

Programa de Doctorado en Matemáticas

TESIS DOCTORAL

Análisis teórico y numérico de problemas diferenciales con quimiotaxis repulsiva

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A mis padres. A mi esposa y mi hijo.

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Resumen

Esta tesis se enmarca en el ámbito del análisis teórico y numérico de Ecuaciones en Derivadas Parciales, con aplicaciones a otras ciencias. Concretamente, aborda el estudio de algunos problemas diferenciales de quimiotaxis de tipo repulsiva-productiva. Los primeros tres capítulos están dedicados al estudio de un modelo de quimiotaxis repulsiva con término de producción cuadrático, y los restantes dos capítulos se enfocan en modelos con términos de producción lineal y potencial (con potencia superlineal y subcuadrática).

En el Capítulo 1, se presentan dos esquemas numéricos discretos solamente en tiempo, energéticamente estables, para un modelo de quimiotaxis repulsiva con término de producción cuadrático, y se estudian algunas propiedades adicionales de estos esquemas tales como la conservación de la cantidad total de masa, positividad, resolubilidad, convergencia hacia soluciones débiles y estimaciones de error.

En el Capítulo 2, se estudia un esquema numérico completamente discreto con elementos finitos, energéticamente estable, asociado al modelo estudiado en el Capítulo 1, basado en la introducción de una variable auxiliar. Nuevamente, se estudian algunas propiedades como resolubilidad, conservación de masa, convergencia hacia soluciones débiles, estimaciones de error, y estimaciones débiles y fuertes del esquema. Adicionalmente, como el esquema bajo estudio es no lineal, se proponen dos métodos iterativos para aproximar las soluciones y se prueba la resolubilidad y la convergencia de ambos esquemas hacia el esquema no lineal.

En el Capítulo 3, se estudia el comportamiento asintótico de las soluciones del modelo estudiado en los Capítulos 1 and 2. En la primera parte, se analiza el comportamiento en tiempo infinito de soluciones débiles del problema continuo y se prueba convergencia exponencial hacia un estado constante. En la segunda parte, se estudia este mismo comportamiento para dos esquemas numéricos completamente discretos asociados a este modelo.

Finalmente, los Capítulos 4 y 5 se centran en el estudio de modelos de quimiotaxis repulsiva con términos de producción lineal y potencial, respectivamente. Aquí, usando una técnica de regularización, se proponen algunos esquemas numéricos completamente discretos con elementos finitos, energéticamente estables, asociados a estos modelos, y se prueban algunas propiedades adicionales tales como la resolubilidad, conservación de la cantidad total de masa, y positividad aproximada de las soluciones.

Abstract

This PhD thesis falls within the scopes of Theoretical and Numerical analysis of Partial Differential Equations, with applications to other sciences. Specifically, it addresses the study of some differential problems of repulsive-productive chemotaxis. The first three chapters are devoted to study a chemo-repulsion model with quadratic production, and other two chapters are focused on models with linear and potential (with a superlinear and subquadratic power) production.

In Chapter 1, we present two unconditionally mass-conservative and energy-stable timediscrete numerical schemes for a chemo-repulsion model with quadratic production, and study some additional properties of the schemes such as positivity, solvability, convergence towards weak solutions and error estimates of these schemes.

In Chapter 2, we study an unconditionally mass-conservative and energy-stable fully discrete FE scheme associated to the problem studied in Chapter 1, in which an auxiliary variable is introduced. Again, we study some properties like solvability, convergence towards weak solutions, error estimates, and weak, strong and more regular a priori estimates of the scheme. Additionally, as the scheme is nonlinear, we propose two different linear iterative methods to approach the solutions and we prove solvability and convergence of both methods to the nonlinear scheme.

In Chapter 3, we focus on the study of the asymptotic behaviour of the solutions of the model studied in Chapters 1 and 2. In the first part, we analyze the large-time behavior of the global weak-strong solutions and we prove the exponential convergence to a constant state as time goes to infinity; and in the second part, we study this same behaviour for two fully discrete FE numerical schemes associated to this model.

Finally, in Chapters 4 and 5 we focus on the study of chemo-repulsion models with linear and potential (superlinear and subquadratic) production, respectively. Here, by using a regularization technique, we propose some unconditionally energy-stable and massconservative fully discrete FE schemes associated to these models, and we prove some additional properties such as solvability and approximated positivity of the solutions.

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Introduction

Chemotaxis is a biological phenomenon which describes the oriented movement of living organisms in response to 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*. At the same time, the presence of living organisms can produce or consume chemical substance. This process allows the bacteria to find food, moving towards the highest concentration of food molecules, or move away from poisonous substances. The typical example for chemotaxis is the amoebae *Dictyostelium*, which is a species of soil-living amoeba belonging to the phylum Mycetozoa. When they are moving towards the nutrients, they produce a chemical substance, cyclic Adenosine Monophosphate, attracting other amoebae.

The main purpose of this thesis is the theoretical and numerical study of repulsiveproductive chemotaxis models, given by the following parabolic PDE's system:

$$\begin{cases} \partial_t u - \Delta u = \nabla \cdot (u \nabla v) & \text{in } \Omega, \ t > 0, \\ \partial_t v - \Delta v + v = f(u) & \text{in } \Omega, \ t > 0, \end{cases}$$
(1)

where $\Omega \subset \mathbb{R}^n$, n = 2, 3, is a bounded domain with boundary $\partial \Omega$, and $u(\boldsymbol{x}, t) \geq 0$ and $v(\boldsymbol{x}, t) \geq 0$ denote the cell density and the chemical concentration, respectively. Moreover, $f(u) \geq 0$ is the production term. Model (1) possesses some properties among which we focus on:

- (i) The blow-up phenomenon is not expected to take place here.
- (ii) Mass-conservation: This problem is conservative in u, because the total mass $\int_{\Omega} u(\cdot, t)$ remains constant in time, that is,

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

(iii) In some cases (for instance, when the production is given by a power of u, that is,

 $f(u) = u^p$, this problem satisfies an energy inequality in the form:

$$\mathcal{E}(u(t_1), v(t_1)) - \mathcal{E}(u(t_0), v(t_0)) + \int_{t_0}^{t_1} D(u(s), v(s)) \, ds \le 0, \tag{3}$$

for a.e. $t_0, t_1 : t_1 \ge t_0 \ge 0$, where $\mathcal{E}(u, v)$ and D(u, v) denote, respectively, the free energy and the physical dissipation terms of the problem. In particular, (3) implies that this problem has a decreasing in time energy.

The motivation of this work was initially based on the study of Finite Element (FE) numerical approximations of problem (1), with production term f(u) = u, conserving at the discrete level the main properties of the continuous model, such as mass-conservation, energy-stability and positivity of the variables. Moreover, as part of the numerical analysis to be developed, we set out the study of the well-posedness, convergence and error estimates of the schemes, among others. However, we find that this is not an easy task, and the main difficulty lies in how to approximate at the discrete level the energy inequality (3) for this case, taking into account that, in the continuous problem, this energy inequality is obtained by testing the *u*-equation by the nonlinear function $F(u) = \ln u$.

Once these difficulties have been pointed out, we decided to focus first in the study of the problem (1) with quadratic production term, that is, $f(u) = u^2$, mainly for the following two reasons: (a) the energy inequality in the continuous problem is obtained by testing the *u*-equation by *u* and the *v*-equation by $-\Delta v$, which it is not so difficult to reproduce for fully discrete FE approximations; and (b) the quadratic production term allows to control an energy in $L^2(\Omega)$ -norm for *u*, which is very useful for performing numerical analysis. In this part, we studied some mass-conservative and energy-stable (in the sense that a discrete energy decreases in time) schemes associated to this problem, for which we also analyzed well-posedness, positivity, convergence towards weak solutions, error estimates and convergence at infinite time.

Later, with the experience obtained in the case of quadratic production, we focused in the case of linear production, that is, f(u) = u. In this case, by using a regularization technique used in previous works, we construct some unconditionally energy-stable fully discrete FE approximations, for which we proved well-posedness and some additional properties such as mass-conservation and approximated positivity of the variables (in the sense that the negative part of the variable tends to 0 as the regularization parameter tends to 0). However, since we could not obtain uniform estimates independent of the discrete and regularization parameters that allowed us to take limits on the discrete problem, the convergence towards weak solutions was not proved.

Finally, in the last part of this work, we have studied the intermediate case, in which $f(u) = u^p$ with $p \in (1, 2)$. Here, we have adapted the ideas used in the case of linear production, in order to obtain mass-conservative and energy-stable fully discrete FE schemes.

This PhD thesis is organized in five chapters, which we expect to correspond to five different papers:

Chapter 1 focuses on the study of numerical approximations of model (1) in the case of $f(u) = u^2$. We present two unconditionally mass-conservative and energy-stable first order time schemes: the (nonlinear) Backward Euler scheme and a linearized coupled version. We analyze positivity, solvability, convergence towards weak solutions and error estimates of these schemes. In particular, uniqueness of the nonlinear scheme is proved assuming small time step with respect to a strong norm of the scheme. This hypothesis is simplified in 2D domains where a global in time strong estimate is proved. Finally, some numerical simulations are made in order to compare the behavior of the schemes.

Chapter 2 is devoted to study a fully discrete FE scheme associated to problem (1) in the case of $f(u) = u^2$. By following the ideas presented in **Chapter 1**, we introduce $\sigma = \nabla v$ as an auxiliary variable, and then the corresponding FE backward Euler scheme is unconditionally mass-conservative and energy-stable. For this nonlinear scheme, we study some properties like solvability, convergence towards weak solutions, error estimates, and weak, strong and more regular a priori estimates of the scheme. Additionally, we propose two different linear iterative methods to approach the nonlinear scheme: an energy-stable Picard's method and the Newton's method. We prove solvability and convergence of both methods to the nonlinear scheme. Finally, we provide some numerical results in agreement with our theoretical analysis about the error estimates.

Chapter 3 is focused on the study of the asymptotic behaviour of the problem (1) in the case of $f(u) = u^2$. In the first part, we analyze the large-time behavior of the global weak-strong solutions and we prove the exponential convergence to a constant state as time goes to infinity. In the second part, we study this same behaviour for two fully discrete numerical schemes associated to this model: the FE backward Euler associated to (1) (with $f(u) = u^2$) and the nonlinear scheme defined in **Chapter 2**. On the way, in order to analyze the asymptotic behaviour for the backward Euler scheme, we prove its solvability and unconditional energy-stability. Finally, we compare the numerical schemes throughout several numerical simulations.

Chapter 4 is devoted to study unconditionally energy-stable and mass-conservative numerical schemes for problem (1) in the case of f(u) = u. By using a regularization

technique (in which, some regularized functions approximating $F(s) = u(\ln u - 1)$ and its first and second derivatives are introduced), we propose three fully discrete FE approximations. The first one is a nonlinear approximation in the variables (u, v); the second one is another nonlinear approximation obtained introducing $\boldsymbol{\sigma} = \nabla v$ as an auxiliary variable; and the third one is a linear approximation constructed by mixing the regularization procedure with the so called Energy Quadratization strategy, in which the energy of the system is transformed into a quadratic form by introducing new auxiliary variables. In addition, we prove the well-posedness of the numerical schemes. In fact, unconditional existence of solution, but conditional uniqueness (for the nonlinear schemes) are proved. Finally, we compare the behavior of the schemes throughout several numerical simulations.

At last, in **Chapter 5** we focus on the study of problem (1) in the case of $f(u) = u^p$, with $p \in (1, 2)$. In the first part, by using a regularization technique, we prove the existence of solutions of the model. In the second part, we propose three fully discrete FE nonlinear approximations, where the first one is defined in the variables (u, v), and the second and third ones by introducing $\boldsymbol{\sigma} = \nabla v$ as an auxiliary variable. We prove some unconditional properties such as mass-conservation, energy-stability and solvability of the schemes. Finally, we compare the behavior of the schemes throughout several numerical simulations.

Chapter 1 On a chemo-repulsion model with quadratic production: The continuous problem and time-discrete numerical schemes

1.1 Introduction

Chemotaxis is understood as the biological process of the movement of living organisms in response to a chemical stimulus which can be given towards a higher (attractive) or lower (repulsive) concentration of a chemical substance. At the same time, the presence of living organisms can produce or consume chemical substance. A repulsive-productive chemotaxis model can be given by the following parabolic PDE's system:

$$\begin{cases} \partial_t u - \Delta u = \nabla \cdot (u \nabla v) & \text{in } \Omega, \ t > 0, \\ \partial_t v - \Delta v + v = f(u) & \text{in } \Omega, \ t > 0, \end{cases}$$
(1.1)

where $\Omega \subset \mathbb{R}^n$, n = 2, 3, is an open bounded domain with boundary $\partial \Omega$. The unknowns for this model are $u(\boldsymbol{x}, t) \geq 0$, the cell density, and $v(\boldsymbol{x}, t) \geq 0$, the chemical concentration. Moreover, f(u) is a function which is nonnegative when $u \geq 0$. In this paper, we consider the particular case in which the production term is quadratic, that is $f(u) = u^2$, and then we focus on the following initial-boundary problem:

$$\begin{cases} \partial_t u - \Delta u = \nabla \cdot (u \nabla v) & \text{in } \Omega, \ t > 0, \\ \partial_t v - \Delta v + v = u^2 & \text{in } \Omega, \ t > 0, \\ \frac{\partial u}{\partial \mathbf{n}} = \frac{\partial v}{\partial \mathbf{n}} = 0 & \text{on } \partial\Omega, \ t > 0, \\ u(\boldsymbol{x}, 0) = u_0(\boldsymbol{x}) \ge 0, \ v(\boldsymbol{x}, 0) = v_0(\boldsymbol{x}) \ge 0 & \text{in } \Omega. \end{cases}$$
(1.2)

The quadratic production term allows to control an energy in $L^2(\Omega)$ -norm for u (see (1.20)-(1.21)), which is very useful for performing numerical analysis. Other production terms will be studied in Chapters 4 and 5.

In the case of linear production term, in [2] the authors proved that model (1.1) with f(u) = u is well-posed in the following sense: there exist global in time weak solutions (based on an energy inequality) and, for 2D domains, there exists a unique global in time strong solution. However, as far as we know, there are not works studying problem (1.2) with quadratic production. In addition, some papers on numerical analysis for chemotaxis models with linear production are [3, 6, 10, 12, 15].

In order to develop our analysis, we reformulate (1.2) introducing the new variable $\boldsymbol{\sigma} = \nabla v$. Then, we rewrite the model (1.2) as follows:

$$\begin{cases} \partial_t u - \nabla \cdot (\nabla u) = \nabla \cdot (u\boldsymbol{\sigma}) & \text{in } \Omega, \ t > 0, \\ \partial_t \boldsymbol{\sigma} - \nabla (\nabla \cdot \boldsymbol{\sigma}) + \operatorname{rot}(\operatorname{rot} \boldsymbol{\sigma}) + \boldsymbol{\sigma} = \nabla (u^2) & \text{in } \Omega, \ t > 0, \\ \frac{\partial u}{\partial \mathbf{n}} = 0 & \text{on } \partial\Omega, \ t > 0, \\ \boldsymbol{\sigma} \cdot \mathbf{n} = 0, \quad [\operatorname{rot} \boldsymbol{\sigma} \times \mathbf{n}]_{tang} = 0 & \text{on } \partial\Omega, \ t > 0, \\ u(\boldsymbol{x}, 0) = u_0(\boldsymbol{x}) \ge 0, \ \boldsymbol{\sigma}(\boldsymbol{x}, 0) = \nabla v_0(\boldsymbol{x}) & \text{in } \Omega, \end{cases}$$
(1.3)

where $(1.3)_2$ was obtained applying the gradient to equation $(1.2)_2$ and adding the term $rot(rot \boldsymbol{\sigma})$ using the fact that $rot \boldsymbol{\sigma} = rot(\nabla v) = 0$. Once solved (1.3), we can recover v from u^2 solving

$$\begin{cases} \partial_t v - \Delta v + v = u^2 & \text{in } \Omega, \ t > 0, \\ \frac{\partial v}{\partial \mathbf{n}} = 0 & \text{on } \partial \Omega, \ t > 0, \\ v(\boldsymbol{x}, 0) = v_0(\boldsymbol{x}) \ge 0 & \text{in } \Omega. \end{cases}$$
(1.4)

We will use the variable σ in order to simplify the notation throughout the chapter. Moreover, for fully discrete schemes by using the Finite Elements Method (which will be analyzed in Chapter 2), it will be very convenient to use the variables (u, σ) in order to obtain an unconditionally energy-stable scheme.

This chapter is organized as follows: In Section 1.2, we give the notation and some preliminary results that will be used along this paper. In Section 1.3, we analyze the continuous problem (1.2), obtaining global in time weak regularity for both two and three dimensions, and global in time strong regularity of the model assuming the regularity criteria (1.32), which is satisfied in 2D domains. In Section 1.4, we analyze the Backward Euler scheme corresponding to problem (1.3)-(1.4), including mass-conservation, unconditional energystability, solvability, positivity and error estimates of the scheme. In particular, uniqueness of solution of the scheme is proved under a hypothesis that relates the time step and a strong norm of the scheme (the discrete version of (1.32)), which can be simplified in the case of 2D domains owing to the strong estimates already obtained for the scheme. Moreover, we prove the existence of weak solutions of model (1.2) throughout the convergence of this scheme when the time step goes to 0. In Section 1.5, we propose a linearized coupled scheme for model (1.3)-(1.4), and again we analyze some properties of this linear scheme as in Section 1.4, comparing to the previous nonlinear scheme. Finally, in Section 1.6, we show some numerical simulations using Finite Elements spatial approximations associated to both time schemes, in order to verify numerically the theoretical results obtained in terms of positivity and unconditional energy-stability.

1.2 Notations and preliminary results

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 the usual notations for norms $\|\cdot\|_m$ and $\|\cdot\|_{L^p}$, respectively. In particular, the $L^2(\Omega)$ -norm will be represented by $\|\cdot\|_0$. Corresponding Sobolev spaces of vector valued functions will be denoted by $H^1(\Omega)$, $L^2(\Omega)$, and so on; and we denote by $H^1_{\sigma}(\Omega) := \{ \boldsymbol{\sigma} \in H^1(\Omega) : \boldsymbol{\sigma} \cdot \mathbf{n} = 0 \text{ on } \partial\Omega \}$ and $H^1_*(\Omega) := \{ h \in H^1(\Omega) : \int_{\Omega} h = 0 \}$. From now on, we will use the following equivalent norms in $H^1(\Omega)$ and $H^1_{\sigma}(\Omega)$, respectively (see [11] and [1, Corollary 3.5], respectively):

$$||u||_{1}^{2} = ||\nabla u||_{0}^{2} + \left(\int_{\Omega} u\right)^{2}, \quad \forall u \in H^{1}(\Omega),$$
(1.5)

$$\|\boldsymbol{\sigma}\|_{1}^{2} = \|\boldsymbol{\sigma}\|_{0}^{2} + \|\operatorname{rot} \boldsymbol{\sigma}\|_{0}^{2} + \|\nabla \cdot \boldsymbol{\sigma}\|_{0}^{2}, \quad \forall \boldsymbol{\sigma} \in \boldsymbol{H}_{\sigma}^{1}(\Omega).$$
(1.6)

In particular, (1.6) implies that, for all $\boldsymbol{\sigma} = \nabla v \in \boldsymbol{H}_{\sigma}^{1}(\Omega)$,

$$\|\nabla v\|_{1}^{2} = \|\nabla v\|_{0}^{2} + \|\Delta v\|_{0}^{2}.$$
(1.7)

If Z is a Banach space, then Z' will denote its topological dual. Moreover, the letters C, K will denote different positive constants always independent of the time step.

