, for the schemes **UV** and **US**, it was proved that $\Pi^h(u_{\varepsilon-}^n) \rightarrow 0$ in $L^2(\Omega)$ as $\varepsilon \rightarrow 0$ (see Remarks 3.12 and 4.5); while for the scheme **UZSW** this fact is not clear. For this reason, in Figure 3 we compare the positivity of the variable u^n in the schemes, taking $\varepsilon = 10^{-3}$, $\varepsilon = 10^{-5}$, and $\varepsilon = 10^{-8}$. For the schemes **UV** and **UZSW** we take the mesh size $h = \frac{1}{40}$, while for the scheme **US** it was necessary to take $h = \frac{1}{80}$, because for coarser meshes we had convergence problems of the corresponding iterative method. In fact, we have checked some meshes with $h > \frac{1}{80}$ and no convergence is observed in all cases when $\varepsilon = 10^{-8}$. Moreover, we have detected that these convergence problems arise from the nonlinear approximation of the self-diffusion term for u , $(\lambda_\varepsilon(u^n) \nabla \Pi^h(F'_\varepsilon(u^n)), \nabla \bar{u})$. Indeed, if we change this term by $(\nabla u^n, \nabla \bar{u})$, then convergence is observed in all cases.

In the case of the schemes **UV** and **US**, we observe that although u^n is negative for some $\mathbf{x} \in \Omega$ in some times $t_n > 0$, when $\varepsilon \rightarrow 0$ these values are closer to 0; while in the case of the scheme **UZSW**, this same behavior is not observed (see Figure 3). Finally, in the case of the scheme **BEUV** we have also observed negative values for the minimum of u^n in some times $t_n > 0$, with values more negative than in the schemes **UV** and **US**.

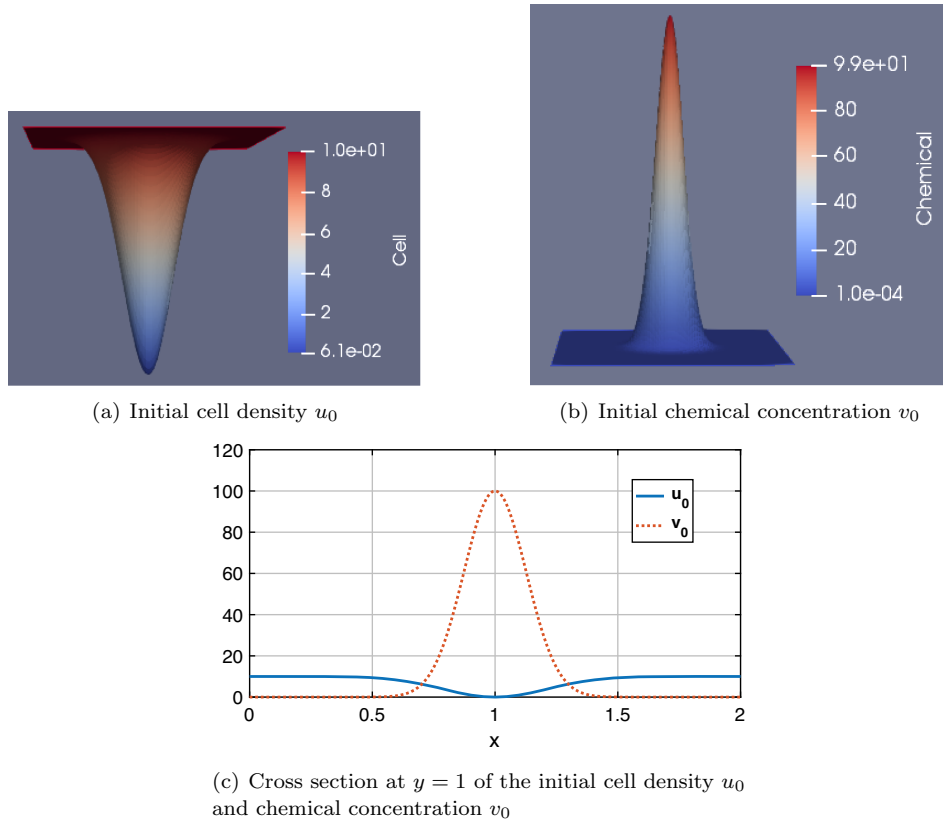


FIGURE 2. Initial conditions.

Remark 6.3. In Figure 3, for the schemes **UV** and **US** there are also negative values of the minimum of u^n for $\varepsilon = 10^{-5}$ and $\varepsilon = 10^{-8}$, but those are of order 10^{-4} and 10^{-7} , respectively, in both schemes.