We define the linear elliptic operators

$$Av = g \quad \Leftrightarrow \quad \begin{cases} -\Delta v + v = g \quad \text{in } \Omega, \\ \frac{\partial v}{\partial \mathbf{n}} = 0 \quad \text{on } \partial \Omega, \end{cases}$$
(1.8)

and

$$B\boldsymbol{\sigma} = \boldsymbol{f} \quad \Leftrightarrow \quad \begin{cases} -\nabla(\nabla \cdot \boldsymbol{\sigma}) + \operatorname{rot} (\operatorname{rot} \boldsymbol{\sigma}) + \boldsymbol{\sigma} = \boldsymbol{f} & \operatorname{in} \Omega, \\ \boldsymbol{\sigma} \cdot \mathbf{n} = 0, \ [\operatorname{rot} \boldsymbol{\sigma} \times \mathbf{n}]_{tang} = \boldsymbol{0} & \operatorname{on} \partial\Omega. \end{cases}$$
(1.9)

The corresponding variational forms are given by $A: H^1(\Omega) \to H^1(\Omega)'$ and $B: \mathbf{H}^1_{\sigma}(\Omega) \to \mathbf{H}^1_{\sigma}(\Omega)'$ such that

$$\langle Av, \bar{v} \rangle = (\nabla v, \nabla \bar{v}) + (v, \bar{v}), \quad \forall v, \bar{v} \in H^{1}(\Omega), \\ \langle B\boldsymbol{\sigma}, \bar{\boldsymbol{\sigma}} \rangle = (\boldsymbol{\sigma}, \bar{\boldsymbol{\sigma}}) + (\nabla \cdot \boldsymbol{\sigma}, \nabla \cdot \bar{\boldsymbol{\sigma}}) + (\operatorname{rot} \boldsymbol{\sigma}, \operatorname{rot} \bar{\boldsymbol{\sigma}}), \quad \forall \boldsymbol{\sigma}, \bar{\boldsymbol{\sigma}} \in \boldsymbol{H}^{1}_{\sigma}(\Omega).$$

We assume the H^2 and H^3 -regularity of problem (1.8) (see for instance [4]). Consequently, we assume the existence of some constants C > 0 such that

$$\|v\|_{2} \le C \|Av\|_{0} \quad \forall v \in H^{2}(\Omega); \quad \|v\|_{3} \le C \|Av\|_{1} \quad \forall v \in H^{3}(\Omega).$$
(1.10)

Then, if the right hand side of problem (1.9) is given by $\mathbf{f} = \nabla h$ with $h \in H^1(\Omega)$, then taking $\boldsymbol{\sigma} = \nabla v$, we will prove the H^2 -regularity of problem (1.9) as follows:

Lemma 1.2.1 If $\mathbf{f} = \nabla h$ with $h \in H^1(\Omega)$, then the solution $\boldsymbol{\sigma}$ of problem (1.9) belongs to $\mathbf{H}^2(\Omega)$. Moreover,

$$\|\boldsymbol{\sigma}\|_2 \le C \, \|\nabla h\|_0. \tag{1.11}$$

Proof. First, we assume that $h \in H^1_*(\Omega)$, hence $\|h\|_1 \leq C \|\nabla h\|_0$. Then, from H^3 -regularity of problem (1.8) taking g = h, we have that $v \in H^3(\Omega)$ with $-\Delta v + v = h$ and $\|v\|_3 \leq C \|h\|_1 \leq C \|\nabla h\|_0$. Then, taking $\boldsymbol{\sigma} = \nabla v$, we have that $\boldsymbol{\sigma} \in \boldsymbol{H}^2(\Omega)$ solves (1.9), and (1.11) holds. Finally, in the general case of $h \in H^1(\Omega)$, we consider $g = h - \frac{1}{|\Omega|} \int_{\Omega} h$ in (1.8), deducing again that $v \in H^3(\Omega)$ and $\|v\|_3 \leq C \|h - \frac{1}{|\Omega|} \int_{\Omega} h\|_1 \leq C \|\nabla (h - \frac{1}{|\Omega|} \int_{\Omega} h)\|_0 = C \|\nabla h\|_0$. Then, taking $\boldsymbol{\sigma} = \nabla v$, we have that $\boldsymbol{\sigma} \in \boldsymbol{H}^2(\Omega)$ solves (1.9) with $\boldsymbol{f} = \nabla (h - \frac{1}{|\Omega|} \int_{\Omega} h) = \nabla h$, and (1.11) holds.

Along this paper, we will use repeatedly the classical interpolations inequalities

$$||u||_{L^4} \le C ||u||_0^{1/2} ||u||_1^{1/2} \quad \forall u \in H^1(\Omega) \quad \text{(in 2D domains)}, \tag{1.12}$$

$$||u||_{L^3} \le C ||u||_0^{1/2} ||u||_1^{1/2} \quad \forall u \in H^1(\Omega) \quad \text{(in 3D domains)}.$$
(1.13)

Finally, in order to obtain uniform in time strong estimates for the continuous problem and the numerical schemes, we will use the following results (see [14] and [13], respectively):

Lemma 1.2.2 (Uniform Gronwall Lemma) Let g = g(t), h = h(t), z = z(t) be three positive locally integrable functions defined in $(0, +\infty)$ with z' also locally integrable in $(0, +\infty)$, such that

$$z'(t) \le g(t)z(t) + h(t) \quad a.e. \ t \ge 0.$$

If for any r > 0 there exist $a_1(r)$, $a_2(r)$ and $a_3(r)$ such that

$$\int_{t}^{t+r} g(s)ds \le a_{1}(r), \quad \int_{t}^{t+r} h(s)ds \le a_{2}(r), \quad \int_{t}^{t+r} z(s)ds \le a_{3}(r) , \quad \forall t \ge 0$$

then,

$$z(t+r) \le \left(a_2(r) + \frac{a_3(r)}{r}\right) \exp(a_1(r)), \quad \forall t \ge 0.$$

Lemma 1.2.3 (Uniform discrete Gronwall lemma) Let k > 0 and $d^n, g^n, h^n \ge 0$ such that

$$\frac{d^{n+1}-d^n}{k} \le g^n d^n + h^n, \quad \forall n \ge 0.$$

$$(1.14)$$

If for any $r \in \mathbb{N}$, there exist $a_1(t_r)$, $a_2(t_r)$ and $a_3(t_r)$ depending on $t_r = kr$, such that

$$k\sum_{n=n_0}^{n_0+r-1} g^n \le a_1(t_r), \quad k\sum_{n=n_0}^{n_0+r-1} h^n \le a_2(t_r), \quad k\sum_{n=n_0}^{n_0+r-1} d^n \le a_3(t_r), \quad \forall n_0 \ge 0,$$

then

$$d^{n} \leq \left(a_{2}(t_{r}) + \frac{a_{3}(t_{r})}{t_{r}}\right) \exp\left\{a_{1}(t_{r})\right\}, \quad \forall n \geq r.$$

As consequence of Lemma 1.2.3 (with an estimate for d^n for any $n \ge r$) and the classical Discrete Gronwall Lemma (estimating d^n for n = 0, ..., r - 1), we will prove the following result:

Corollary 1.2.4 Assume hypothesis of Lemma 1.2.3. Let $k_0 > 0$ be fixed, then the following estimate holds for all $k \leq k_0$

$$d^n \le C(d^0, k_0) \quad \forall n \ge 0.$$
(1.15)

Proof. We fix $T = 2k_0$ and choose $r_0 \in \mathbb{N}$ such that $k(r_0 - 1) < T \leq kr_0 := t_{r_0}$. Then, from Lemma 1.2.3 we have

$$d^{n} \leq \left(a_{2}(t_{r_{0}}) + \frac{a_{3}(t_{r_{0}})}{t_{r_{0}}}\right) \exp\left\{a_{1}(t_{r_{0}})\right\}$$
$$\leq \left(a_{2}(t_{r_{0}}) + \frac{a_{3}(t_{r_{0}})}{T}\right) \exp\left\{a_{1}(t_{r_{0}})\right\} := C_{1}(k_{0}), \quad \forall n \geq r_{0}.$$
(1.16)

On the other hand, applying the Discrete Gronwall Lemma to (1.14), one has

$$d^{n} \leq \left(a_{2}(t_{r_{0}}) + d^{0}\right) \exp\left\{a_{1}(t_{r_{0}})\right\} := C_{2}(d^{0}, k_{0}), \quad \forall n < r_{0}.$$

$$(1.17)$$

Therefore, from (1.16)-(1.17) we deduce (1.15).

1.3 Analysis of the continuous model

In this section, we analyze the weak and strong regularity of problem (1.2). With this aim, we will start giving the following definition of weak-strong solutions for problem (1.2).

Definition 1.3.1 (Weak-strong solutions of (1.2)) Given $(u_0, v_0) \in L^2(\Omega) \times H^1(\Omega)$ with $u_0 \geq 0, v_0 \geq 0$ a.e. $\boldsymbol{x} \in \Omega$, a pair (u, v) is called weak-strong solution of problem (1.2) in $(0, +\infty)$, if $u \geq 0, v \geq 0$ a.e. $(t, \boldsymbol{x}) \in (0, +\infty) \times \Omega$,

$$(u,v) \in L^{\infty}(0,+\infty; L^{2}(\Omega) \times H^{1}(\Omega)) \cap L^{2}(0,T; H^{1}(\Omega) \times H^{2}(\Omega)), \quad \forall T > 0,$$
$$(\partial_{t}u, \partial_{t}v) \in L^{q'}(0,T; H^{1}(\Omega)' \times L^{2}(\Omega)), \quad \forall T > 0,$$

where q' = 2 in the 2-dimensional case (2D) and q' = 4/3 in the 3-dimensional case (3D) (q' is the conjugate exponent of q = 2 in 2D and q = 4 in 3D); the following variational formulation holds

$$\int_0^T \langle \partial_t u, \bar{u} \rangle + \int_0^T (\nabla u, \nabla \bar{u}) + \int_0^T (u \nabla v, \nabla \bar{u}) = 0, \quad \forall \bar{u} \in L^q(0, T; H^1(\Omega)), \quad \forall T > 0, \quad (1.18)$$

the following equation holds pointwisely

$$\partial_t v + Av = u^2 \quad a.e. \ (t, \boldsymbol{x}) \in (0, +\infty) \times \Omega,$$
(1.19)

the initial conditions $(1.2)_4$ are satisfied and the following energy inequality (in integral version) holds for a.e. t_0, t_1 with $t_1 \ge t_0 \ge 0$:

$$\mathcal{E}(u(t_1), v(t_1)) - \mathcal{E}(u(t_0), v(t_0)) + \int_{t_0}^{t_1} \left(\|\nabla u(s)\|_0^2 + \frac{1}{2} \|\nabla v(s)\|_1^2 \right) \, ds \le 0, \tag{1.20}$$

where

$$\mathcal{E}(u,v) = \frac{1}{2} \|u\|_0^2 + \frac{1}{4} \|\nabla v\|_0^2.$$
(1.21)

Remark 1.3.2 In 2D domains, we can take $\bar{u} = u$ in (1.18), test (1.19) by $-\frac{1}{2}\Delta v$, integrating by parts and using (1.7), we arrive at the following equality energy law (in differential version):

$$\frac{d}{dt}\mathcal{E}(u(t),v(t)) + \|\nabla u(t)\|_0^2 + \frac{1}{2}\|\nabla v(t)\|_1^2 = 0 \quad a.e. \ t > 0.$$
(1.22)

Moreover, this equality is also true in 3D domains for regular enough solutions.

Moreover, we also give the definition of weak solutions for the reformulated problem (1.3):

Definition 1.3.3 (Weak solutions of (1.3)) Given $(u_0, \sigma_0) \in L^2(\Omega) \times L^2(\Omega)$ with $u_0 \ge 0$ a.e. $\boldsymbol{x} \in \Omega$, a pair (u, σ) is called weak solution of problem (1.3) in $(0, +\infty)$, if $u \ge 0$ a.e. $(t, \boldsymbol{x}) \in (0, +\infty) \times \Omega$,

$$(u, \boldsymbol{\sigma}) \in L^{\infty}(0, +\infty; L^{2}(\Omega) \times \boldsymbol{L}^{2}(\Omega)) \cap L^{2}(0, T; H^{1}(\Omega) \times \boldsymbol{H}^{1}(\Omega)), \quad \forall T > 0,$$
$$(\partial_{t}u, \partial_{t}\boldsymbol{\sigma}) \in L^{q'}(0, T; H^{1}(\Omega)' \times \boldsymbol{H}^{1}(\Omega)'), \quad \forall T > 0,$$

where q is as in Definition 1.3.1; the following variational formulations hold

$$\int_0^T \langle \partial_t u, \bar{u} \rangle + \int_0^T (\nabla u, \nabla \bar{u}) + \int_0^T (u\boldsymbol{\sigma}, \nabla \bar{u}) = 0, \quad \forall \bar{u} \in L^q(0, T; H^1(\Omega)), \quad \forall T > 0, \quad (1.23)$$

$$\int_0^T \langle \partial_t \boldsymbol{\sigma}, \bar{\boldsymbol{\sigma}} \rangle + \int_0^T \langle B \boldsymbol{\sigma}, \bar{\boldsymbol{\sigma}} \rangle = 2 \int_0^T (u \nabla u, \bar{\boldsymbol{\sigma}}), \ \forall \bar{\boldsymbol{\sigma}} \in L^q(0, T; \boldsymbol{H}^1(\Omega)), \ \forall T > 0, \quad (1.24)$$

the initial conditions $(1.3)_5$ are satisfied and the following energy inequality (in integral version) holds for a.e. t_0, t_1 with $t_1 \ge t_0 \ge 0$:

$$\mathcal{E}(u(t_1), \boldsymbol{\sigma}(t_1)) - \mathcal{E}(u(t_0), \boldsymbol{\sigma}(t_0)) + \int_{t_0}^{t_1} (\|\nabla u(s)\|_0^2 + \frac{1}{2} \|\boldsymbol{\sigma}(s)\|_1^2) \, ds \le 0,$$
(1.25)

where

$$\mathcal{E}(u, \boldsymbol{\sigma}) = \frac{1}{2} \|u\|_0^2 + \frac{1}{4} \|\boldsymbol{\sigma}\|_0^2.$$
(1.26)

Lemma 1.3.4 If $\sigma_0 = \nabla v_0$, problems (1.2) and (1.3)-(1.4) are equivalents in the following sense: If (u, v) is a weak-strong solution of (1.2) then (u, σ) with $\sigma = \nabla v$ is a weak solution of (1.3); and reciprocally, if (u, σ) is a weak solution of (1.3) and $v = v(u^2)$ is the unique strong solution of problem (1.4) (i.e. $v \in L^p(0, T; W^{2,p}(\Omega)) \cap L^{\infty}(0, T; W^{1,p}(\Omega)) \cap L^{q'}(0, T; H^2(\Omega))$ since $u^2 \in L^p(0, T; L^p(\Omega)) \cap L^{q'}(0, T; L^2(\Omega))$ for p = 5/3 in 3D, p = 2 in 2D and q' is as in Definition 1.3.1, see [5, Theorem 10.22]), then $\sigma = \nabla v$ and (u, v) is a weak-strong solution of (1.2).

Proof. Suppose that (u, v) is a weak-strong solution of (1.2), then testing (1.19) by $-\nabla \cdot \overline{\mathbf{w}}$, for any $\overline{\mathbf{w}} \in L^q(0, T; \mathbf{H}^1(\Omega))$, and taking into account that $\operatorname{rot}(\nabla v) = 0$, we obtain

$$\int_{0}^{T} \langle \partial_t \nabla v, \overline{\mathbf{w}} \rangle + \int_{0}^{T} \langle B \nabla v, \overline{\mathbf{w}} \rangle = 2 \int_{0}^{T} (u \nabla u, \overline{\mathbf{w}}), \quad \forall \, \overline{\mathbf{w}} \in L^q(0, T; \boldsymbol{H}^1(\Omega)).$$
(1.27)

Then, defining $\boldsymbol{\sigma} = \nabla v$ and assuming the hypothesis $\boldsymbol{\sigma}_0 = \nabla v_0$, from (1.27) we conclude that $(u, \boldsymbol{\sigma})$ is a weak solution of (1.3). By other hand, if $(u, \boldsymbol{\sigma})$ is a weak solution of (1.3) and $v = v(u^2)$ is the unique strong solution of problem (1.4), reasoning as above, we conclude that ∇v satisfies (1.27). Therefore, from (1.24) and (1.27), we obtain

$$\int_{0}^{T} \langle \partial_{t}(\boldsymbol{\sigma} - \nabla v), \overline{\boldsymbol{\sigma}} \rangle + \int_{0}^{T} \langle B(\boldsymbol{\sigma} - \nabla v), \overline{\boldsymbol{\sigma}} \rangle = 0, \quad \forall \, \overline{\boldsymbol{\sigma}} \in L^{q}(0, T; \boldsymbol{H}^{1}(\Omega)).$$
(1.28)

Then, since $\boldsymbol{\sigma} - \nabla v \in L^{\infty}(0,T; \boldsymbol{L}^{p}(\Omega))$, taking $\overline{\boldsymbol{\sigma}} = B^{-1}(\boldsymbol{\sigma} - \nabla v) \in L^{\infty}(0,T; \boldsymbol{W}^{2,p}(\Omega)) \hookrightarrow L^{q}(0,T; \boldsymbol{H}^{1}(\Omega))$ in (1.28), we deduce

$$\frac{1}{2} \|B^{-1}(\boldsymbol{\sigma}(T) - \nabla v(T))\|_{1}^{2} + \int_{0}^{T} \|\boldsymbol{\sigma} - \nabla v\|_{0}^{2} = \frac{1}{2} \|B^{-1}(\boldsymbol{\sigma}(0) - \nabla v(0))\|_{1}^{2} = 0,$$

where, in the last equality, the relation $\boldsymbol{\sigma}(0) = \nabla v(0)$ was used, and therefore we deduce $\boldsymbol{\sigma} = \nabla v$. Thus, (u, v) is a weak-strong solution of (1.2).

Remark 1.3.5 Since $v_0 \ge 0$ in Ω , then the unique strong solution $v = v(u^2)$ of problem (1.4) satisfies $v \ge 0$ in $(0, +\infty) \times \Omega$.

Later, in Section 1.4 we will prove the existence of solutions of a discrete in time scheme that approximates problem (1.3)-(1.4) and we will obtain uniform estimates of the discrete solutions, which will allow us to pass to the limit in the discrete problem in order to obtain the existence of weak solutions of problem (1.3) (in the sense of Definition 1.3.3) and strong solution of (1.4). Finally, taking into account Lemma 1.3.4, the existence of weak-strong solutions of problem (1.2) (in the sense of Definition 1.3.1) will be obtained.

Observe that any weak-strong solution of (1.2) (or weak solution of (1.3)) is conservative in u, because the total mass $\int_{\Omega} u(t)$ remains constant in time, as we can check taking $\bar{u} = 1$ in (1.18),

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

Moreover, integrating $(1.2)_2$ (or $(1.4)_1$) in Ω we deduce the following behavior of $\int_{\Omega} v$,

$$\frac{d}{dt}\left(\int_{\Omega} v\right) = \int_{\Omega} u^2 - \int_{\Omega} v.$$
(1.29)

1.3.1 Weak-Strong Regularity

Observe that from the energy law (1.20), and using (1.7), we deduce

$$\begin{cases} (u, \nabla v) \in L^{\infty}(0, +\infty; L^{2}(\Omega) \times \boldsymbol{L}^{2}(\Omega)), \\ (\nabla u, \nabla v) \in L^{2}(0, +\infty; \boldsymbol{L}^{2}(\Omega) \times \boldsymbol{H}^{1}(\Omega)). \end{cases}$$
(1.30)

From (1.30), we have

$$u \in L^2(0,T; H^1(\Omega)), \quad \forall T > 0.$$

From (1.29), we observe that the function $y(t) = \int_{\Omega} v(\boldsymbol{x}, t) d\boldsymbol{x} = \|v(t)\|_{L^1}$ (where Remark 1.3.5 has been taken into account) satisfies y'(t) + y(t) = z(t), with $z(t) = \int_{\Omega} u(\boldsymbol{x}, t)^2 d\boldsymbol{x} = \|u(t)\|_{L^2}^2$. Therefore, $y(t) = y(0) e^{-t} + \int_{\Omega}^{t} e^{-(t-s)} z(s) ds$, and using $(1.30)_1$,

$$\|v(t)\|_{L^{1}} \le e^{-t} \|v_{0}\|_{L^{1}} + \int_{0}^{t} e^{-(t-s)} \|u(s)\|_{0}^{2} ds \le \|v_{0}\|_{L^{1}} + \|u\|_{L^{\infty}(0,+\infty;L^{2})}^{2}, \quad \forall t \ge 0.$$
(1.31)

Then, from (1.31) we conclude that $v \in L^{\infty}(0, +\infty; L^{1}(\Omega))$ which, together with (1.30), implies that

$$v \in L^{\infty}(0, +\infty; H^1(\Omega)) \cap L^2(0, T; H^2(\Omega)), \quad \forall T > 0.$$

Remark 1.3.6 In 2D domains, by using the interpolation inequality (1.12) (proceeding for instance as for the Navier-Stokes equations [8]), one can deduce the uniqueness of weak-strong solutions of (1.2).

1.3.2 A regularity criterium implying global in time strong regularity

We are going to obtain strong regularity in a formal manner, assuming a regular enough solution. In fact, a rigorous proof could be made via a regularization argument or a Galerkin approximation, using the eigenfunctions of the operator A.

We will assume the following regularity criterium:

$$(u, \nabla v) \in L^{\infty}(0, +\infty; H^1(\Omega) \times \boldsymbol{H}^1(\Omega)).$$
(1.32)

Later, at the end of this Subsection, we will show that (1.32) holds, at least, in 2D domains.

First, we make $(\nabla(1.2)_1, \nabla u) + \frac{1}{2}(\Delta(1.2)_2, \Delta v)$, integrating by parts, using the Hölder and Young inequalities and the 3D interpolation inequality (1.13), one has

$$\frac{1}{2} \frac{d}{dt} \left(\|\nabla u\|_{0}^{2} + \frac{1}{2} \|\Delta v\|_{0}^{2} \right) + \|\Delta u\|_{0}^{2} + \frac{1}{2} \|\Delta v\|_{0}^{2} + \frac{1}{2} \|\nabla (\Delta v)\|_{0}^{2} \\
= (\partial_{i} \partial_{j} (u \partial_{j} v), \partial_{i} u) + (\partial_{i} (u \partial_{i} u), \partial_{j} \partial_{j} v) = (\partial_{i} (\partial_{j} u \partial_{j} v), \partial_{i} u) + (\partial_{i} u \partial_{i} u, \partial_{j} \partial_{j} v) \\
= (\partial_{j} u \partial_{i} \partial_{j} v, \partial_{i} u) + \frac{1}{2} (\partial_{i} u \partial_{i} u, \partial_{j} \partial_{j} v) = \left((\nabla u \cdot \nabla) (\nabla v), \nabla u \right) + \frac{1}{2} \left(|\nabla u|^{2}, \Delta v \right) \\
\leq C \|\nabla u\|_{L^{3}} \|\nabla u\|_{L^{6}} \|\nabla^{2} v\|_{0} \leq C \|\nabla u\|_{0}^{1/2} \|\nabla u\|_{1}^{3/2} \|\nabla v\|_{1} \leq \varepsilon \|\nabla u\|_{1}^{2} + C_{\varepsilon} \|\nabla u\|_{0}^{2} \|\nabla v\|_{1}^{4}. \tag{1.33}$$

Therefore, if we add (1.22) and (1.33), use (1.7) and take ε small enough, we have

$$\frac{d}{dt} \left(\|u\|_1^2 + \frac{1}{2} \|\nabla v\|_1^2 \right) + \|\nabla u\|_1^2 + \|\nabla v\|_2^2 \le C \|\nabla u\|_0^2 \|\nabla v\|_1^4$$
(1.34)

Then, integrating in time (1.34), since $\|\nabla u\|_0^2 \|\nabla v\|_1^4 \in L^1(0, +\infty)$ (owing to (1.30) and (1.32)), we deduce

$$\begin{cases} (\nabla u, \nabla v) \in L^2(0, +\infty; \boldsymbol{H}^1(\Omega) \times \boldsymbol{H}^2(\Omega)), \\ (u, v) \in L^2(0, T; H^2(\Omega) \times H^3(\Omega)), \quad \forall T > 0. \end{cases}$$
(1.35)

On the other hand, making $(\Delta(1.2)_1, \Delta u)$ and using the Hölder and Young inequalities, we have

$$\frac{d}{dt} \|\Delta u\|_{0}^{2} + \|\nabla(\Delta u)\|_{0}^{2} \leq \|\nabla(\nabla \cdot (u\nabla v))\|_{0}^{2}
\leq C \left(\|u\|_{L^{\infty}}^{2} \|\nabla(\Delta v)\|_{0}^{2} + \|\nabla^{2}u\|_{0}^{2} \|\nabla v\|_{L^{\infty}}^{2} + \|\nabla u\|_{L^{4}}^{2} \|\nabla^{2}v\|_{L^{4}}^{2} \right).$$
(1.36)

Therefore, summing (1.34) to (1.36) and using (1.7), we have

$$\frac{d}{dt} \left(\|u\|_2^2 + \frac{1}{2} \|\nabla v\|_1^2 \right) + \|\nabla u\|_2^2 + \|\nabla v\|_2^2 \le C \|\nabla v\|_2^2 \|u\|_2^2 + C \|\nabla u\|_0^2 \|\nabla v\|_1^4$$
(1.37)

and thus, since $\|\nabla v\|_2^2 \in L^1(0, +\infty)$ (owing to (1.35)) and $\|\nabla u\|_0^2 \|\nabla v\|_1^4 \in L^1(0, +\infty)$, Lemma 1.2.2 implies

$$u \in L^{\infty}(0, +\infty; H^2(\Omega)).$$
(1.38)

Moreover, integrating in time (1.37), and using $\|\nabla v\|_2^2 \|u\|_2^2 \in L^1(0, +\infty)$ (owing to (1.35) and (1.38)), we deduce

$$\nabla u \in L^2(0, +\infty; \mathbf{H}^2(\Omega)), \text{ hence } u \in L^2(0, T; H^3(\Omega)), \forall T > 0.$$

In particular, from (1.32) and (1.38), we deduce

$$(u, v) \in L^{\infty}(0, +\infty; L^{\infty}(\Omega) \times L^{\infty}(\Omega)).$$

Therefore, one has that any global in time weak-strong solution satisfying (1.32) does not blow-up, neither at finite time nor infinite one. Finally, from equation $(1.2)_1$ and taking into account (1.32) and (1.35), we deduce

$$\partial_t u \in L^2(0, +\infty; L^2(\Omega)). \tag{1.39}$$

Moreover, taking the time derivative of $(1.2)_2$ and testing by $\partial_t v$, we obtain

$$\frac{1}{2} \frac{d}{dt} \|\partial_t v\|_0^2 + \|\partial_t v\|_1^2 = 2(u \,\partial_t u, \partial_t v) \le 2\|u\|_{L^6} \|\partial_t u\|_0 \|\partial_t v\|_{L^3}$$

$$\le \varepsilon \|\partial_t v\|_1^2 + C_\varepsilon \|u\|_1^2 \|\partial_t u\|_0^2 \in L^1(0, +\infty),$$

hence we arrive at

$$\partial_t v \in L^{\infty}(0, +\infty; L^2(\Omega)) \cap L^2(0, +\infty; H^1(\Omega)).$$
(1.40)

1.3.3 Higher global in time regularity

Denote by $\widetilde{u} = \partial_t u$ and $\widetilde{v} = \partial_t v$. Then, from (1.2) we deduce that $(\widetilde{u}, \widetilde{v})$ satisfies

$$\begin{cases} \partial_t \widetilde{u} - \Delta \widetilde{u} - \nabla \cdot (\widetilde{u} \nabla v) - \nabla \cdot (u \nabla \widetilde{v}) = 0, \\ \partial_t \widetilde{v} - \Delta \widetilde{v} + \widetilde{v} = 2u \widetilde{u}. \end{cases}$$
(1.41)

Testing by \tilde{u} in $(1.41)_1$ and $-\frac{1}{2}\Delta \tilde{v}$ in $(1.41)_2$, taking into account that $\int_{\Omega} \tilde{u} = 0$ and using the 3D interpolation inequality (1.13), we deduce

$$\frac{1}{2} \frac{d}{dt} \left(\|\widetilde{u}\|_{0}^{2} + \frac{1}{2} \|\nabla\widetilde{v}\|_{0}^{2} \right) + \|\widetilde{u}\|_{1}^{2} + \frac{1}{2} \|\nabla\widetilde{v}\|_{1}^{2}
= -(\widetilde{u}\nabla v, \nabla\widetilde{u}) + (\widetilde{u}\nabla u, \nabla\widetilde{v}) \leq \|\widetilde{u}\|_{L^{3}} \left(\|\nabla v\|_{L^{6}} \|\nabla\widetilde{u}\|_{0} + \|\nabla\widetilde{v}\|_{L^{6}} \|\nabla u\|_{0} \right)
\leq \frac{1}{2} \left(\|\widetilde{u}\|_{1}^{2} + \frac{1}{2} \|\nabla\widetilde{v}\|_{1}^{2} \right) + C \|\nabla v\|_{1}^{4} \|\widetilde{u}\|_{0}^{2} + C \|\nabla u\|_{0}^{4} \|\widetilde{u}\|_{0}^{2}.$$
(1.42)

Therefore, since $\|\nabla v\|_1^4$ and $\|\nabla u\|_0^4 \in L^1(0, +\infty)$ (owing to (1.30)₂ and (1.32)), Lemma 1.2.2 and (1.40) imply

$$(\partial_t u, \partial_t v) \in L^{\infty}(0, +\infty; L^2(\Omega) \times H^1(\Omega)).$$
(1.43)

Moreover, integrating in time (1.42) and using (1.40) and (1.43), we deduce

$$(\partial_t u, \partial_t v) \in L^2(0, +\infty; H^1(\Omega) \times H^2(\Omega)).$$
(1.44)

Finally, applying time derivative to equations $(1.2)_1$ and $(1.2)_2$, and taking into account (1.32)-(1.35), (1.38) and (1.43)-(1.44), we can deduce the following regularity for $\partial_{tt}u$ and $\partial_{tt}v$:

$$(\partial_{tt}u, \partial_{tt}v) \in L^2(0, +\infty; H^1(\Omega)' \times L^2(\Omega)).$$
(1.45)

By following with a bootstrap argument, it is possible to obtain more regularity for (u, v). However, the regularity obtained so far is sufficient to guarantee the hypothesis required later to prove error estimates (see Theorem 1.4.21 and Theorem 1.5.6).

1.3.4 Proof of (1.32) in 2D domains

In order to prove (1.32) in 2D domains, we make $(\nabla(1.2)_1, \nabla u) + \frac{1}{2}(\Delta(1.2)_2, \Delta v)$, integrating by parts, and arguing as in (1.33), but in this case using the 2D interpolation inequality (1.12), one has

$$\frac{1}{2} \frac{d}{dt} \left(\|\nabla u\|_{0}^{2} + \frac{1}{2} \|\Delta v\|_{0}^{2} \right) + \|\Delta u\|_{0}^{2} + \frac{1}{2} \|\nabla v\|_{0}^{2} + \frac{1}{2} \|\nabla (\Delta v)\|_{0}^{2} \\
\leq C \|\nabla u\|_{L^{4}}^{2} \|\nabla^{2} v\|_{0} \leq C \|\nabla u\|_{0} \|\nabla u\|_{1} \|\nabla v\|_{1} \leq \varepsilon \|\nabla u\|_{1}^{2} + C_{\varepsilon} \|\nabla u\|_{0}^{2} \|\nabla v\|_{1}^{2}.$$
(1.46)

Therefore, if we add (1.22) and (1.46), use (1.7) and take ε small enough, we have

$$\frac{d}{dt}\left(\|u\|_{1}^{2} + \frac{1}{2}\|\nabla v\|_{1}^{2}\right) + \|\nabla u\|_{1}^{2} + \|\nabla v\|_{2}^{2} \le C\|\nabla u\|_{0}^{2}\|\nabla v\|_{1}^{2}$$

and thus, since $\|\nabla u\|_0^2 \in L^1(0, +\infty)$, Lemma 1.2.2 implies (1.32).

1.4 Euler time discretization

In this section, we study the Euler time discretization for the problem (1.3)-(1.4), and we analyze the unconditional stability (in weak norms, see Definition 1.4.5 below) and solvability

of the scheme, as well as its convergence towards weak solutions. We also study some additional properties as positivity of the cell and chemical variables, mass-conservation of cells, and error estimates. Additionally, we prove uniqueness of solution of the scheme under a hypothesis that relates the time step and strong norms of the scheme, which is simplified in the case of 2D domains owing to a strong estimate obtained for the scheme (the discrete version of (1.32)).

Let us consider a fixed partition of the time interval $[0, +\infty)$ given by $t_n = nk$, where k > 0 denotes the time step (that we take constant for simplicity). First, taking into account the (u, v)-problem (1.2), we consider the following first order, nonlinear and coupled scheme (Backward Euler):

• <u>Scheme</u> UV:

Initialization: We fix $u_0 = u(0)$ and $v_0 = v(0)$.

Time step n: Given $(u_{n-1}, v_{n-1}) \in H^1(\Omega) \times H^2(\Omega)$ with $u_{n-1} \ge 0$ and $v_{n-1} \ge 0$, compute $(u_n, v_n) \in H^1(\Omega) \times H^2(\Omega)$ with $u_n \ge 0$ and $v_n \ge 0$ and solving

$$\begin{cases} (\delta_t u_n, \bar{u}) + (\nabla u_n, \nabla \bar{u}) + (u_n \nabla v_n, \nabla \bar{u}) = 0, \quad \forall \bar{u} \in H^1(\Omega), \\ \delta_t v_n + A v_n - u_n^2 = 0, \quad \text{a.e. } \boldsymbol{x} \in \Omega, \end{cases}$$
(1.47)

where, in general, we denote $\delta_t a_n = \frac{a_n - a_{n-1}}{k}$.

On the other hand, we can consider the following Backward Euler scheme related to the reformulation in the (u, σ) -problem (1.3). Then, one also has the following first order, nonlinear and coupled scheme:

• <u>Scheme US</u>:

Initialization: We fix $v_0 = v(0)$ and $(u_0, \boldsymbol{\sigma}_0) = (u(0), \boldsymbol{\sigma}(0))$, with $\boldsymbol{\sigma}_0 = \nabla v_0$. **Time step** n: Given $(u_{n-1}, \boldsymbol{\sigma}_{n-1}) \in H^1(\Omega) \times \boldsymbol{H}^1_{\sigma}(\Omega)$ with $u_{n-1} \geq 0$, compute $(u_n, \boldsymbol{\sigma}_n) \in H^1(\Omega) \times \boldsymbol{H}^1_{\sigma}(\Omega)$ with $u_n \geq 0$ and solving

$$\begin{cases} (\delta_t u_n, \bar{u}) + (\nabla u_n, \nabla \bar{u}) + (u_n \boldsymbol{\sigma}_n, \nabla \bar{u}) = 0, \quad \forall \bar{u} \in H^1(\Omega), \\ (\delta_t \boldsymbol{\sigma}_n, \bar{\boldsymbol{\sigma}}) + \langle B \boldsymbol{\sigma}_n, \bar{\boldsymbol{\sigma}} \rangle - 2(u_n \nabla u_n, \bar{\boldsymbol{\sigma}}) = 0, \quad \forall \bar{\boldsymbol{\sigma}} \in \boldsymbol{H}^1_{\sigma}(\Omega). \end{cases}$$
(1.48)

Once the Scheme **US** is solved, given $v_{n-1} \in H^2(\Omega)$ with $v_{n-1} \ge 0$, we can recover $v_n = v_n(u_n^2) \in H^2(\Omega)$ (with $v_n \ge 0$) solving:

$$\delta_t v_n + A v_n = u_n^2, \quad \text{a.e. } \boldsymbol{x} \in \Omega.$$
(1.49)

Remark 1.4.1 (Positivity and regularity of v_n) It is not difficult to prove that, given $u_n \in H^1(\Omega)$ and $v_{n-1} \in H^2(\Omega)$, there exists a unique $v_n \in H^2(\Omega)$ solution of (1.49). Even more, using the H³-regularity of problem (1.8), we can prove that $v_n \in H^3(\Omega)$. Moreover, if $v_{n-1} \ge 0$ then $v_n \ge 0$. Indeed, testing by $(v_n)_- = \min\{v_n, 0\} \le 0$ in (1.49), and taking into account that $(v_n)_- = 0$ if $(v_n) \ge 0$, as well as $(v_n)_- \in H^1(\Omega)$ with $\nabla((v_n)_-) = \nabla(v_n)$ if $(v_n) \le 0$, and $\nabla((v_n)_-) = 0$ if $(v_n) > 0$, we obtain

$$\frac{1}{k} \|(v_n)_-\|_0^2 - \frac{1}{k} \int_{\Omega} v_{n-1}(v_n)_- + \|\nabla((v_n)_-)\|_0^2 + \|((v_n)_-)\|_0^2 = \int_{\Omega} u_n^2((v_n)_-) \le 0.$$
(1.50)

Then, as $v_{n-1} \ge 0$, from (1.50) we conclude $||(v_n)_-||_1^2 \le 0$, which implies that $(v_n)_- \equiv 0$ a.e. $\boldsymbol{x} \in \Omega$, and thus, $v_n \ge 0$ in Ω .

Lemma 1.4.2 If $\sigma_{n-1} = \nabla v_{n-1}$, the schemes UV and US are equivalents in the following sense: If (u_n, v_n) is a solution of scheme UV then (u_n, σ_n) with $\sigma_n = \nabla v_n$ solves scheme US; and reciprocally, if (u_n, σ_n) is a solution of the scheme US and $v_n = v_n(u_n^2)$ is the unique solution of (1.49), then $\sigma_n = \nabla v_n$, and therefore (u_n, v_n) is a solution of the scheme UV.

Proof. Suppose that (u_n, v_n) is a solution of the scheme **UV**, then testing $(1.47)_2$ by $-\nabla \cdot \bar{\mathbf{w}}$, for any $\bar{\mathbf{w}} \in \boldsymbol{H}^1_{\sigma}(\Omega)$, and taking into account that $\operatorname{rot}(\nabla v_n) = 0$, we obtain

$$(\delta_t \nabla v_n, \bar{\mathbf{w}}) + \langle B \nabla v_n, \bar{\mathbf{w}} \rangle = 2(u_n \nabla u_n, \bar{\mathbf{w}}), \quad \forall \, \bar{\mathbf{w}} \in \boldsymbol{H}^1_{\sigma}(\Omega).$$
(1.51)

Then, defining $\sigma_n = \nabla v_n$ and assuming the hypothesis $\sigma_{n-1} = \nabla v_{n-1}$, from (1.51) we conclude that (u_n, σ_n) is solution of the scheme **US**. On the other hand, if (u_n, σ_n) is a solution of the scheme **US** and v_n satisfies (1.49), reasoning as above, we conclude that ∇v_n satisfies (1.51). Therefore, from (1.48)₂ and (1.51), we obtain

$$(\delta_t(\boldsymbol{\sigma}_n - \nabla v_n), \bar{\boldsymbol{\sigma}}) + \langle B(\boldsymbol{\sigma}_n - \nabla v_n), \bar{\boldsymbol{\sigma}} \rangle = 0, \quad \forall \, \bar{\boldsymbol{\sigma}} \in \boldsymbol{H}^1_{\boldsymbol{\sigma}}(\Omega).$$
(1.52)

Then, taking $\bar{\boldsymbol{\sigma}} = \boldsymbol{\sigma}_n - \nabla v_n$ in (1.52) and using the formula $a(a-b) = \frac{1}{2}(a^2-b^2) + \frac{1}{2}(a-b)^2$, we deduce

$$\delta_t \left(\frac{1}{2} \|\boldsymbol{\sigma}_n - \nabla v_n\|_0^2 \right) + \frac{k}{2} \|\delta_t (\boldsymbol{\sigma}_n - \nabla v_n)\|_0^2 + \|\boldsymbol{\sigma}_n - \nabla v_n\|_1^2 = 0,$$

which implies that $\boldsymbol{\sigma}_n = \nabla v_n$ using that $\boldsymbol{\sigma}_{n-1} = \nabla v_{n-1}$. Thus, we conclude that (u_n, v_n) is solution of the scheme UV.