6.1.2. Influence of the mesh size h . In the case of only time-discrete approximations of the schemes, following the ideas of [11, Theorem 4.3], it is possible to prove the existence of the $u^n \geq 0$ (and the $v^n \geq 0$) solution of the scheme **BEUV**; while for the schemes **UV**, **US**, and **UZSW** this fact it is not clear due to the approximation of the chemotaxis velocity by the truncated function $\lambda_\varepsilon(u)$ instead of u (basically because $\lambda_\varepsilon(u) \neq 0$ if $u < 0$). For this reason, in Figure 4 we compare the positivity of the variable u^n in the schemes, taking $h = \frac{1}{60}$, $h = \frac{1}{80}$, and $h = \frac{1}{100}$. We consider the regularization parameter $\varepsilon = 10^{-3}$.

In the case of the scheme **BEUV**, we observe that although u^n is negative for some $\mathbf{x} \in \Omega$ in some times $t_n > 0$, when $h \rightarrow 0$ these values are closer to 0; while in the case of the schemes **UV**, **US**, and **UZSW**, this same behavior is not observed (see Figure 4).

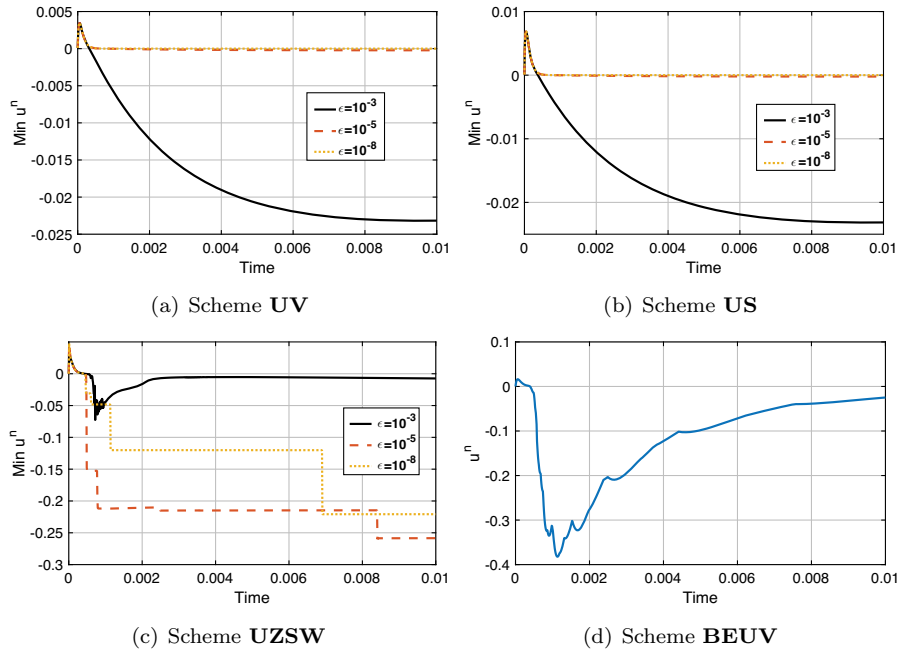


FIGURE 3. Behavior of the minimum of u^n , taking k and h fixed and ϵ variable.

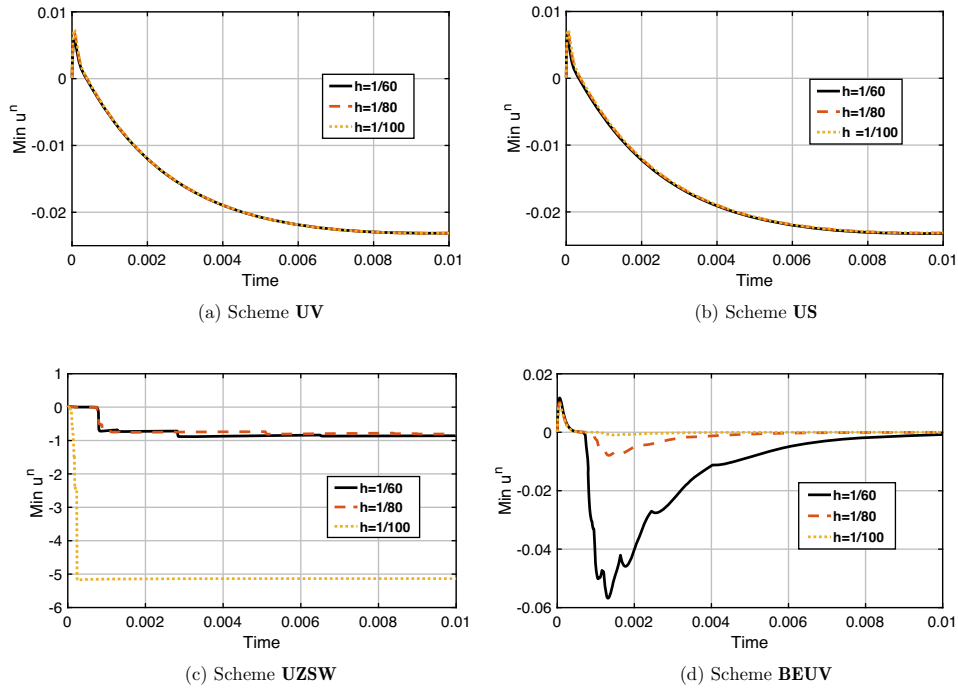


FIGURE 4. Behavior of the minimum of u^n , taking k and ϵ fixed and h variable.