Although, as it was said at the beginning, both time schemes **UV** and **US** are equivalent, we will study the scheme **US** with the variable σ_n in order to facilitate the notation throughout the paper. Moreover, both schemes furnish different fully discrete schemes considering for instance the spatial approximation by Finite Elements, which will be analyzed in Chapter 2. In fact, it will be necessary to use the variable σ_n in order to obtain a fully discrete unconditional energy-stable scheme.

1.4.1 Solvability, Energy-Stability and Convergence

Taking $\bar{u} = 1$ in $(1.48)_1$ we see that the scheme **US** is conservative, that is:

$$\int_{\Omega} u_n = \int_{\Omega} u_{n-1} = \dots = \int_{\Omega} u_0.$$
(1.53)

Moreover, integrating (1.49) in Ω , we deduce the following discrete in time equation for $\int_{\Omega} v_n$:

$$\delta_t \left(\int_{\Omega} v_n \right) + \int_{\Omega} v_n = \int_{\Omega} u_n^2. \tag{1.54}$$

Theorem 1.4.3 (Unconditional existence and conditional uniqueness) There exists $(u_n, \sigma_n) \in H^1(\Omega) \times H^1_{\sigma}(\Omega)$ solution of the scheme **US**, such that $u_n \ge 0$. Moreover, if

$$k \| (u_n, \boldsymbol{\sigma}_n) \|_1^4 \quad is \ small \ enough \tag{1.55}$$

then the solution of the scheme **US** is unique.

Proof. Let $(u_{n-1}, \sigma_{n-1}) \in H^1(\Omega) \times H^1_{\sigma}(\Omega)$ be given, with $u_{n-1} \ge 0$. The proof is divided into two parts.

<u>Part 1:</u> In order to prove the existence of $(u_n, \sigma_n) \in H^1(\Omega) \times H^1_{\sigma}(\Omega)$ solution of the scheme **US**, such that $u_n \geq 0$, we consider the following auxiliary problem:

$$\begin{cases} (\delta_t u_n, \bar{u}) + (\nabla u_n, \nabla \bar{u}) + ((u_n)_+ \boldsymbol{\sigma}_n, \nabla \bar{u}) = 0, \quad \forall \bar{u} \in H^1(\Omega), \\ (\delta_t \boldsymbol{\sigma}_n, \bar{\boldsymbol{\sigma}}) + \langle B \boldsymbol{\sigma}_n, \bar{\boldsymbol{\sigma}} \rangle - 2(u_n \nabla u_n, \bar{\boldsymbol{\sigma}}) = 0, \quad \forall \bar{\boldsymbol{\sigma}} \in \boldsymbol{H}^1_{\boldsymbol{\sigma}}(\Omega), \end{cases}$$
(1.56)

where $(u_n)_+ = \max\{u_n, 0\}$. In fact, it is the same scheme **US** but changing u_n by $(u_n)_+$ in the chemotaxis term.

A. Positivity of u_n : First, we will see that if $(u_n, \boldsymbol{\sigma}_n)$ is a solution of (1.56), then $u_n \ge 0$. Testing by $\bar{u} = (u_n)_- = \min\{u_n, 0\} \le 0$ in (1.56), and using that $((u_n)_+\boldsymbol{\sigma}_n, \nabla((u_n)_-)) = 0$, we obtain

$$\frac{1}{k} \|(u_n)_-\|_0^2 - \frac{1}{k} \int_{\Omega} u_{n-1}(u_n)_- + \|\nabla((u_n)_-)\|_0^2 = 0.$$

Then, using the fact that $u_{n-1} \ge 0$, one has that $||(u_n)_-||_1^2 \le 0$, and thus $(u_n)_- \equiv 0$ a.e. $\boldsymbol{x} \in \Omega$. Therefore, $u_n \ge 0$ in Ω .

B. Existence of solution of (1.56): It can be proven by using the Leray-Schauder fixed-point theorem. (See Appendix A).

Then, from parts A and B, we conclude that there exists $(u_n, \boldsymbol{\sigma}_n)$ solution of (1.56) with $u_n \geq 0$. In particular, taking into account that $u_n = (u_n)_+$, we conclude that $(u_n, \boldsymbol{\sigma}_n)$ is also a solution of the scheme **US**, with $u_n \geq 0$.

<u>Part 2:</u> In order to prove the uniqueness of solution $(u_n, \boldsymbol{\sigma}_n)$ of the scheme **US**, we suppose that there exist $(u_n^1, \boldsymbol{\sigma}_n^1), (u_n^2, \boldsymbol{\sigma}_n^2) \in H^1(\Omega) \times \boldsymbol{H}_{\sigma}^1(\Omega)$ two possible solutions of (1.48). Then, defining $u_n = u_n^1 - u_n^2$ and $\boldsymbol{\sigma}_n = \boldsymbol{\sigma}_n^1 - \boldsymbol{\sigma}_n^2$, we have that $(u_n, \boldsymbol{\sigma}_n) \in H^1(\Omega) \times \boldsymbol{H}_{\sigma}^1(\Omega)$ satisfies

$$\frac{1}{k}(u_n,\bar{u}) + (\nabla u_n,\nabla\bar{u}) + (u_n^1\boldsymbol{\sigma}_n,\nabla\bar{u}) + (u_n\boldsymbol{\sigma}_n^2,\nabla\bar{u}) = 0, \ \forall \bar{u} \in H^1(\Omega), \tag{1.57}$$

$$\frac{1}{k}(\boldsymbol{\sigma}_n, \bar{\boldsymbol{\sigma}}) + \langle B\boldsymbol{\sigma}_n, \bar{\boldsymbol{\sigma}} \rangle - 2(u_n^1 \nabla u_n, \bar{\boldsymbol{\sigma}}) - 2(u_n \nabla u_n^2, \bar{\boldsymbol{\sigma}}) = 0, \ \forall \bar{\boldsymbol{\sigma}} \in \boldsymbol{H}_{\sigma}^1(\Omega).$$
(1.58)

Taking $\bar{u} = u_n$, $\bar{\sigma} = \frac{1}{2}\sigma_n$ in (1.57)-(1.58) and adding the resulting expressions, the terms $(u_n^1 \sigma_n, \nabla u_n)$ cancel, and using the fact that $\int_{\Omega} u_n = 0$, we obtain

$$\frac{1}{2k} \|(u_n, \boldsymbol{\sigma}_n)\|_0^2 + \frac{1}{2} \|(u_n, \boldsymbol{\sigma}_n)\|_1^2 \\
\leq \|u_n\|_{L^3} \|\boldsymbol{\sigma}_n^2\|_{L^6} \|\nabla u_n\|_0 + \|u_n\|_{L^3} \|\nabla u_n^2\|_0 \|\boldsymbol{\sigma}_n\|_{L^6} \\
\leq C \|u_n\|_0^{1/2} \|\boldsymbol{\sigma}_n^2\|_{L^6} \|u_n\|_1^{3/2} + C \|u_n\|_0^{1/2} \|u_n\|_1^{1/2} \|\nabla u_n^2\|_0 \|\boldsymbol{\sigma}_n\|_1^2 \\
\leq \frac{1}{4} \|(u_n, \boldsymbol{\sigma}_n)\|_1^2 + C \|u_n\|_0^2 \|\boldsymbol{\sigma}_n^2\|_1^4 + C \|u_n\|_0^2 \|\nabla u_n^2\|_0^4,$$

which implies that

$$\frac{1}{2} \| (u_n, \boldsymbol{\sigma}_n) \|_0^2 + \frac{k}{4} \| (u_n, \boldsymbol{\sigma}_n) \|_1^2 \le C k \left(\| \nabla u_n^2 \|_0^4 + \| \boldsymbol{\sigma}_n^2 \|_1^4 \right) \| (u_n, \boldsymbol{\sigma}_n) \|_0^2.$$

Therefore, since $k(\|\nabla u_n^2\|_0^4 + \|\boldsymbol{\sigma}_n^2\|_1^4)$ is small enough (from hypothesis (1.55)), we conclude that $\|(u_n, \boldsymbol{\sigma}_n)\|_1 = 0$, thus $u_n^1 = u_n^2$ and $\boldsymbol{\sigma}_n^1 = \boldsymbol{\sigma}_n^2$.
Remark 1.4.4 In the case of 2D domains, using estimate (1.75) (see Theorem 1.4.20 below), the uniqueness restriction (1.55) can be relaxed to $k K_0^2$ small enough, where K_0 is the constant appearing in (1.75) which depends on data (Ω, u_0, σ_0), but is independent of n.

Definition 1.4.5 A numerical scheme with solution (u_n, σ_n) is called energy-stable with respect to the energy $\mathcal{E}(u, \sigma)$ given in (1.26) if this energy is time decreasing, that is

$$\mathcal{E}(u_n, \boldsymbol{\sigma}_n) \le \mathcal{E}(u_{n-1}, \boldsymbol{\sigma}_{n-1}), \quad \forall n.$$
(1.59)

In the next Lemma, we obtain unconditional energy-stability for the scheme US.

Lemma 1.4.6 (Unconditional stability) The scheme **US** is unconditionally energy-stable with respect to $\mathcal{E}(u, \boldsymbol{\sigma})$. In fact, for any $(u_n, \boldsymbol{\sigma}_n)$ solution of scheme **US**, the following discrete energy law holds

$$\delta_t \mathcal{E}(u_n, \boldsymbol{\sigma}_n) + \frac{k}{2} \|\delta_t u_n\|_0^2 + \frac{k}{4} \|\delta_t \boldsymbol{\sigma}_n\|_0^2 + \|\nabla u_n\|_0^2 + \frac{1}{2} \|\boldsymbol{\sigma}_n\|_1^2 = 0.$$
(1.60)

Proof. Taking $\bar{u} = u_n$ in $(1.48)_1$ and $\bar{\sigma} = \frac{1}{2}\sigma_n$ in $(1.48)_2$ and adding the resulting expressions, the chemotaxis and production terms cancel, obtaining (1.60).

Remark 1.4.7 Comparing the energy law (1.22) of the continuous problem, and the discrete version (1.60), we can say that the scheme **US** introduces the following two first order "numerical dissipation terms":

$$\frac{k}{2} \|\delta_t u_n\|_0^2 \quad and \quad \frac{k}{4} \|\delta_t \boldsymbol{\sigma}_n\|_0^2.$$

From the (local in time) discrete energy law (1.60), we deduce the following global in time estimates for any (u_n, σ_n) solution of the scheme **US**:

Theorem 1.4.8 (Uniform Weak estimates) Let (u_n, σ_n) be a solution of the scheme **US**. Then, the following estimates hold

$$\|(u_n, \boldsymbol{\sigma}_n)\|_0^2 + k^2 \sum_{m=1}^n \|(\delta_t u_m, \delta_t \boldsymbol{\sigma}_m)\|_0^2 + k \sum_{m=1}^n \|(\nabla u_m, \boldsymbol{\sigma}_m)\|_{L^2 \times H^1}^2 \le C_0, \quad \forall n \ge 1, \quad (1.61)$$
$$k \sum_{m=n_0+1}^{n_0+n} \|(u_m, \boldsymbol{\sigma}_m)\|_1^2 \le C_0 + C_1(nk), \quad \forall n \ge 1, \quad (1.62)$$

where $n_0 \ge 0$ is any integer and C_0, C_1 are positive constants depending on the data $(u_0, \boldsymbol{\sigma}_0)$ and (Ω, u_0) respectively, but independent of n_0 , k and n. *Proof.* Observe that from the discrete energy law (1.60), we have

$$\frac{1}{4} \| (u_n, \boldsymbol{\sigma}_n) \|_0^2 + \frac{k^2}{4} \sum_{m=1}^n \| (\delta_t u_m, \delta_t \boldsymbol{\sigma}_m) \|_0^2 + \frac{k}{2} \sum_{m=1}^n \| (\nabla u_m, \boldsymbol{\sigma}_m) \|_{L^2 \times H^1}^2 \le \frac{1}{2} \| (u_0, \boldsymbol{\sigma}_0) \|_0^2,$$

which implies (1.61). Moreover, starting again from (1.60), but now summing for m from $n_0 + 1$ to $n + n_0$, using (1.61) and the Poincaré inequality for the zero-mean value function $u_m - m_0$, where $m_0 = \frac{1}{|\Omega|} \int_{\Omega} u_0 = \frac{1}{|\Omega|} \int_{\Omega} u_m$, we have $k \sum_{m=n_0+1}^{n_0+n} \|(u_m - m_0, \boldsymbol{\sigma}_m)\|_1^2 \leq C_0,$

and thus, we deduce (1.62).

Remark 1.4.9 The proofs of solvability (without positivity) and unconditional energy-stability of the scheme **US** (see Theorems 1.4.3 and 1.4.8, and Lemma 1.4.6) can be followed almost line by line if we consider a fully discrete scheme corresponding to a Finite Element approximation of **US**, that is, if we take any finite-dimensional subspaces $U_h \subset H^1(\Omega)$ and $\Sigma_h \subset H^1_{\sigma}(\Omega)$ instead of $H^1(\Omega)$ and $H^1_{\sigma}(\Omega)$ respectively.

Corollary 1.4.10 (Estimates for v_n) If $v_n = v_n(u_n^2)$ is the solution of (1.49), it holds

$$\|v_n\|_{L^1} \le K_0, \quad \forall n \ge 0,$$
 (1.63)

where $K_0 > 0$ depends on the data (u_0, σ_0, v_0) , but independent of k and n. Moreover, the following estimates hold

$$\|v_n\|_1^2 \le K_0, \quad and \quad k \sum_{m=n_0+1}^{n_0+n} \|v_m\|_2^2 \le K_0 + K_1(nk), \quad \forall n \ge 1,$$
 (1.64)

with $K_1 > 0$ depending on the data $u_0, \boldsymbol{\sigma}_0, v_0, \Omega$, but independent of n_0, k and n.

Proof. From (1.54) and (1.61) we have

$$(1+k)\|v_i\|_{L^1} - \|v_{i-1}\|_{L^1} = k\|u_i\|_0^2 \le kC_0.$$
(1.65)

Then, multiplying (1.65) by $(1+k)^{i-1}$ and summing for $i = 1, \dots, n$, we obtain

$$(1+k)^n \|v_n\|_{L^1} \le \|v_0\|_{L^1} + k C_0 \sum_{i=0}^{n-1} (1+k)^i$$

and taking into account that

$$\sum_{i=0}^{n-1} (1+k)^i = \frac{1-(1+k)^n}{1-(1+k)} = \frac{1}{k}((1+k)^n - 1) \le \frac{1}{k}(1+k)^n,$$

we conclude

$$||v_n||_{L^1} \le (1+k)^{-n} ||v_0||_{L^1} + C_0 \le ||v_0||_{L^1} + C_0,$$

which implies (1.63). Finally, taking into account the relation $\sigma_n = \nabla v_n$, from (1.61)-(1.63), we can deduce (1.64).

Starting from the previous stability estimates, following the ideas of [9] we can prove the convergence towards weak solutions. For this, let us to introduce the functions:

- $(\widetilde{u}_k, \widetilde{\boldsymbol{\sigma}}_k)$ are continuous functions on $[0, +\infty)$, linear on each interval (t_{n-1}, t_n) and equal to $(u_n, \boldsymbol{\sigma}_n)$ at $t = t_n, n \ge 0$;
- (u_k^r, σ_k^r) as the piecewise constant functions taking values (u_n, σ_n) on $(t_{n-1}, t_n]$, $n \ge 1$.

Theorem 1.4.11 (Convergence) There exists a subsequence (k') of (k), with $k' \downarrow 0$, and a weak solution (u, σ) of (1.3) in $(0, +\infty)$, such that $(\tilde{u}_{k'}, \tilde{\sigma}_{k'})$ and $(u_{k'}^r, \sigma_{k'}^r)$ converge to (u, σ) weakly- \star in $L^{\infty}(0, +\infty; L^2(\Omega) \times L^2(\Omega))$, weakly in $L^2(0, T; H^1(\Omega) \times H^1(\Omega))$ and strongly in $L^2(0, T; L^2(\Omega) \times L^2(\Omega))$, for any T > 0.

Proof. Observe that (1.48) can be rewritten as:

$$\begin{cases} \left(\frac{d}{dt}\tilde{u}_{k}(t),\bar{u}\right) + \left(\nabla u_{k}^{r}(t),\nabla\bar{u}\right) + \left(u_{k}^{r}(t)\boldsymbol{\sigma}_{k}^{r}(t),\nabla\bar{u}\right) = 0, \quad \forall \bar{u} = \bar{u}(t), \quad \text{for } t \in [0,+\infty) \setminus \{t_{n}\}, \\ \left(\frac{d}{dt}\tilde{\boldsymbol{\sigma}}_{k}(t),\bar{\boldsymbol{\sigma}}\right) + \left\langle B\boldsymbol{\sigma}_{k}^{r}(t),\bar{\boldsymbol{\sigma}}\right\rangle - 2\left(u_{k}^{r}(t)\nabla u_{k}^{r}(t),\bar{\boldsymbol{\sigma}}\right) = 0, \quad \forall \bar{\boldsymbol{\sigma}} = \bar{\boldsymbol{\sigma}}(t), \quad \text{for } t \in [0,+\infty) \setminus \{t_{n}\}, \end{cases}$$

$$(1.66)$$

where $\bar{u}(t)|_{I_n} = \bar{u}_n \in H^1(\Omega)$ and $\bar{\boldsymbol{\sigma}}(t)|_{I_n} = \bar{\boldsymbol{\sigma}}_n \in \boldsymbol{H}^1_{\boldsymbol{\sigma}}(\Omega)$, with $I_n := [t_{n-1}, t_n]$. From Theorem 1.4.8 we have that $(\tilde{u}_k, \tilde{\boldsymbol{\sigma}}_k)$ and $(u_k^r, \boldsymbol{\sigma}_k^r)$ are bounded in $L^{\infty}(0, +\infty; L^2(\Omega) \times \boldsymbol{L}^2(\Omega)) \cap L^2(0, T; H^1(\Omega) \times \boldsymbol{H}^1(\Omega))$. Moreover, using (1.61), it is not difficult to prove that $\tilde{u}_k - u_k^r$ and $\tilde{\boldsymbol{\sigma}}_k - \boldsymbol{\sigma}_k^r$ converge to 0 in $L^2(0, T; L^2(\Omega))$ as $k \to 0$, for any T > 0. More precisely, we have $\|\tilde{u}_k - u_k^r, \tilde{\boldsymbol{\sigma}}_k - \boldsymbol{\sigma}_k^r\|_{L^2(0,T; L^2(\Omega))} \leq (C_0 k/3)^{1/2}$. Therefore, there exists a subsequence (k')of (k) and limit functions u and $\boldsymbol{\sigma}$ verifying the following convergence as $k' \to 0$:

$$(\widetilde{u}_{k'}, \widetilde{\boldsymbol{\sigma}}_{k'}) \to u, \quad (u_{k'}^r, \boldsymbol{\sigma}_{k'}^r) \to u \quad \text{in} \quad \begin{cases} L^{\infty}(0, +\infty; L^2(\Omega) \times \boldsymbol{L}^2(\Omega)) - \text{weak}^* \\ L^2(0, T; H^1(\Omega) \times \boldsymbol{H}^1(\Omega)) - \text{weak}. \end{cases}$$

Moreover, we can deduce $\frac{d}{dt}(\tilde{u}_{k'}, \tilde{\boldsymbol{\sigma}}_{k'})$ is bounded in $L^{4/3}(0, T; H^1(\Omega)' \times \boldsymbol{H}^1(\Omega)')$. Therefore, a compactness result of Aubin-Lions type implies that the sequence is compact in $L^2(0, T; L^2(\Omega) \times \boldsymbol{L}^2(\Omega))$. This implies the strong convergence of both subsequences $(\tilde{u}_k, \tilde{\boldsymbol{\sigma}}_k)$ and $(u_k^r, \boldsymbol{\sigma}_k^r)$ in $L^2(0, T; L^2(\Omega) \times \boldsymbol{L}^2(\Omega))$; and passing to the limit in (1.66), we obtain that $(u, \boldsymbol{\sigma})$ satisfies (1.23)-(1.24).

Now, in order to obtain that (u, σ) satisfies energy inequality (1.25), we test (1.66)₁ by $\bar{u} = u_k^r(t)$ and (1.66)₂ by $\bar{\sigma} = \frac{1}{2}\sigma_k^r(t)$, and taking into account that $\tilde{u}_k|_{I_n} = u_n + \frac{t_n - t}{k}(u_{n-1} - u_n)$ (and $\tilde{\sigma}_k$ is defined in the same way), we obtain

$$\frac{d}{dt}\left(\frac{1}{2}\|\widetilde{u}_k(t)\|_0^2 + \frac{1}{4}\|\widetilde{\boldsymbol{\sigma}}_k(t)\|_0^2\right) + (t_n - t)\|(\delta_t u_n, \delta_t \boldsymbol{\sigma}_n)\|_0^2 + \|\nabla u_k^r(t)\|_0^2 + \frac{1}{2}\|\boldsymbol{\sigma}_k^r(t)\|_1^2 = 0,$$

for any $t \in (t_{n-1}, t_n)$, which implies that

$$\frac{d}{dt}\mathcal{E}(\widetilde{u}_{k}(t),\widetilde{\boldsymbol{\sigma}}_{k}(t)) + \|\nabla u_{k}^{r}(t)\|_{0}^{2} + \frac{1}{2}\|\boldsymbol{\sigma}_{k}^{r}(t)\|_{1}^{2} \le 0, \text{ for } t \in [0,+\infty) \setminus \{t_{n}\}.$$
(1.67)

Then, integrating (1.67) in time from t_0 to t_1 , with $t_0, t_1 \in [0, +\infty)$, and taking into account that

$$\int_{t_0}^{t_1} \frac{d}{dt} \mathcal{E}(\widetilde{u}_k(t), \widetilde{\boldsymbol{\sigma}}_k(t)) = \mathcal{E}(\widetilde{u}_k(t_1), \widetilde{\boldsymbol{\sigma}}_k(t_1)) - \mathcal{E}(\widetilde{u}_k(t_0), \widetilde{\boldsymbol{\sigma}}_k(t_0)) \quad \forall t_0 < t_1$$

since $\mathcal{E}(\widetilde{u}_k(t), \widetilde{\boldsymbol{\sigma}}_k(t))$ is continuous in time, we deduce

$$\mathcal{E}(\widetilde{u}_{k}(t_{1}),\widetilde{\boldsymbol{\sigma}}_{k}(t_{1})) - \mathcal{E}(\widetilde{u}_{k}(t_{0}),\widetilde{\boldsymbol{\sigma}}_{k}(t_{0})) + \int_{t_{0}}^{t_{1}} (\|\nabla u_{k}^{r}(t)\|_{0}^{2} + \frac{1}{2}\|\boldsymbol{\sigma}_{k}^{r}(t)\|_{1}^{2})dt \leq 0, \quad \forall t_{0} < t_{1}.$$
(1.68)

Finally, we will prove that

$$\mathcal{E}(\widetilde{u}_{k'}(t), \widetilde{\boldsymbol{\sigma}}_{k'}(t)) \to \mathcal{E}(u(t), \boldsymbol{\sigma}(t)), \text{ a.e. } t \in [0, +\infty).$$
 (1.69)

Indeed, for any T > 0,

$$\begin{aligned} \|\mathcal{E}(\widetilde{u}_{k'}(t),\widetilde{\boldsymbol{\sigma}}_{k'}(t)) - \mathcal{E}(u(t),\boldsymbol{\sigma}(t))\|_{L^{1}(0,T)} &= \int_{0}^{T} |\mathcal{E}(\widetilde{u}_{k'}(t),\widetilde{\boldsymbol{\sigma}}_{k'}(t)) - \mathcal{E}(u(t),\boldsymbol{\sigma}(t))| dt \\ &= \int_{0}^{T} \left| \frac{1}{2} \left(\|\widetilde{u}_{k'}(t)\|_{0}^{2} - \|u(t)\|_{0}^{2} \right) + \frac{1}{4} \left(\|\widetilde{\boldsymbol{\sigma}}_{k'}(t)\|_{0}^{2} - \|\boldsymbol{\sigma}(t)\|_{0}^{2} \right) \right| dt \\ &\leq \frac{1}{2} \|\widetilde{u}_{k'} - u\|_{L^{2}(0,T;L^{2})} (\|\widetilde{u}_{k'}\|_{L^{2}(0,T;L^{2})} + \|u\|_{L^{2}(0,T;L^{2})}) \\ &+ \frac{1}{4} \|\widetilde{\boldsymbol{\sigma}}_{k'} - \boldsymbol{\sigma}\|_{L^{2}(0,T;L^{2})} (\|\widetilde{\boldsymbol{\sigma}}_{k'}\|_{L^{2}(0,T;L^{2})} + \|\boldsymbol{\sigma}\|_{L^{2}(0,T;L^{2})}), \end{aligned}$$
(1.70)

and taking into account that $(\tilde{u}_{k'}, \tilde{\boldsymbol{\sigma}}_{k'}) \to (u, \boldsymbol{\sigma})$ strongly in $L^2(0, T; L^2(\Omega))$ for any T > 0, from (1.70) we conclude that $\mathcal{E}(\tilde{u}_{k'}(t), \tilde{\boldsymbol{\sigma}}_{k'}(t)) \to \mathcal{E}(u(t), \boldsymbol{\sigma}(t))$ strongly in $L^1(0, T)$ for all T > 0, which implies (1.69). Then, taking into account that $(u_{k'}^r, \boldsymbol{\sigma}_{k'}^r) \to (u, \boldsymbol{\sigma})$ weakly in $L^2(0, T; H^1(\Omega) \times \boldsymbol{H}^1(\Omega))$, we deduce

$$\liminf_{k' \to 0} \int_{t_0}^{t_1} (\|\nabla u_{k'}^r(t)\|_0^2 + \frac{1}{2} \|\boldsymbol{\sigma}_{k'}^r(t)\|_1^2) dt \ge \int_{t_0}^{t_1} (\|\nabla u(t)\|_0^2 + \frac{1}{2} \|\boldsymbol{\sigma}(t)\|_1^2) dt \quad \forall t_1 \ge t_0 \ge 0$$

and, owing to (1.69),

$$\liminf_{k'\to 0} \left[\mathcal{E}(\widetilde{u}_{k'}(t_1), \widetilde{\boldsymbol{\sigma}}_{k'}(t_1)) - \mathcal{E}(\widetilde{u}_{k'}(t_0), \widetilde{\boldsymbol{\sigma}}_{k'}(t_0)) \right] = \mathcal{E}(u(t_1), \boldsymbol{\sigma}(t_1)) - \mathcal{E}(u(t_0), \boldsymbol{\sigma}(t_0)),$$

for a.e. $t_1, t_0 : t_1 \ge t_0 \ge 0$. Thus, taking lim inf as $k' \to 0$ in the inequality (1.68), we deduce the energy inequality (1.25) for a.e. $t_0, t_1 : t_1 \ge t_0 \ge 0$.

Analogously, if we introduce the functions:

- \widetilde{v}_k are continuous functions on $[0, +\infty)$, linear on each interval (t_{n-1}, t_n) and equal to v_n , at $t = t_n$, $n \ge 0$;
- v_k^r as the piecewise constant functions taking values v_n on $(t_{n-1}, t_n], n \ge 1$,

the following result can be proved:

Lemma 1.4.12 There exists a subsequence (k') of (k), with $k' \downarrow 0$, and a strong solution v of (1.4) in $(0, +\infty)$, such that $\tilde{v}_{k'}$ and $v_{k'}^r$ converge to v weakly- \star in $L^{\infty}(0, +\infty; H^1(\Omega))$, weakly in $L^2(0, T; H^2(\Omega))$ and strongly in $L^2(0, T; H^1(\Omega)) \cap C([0, T]; L^p(\Omega))$, for $1 \le p < 6$ and any T > 0.

Proof. Observe that (1.49) can be rewritten as:

$$\frac{d}{dt}\widetilde{v}_k(t) + Av_k^r(t) = (u_k^r(t))^2, \text{ for } t \in [0, +\infty) \setminus \{t_n\},$$
(1.71)

From estimate (1.64) we have that \tilde{v}_k and v_k^r are bounded in $L^{\infty}(0, +\infty; H^1(\Omega)) \cap L^2(0, T; H^2(\Omega))$. Moreover, it is not difficult to prove that $\tilde{v}_k - v_k^r$ converge to 0 in $L^2(0, T; H^1(\Omega))$ as $k \to 0$, for any T > 0. Therefore, there exists a subsequence (k') of (k) and a limit function vverifying the following convergence as $k' \to 0$:

$$\widetilde{v}_{k'} \to v, \quad v_{k'}^r \to v \quad \text{in} \quad \begin{cases} L^{\infty}(0, +\infty; H^1(\Omega)) \text{-weak}^* \\ L^2(0, T; H^2(\Omega)) \text{-weak}. \end{cases}$$

Moreover, we can deduce that $\frac{d}{dt} \tilde{v}_{k'}$ is bounded in $L^{4/3}(0,T;L^2(\Omega))$. Therefore, a compactness result of Aubin-Lions type implies that the sequence is compact in $L^2(0,T;H^1(\Omega)) \cap C([0,T];L^p(\Omega))$, for $1 \leq p < 6$. This implies the strong convergence of both subsequences \tilde{v}_k and v_k^r in $L^2(0,T;H^1(\Omega)) \cap C([0,T];L^p(\Omega))$; and passing to the limit in (1.71), we obtain that v satisfies (1.19).

1.4.2 Uniform strong estimates

In this section, we are going to obtain a priori estimates in strong norms for $(u_n, \boldsymbol{\sigma}_n)$ solution of the scheme **US**. First, in the following proposition, we shall show H^2 -regularity for $(u_n, \boldsymbol{\sigma}_n)$.

Proposition 1.4.13 Let $(u_{n-1}, \sigma_{n-1}) \in H^1(\Omega) \times H^1_{\sigma}(\Omega)$. If $(u_n, \sigma_n) \in H^1(\Omega) \times H^1_{\sigma}(\Omega)$ is solution of the scheme **US**, then $(u_n, \sigma_n) \in H^2(\Omega) \times H^2(\Omega)$. Moreover, the following estimate holds

$$\|(u_n, \boldsymbol{\sigma}_n)\|_2 \le C\left(\|(\delta_t u_n, \delta_t \boldsymbol{\sigma}_n)\|_0 + \|(u_n, \boldsymbol{\sigma}_n)\|_1^3 + \|u_n\|_0\right),$$
(1.72)

where C is a constant depending on data $(\Omega, u_0, \boldsymbol{\sigma}_0)$, but independent of k and n.

Proof. Recall that we have assumed the H^2 and H^3 -regularity of problem (1.8), which implies the H^2 -regularity of problem (1.9) in the case of $\mathbf{f} = \nabla h$ for some $h \in H^1(\Omega)$. Moreover, observe that scheme **US** can be rewrite in terms of the operators A and B as follows

$$\begin{cases} Au_n = u_n - \delta_t u_n + \nabla \cdot (u_n \boldsymbol{\sigma}_n), \\ B\boldsymbol{\sigma}_n = -\delta_t \boldsymbol{\sigma}_n + 2u_n \nabla u_n. \end{cases}$$

Now, since $(u_n, \boldsymbol{\sigma}_n) \in H^1(\Omega) \times \boldsymbol{H}^1_{\boldsymbol{\sigma}}(\Omega)$, we have that $\nabla u_n \in \mathbf{L}^2(\Omega)$, $\nabla \cdot \boldsymbol{\sigma}_n \in L^2(\Omega)$ and, from Sobolev embeddings, $(u_n, \boldsymbol{\sigma}_n) \in L^6(\Omega) \times \mathbf{L}^6(\Omega)$. Consequently, we get $\nabla \cdot (u_n \boldsymbol{\sigma}_n) =$ $\boldsymbol{\sigma}_n \cdot \nabla u_n + u_n \nabla \cdot \boldsymbol{\sigma}_n \in L^{3/2}(\Omega)$ and, using the fact that $u_n, \delta_t u_n \in L^2(\Omega) \hookrightarrow L^{3/2}(\Omega)$, from classical elliptic regularity we conclude that $u_n \in W^{2,3/2}(\Omega)$. Analogously, since $u_n \in$ $W^{2,3/2}(\Omega)$, we have $\nabla u_n \in \boldsymbol{W}^{1,3/2}(\Omega) \hookrightarrow \boldsymbol{L}^3(\Omega)$, and therefore $u_n \nabla u_n \in \boldsymbol{L}^2(\Omega)$. Thus, using the fact that $\delta_t \boldsymbol{\sigma}_n \in L^2(\Omega)$ and taking into account that $-\delta_t \boldsymbol{\sigma}_n + 2u_n \nabla u_n = \nabla(-\delta_t v_n + u_n^2)$, with $-\delta_t v_n + u_n^2 \in H^1(\Omega)$, we conclude that $\boldsymbol{\sigma}_n \in \boldsymbol{H}^2(\Omega)$. Finally, taking into account that $\boldsymbol{\sigma}_n \in \boldsymbol{H}^2(\Omega)$ and $u_n \in W^{2,3/2}(\Omega)$, we deduce that $\nabla \cdot (u_n \boldsymbol{\sigma}_n) \in L^2(\Omega)$, and thus, since $u_n, \delta_t u_n \in L^2(\Omega)$, we conclude that $u_n \in H^2(\Omega)$. Besides, from (1.10)₁-(1.11), the interpolation inequality (1.13), using the Hölder and Young inequalities, we have

$$\begin{aligned} \|u_n\|_2 &\leq C \left(\|\delta_t u_n\|_0 + \|u_n \nabla \cdot \boldsymbol{\sigma}_n\|_0 + \|\boldsymbol{\sigma}_n \cdot \nabla u_n\|_0 + \|u_n\|_0 \right) \\ &\leq C \left(\|\delta_t u_n\|_0 + \|u_n\|_0 \right) + \frac{1}{2} \|\boldsymbol{\sigma}_n\|_2 + C \|u_n\|_1^2 \|\boldsymbol{\sigma}_n\|_1 + \frac{1}{4} \|u_n\|_2 + C \|u_n\|_1 \|\boldsymbol{\sigma}_n\|_1^2.73) \end{aligned}$$

and

$$\|\boldsymbol{\sigma}_{n}\|_{2} \leq C\left(\|\delta_{t}\boldsymbol{\sigma}_{n}\|_{0} + \|u_{n}\nabla u_{n}\|_{0}\right) \leq C\left(\|\delta_{t}\boldsymbol{\sigma}_{n}\|_{0} + \|u_{n}\|_{L^{6}}\|\nabla u_{n}\|_{L^{3}}\right)$$

$$\leq C\|\delta_{t}\boldsymbol{\sigma}_{n}\|_{0} + \frac{1}{4}\|u_{n}\|_{2} + C\|u_{n}\|_{1}^{3}.$$
 (1.74)

Then, adding (1.73) and (1.74), we conclude (1.72).

Now, assuming the estimate

$$\|(u_n, \boldsymbol{\sigma}_n)\|_1^2 \le K_0, \quad \forall n \ge 0, \tag{1.75}$$

with $K_0 > 0$ independent of k and n, we will prove uniform strong and more regular estimates for the scheme **US**. Later, in the next section, we will prove that condition (1.75) holds, at least, in 2D domains.

Theorem 1.4.14 (Strong estimates) Let (u_n, σ_n) be a solution of the scheme **US** satisfying the assumption (1.75). Then, the following estimate holds

$$k \sum_{m=n_0+1}^{n_0+n} (\|(\delta_t u_m, \delta_t \boldsymbol{\sigma}_m)\|_0^2 + \|(u_m, \boldsymbol{\sigma}_m)\|_2^2) \le K_1 + K_2(nk), \quad \forall n \ge 1,$$
(1.76)

for any integer $n_0 \ge 0$, with positive constants K_1, K_2 depending on $(\Omega, u_0, \boldsymbol{\sigma}_0)$, but independent of n_0 , k and n.

Proof. Testing (1.48) by $\bar{u} = \delta_t u_n$ and $\bar{\sigma} = \delta_t \sigma_n$, and taking into account that from (1.53) we have $||u_n||_1^2 - ||u_{n-1}||_1^2 = ||\nabla u_n||_0^2 - ||\nabla u_{n-1}||_0^2$, we can deduce

$$\frac{1}{2} \| (\delta_t u_n, \delta_t \boldsymbol{\sigma}_n) \|_0^2 + \delta_t \left(\frac{1}{2} \| (u_n, \boldsymbol{\sigma}_n) \|_1^2 \right) + \frac{k}{2} \| (\delta_t u_n, \delta_t \boldsymbol{\sigma}_n) \|_1^2 \le C(\|\nabla \cdot (u_n \boldsymbol{\sigma}_n) \|_0^2 + \|2u_n \nabla u_n\|_0^2).$$
(1.77)

Moreover, using (1.13), (1.61), (1.72) and (1.75), we obtain

$$\begin{aligned} \|\boldsymbol{\sigma}_{n} \cdot \nabla u_{n}\|_{0}^{2} + \|u_{n} \nabla \cdot \boldsymbol{\sigma}_{n}\|_{0}^{2} + \|2u_{n} \nabla u_{n}\|_{0}^{2} &\leq C \|(u_{n}, \boldsymbol{\sigma}_{n})\|_{1}^{3} \|(u_{n}, \boldsymbol{\sigma}_{n})\|_{2} \\ &\leq C \|(\delta_{t} u_{n}, \delta_{t} \boldsymbol{\sigma}_{n})\|_{0} + C \leq \frac{1}{4} \|(\delta_{t} u_{n}, \delta_{t} \boldsymbol{\sigma}_{n})\|_{0}^{2} + C, \ (1.78) \end{aligned}$$

where the constant C is independent of k and n. Therefore, from (1.77)-(1.78), we deduce

$$\delta_t(\|(u_n, \boldsymbol{\sigma}_n)\|_1^2) + k\|(\delta_t u_n, \delta_t \boldsymbol{\sigma}_n)\|_1^2 + \frac{1}{2}\|(\delta_t u_n, \delta_t \boldsymbol{\sigma}_n)\|_0^2 \le C.$$
(1.79)

Then, multiplying (1.79) by k, summing for m from $n_0 + 1$ to $n + n_0$ and using (1.75), we have $n_0 + n$

$$k \sum_{m=n_0+1}^{N_0+n} \| (\delta_t u_m, \delta_t \boldsymbol{\sigma}_m) \|_0^2 \le K_0 + K_1(nk),$$

which, taking into account (1.72), implies (1.76).

From Theorem 1.4.14 and Corollary 1.4.10, we deduce strong estimates for v_n .

Corollary 1.4.15 Let v_n be the solution of (1.49). Under the hypothesis of Theorem 1.4.14, the following estimates hold

$$\|v_n\|_2^2 \le K_0 \quad and \quad k \sum_{m=n_0+1}^{n_0+n} \|v_n\|_3^2 \le K_0 + K_1(nk), \quad \forall n \ge 1,$$
 (1.80)

for any integer $n_0 \geq 0$, with positive constants K_0, K_1 depending on $(\Omega, u_0, \boldsymbol{\sigma}_0, v_0)$, but independent of n_0 , k and n.