6.2. Energy-stability. In this subsection, we compare numerically the stability of the schemes **UV**, **UZSW**, **US**, and **BEUV** with respect to the “exact” energy

$$(64) \quad \mathcal{E}_e(u, v) = \int_{\Omega} F_0(u(\mathbf{x})) d\mathbf{x} + \frac{1}{2} \|\nabla v\|_0^2,$$

where

$$F_0(u) := F(u_+) = \begin{cases} 1, & \text{if } u \leq 0, \\ u \ln(u) - u + 1, & \text{if } u > 0. \end{cases}$$

We recall it was proved that the schemes **UV**, **UZSW**, and **US** are unconditionally energy-stable with respect to modified energies obtained in terms of the variables of each scheme. Even more, some energy inequalities are satisfied (see Theorems 3.8, 4.3, and 5.4). However, it is not clear how to prove the energy-stability of these schemes with respect to the “exact” energy $\mathcal{E}_e(u, v)$ given in (64), which comes from the continuous problem (1) (see (3)). Therefore, it is interesting to compare numerically the schemes with respect to this energy $\mathcal{E}_e(u, v)$, and to study the behavior of the corresponding discrete residual of the energy law (3):

$$(65) \quad RE_e^n := \delta_t \mathcal{E}_e(u^n, v^n) + 4 \int_{\Omega} |\nabla \sqrt{u_+^n}|^2 d\mathbf{x} + \|(A_h - I)v^n\|_0^2 + \|\nabla v^n\|_0^2.$$

Then, the aim of this subsection is to see numerically how the mesh size, the time step, and the regularization parameter ε influence the stability of the schemes with respect to the energy $\mathcal{E}_e(u, v)$. In all numerical simulations, we consider the following initial conditions (see Figure 5):

$$u_0 = 10w + 11 \quad \text{and} \quad v_0 = -10w + 11,$$

where $w := \cos(2\pi x) \cos(2\pi y)$.

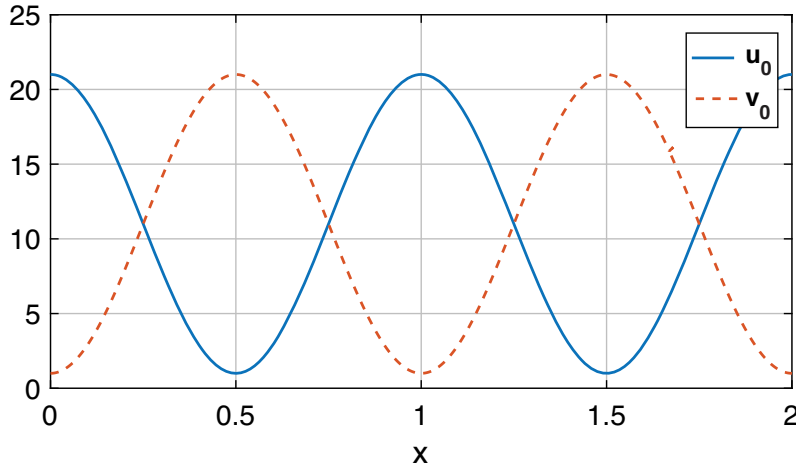


FIGURE 5. Cross section at $y = 0$ of the initial cell density u_0 and chemical concentration v_0

6.2.1. *Influence of the regularization parameter ε .* In Figures 6–7 we compare the energy-stability of the schemes with respect to the energy $\mathcal{E}_\varepsilon(u, v)$, taking $\varepsilon = 10^{-3}$, $\varepsilon = 10^{-5}$, and $\varepsilon = 10^{-8}$. We consider the time step $k = 10^{-3}$ and the mesh size $h = \frac{1}{20}$. Then, we obtain that:

- (i) The schemes **BEUV**, **UV**, and **US** satisfy the energy decreasing in time property (independently of the choice of ε) for the exact energy $\mathcal{E}_\varepsilon(u, v)$ (see Figure 6(a),(c),(d)), that is,

$$(66) \quad \mathcal{E}_\varepsilon(u^n, v^n) \leq \mathcal{E}_\varepsilon(u^{n-1}, v^{n-1}) \quad \forall n.$$

In the case of the scheme **UZSW**, this property (66) is not satisfied for any value of ε . Indeed, increasing energies are obtained for different values of ε (see Figure 6(b)).

- (ii) The schemes **BEUV**, **UV**, and **US** satisfy the discrete energy inequality $RE_e^n \leq 0$ for RE_e^n defined in (65) independently of the choice of ε (see Figure 7(a)). In the case of the scheme **UZSW**, it is observed that this discrete energy inequality is not satisfied for any value of ε . Indeed, the residual RE_e^n obtained for each ε reaches very large positive values (see Figure 7(b)).

Therefore, we can conclude that the energy behavior of the schemes is practically ε -independent.

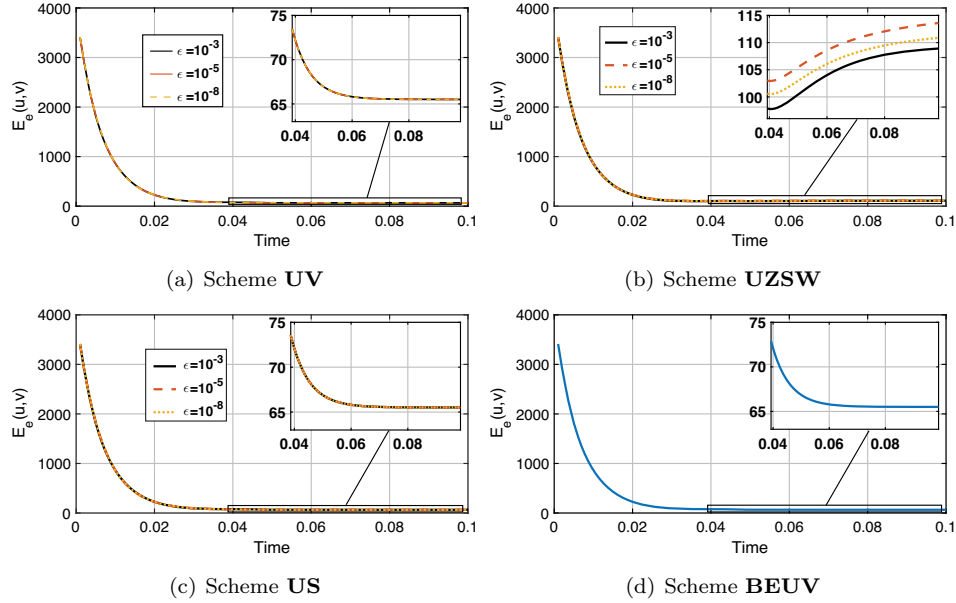


FIGURE 6. Behavior of the exact energy $\mathcal{E}_\varepsilon(u, v)$, taking k and h fixed and ε variable.

6.2.2. *Influence of the time step k .* In Figures 8–9 we compare the energy-stability of the schemes with respect to $\mathcal{E}_\varepsilon(u, v)$, taking $k = 10^{-3}$, $k = 10^{-4}$, and $k = 10^{-5}$. We consider the mesh size $h = \frac{1}{20}$ and the regularization parameter $\varepsilon = 10^{-5}$. Then, we obtain that:

- (i) The schemes **BEUV**, **UV**, and **US** satisfy the energy decreasing in time property (66) independently of the value of k (see Figure 8(a),(c),(d)). In the case of the scheme **UZSW**, this property (66) is not satisfied for $k = 10^{-3}$, but this property holds taking smaller time steps $k = 10^{-4}, 10^{-5}$ (see Figure 8(b)).
- (ii) The schemes **UV** and **US** satisfy the discrete energy inequality $RE_e^n \leq 0$ for RE_e^n defined in (65) independently of the choice of h (see Figure 9(a),(b)). In the case of the schemes **BEUV** the discrete energy inequality is satisfied only for $k = 10^{-3}, 10^{-4}$, while some positive values for RE_e^n are obtained in the case when $k = 10^{-5}$ (see Figure 9(e)). Finally, for the scheme **UZSW**, we also observe some positive values for RE_e^n for the different values taken for k , but it is observed that this residual RE_e^n is closer to 0 when k decreases (see Figure 9(c),(d)).

6.2.3. *Influence of the mesh size h .* In Figures 10–11 we compare the energy-stability of the the schemes with respect to $\mathcal{E}_e(u, v)$, taking $h = \frac{1}{20}$, $h = \frac{1}{40}$, and $h = \frac{1}{60}$. We consider the time step $k = 10^{-5}$ and the regularization parameter $\varepsilon = 10^{-5}$. Then, we obtain that:

- (i) All the schemes (**BEUV**, **UV**, **US**, and **UZSW**) satisfy the energy decreasing in time property (66) independently of the value of h (see Figure 10).
- (ii) The schemes **UV** and **US** satisfy the discrete energy inequality $RE_e^n \leq 0$ for RE_e^n defined in (65) independently of the choice of h (see Figure 11(a),(b)). In the case of the schemes **BEUV** and **UZSW**, we observe some positive values for RE_e^n in the cases $h = \frac{1}{20}, \frac{1}{40}$, but these values are closer to 0 when h decreases (see Figure 11(c),(d)).