Theorem 1.4.16 (More regular estimates) Assume that $(u_0, \sigma_0) \in H^2(\Omega) \times H^2(\Omega)$. Under the hypothesis of Theorem 1.4.14, the following estimates hold

$$\|(\delta_t u_n, \delta_t \boldsymbol{\sigma}_n)\|_0^2 \le C_3, \quad \forall n \ge 1,$$
(1.81)

$$k \sum_{m=n_0+1}^{n_0+n} \| (\delta_t u_m, \delta_t \boldsymbol{\sigma}_m) \|_1^2 \le C_4 + C_5(nk), \quad \forall n \ge 1,$$
(1.82)

$$\|(u_n, \boldsymbol{\sigma}_n)\|_2 \le C_6, \quad \forall n \ge 0, \tag{1.83}$$

for any integer $n_0 \ge 0$, with positive constants C_3, C_4, C_5, C_6 depending on data $(\Omega, u_0, \boldsymbol{\sigma}_0)$, but independent of n_0 , k and n.

Remark 1.4.17 In particular, from (1.83) one has $||(u_n, \sigma_n)||_{L^{\infty}} \leq C_7$ for all $n \geq 0$, with $C_7 > 0$ a constant independent of k and n.

Proof. Denote by $\tilde{u}_n = \delta_t u_n$ and $\tilde{\boldsymbol{\sigma}}_n = \delta_t \boldsymbol{\sigma}_n$. Then, making the time discrete derivative of (1.48), and using the equality $\delta_t(a_n b_n) = (\delta_t a_n)b_{n-1} + a_n(\delta_t b_n)$, we obtain that $(\tilde{u}_n, \tilde{\boldsymbol{\sigma}}_n)$ satisfies

$$\begin{cases} (\delta_t \widetilde{u}_n, \overline{u}) + (\nabla \widetilde{u}_n, \nabla \overline{u}) + (\widetilde{u}_n \boldsymbol{\sigma}_{n-1}, \nabla \overline{u}) + (u_n \widetilde{\boldsymbol{\sigma}}_n, \nabla \overline{u}) = 0, \\ (\delta_t \widetilde{\boldsymbol{\sigma}}_n, \overline{\boldsymbol{\sigma}}) + \langle B \widetilde{\boldsymbol{\sigma}}_n, \overline{\boldsymbol{\sigma}} \rangle = 2(\widetilde{u}_n \nabla u_{n-1}, \overline{\boldsymbol{\sigma}}) + 2(u_n \nabla \widetilde{u}_n, \overline{\boldsymbol{\sigma}}), \end{cases}$$
(1.84)

for all $(\bar{u}, \bar{\sigma}) \in H^1(\Omega) \times H^1_{\sigma}(\Omega)$. Taking $\bar{u} = \tilde{u}_n$ and $\bar{\sigma} = \frac{1}{2}\tilde{\sigma}_n$ in (1.84) and adding the resulting expressions, the terms $(u_n \tilde{\sigma}_n, \nabla \tilde{u}_n)$ cancel, and taking into account that $\int_{\Omega} \tilde{u}_n = 0$, we deduce

$$\begin{split} \delta_t & \left(\frac{1}{2} \| \widetilde{u}_n \|_0^2 + \frac{1}{4} \| \widetilde{\boldsymbol{\sigma}}_n \|_0^2 \right) + \frac{k}{4} \| (\delta_t \widetilde{u}_n, \delta_t \widetilde{\boldsymbol{\sigma}}_n) \|_0^2 + \frac{1}{2} \| (\widetilde{u}_n, \widetilde{\boldsymbol{\sigma}}_n) \|_1^2 \\ & \leq \| \widetilde{u}_n \|_{L^3} \| \boldsymbol{\sigma}_{n-1} \|_{L^6} \| \nabla \widetilde{u}_n \|_0 + \| \widetilde{u}_n \|_{L^6} \| \widetilde{\boldsymbol{\sigma}}_n \|_{L^3} \| \nabla u_{n-1} \|_0 \\ & \leq \frac{1}{8} \| \widetilde{u}_n \|_1^2 + K_0^2 C \| \widetilde{u}_n \|_0^2 + \frac{1}{8} \| \widetilde{u}_n \|_1^2 + \frac{1}{4} \| \widetilde{\boldsymbol{\sigma}}_n \|_1^2 + K_0^2 C \| \widetilde{\boldsymbol{\sigma}}_n \|_0^2 \end{split}$$

where (1.13) and (1.75) have been used in the first and second inequalities respectively. Thus, we deduce

$$\delta_t \left(\frac{1}{2} \| \widetilde{u}_n \|_0^2 + \frac{1}{4} \| \widetilde{\boldsymbol{\sigma}}_n \|_0^2 \right) + \frac{k}{4} \| (\delta_t \widetilde{u}_n, \delta_t \widetilde{\boldsymbol{\sigma}}_n) \|_0^2 + \frac{1}{4} \| (\widetilde{u}_n, \widetilde{\boldsymbol{\sigma}}_n) \|_1^2 \le K_0^2 C \| (\widetilde{u}_n, \widetilde{\boldsymbol{\sigma}}_n) \|_0^2.$$
(1.85)

In particular,

$$\frac{1}{2} \|\widetilde{u}_n\|_0^2 + \frac{1}{4} \|\widetilde{\boldsymbol{\sigma}}_n\|_0^2 - \left(\frac{1}{2} \|\widetilde{u}_{n-1}\|_0^2 + \frac{1}{4} \|\widetilde{\boldsymbol{\sigma}}_{n-1}\|_0^2\right) \le kC \|(\widetilde{u}_n, \widetilde{\boldsymbol{\sigma}}_n)\|_0^2.$$
(1.86)

Moreover, observe that from (1.48) we have that, for all $(\bar{u}, \bar{\sigma}) \in H^1(\Omega) \times H^1_{\sigma}(\Omega)$,

$$\begin{cases} (\delta_t u_1, \bar{u}) + (\nabla(u_1 - u_0), \nabla \bar{u}) + (\nabla u_0, \nabla \bar{u}) = -(u_1(\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_0), \nabla \bar{u}) - (u_1 \boldsymbol{\sigma}_0, \nabla \bar{u}), \\ (\delta_t \boldsymbol{\sigma}_1, \bar{\boldsymbol{\sigma}}) + \langle B(\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_0), \bar{\boldsymbol{\sigma}} \rangle + \langle B \boldsymbol{\sigma}_0, \bar{\boldsymbol{\sigma}} \rangle = 2(u_1 \nabla(u_1 - u_0), \bar{\boldsymbol{\sigma}}) + 2(u_1 \nabla u_0, \bar{\boldsymbol{\sigma}}). \end{cases}$$
(1.87)

Then, testing (1.87) by $\bar{u} = \delta_t u_1$, $\bar{\boldsymbol{\sigma}} = \frac{1}{2} \delta_t \boldsymbol{\sigma}_1$ and adding, the terms $\frac{1}{k} (u_1 \nabla (u_1 - u_0), \boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_0)$ cancel, and using the Hölder and Young inequalities and (1.75), we can deduce

$$\|(\delta_t u_1, \delta_t \boldsymbol{\sigma}_1)\|_0^2 \le C \,\|(u_0, \boldsymbol{\sigma}_0)\|_2^2.$$
(1.88)

Therefore, taking into account (1.76) and (1.88), applying Corollary 1.2.4 in (1.86) we conclude (1.81). Moreover, multiplying (1.85) by k, adding from $m = n_0 + 1$ to $m = n_0 + n$, and using (1.81), we deduce (1.82). Finally, from (1.61), (1.75), (1.81) and (1.72), we conclude (1.83).

From Theorem 1.4.16 and Corollary 1.4.10, we deduce a more regular estimate for v_n .

Corollary 1.4.18 Let v_n be the solution of (1.49). Under hypothesis of Theorem 1.4.16, the following estimate holds

$$\|v_n\|_3^2 \le K_0, \quad \forall n \ge 0, \tag{1.89}$$

where $K_0 > 0$ is a constant depending on $(\Omega, u_0, \sigma_0, v_0)$, but independent of k and n.

1.4.3 Proof of (1.75) in 2D domains

In this section, we will prove that estimate (1.75) holds in 2D domains. With this aim, first we consider a preliminar result.

Proposition 1.4.19 Let (u_n, σ_n) be any solution of the scheme **US**. Then, in 2D domains, the following estimate holds

$$\|(u_n, \boldsymbol{\sigma}_n)\|_1^2 \le K_1 \|(u_{n-1}, \boldsymbol{\sigma}_{n-1})\|_1^2,$$
(1.90)

where K_1 is a constant depending on data $(\Omega, u_0, \boldsymbol{\sigma}_0)$, but independent of k and n.

Proof. We take $\bar{u} = u_n - u_{n-1}$ and $\bar{\sigma} = \frac{1}{2}(\sigma_n - \sigma_{n-1})$ in (1.48), and recalling that from (1.53) we have $||u_n||_1^2 - ||u_{n-1}||_1^2 = ||\nabla u_n||_0^2 - ||\nabla u_{n-1}||_0^2$, we obtain

$$\frac{1}{2k} \| (u_n - u_{n-1}, \boldsymbol{\sigma}_n - \boldsymbol{\sigma}_{n-1}) \|_0^2 + \frac{1}{4} \| (u_n, \boldsymbol{\sigma}_n) \|_1^2 - \frac{1}{2} \| (u_{n-1}, \boldsymbol{\sigma}_{n-1}) \|_1^2 + \frac{1}{4} \| (u_n - u_{n-1}, \boldsymbol{\sigma}_n - \boldsymbol{\sigma}_{n-1}) \|_1^2 \\
\leq | (u_n \nabla u_n, \boldsymbol{\sigma}_n - \boldsymbol{\sigma}_{n-1}) - (u_n \boldsymbol{\sigma}_n, \nabla (u_n - u_{n-1})) | \\
= | (u_n \nabla u_{n-1}, \boldsymbol{\sigma}_n - \boldsymbol{\sigma}_{n-1}) - (u_n \boldsymbol{\sigma}_{n-1}, \nabla (u_n - u_{n-1})) |.$$
(1.91)

Then, by using the Hölder and Young inequalities as well as the 2D interpolation inequality (1.12) and estimate (1.61), we find

$$\begin{aligned} |(u_{n}\nabla u_{n-1},\boldsymbol{\sigma}_{n}-\boldsymbol{\sigma}_{n-1})-(u_{n}\boldsymbol{\sigma}_{n-1},\nabla(u_{n}-u_{n-1}))| \\ &\leq \|\nabla u_{n-1}\|_{0}\|u_{n}\|_{L^{4}}\|\boldsymbol{\sigma}_{n}-\boldsymbol{\sigma}_{n-1}\|_{L^{4}}+\|\nabla(u_{n}-u_{n-1})\|_{0}\|u_{n}\|_{L^{4}}\|\boldsymbol{\sigma}_{n-1}\|_{L^{4}} \\ &\leq \frac{1}{8}\|(u_{n}-u_{n-1},\boldsymbol{\sigma}_{n}-\boldsymbol{\sigma}_{n-1})\|_{1}^{2}+\frac{1}{8}\|u_{n}\|_{1}^{2}+C\|(u_{n-1},\boldsymbol{\sigma}_{n-1})\|_{1}^{2}. \end{aligned}$$
(1.92)

Therefore, from (1.91)-(1.92) we deduce

$$\frac{k}{2} \| (\delta_t u_n, \delta_t \boldsymbol{\sigma}_n) \|_0^2 + \frac{1}{8} \| (u_n, \boldsymbol{\sigma}_n) \|_1^2 + \frac{1}{8} \| (u_n - u_{n-1}, \boldsymbol{\sigma}_n - \boldsymbol{\sigma}_{n-1}) \|_1^2 \le \left(\frac{1}{2} + C \right) \| (u_{n-1}, \boldsymbol{\sigma}_{n-1}) \|_1^2,$$

hence (1.90) is deduced.

Now, taking into account that from Proposition 1.4.13 we have $(u_n, \sigma_n) \in H^2(\Omega) \times H^2(\Omega)$, we will consider the following pointwise differential formulation of the scheme US:

$$\begin{cases} \delta_t u_n + A u_n - u_n - \nabla \cdot (u_n \boldsymbol{\sigma}_n) = 0, \quad \text{a.e. } \boldsymbol{x} \in \Omega, \\ \delta_t \boldsymbol{\sigma}_n + B \boldsymbol{\sigma}_n = 2 u_n \nabla u_n, \quad \text{a.e. } \boldsymbol{x} \in \Omega. \end{cases}$$
(1.93)

Theorem 1.4.20 Let (u_n, σ_n) be a solution of the scheme US. Then, in 2D domains, the estimate (1.75) holds.

Proof. Testing $(1.93)_1$ by Au_n and $(1.93)_2$ by $B\boldsymbol{\sigma}_n$, we can deduce

$$\delta_t \Big(\|(u_n, \boldsymbol{\sigma}_n)\|_1^2 \Big) + k \|(\delta_t u_n, \delta_t \boldsymbol{\sigma}_n)\|_1^2 + \|(Au_n, B\boldsymbol{\sigma}_n)\|_0^2 \le C(\|\nabla \cdot (u_n \boldsymbol{\sigma}_n)\|_0^2 + \|u_n \nabla u_n\|_0^2 + \|u_n\|_0^2).$$
(1.94)

Moreover, using the 2D inequality (1.12) jointly to (1.61), $(1.10)_1$, (1.11) and (1.90), we obtain

$$\|\boldsymbol{\sigma}_{n} \cdot \nabla u_{n}\|_{0}^{2} + \|u_{n} \nabla \cdot \boldsymbol{\sigma}_{n}\|_{0}^{2} + \|2u_{n} \nabla u_{n}\|_{0}^{2} + \|u_{n}\|_{0}^{2} \leq C \|(u_{n}, \boldsymbol{\sigma}_{n})\|_{1}^{2} \|(u_{n}, \boldsymbol{\sigma}_{n})\|_{2} + C_{0}$$

$$\leq \frac{1}{2} \|(Au_{n}, B\boldsymbol{\sigma}_{n})\|_{0}^{2} + C \|(u_{n-1}, \boldsymbol{\sigma}_{n-1})\|_{1}^{4} + C_{0}.$$
(1.95)

Therefore, from (1.94)-(1.95), we deduce

$$\delta_t \Big(\|(u_n, \boldsymbol{\sigma}_n)\|_1^2 \Big) + k \|(\delta_t u_n, \delta_t \boldsymbol{\sigma}_n)\|_1^2 + \frac{1}{2} \|(Au_n, B\boldsymbol{\sigma}_n)\|_0^2 \le C \|(u_{n-1}, \boldsymbol{\sigma}_{n-1})\|_1^4 + C.$$

In particular,

$$\|(u_n, \boldsymbol{\sigma}_n)\|_1^2 - \|(u_{n-1}, \boldsymbol{\sigma}_{n-1})\|_1^2 \le kC \|(u_{n-1}, \boldsymbol{\sigma}_{n-1})\|_1^4 + kC.$$
(1.96)

Then, taking into account (1.96) and (1.62), applying the Corollary 1.2.4 we deduce (1.75).

1.4.4 Error estimates in weak norms in finite time

Error estimates for the scheme US

We will obtain error estimates for $(u_n, \boldsymbol{\sigma}_n)$ solution of the scheme **US** with respect to a sufficiently regular solution $(u, \boldsymbol{\sigma})$ of (1.3). For this, we introduce the following notations for the errors in $t = t_n$: $e_u^n = u(t_n) - u_n$ and $e_{\boldsymbol{\sigma}}^n = \boldsymbol{\sigma}(t_n) - \boldsymbol{\sigma}_n$, and for the discrete in time derivative of these errors: $\delta_t e_u^n = \frac{e_u^n - e_u^{n-1}}{k}$ and $\delta_t e_{\boldsymbol{\sigma}}^n = \frac{e_{\boldsymbol{\sigma}}^n - e_{\boldsymbol{\sigma}}^{n-1}}{k}$. Then, subtracting (1.3) at $t = t_n$ and the scheme **US**, we have that $(e_u^n, e_{\boldsymbol{\sigma}}^n)$ satisfies

$$(\delta_t e_u^n, \bar{u}) + (\nabla e_u^n, \nabla \bar{u}) + (e_u^n \boldsymbol{\sigma}(t_n) + u_n e_{\boldsymbol{\sigma}}^n, \nabla \bar{u}) = (\xi_1^n, \bar{u}), \quad \forall \bar{u} \in H^1(\Omega),$$
(1.97)

$$(\delta_t e^n_{\boldsymbol{\sigma}}, \bar{\boldsymbol{\sigma}}) + \langle B e^n_{\boldsymbol{\sigma}}, \bar{\boldsymbol{\sigma}} \rangle = 2(e^n_u \nabla u(t_n) + u_n \nabla e^n_u, \bar{\boldsymbol{\sigma}}) + (\xi^n_2, \bar{\boldsymbol{\sigma}}), \quad \forall \bar{\boldsymbol{\sigma}} \in \boldsymbol{H}^1_{\boldsymbol{\sigma}}(\Omega),$$
(1.98)

where ξ_1^n, ξ_2^n are the consistency errors associated to the scheme **US**, that is, $\xi_1^n = \delta_t(u(t_n)) - u_t(t_n)$ and $\xi_2^n = \delta_t(\boldsymbol{\sigma}(t_n)) - \boldsymbol{\sigma}_t(t_n)$.

Theorem 1.4.21 Let (u_n, σ_n) be a solution of the scheme **US** and assume the following regularity for the exact solution (u, σ) of (1.3):

$$(u,\boldsymbol{\sigma}) \in L^{\infty}(0,T; H^{1}(\Omega) \times \boldsymbol{H}^{1}(\Omega)) \quad and \quad (u_{tt},\boldsymbol{\sigma}_{tt}) \in L^{2}(0,T; H^{1}_{*}(\Omega)' \times \boldsymbol{H}^{1}_{\sigma}(\Omega)').$$
(1.99)

Assuming that

$$k \| (\nabla u, \nabla \cdot \boldsymbol{\sigma}) \|_{L^{\infty}(L^2)}^4 \quad is \ small \ enough, \tag{1.100}$$

then the a priori error estimate

$$\|(e_u^n, e_{\sigma}^n)\|_{l^{\infty}L^2 \cap l^2 H^1} \le C(T) k \tag{1.101}$$

holds, where $C(T) = K_1 exp(K_2T)$, with $K_1, K_2 > 0$ independent of k.