7. CONCLUSIONS

In this paper we have developed three new mass-conservative and unconditionally energy-stable fully discrete FE schemes for the chemo-repulsion production model (1), namely **UV**, **US**, and **UZSW**. From the theoretical point of view we have obtained:

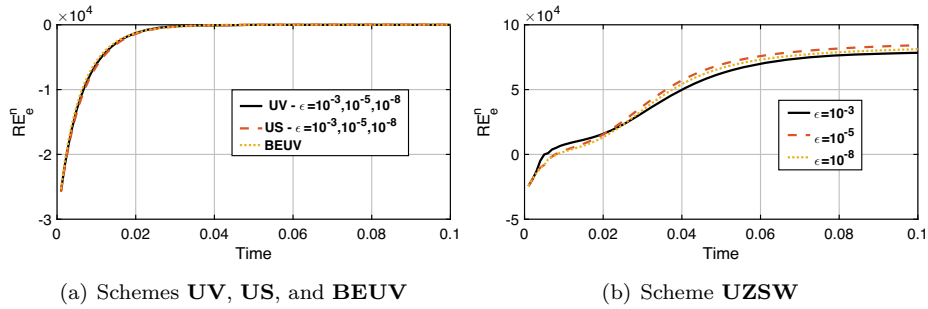


FIGURE 7. Behavior of the discrete residual RE_e^n , taking k and h fixed and ε variable.

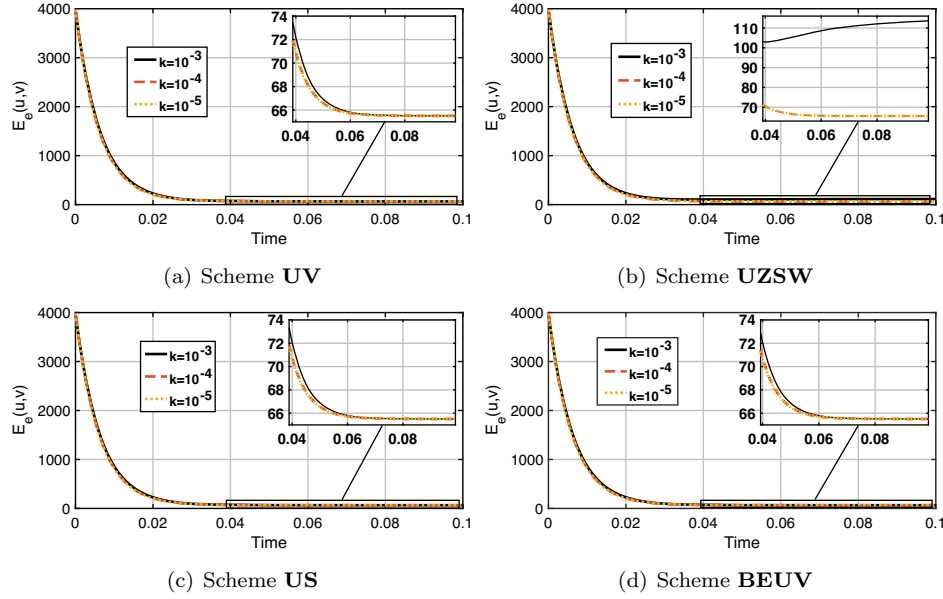


FIGURE 8. Behavior of the exact energy $\mathcal{E}_e(u, v)$, taking h and ε fixed and k variable.

- (i) The well-posedness of the numerical schemes (with conditional uniqueness for the nonlinear schemes **UV** and **US**).
- (ii) The nonlinear scheme **UV** is energy stable with respect to the energy $\mathcal{E}_\varepsilon^h(u, v)$ given in (20), under the constraint **(H)** on the space triangulation related with the right angles and assuming that U_h is approximated by \mathbb{P}_1 -continuous FE.
- (iii) The nonlinear scheme **US** and the linear scheme **UZSW** are unconditional energy stable with respect to the modified energies $\mathcal{E}_\varepsilon^h(u, \sigma)$ (given in (46)) and $\mathcal{E}(w, \sigma)$ (given in (59)), respectively, without the constraint on the triangulation related with the right-angle simplices and assuming that U_h can be approximated by \mathbb{P}_1 -continuous and \mathbb{P}_k -continuous FE, respectively, for any $k \geq 1$.
- (iv) It is not clear how to prove the energy-stability of the nonlinear scheme **BEUV** with respect to the energy $\mathcal{E}_e(u, v)$ (given in (64)) or some modified energy (see Remark 6.1).
- (v) In the schemes **UV** and **US** there is a control for $\Pi^h(u_\varepsilon^n_-)$ in the L^2 -norm which tends to 0 as $\varepsilon \rightarrow 0$. This allows us to conclude the nonnegativity of the solution u_ε^n in the limit when $\varepsilon \rightarrow 0$. This property is not clear for the linear scheme **UZSW**.