Proof. Since $u_0 = u(t_0)$, then $\int_{\Omega} e_u^n = \int_{\Omega} e_u^0 = 0$. Moreover, taking $\bar{u} = e_u^n$ in (1.97), $\bar{\sigma} = \frac{1}{2} e_{\sigma}^n$ in (1.98), and adding the resulting expressions, the terms $(u_n e_{\sigma}^n, \nabla e_u^n)$ cancel, and using the Hölder and Young inequalities and (1.13), we obtain

$$\delta_t \left(\frac{1}{2} \| e_u^n \|_0^2 + \frac{1}{4} \| e_{\sigma}^n \|_0^2 \right) + \frac{k}{4} \| (\delta_t e_u^n, \delta_t e_{\sigma}^n) \|_0^2 + \frac{1}{2} \| (e_u^n, e_{\sigma}^n) \|_1^2$$

$$\leq \frac{1}{8} \| (e_u^n, e_{\sigma}^n) \|_1^2 + C \| (\xi_1^n, \xi_2^n) \|_{(H_*^1)' \times (H_{\sigma}^1)'}^2 + \frac{1}{8} \| (e_u^n, e_{\sigma}^n) \|_1^2 + C \| (\nabla u(t_n), \nabla \cdot \boldsymbol{\sigma}(t_n)) \|_0^4 \| e_u^n \|_0^2,$$

and therefore

$$\delta_t \left(\frac{1}{2} \| e_u^n \|_0^2 + \frac{1}{4} \| e_{\sigma}^n \|_0^2 \right) + \frac{1}{4} \| (e_u^n, e_{\sigma}^n) \|_1^2 \\ \leq C \| (\xi_1^n, \xi_2^n) \|_{(H^1_*)' \times (H^1_{\sigma})'}^2 + C \| (\nabla u(t_n), \nabla \cdot \boldsymbol{\sigma}(t_n)) \|_0^4 \| e_u^n \|_{\mathbf{0}}^2 \mathbf{1}.102)$$

Now, taking into account that

$$(\xi_1^n, \xi_2^n) = -\frac{1}{k} \int_{t_{n-1}}^{t_n} (t - t_{n-1}) (u_{tt}(t), \boldsymbol{\sigma}_{tt}(t)) dt,$$

using the Hölder inequality, we can deduce

$$C\|(\xi_1^n,\xi_2^n)\|_{(H^1_*)'\times(H^1_{\sigma})'}^2 \le Ck \int_{t_{n-1}}^{t_n} \|(u_{tt}(t),\boldsymbol{\sigma}_{tt}(t))\|_{(H^1_*)'\times(H^1_{\sigma})'}^2 dt.$$
(1.103)

Therefore, from (1.102) and (1.103) we deduce

$$\delta_t \left(\frac{1}{2} \| e_u^n \|_0^2 + \frac{1}{4} \| e_{\sigma}^n \|_0^2 \right) + \frac{1}{4} \| (e_u^n, e_{\sigma}^n) \|_1^2$$

$$\leq Ck \int_{t_{n-1}}^{t_n} \| (u_{tt}(t), \boldsymbol{\sigma}_{tt}(t)) \|_{(H^1_*)' \times (H^1_{\sigma})'}^2 dt + C \| (\nabla u(t_n), \nabla \cdot \boldsymbol{\sigma}(t_n)) \|_0^4 \| e_u^n \|_0^2.$$
(1.104)

Then, multiplying (1.104) by k and adding from n = 1 to n = r, we obtain (recall that $e_u^0 = e_{\sigma}^0 = 0$):

$$\left[\frac{1}{4} - Ck \| (\nabla u, \nabla \cdot \boldsymbol{\sigma}) \|_{L^{\infty}L^{2}}^{4} \right] \| (e_{u}^{r}, e_{\boldsymbol{\sigma}}^{r}) \|_{0}^{2} + \frac{k}{4} \sum_{n=1}^{r} \| (e_{u}^{n}, e_{\boldsymbol{\sigma}}^{n}) \|_{1}^{2}$$

$$\leq Ck^{2} \int_{0}^{t_{r}} \| (u_{tt}(t), \boldsymbol{\sigma}_{tt}(t)) \|_{(H^{1}_{*})' \times (H^{1}_{\boldsymbol{\sigma}})'}^{2} dt + C \| (\nabla u, \nabla \cdot \boldsymbol{\sigma}) \|_{L^{\infty}L^{2}}^{4} k \sum_{n=0}^{r-1} \| (e_{u}^{n}, e_{\boldsymbol{\sigma}}^{n}) \|_{0}^{2} (1.105)$$

Therefore, if hypothesis (1.100) is satisfied, using the Discrete Gronwall Lemma (see [7], p. 369) in (1.105), and taking into account (1.99), we conclude (1.101).

Remark 1.4.22 From (1.101), we deduce $||(u_n, \sigma_n)||_1 \leq C(T)$, for all n = 1, ..., N. In particular, this implies that in 3D domains, for finite time, the hypothesis (1.55) assuring the uniqueness of solution (u_n, σ_n) can be relaxed to $k C(T)^4$ small enough.

Error estimates for v_n solution of (1.49)

We will obtain error estimates for v_n solution of (1.49) with respect to a sufficiently regular solution v of (1.4). For this, we introduce the following notation for the error in $t = t_n$: $e_v^n = v(t_n) - v_n$ and for the discrete in time derivative of this error: $\delta_t e_v^n = \frac{e_v^n - e_v^{n-1}}{k}$. Then, subtracting (1.4) at $t = t_n$ and (1.49), we obtain that e_v^n satisfies

$$\delta_t e_v^n + A e_v^n = (u(t_n) + u_n) e_u^n + \xi_3^n, \quad \text{a.e.} \quad \boldsymbol{x} \in \Omega,$$
(1.106)

where ξ_3^n is the consistency error associated to (1.49), that is,

$$\xi_3^n = \delta_t(v(t_n)) - v_t(t_n) = -\frac{1}{k} \int_{t_{n-1}}^{t_n} (t - t_{n-1}) v_{tt}(t) dt.$$
(1.107)

Theorem 1.4.23 Under hypothesis of Theorem 1.4.21. Let v_n be the solution of (1.49) and assume the following regularity for the exact solution v of (1.4):

$$v_{tt} \in L^1(0, T; H^1(\Omega)').$$
 (1.108)

Then the a priori error estimate holds

$$\|e_v^n\|_{l^{\infty}H^1 \cap l^2 H^2} \le C(T) k \tag{1.109}$$

where $C(T) = K_1 exp(K_2T)$, with $K_1, K_2 > 0$ independent of k.

Proof. From the relation $e_{\sigma}^n = \nabla e_v^n$, taking into account (1.101), we only need to prove the following estimate

$$\left| \int_{\Omega} e_v^n \right| \le C(T) \, k. \tag{1.110}$$

With this aim, if we integrate (1.106) in Ω ,

$$\delta_t \left(\int_{\Omega} e_v^n \right) + \int_{\Omega} e_v^n = \int_{\Omega} (u(t_n) + u_n) e_u^n + \int_{\Omega} \xi_3^n, \qquad (1.111)$$

and therefore, multiplying (1.111) by k and using (1.107), we have

$$(1+k)\left|\int_{\Omega} e_{v}^{n}\right| - \left|\int_{\Omega} e_{v}^{n-1}\right| \leq k\left|\int_{\Omega} (u(t_{n})+u_{n})e_{u}^{n}\right| + \left|\int_{t_{n-1}}^{t_{n}} \int_{\Omega} (t-t_{n-1})v_{tt}(\boldsymbol{x},t)d\boldsymbol{x}dt\right|$$
$$\leq k \left\|u(t_{n})+u_{n}\right\|_{0}\left\|e_{u}^{n}\right\|_{0} + k \left|\Omega\right|^{1/2} \int_{t_{n-1}}^{t_{n}} \|v_{tt}(t)\|_{(H^{1})'}. (1.112)$$

Then, adding from n = 1 to n = r in (1.112) and taking into account that $u(t_n) + u_n$ is bounded in $l^{\infty}L^2$, we obtain (recall that $e_v^0 = 0$)

$$\left| \int_{\Omega} e_v^r \right| + k \sum_{n=1}^r \left| \int_{\Omega} e_v^n \right| \le Ck \| v_{tt}(t) \|_{L^1(H^1)'} + kC \sum_{n=1}^r \| e_u^n \|_0.$$
(1.113)

Thus, using (1.108) and (1.101) in (1.113), we deduce (1.110).

1.5 A linear scheme

In this section, we propose the following first order in time, linear coupled scheme for model (1.3):

• <u>Scheme LC</u>:

Initialization: We fix $v_0 = v(0)$ and $(u_0, \sigma_0) = u(0), \sigma(0)$, with $\sigma_0 = \nabla v_0$. Time step n: Given $(u_{n-1}, \sigma_{n-1}) \in H^1(\Omega) \times H^1_{\sigma}(\Omega)$, compute $(u_n, \sigma_n) \in H^1(\Omega) \times H^1_{\sigma}(\Omega)$ solving

$$\begin{cases} (\delta_t u_n, \bar{u}) + (\nabla u_n, \nabla \bar{u}) = -(u_{n-1}\boldsymbol{\sigma}_n, \nabla \bar{u}), & \forall \bar{u} \in H^1(\Omega), \\ (\delta_t \boldsymbol{\sigma}_n, \bar{\boldsymbol{\sigma}}) + \langle B \boldsymbol{\sigma}_n, \bar{\boldsymbol{\sigma}} \rangle = 2(u_{n-1}\nabla u_n, \bar{\boldsymbol{\sigma}}), & \forall \bar{\boldsymbol{\sigma}} \in \boldsymbol{H}^1_{\sigma}(\Omega). \end{cases}$$
(1.114)

Again, once solved the scheme **LC**, given $v_{n-1} \in H^2(\Omega)$ with $v_{n-1} \ge 0$, we can recover $v_n = v_n(u_n^2) \in H^2(\Omega)$ solving (1.49).

1.5.1 Unconditional energy-stability and Unique Solvability

Observe that scheme **LC** is also conservative in u (satisfying (1.53)) and also has the behavior for $\int_{\Omega} v_n$ given in (1.54).

Theorem 1.5.1 (Unconditional Unique Solvability) There exists a unique (u_n, σ_n) solution of the scheme *LC*.

Proof. Let $(u_{n-1}, \sigma_{n-1}) \in \mathbb{H} := H^1(\Omega) \times H^1_{\sigma}(\Omega)$ be given, and consider the following bilinear form $a : \mathbb{H} \times \mathbb{H} \to \mathbb{R}$, and the linear operator $l : \mathbb{H} \to \mathbb{R}$ given by

$$a((u_n, \boldsymbol{\sigma}_n), (\bar{u}, \bar{\boldsymbol{\sigma}})) = \frac{2}{k}(u_n, \bar{u}) + \frac{1}{k}(\boldsymbol{\sigma}_n, \bar{\boldsymbol{\sigma}}) + 2(\nabla u_n, \nabla \bar{u}) + \langle B\boldsymbol{\sigma}_n, \bar{\boldsymbol{\sigma}} \rangle + 2(u_{n-1}\boldsymbol{\sigma}_n, \nabla \bar{u}) - 2(u_{n-1}\nabla u_n, \bar{\boldsymbol{\sigma}}), l((\bar{u}, \bar{\boldsymbol{\sigma}})) = \frac{2}{k}(u_{n-1}, \bar{u}) + \frac{1}{k}(\boldsymbol{\sigma}_{n-1}, \bar{\boldsymbol{\sigma}}),$$

for all $(u_n, \boldsymbol{\sigma}_n), (\bar{u}, \bar{\boldsymbol{\sigma}}) \in \mathbb{H}$. Then, using the Hölder inequality and Sobolev embeddings, we can verify that $a(\cdot, \cdot)$ is continuous and coercive on \mathbb{H} , and $l \in \mathbb{H}'$. Thus, from Lax-Milgram theorem, there exists a unique $(u_n, \boldsymbol{\sigma}_n) \in \mathbb{H}$ such that

$$a((u_n, \boldsymbol{\sigma}_n), (\bar{u}, \bar{\boldsymbol{\sigma}})) = l((\bar{u}, \bar{\boldsymbol{\sigma}})), \quad \forall (\bar{u}, \bar{\boldsymbol{\sigma}}) \in \mathbb{H}.$$

Finally, taking first $\bar{\boldsymbol{\sigma}} = 0$ and then $\bar{u} = 0$, implies that $(u_n, \boldsymbol{\sigma}_n) \in H^1(\Omega) \times \boldsymbol{H}^1_{\boldsymbol{\sigma}}(\Omega)$ is the unique solution of (1.114).

Moreover, following the proof of Lemma 1.4.6, we can prove unconditional energy-stability of the scheme **LC**.

Lemma 1.5.2 (Unconditional energy-stability) The scheme LC is unconditionally energystable for $\mathcal{E}(u, \sigma)$. In fact, the same discrete energy law (1.60) holds.

Remark 1.5.3 If we consider the fully discrete scheme corresponding to LC via a spatial approximation by using the Finite Elements method, i.e. taking $U_h \subset H^1(\Omega)$ and $\Sigma_h \subset H^1_{\sigma}(\Omega)$ instead of $H^1(\Omega)$ and $H^1_{\sigma}(\Omega)$ respectively, then the proofs of solvability and unconditional energy-stability of this fully discrete scheme can be followed line by line from Theorem 1.5.1 and Lemma 1.5.2.

Remark 1.5.4 We can prove weak estimates for the solution (u_n, σ_n) of the scheme **LC** analogously to Theorem 1.4.8. Moreover, assuming the H^2 -regularity for problem (1.9) in the case that the right hand side is not the gradient of a function, we can deduce strong and more regular estimates for this solution (u_n, σ_n) as in Subsection 1.4.2. **Remark 1.5.5** Unlike the scheme US, in the scheme LC it is not clear how to prove the nonnegativity of u_n . In fact, in some numerical simulations, very negative cell densities are obtained when $h \rightarrow 0$, where h is the spatial parameter (see Subsection 1.6.1).

1.5.2 Error estimates in weak norms

Theorem 1.5.6 (Error estimates for the scheme LC) Let (u_n, σ_n) be a solution of the scheme **LC**, and assume the regularity (1.99). Then, the a priori error estimate (1.101) holds.

Proof. The proof follows as in Theorem 1.4.21, but we recall that in this case we do not need to impose hypothesis of small time step given in (1.100) in order to apply the Discrete Gronwall Lemma, since we use the form of the terms $(u_{n-1}\sigma_n, \nabla \bar{u})$ and $(u_{n-1}\nabla u_n, \bar{\sigma})$ to bound them in a suitable way.

Moreover, although in this linear scheme **LC** it is not clear if the relation $\sigma_n = \nabla v_n$ holds, it will be possible to obtain error estimates for v_n .

Theorem 1.5.7 (Error estimates for v_n) Under hypothesis of Theorem 1.5.6. Let v_n be the solution of (1.49) (corresponding to the scheme **LC**), and assume the regularity:

$$v_{tt} \in L^2(0, T; L^2(\Omega)).$$
 (1.115)

Then, the a priori error estimate (1.109) holds.

Proof. Since in the scheme **LC** it is not clear the relation $\sigma_n = \nabla v_n$, we will argue in a different way of Theorem 1.4.23. Indeed, we test (1.106) by Ae_v^n , and using the Hölder and Young inequalities, we obtain

$$\frac{1}{2}\delta_t\left(\|e_v^n\|_1^2\right) + \frac{k}{2}\|\delta_t e_v^n\|_1^2 + \frac{1}{2}\|Ae_v^n\|_0^2 \le C(\|u(t_n) + u_n\|_1^2\|e_u^n\|_1^2 + \|\xi_3^n\|_0^2).$$
(1.116)

Observe that from (1.101) we have $\sum_{n=1}^{r} ||u(t_n) - u_n||_1^2 \leq C(T)k$, which implies that

$$||u_n||_1 \le C + ||u(t_n)||_1.$$
(1.117)

Then, multiplying (1.116) by k, adding from n = 1 to n = r and using (1.117), we obtain (recall that $e_v^0 = 0$)

$$\|e_v^r\|_1^2 + k \sum_{n=1}^r \|Ae_v^n\|_0^2 \le \left(C + C\|u!^{\epsilon}\|_{L^{\infty}H^1}^2\right) k \sum_{n=1}^r \|e_u^n\|_1^2 + Ck^2 \int_0^{t_r} \|v_{tt}(t)\|_0^2 dt.$$
(1.118)

Therefore, taking into account (1.99), (1.115) and (1.101), from (1.118) we conclude (1.109).

1.6 Numerical simulations

The aim of this section is to compare the results of several numerical simulations that we have carried out using the schemes derived through the paper. We are considering a finite element discretization in space associated to the variational formulation of schemes **US**, **LC** and **UV**, where the \mathcal{P}_1 -continuous approximation is taken for u_h , σ_h and v_h (where h is the spatial parameter). Moreover, we have chosen the 2D domain $\Omega = [0, 2]^2$ using a structured mesh, and all the simulations are carried out using **FreeFem**++ software. The linear iterative method used to approach the nonlinear schemes **US** and **UV** is the Newton Method, and in all the cases, the iterative method stops when the relative error in L^2 -norm is less than $\varepsilon = 10^{-6}$.

1.6.1 Positivity

In this subsection, we compare the schemes **US** and **LC** in terms of positivity. For the fully discretization of both schemes is not clear the positivity of the variable u_h . In fact, for the time-discrete scheme **US** the existence of nonnegative solution (u_n, v_n) was proved (see Theorem 1.4.3 and Remark 1.4.1), but for the time-discrete scheme **LC**, although we can prove that v_n is nonnegative, the nonnegativity of u_n is not clear. For this reason, in Figures 1.2-1.5, we compare the positivity of the variables u_h and v_h in both schemes taking meshes in space increasingly thinner $(h = \frac{1}{35}, h = \frac{1}{75} \text{ and } h = \frac{1}{150})$. In all the cases, we choose $k = 10^{-5}$ and the initial conditions are (see Figure 1.1)

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

and

$$v_0 = 200xy(2-x)(2-y)exp(-30(y-1)^2 - 30(x-1)^2) + 0.0001.$$

In the case of the scheme **US**, we observe that although u_h is negative for some $\boldsymbol{x} \in \Omega$ in some times $t_n > 0$, when $h \to 0$ these values are closer to 0; while in the case of the scheme **LC**, when $h \to 0$ very negative cell densities u_h are obtained for some $\boldsymbol{x} \in \Omega$ in some times $t_n > 0$ (see Figures 1.2-1.4). On the other hand, the same behavior is observed for the minimum of v_h in both schemes. In fact, independently of h, if v_0 is positive, then v_h also is positive (we show this behavior in Figure 1.5 for the case $h = \frac{2}{70}$, but the same holds for the cases $h = \frac{2}{150}$ and $h = \frac{2}{300}$).





(b) Initial chemical concentration v_0

Figure 1.1: Initial conditions.

Remark 1.6.1 In Figures 1.3 and 1.4 there are also negative values of minimum of u_h for the scheme **US**, but those are of order 10^{-2} and 10^{-4} respectively.

1.6.2 Unconditional Stability

In this subsection, we compare numerically the stability with respect to two energies $\mathcal{E}(u, \sigma)$ and $\mathcal{E}(u, v)$. Following line to line the proof of Lemma 1.4.6, we deduce the unconditional energy-stability for the fully discrete schemes corresponding to schemes **US** and **LC** (for the modified energy $\mathcal{E}(u, \sigma)$). In fact, if (u_n, σ_n) is any solution of the fully discrete schemes corresponding to schemes **US** or **LC**, the following relation holds

$$RE(u_n, \boldsymbol{\sigma}_n) := \delta_t \mathcal{E}(u_n, \boldsymbol{\sigma}_n) + \|\nabla u_n\|_0^2 + \frac{1}{2} \|\boldsymbol{\sigma}_n\|_1^2 \le 0, \quad \forall n.$$
(1.119)

However, considering the "exact" energy (1.21), in the case of fully discrete schemes, it is not clear how to prove unconditional energy-stability of schemes **US**, **LC** and **UV** with respect to this energy. Moreover, it is interesting to study the behaviour of the corresponding residual

$$RE(u_n, v_n) := \delta_t \mathcal{E}(u_n, v_n) + \|\nabla u_n\|_0^2 + \frac{1}{2} \|\Delta_h v_n\|_0^2 + \frac{1}{2} \|\nabla v_n\|_0^2$$

Indeed, taking $k = 10^{-6}$, $h = \frac{2}{50}$ and the initial conditions

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

and

$$v_0 = 20xy(2-x)(2-y)exp(-30(y-1)^2 - 30(x-1)^2) + 0.0001,$$

we obtain that:



Figure 1.2: Minimum values of u_h , with $h = \frac{1}{35}$.

- (a) The schemes **US** and **LC** satisfy the energy decreasing in time property (1.59) for the modified energy $\mathcal{E}(u, \boldsymbol{\sigma})$, see Figure 1.6.
- (b) The schemes **US** and **LC** satisfy (1.119), see Figure 1.7.
- (c) The schemes **US**, **LC** and **UV** satisfy the energy decreasing in time property for the exact energy $\mathcal{E}(u, v)$, that is, $\mathcal{E}(u_n, v_n) \leq \mathcal{E}(u_{n-1}, v_{n-1})$ for all n, see Figure 1.8.
- (d) The schemes **US**, **LC** and **UV** have $RE(u_n, v_n) > 0$ for some $t_n \ge 0$. However, it is observed that the residues $RE(u_n, v_n)$ of the schemes **US** and **LC** in those times t_n where each residue is positive, its values are less than the residues of the scheme **UV**, see Figure 1.9.