On the other hand, from the numerical simulations, we can conclude:

- (i) For the three compared nonlinear schemes (**UV**, **US**, and **BEUV**), only the scheme **US** has convergence problems for the linear iterative method. However, these problems are overcome considering finer meshes.

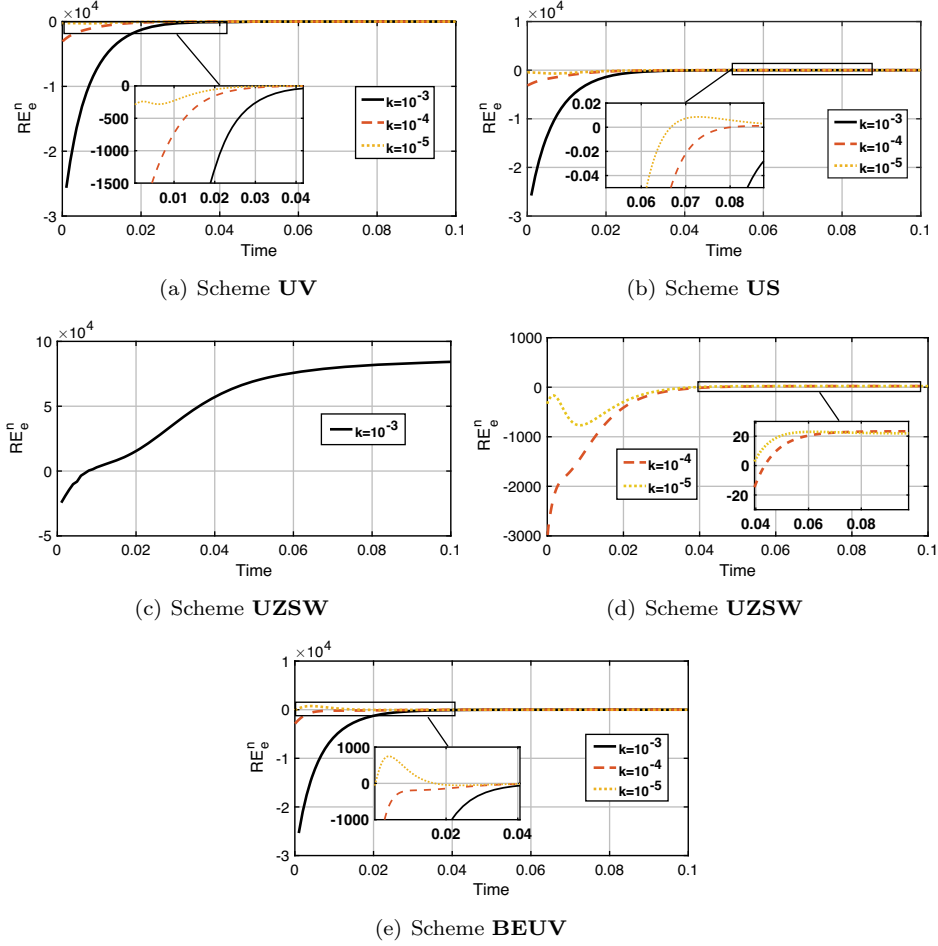


FIGURE 9. Behavior of the discrete residual RE_e^n , taking h and ε fixed and k variable.

- (ii) The schemes **UV** and **US** have decreasing in time energy $\mathcal{E}_e(u, v)$ independently of the choice of ε, k , and h . In fact, the discrete energy inequality $RE_e^n \leq 0$ is satisfied in all cases, for RE_e^n defined in (65).
- (iii) The scheme **UZSW** is not energy stable with respect to the energy $\mathcal{E}_e(u, v)$ (that is, the decreasing in time property (66) is not satisfied) for coarse time and space discretizations (independently of the choice of ε). However, for finer time discretizations, this energy-stability property holds; and the discrete energy inequality $RE_e^n \leq 0$ is satisfied for finer time and space discretizations.
- (iv) The scheme **BEUV** has decreasing in time energy $\mathcal{E}_e(u, v)$ independently of the choice of k and h ; but the discrete energy inequality $RE_e^n \leq 0$ is not satisfied for coarse spatial and fine time discretizations.

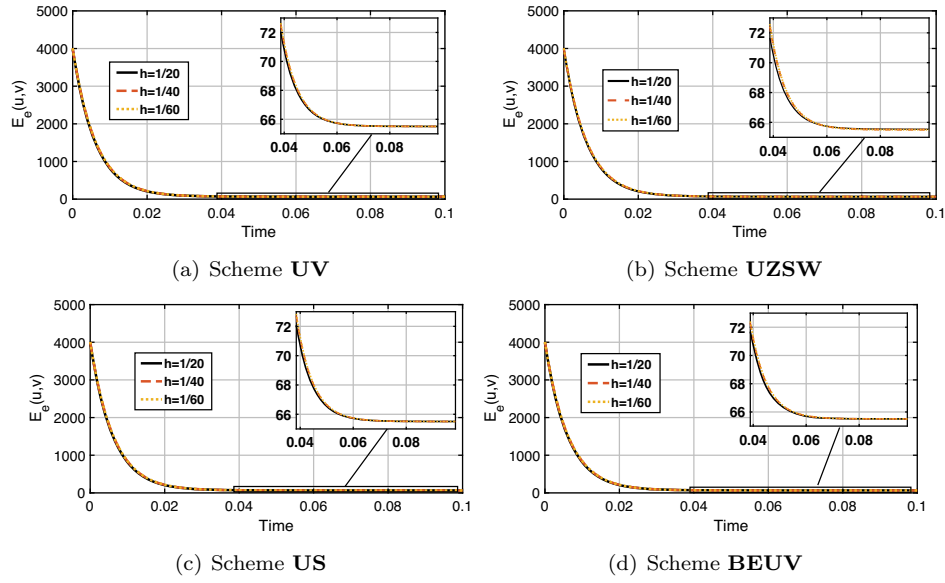


FIGURE 10. Behavior of the exact energy $\mathcal{E}_e(u, v)$, taking k and ε fixed and h variable.

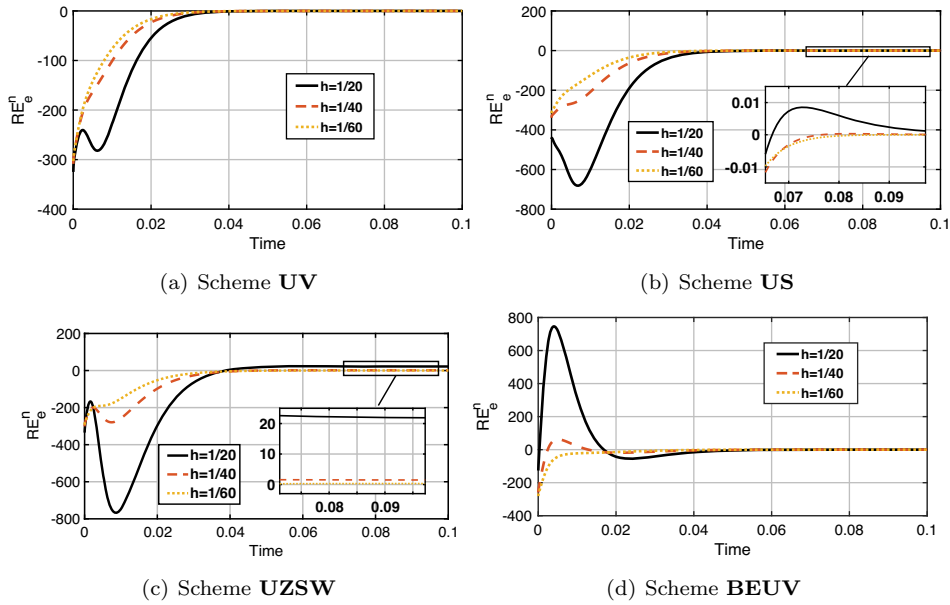


FIGURE 11. Behavior of the discrete residual RE_e^n , taking k and ε fixed and h variable.

- (v) Finally, it was observed numerically that, for the schemes **UV** and **US**, $u_{\varepsilon-}^n \rightarrow 0$ as $\varepsilon \rightarrow 0$; while for the scheme **UZW** this behavior was not observed.

REFERENCES

- [1] C. Amrouche and N. E. H. Seloula, *L^p -theory for vector potentials and Sobolev's inequalities for vector fields: application to the Stokes equations with pressure boundary conditions*, Math. Models Methods Appl. Sci. **23** (2013), no. 1, 37–92, DOI 10.1142/S0218202512500455. MR2997467
- [2] S. Badia, F. Guillén-González, and J. V. Gutiérrez-Santacreu, *Finite element approximation of nematic liquid crystal flows using a saddle-point structure*, J. Comput. Phys. **230** (2011), no. 4, 1686–1706, DOI 10.1016/j.jcp.2010.11.033. MR2753385
- [3] J. W. Barrett and J. F. Blowey, *Finite element approximation of a nonlinear cross-diffusion population model*, Numer. Math. **98** (2004), no. 2, 195–221, DOI 10.1007/s00211-004-0540-y. MR2092740
- [4] R. Becker, X. Feng, and A. Prohl, *Finite element approximations of the Ericksen-Leslie model for nematic liquid crystal flow*, SIAM J. Numer. Anal. **46** (2008), no. 4, 1704–1731, DOI 10.1137/07068254X. MR2399392
- [5] M. Bessemoulin-Chatard and A. Jüngel, *A finite volume scheme for a Keller-Segel model with additional cross-diffusion*, IMA J. Numer. Anal. **34** (2014), no. 1, 96–122, DOI 10.1093/imanum/drs061. MR3168280
- [6] G. Chamoun, M. Saad, and R. Talhouk, *Monotone combined edge finite volume-finite element scheme for anisotropic Keller-Segel model*, Numer. Methods Partial Differential Equations **30** (2014), no. 3, 1030–1065, DOI 10.1002/num.21858. MR3190349
- [7] T. Cieślak, P. Laurençot, and C. Morales-Rodrigo, *Global existence and convergence to steady states in a chemorepulsion system*, Parabolic and Navier-Stokes Equations. Part 1, Banach Center Publ., vol. 81, Polish Acad. Sci. Inst. Math., Warsaw, 2008, pp. 105–117, DOI 10.4064/bc81-0-7. MR2549326
- [8] Y. Epshteyn and A. Izmirliglu, *Fully discrete analysis of a discontinuous finite element method for the Keller-Segel chemotaxis model*, J. Sci. Comput. **40** (2009), no. 1-3, 211–256, DOI 10.1007/s10915-009-9281-5. MR2511733
- [9] F. Filbet, *A finite volume scheme for the Patlak-Keller-Segel chemotaxis model*, Numer. Math. **104** (2006), no. 4, 457–488, DOI 10.1007/s00211-006-0024-3. MR2249674
- [10] G. Galiano and V. Selgas, *On a cross-diffusion segregation problem arising from a model of interacting particles*, Nonlinear Anal. Real World Appl. **18** (2014), 34–49, DOI 10.1016/j.nonrwa.2014.02.001. MR3176295
- [11] F. Guillén-González, M.A. Rodríguez-Bellido and D.A. Rueda-Gómez, *Study of a chemorepulsion model with quadratic production. Part I: Analysis of the continuous problem and time-discrete numerical schemes*, submitted.
- [12] F. Guillén-González, M.A. Rodríguez-Bellido and D.A. Rueda-Gómez, *Study of a chemorepulsion model with quadratic production. Part II: Analysis of an unconditional energy-stable fully discrete scheme*, submitted.
- [13] Y. He and K. Li, *Asymptotic behavior and time discretization analysis for the non-stationary Navier-Stokes problem*, Numer. Math. **98** (2004), no. 4, 647–673, DOI 10.1007/s00211-004-0532-y. MR2099315
- [14] A. Marrocco, *Numerical simulation of chemotactic bacteria aggregation via mixed finite elements*, M2AN Math. Model. Numer. Anal. **37** (2003), no. 4, 617–630, DOI 10.1051/m2an:2003048. MR2018433
- [15] J. Nečas, *Les Méthodes Directes en Théorie des Équations Elliptiques* (French), Masson et Cie, Éditeurs, Paris; Academia, Éditeurs, Prague, 1967. MR0227584
- [16] N. Saito, *Conservative upwind finite-element method for a simplified Keller-Segel system modelling chemotaxis*, IMA J. Numer. Anal. **27** (2007), no. 2, 332–365, DOI 10.1093/imanum/drl018. MR2317007
- [17] N. Saito, *Error analysis of a conservative finite-element approximation for the Keller-Segel system of chemotaxis*, Commun. Pure Appl. Anal. **11** (2012), no. 1, 339–364, DOI 10.3934/cpaa.2012.11.339. MR2833351

- [18] X. Yang, J. Zhao, and Q. Wang, *Numerical approximations for the molecular beam epitaxial growth model based on the invariant energy quadratization method*, J. Comput. Phys. **333** (2017), 104–127, DOI 10.1016/j.jcp.2016.12.025. MR3599396
- [19] J. Zhang, J. Zhu, and R. Zhang, *Characteristic splitting mixed finite element analysis of Keller-Segel chemotaxis models*, Appl. Math. Comput. **278** (2016), 33–44, DOI 10.1016/j.amc.2016.01.021. MR3457640
- [20] J. Zhao, X. Yang, Y. Gong, X. Zhao, X. Yang, J. Li, and Q. Wang, *A general strategy for numerical approximations of non-equilibrium models—part I: thermodynamical systems*, Int. J. Numer. Anal. Model. **15** (2018), no. 6, 884–918. MR3813735
- [21] J. Zhao, X. Yang, Y. Gong, and Q. Wang, *A novel linear second order unconditionally energy stable scheme for a hydrodynamic \mathbf{Q} -tensor model of liquid crystals*, Comput. Methods Appl. Mech. Engrg. **318** (2017), 803–825, DOI 10.1016/j.cma.2017.01.031. MR3627201

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