1.7 Appendix A

In order to prove the solvability of (1.56), we will use the Leray-Schauder fixed point theorem. With this aim, we define the operator $R: L^4(\Omega) \times \mathbf{L}^4(\Omega) \to L^4(\Omega) \times \mathbf{L}^4(\Omega)$ by $R(\tilde{u}, \tilde{\sigma}) =$



Figure 1.3: Minimum values of u_h , with $h = \frac{1}{75}$.

 (u, σ) , such that (u, σ) solves the following linear decoupled problems

$$\begin{cases} \frac{1}{k}(u,\bar{u}) + (\nabla u,\nabla\bar{u}) = \frac{1}{k}(u_{n-1},\bar{u}) - (\tilde{u}_{+}\tilde{\boldsymbol{\sigma}},\nabla\bar{u}), \quad \forall \bar{u} \in H^{1}(\Omega), \\ \frac{1}{k}(\boldsymbol{\sigma},\bar{\boldsymbol{\sigma}}) + \langle B\boldsymbol{\sigma},\bar{\boldsymbol{\sigma}} \rangle = \frac{1}{k}(\boldsymbol{\sigma}_{n-1},\bar{\boldsymbol{\sigma}}) - (\tilde{u}^{2},\nabla\cdot\bar{\boldsymbol{\sigma}}), \quad \forall \bar{\boldsymbol{\sigma}} \in \boldsymbol{H}^{1}_{\sigma}(\Omega). \end{cases}$$
(1.120)

1. *R* is well defined. Let $(\tilde{u}, \tilde{\sigma}) \in L^4(\Omega) \times \mathbf{L}^4(\Omega)$ and consider the following bilinear forms $\tilde{a} : H^1(\Omega) \times H^1(\Omega) \to \mathbb{R}$, $\tilde{b} : H^1_{\sigma}(\Omega) \times H^1_{\sigma}(\Omega) \to \mathbb{R}$, and the linear operators $l_1 : H^1(\Omega) \to \mathbb{R}$ and $l_2 : H^1_{\sigma}(\Omega) \to \mathbb{R}$ given by

$$\widetilde{a}(u,\bar{u}) = \frac{1}{k}(u,\bar{u}) + (\nabla u,\nabla\bar{u}), \quad \widetilde{b}(\boldsymbol{\sigma},\bar{\boldsymbol{\sigma}}) = \frac{1}{k}(\boldsymbol{\sigma},\bar{\boldsymbol{\sigma}}) + \langle B\boldsymbol{\sigma},\bar{\boldsymbol{\sigma}}\rangle,$$
$$l_1(\bar{u}) = \frac{1}{k}\int_{\Omega} u_{n-1}\bar{u} - \int_{\Omega} \widetilde{u}_+\widetilde{\boldsymbol{\sigma}}\cdot\nabla\bar{u} \text{ and } l_2(\bar{\boldsymbol{\sigma}}) = \frac{1}{k}\int_{\Omega} \boldsymbol{\sigma}_{n-1}\bar{\boldsymbol{\sigma}} - \int_{\Omega} \widetilde{u}^2\nabla\cdot\bar{\boldsymbol{\sigma}},$$

for all $u, \bar{u} \in H^1(\Omega)$ and $\sigma, \bar{\sigma} \in H^1_{\sigma}(\Omega)$. Then, using the Hölder inequality and Sobolev embeddings, we can verify that \tilde{a} and \tilde{b} are continuous and coercive on $H^1(\Omega)$ and $H^1_{\sigma}(\Omega)$ respectively, and $l_1 \in H^1(\Omega)'$ and $l_2 \in H^1_{\sigma}(\Omega)'$. Thus, from Lax-Milgram theorem, there exists a unique $(u, \sigma) \in H^1(\Omega) \times H^1_{\sigma}(\Omega) \hookrightarrow L^4(\Omega) \times L^4(\Omega)$ solution of (1.120).



Figure 1.4: Minimum values of u_h , with $h = \frac{1}{150}$.

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

$$\begin{cases} \frac{1}{\lambda}\widetilde{a}(u,\bar{u}) = \frac{1}{k}(u_{n-1},\bar{u}) - (u_{+}\boldsymbol{\sigma},\nabla\bar{u}), \quad \forall \bar{u} \in H^{1}(\Omega), \\ \frac{1}{\lambda}\widetilde{b}(\boldsymbol{\sigma},\bar{\boldsymbol{\sigma}}) = \frac{1}{k}(\boldsymbol{\sigma}_{n-1},\bar{\boldsymbol{\sigma}}) - (u^{2},\nabla\cdot\bar{\boldsymbol{\sigma}}), \quad \forall \bar{\boldsymbol{\sigma}} \in \boldsymbol{H}^{1}_{\sigma}(\Omega), \end{cases}$$
(1.121)

(because $\lambda R(u, \boldsymbol{\sigma}) = (u, \boldsymbol{\sigma})$ implies $R(u, \boldsymbol{\sigma}) = (\frac{1}{\lambda}u, \frac{1}{\lambda}\boldsymbol{\sigma})$). Proceeding as in Part A of the proof of Theorem 1.4.3, we can prove that if $(u, \boldsymbol{\sigma})$ is a solution of (1.121), then $u \geq 0$, which implies that $u = u_+$. Then, multiplying $(1.121)_1$ and $(1.121)_2$ by λ , testing by $\bar{u} = u$ and $\bar{\boldsymbol{\sigma}} = \frac{1}{2}\boldsymbol{\sigma}$ and taking into account that $\lambda \in (0, 1]$, we obtain

$$\frac{1}{4} \| (u, \boldsymbol{\sigma}) \|_{0}^{2} + \frac{k}{2} \| (\nabla u, \boldsymbol{\sigma}) \|_{L^{2} \times H^{1}}^{2} \leq C \lambda^{2} \| (u_{n-1}, \boldsymbol{\sigma}_{n-1}) \|_{0}^{2} \equiv C(u_{n-1}, \boldsymbol{\sigma}_{n-1}).$$

Thus, we deduce that $||(u, \boldsymbol{\sigma})||_{L^4} \leq C||(u, \boldsymbol{\sigma})||_1 \leq C$, where the constant C depends on data $(\Omega, u_{n-1}, \boldsymbol{\sigma}_{n-1})$.

3. We prove that R is continuous. Let $\{(\widetilde{u}^l, \widetilde{\boldsymbol{\sigma}}^l)\}_{l \in \mathbb{N}} \subset L^4(\Omega) \times \mathbf{L}^4(\Omega)$ be a sequence such that

$$(\widetilde{u}^l, \widetilde{\boldsymbol{\sigma}}^l) \to (\widetilde{u}, \widetilde{\boldsymbol{\sigma}}) \text{ in } L^4(\Omega) \times \mathbf{L}^4(\Omega), \text{ as } l \to +\infty.$$
 (1.122)



Figure 1.5: Minimum values of v_h , with $h = \frac{1}{35}$.

Therefore, $\{(\widetilde{u}^l, \widetilde{\boldsymbol{\sigma}}^l)\}_{l \in \mathbb{N}}$ is bounded in $L^4(\Omega) \times \mathbf{L}^4(\Omega)$, and from item 1 we deduce that $\{(u^l, \boldsymbol{\sigma}^l) = R(\widetilde{u}^l, \widetilde{\boldsymbol{\sigma}}^l)\}_{l \in \mathbb{N}}$ is bounded in $H^1(\Omega) \times H^1(\Omega)$. Then, there exists a subsequence $\{R(\widetilde{u}^{l^r}, \widetilde{\boldsymbol{\sigma}}^{l^r})\}_{r \in \mathbb{N}}$ such that

$$R(\tilde{u}^{l^r}, \tilde{\boldsymbol{\sigma}}^{l^r}) \to (u', \boldsymbol{\sigma}') \quad \text{weakly in } H^1(\Omega) \times \boldsymbol{H}^1(\Omega) \text{ and strongly in } L^4(\Omega) \times \mathbf{L}^4(\Omega).$$
(1.123)

Then, from (1.122)-(1.123), a standard procedure allows us to pass to the limit, as r goes to $+\infty$, in (1.120) (with $(\tilde{u}^{l^r}, \tilde{\boldsymbol{\sigma}}^{l^r})$ and $(u^{l^r}, \boldsymbol{\sigma}^{l^r})$ instead of $(\tilde{u}, \tilde{\boldsymbol{\sigma}})$ and $(u, \boldsymbol{\sigma})$ respectively), and we deduce that $R(\tilde{u}, \tilde{\boldsymbol{\sigma}}) = (u', \boldsymbol{\sigma}')$. Therefore, we have proved that any convergent subsequence of $\{R(\tilde{u}^l, \tilde{\boldsymbol{\sigma}}^l)\}_{l \in \mathbb{N}}$ converges to $R(\tilde{u}, \tilde{\boldsymbol{\sigma}})$ strong in $L^4(\Omega) \times$ $\mathbf{L}^4(\Omega)$, and from uniqueness of $R(\tilde{u}, \tilde{\boldsymbol{\sigma}})$, we conclude that $R(\tilde{u}^l, \tilde{\boldsymbol{\sigma}}^l) \to R(\tilde{u}, \tilde{\boldsymbol{\sigma}})$ in $L^4(\Omega) \times \mathbf{L}^4(\Omega)$. Thus, R is continuous.

4. *R* is compact. In fact, if $\{(\widetilde{u}^l, \widetilde{\boldsymbol{\sigma}}^l)\}_{l \in \mathbb{N}}$ is a bounded sequence in $L^4(\Omega) \times \mathbf{L}^4(\Omega)$ and we denote $(u^l, \boldsymbol{\sigma}^l) = R(\widetilde{u}^l, \widetilde{\boldsymbol{\sigma}}^l)$, then we can deduce

$$\frac{1}{2k} \| (u^l, \boldsymbol{\sigma}^l) \|_0^2 + \frac{1}{2} \| (\nabla u^l, \boldsymbol{\sigma}^l) \|_{L^2 \times H^1}^2 \le \frac{1}{2k} \| (u_{n-1}, \boldsymbol{\sigma}_{n-1}) \|_0^2 + \frac{1}{2} \| \widetilde{u}^l \|_{L^4}^2 \| \widetilde{\boldsymbol{\sigma}}^l \|_{L^4}^2 + \frac{1}{2} \| \widetilde{u}^l \|_{L^4}^4 \le C_{\mathbf{n}}^{-1} \| \widetilde{\boldsymbol{\sigma}}^l \|_{L^4}^2 + \frac{1}{2} \| \widetilde{u}^l \|_{L^4}^4 \le C_{\mathbf{n}}^{-1} \| \widetilde{\boldsymbol{\sigma}}^l \|_{L^4}^2 + \frac{1}{2} \| \widetilde{u}^l \|_{L^4}^4 \le C_{\mathbf{n}}^{-1} \| \widetilde{\boldsymbol{\sigma}}^l \|_{L^4}^2 + \frac{1}{2} \| \widetilde{u}^l \|_{L^4}^4 \le C_{\mathbf{n}}^{-1} \| \widetilde{\boldsymbol{\sigma}}^l \|_{L^4}^2 + \frac{1}{2} \| \widetilde{u}^l \|_{L^4}^4 \le C_{\mathbf{n}}^{-1} \| \widetilde{\boldsymbol{\sigma}}^l \|_{L^4}^2 + \frac{1}{2} \| \widetilde{\boldsymbol{\sigma}}^l \|_{L^4}^2 + \frac{1}{2} \| \widetilde{\boldsymbol{\sigma}}^l \|_{L^4}^4 \le C_{\mathbf{n}}^{-1} \| \widetilde{\boldsymbol{\sigma}}^l \|_{L^4}^2 + \frac{1}{2} \| \widetilde{\boldsymbol{\sigma}}^l \|_{L^4}^4 + \frac{1}{2} \| \widetilde{\boldsymbol{\sigma}^l \|_{L^4}^4 + \frac{1}{2} \| \widetilde{\boldsymbol{\sigma}^l \|_{L^4}^4 + \frac{1}{2} \| \widetilde{\boldsymbol{\sigma}}^l \|_{L^4}^4 + \frac{1}{2} \| \widetilde{\boldsymbol{\sigma}^l \|_{L^4}^4 + \frac{1}{2} \| \widetilde$$

where C is a constant independent of $l \in \mathbb{N}$. Therefore, we conclude that $\{R(\tilde{u}^l, \tilde{\sigma}^l)\}_{l \in \mathbb{N}}$ is bounded in $H^1(\Omega) \times H^1(\Omega)$ which is compactly embedded in $L^4(\Omega) \times L^4(\Omega)$, and thus R is compact.



Figure 1.6: Energy $\mathcal{E}(u_n, \boldsymbol{\sigma}_n)$ of schemes **US** and **LC**.

Therefore, the hypotheses of the Leray-Schauder fixed point theorem are satisfied and we conclude that the map $R(\tilde{u}, \tilde{\sigma})$ has a fixed point. This fixed point $R(u, \sigma) = (u, \sigma)$ is a solution of nonlinear scheme (1.56).



Figure 1.7: Residue $RE(u_n, \boldsymbol{\sigma}_n)$ of schemes **US** and **LC**.



Figure 1.8: Energy $\mathcal{E}(u_n, v_n)$ of schemes **US**, **LC** and **UV**.



Figure 1.9: Residue $RE(u_n, v_n)$ of schemes **US**, **LC** and **UV**.

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Chapter 2 Energy-stable fully discrete approximation for a chemo-repulsion model with quadratic production

2.1 Introduction

The aim of this paper is to study an unconditional energy-stable fully discrete scheme for the following parabolic-parabolic repulsive-productive chemotaxis model (with quadratic production term):

$$\begin{cases} \partial_t u - \Delta u = \nabla \cdot (u \nabla v) & \text{in } \Omega, \ t > 0, \\ \partial_t v - \Delta v + v = u^2 & \text{in } \Omega, \ t > 0, \\ \frac{\partial u}{\partial \mathbf{n}} = \frac{\partial v}{\partial \mathbf{n}} = 0 & \text{on } \partial\Omega, \ t > 0, \\ u(\boldsymbol{x}, 0) = u_0(\boldsymbol{x}) \ge 0, \ v(\boldsymbol{x}, 0) = v_0(\boldsymbol{x}) \ge 0 & \text{in } \Omega, \end{cases}$$
(2.1)

where Ω is a *n*-dimensional open bounded domain, n = 2, 3, with boundary $\partial \Omega$. The unknowns for this model are $u(\boldsymbol{x},t) \geq 0$, the cell density, and $v(\boldsymbol{x},t) \geq 0$, the chemical concentration. Problem (2.1) is conservative in u, because the total mass $\int_{\Omega} u(t)$ remains constant in time, as we can check integrating equation $(2.1)_1$ in Ω ,

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

In Chapter 1 was proved that problem (2.1) is well-posed, because there exists global in time "weak-strong" solutions in the following sense: $u \ge 0$ and $v \ge 0$ a.e. $(t, \mathbf{x}) \in$

 $(0, +\infty) \times \Omega,$

$$(u,v) \in L^{\infty}(0,+\infty; L^{2}(\Omega) \times H^{1}(\Omega)) \cap L^{2}(0,T; H^{1}(\Omega) \times H^{2}(\Omega)), \quad \forall T > 0,$$

$$(\partial_{t}u, \partial_{t}v) \in L^{q'}(0,T; H^{1}(\Omega)' \times L^{2}(\Omega)), \quad \forall T > 0,$$

$$(\nabla u, \nabla v) \in L^{2}(0,+\infty; \boldsymbol{L}^{2}(\Omega) \times \boldsymbol{H}^{1}(\Omega)),$$
(2.2)

where q' = 2 in the 2-dimensional case (2D) and q' = 4/3 in the 3-dimensional case (3D) (q' is the conjugate exponent of q = 2 in 2D and q = 4 in 3D), satisfying the *u*-equation (2.1)₁ in a variational sense, the *v*-equation (2.1)₂ a.e. $(t, \boldsymbol{x}) \in (0, +\infty) \times \Omega$, and the following energy inequality for a.e. $t_0, t_1 : t_1 \ge t_0 \ge 0$:

$$\mathcal{E}(u(t_1), v(t_1)) - \mathcal{E}(u(t_0), v(t_0)) + \int_{t_0}^{t_1} (\|\nabla u(s)\|_{L^2}^2 + \frac{1}{2} \|\Delta v(s)\|_{L^2}^2 + \frac{1}{2} \|\nabla v(s)\|_{L^2}^2) \, ds \le 0, \quad (2.3)$$

where $\mathcal{E}(u, v) = \frac{1}{2} ||u||_{L^2}^2 + \frac{1}{4} ||\nabla v||_{L^2}^2$. Moreover, assuming that the following regularity criteria is satisfied:

$$(u, \nabla v) \in L^{\infty}(0, +\infty; H^{1}(\Omega) \times \boldsymbol{H}^{1}(\Omega)), \qquad (2.4)$$

(which, at least in 2D domains, is always true), it was proved that there exists a unique global in time strong solution of (2.1) satisfying

$$\begin{cases}
(u,v) \in L^{\infty}(0,+\infty; H^{2}(\Omega)^{2}) \cap L^{2}(0,T; H^{3}(\Omega)^{2}), \\
(\partial_{t}u, \partial_{t}v) \in L^{\infty}(0,+\infty; L^{2}(\Omega) \times H^{1}(\Omega)) \cap L^{2}(0,+\infty; H^{1}(\Omega) \times H^{2}(\Omega)), \\
(\partial_{tt}u, \partial_{tt}v) \in L^{2}(0,+\infty; H^{1}(\Omega)' \times L^{2}(\Omega)).
\end{cases}$$
(2.5)

In particular, $(2.5)_1$ implies

$$\|(u,v)\|_{L^{\infty}(0,+\infty;L^{\infty}\times L^{\infty})} \le C.$$
 (2.6)

Therefore, it is desired to design numerical methods for the model (2.1) conserving at the discrete level the main properties of the continuous model, such as mass-conservation, energy-stability, positivity and regularity.

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 [4] the existence of discrete solutions and the convergence of a finite volume scheme. Saito, in [8, 9], proved error estimates for a conservative Finite Element (FE) approximation. A mixed FE approximation is studied in [6]. In [3], some error estimates are proved for a fully discrete discontinuous FE method. However, as far as we know, there are not works studying

FE schemes satisfying the property of energy-stability related to the energy inequality (2.3).

In this paper, we propose an unconditional energy-stable fully discrete scheme, which inherit some properties from the continuous model, such as mass-conservation, and weak and strong estimates analogues to (2.2) and (2.5)-(2.6). Moreover, with respect to the nonnegativity of the discrete cell and chemical variables, u_h^n and v_h^n , we can deduce that $v_h^n \ge 0$ (see Remark 2.3.2), but the cell density nonnegativity $u_h^n \ge 0$ can not be assured.

In order to design the scheme, we follow the ideas presented in Chapter 1, and we reformulate (2.1) introducing a new variable $\boldsymbol{\sigma} = \nabla v$ instead of v. Then, model (2.1) is rewritten as:

$$\begin{aligned}
& (\partial_t u - \nabla \cdot (\nabla u) = \nabla \cdot (u\boldsymbol{\sigma}) & \text{in } \Omega, \ t > 0, \\
& \partial_t \boldsymbol{\sigma} - \nabla (\nabla \cdot \boldsymbol{\sigma}) + \boldsymbol{\sigma} + \text{rot}(\text{rot } \boldsymbol{\sigma}) = \nabla (u^2) & \text{in } \Omega, \ t > 0, \\
& \frac{\partial u}{\partial \mathbf{n}} = 0 & \text{on } \partial\Omega, \ t > 0, \\
& \boldsymbol{\sigma} \cdot \mathbf{n} = 0, \quad [\text{rot } \boldsymbol{\sigma} \times \mathbf{n}]_{tang} = 0 & \text{on } \partial\Omega, \ t > 0, \\
& u(\boldsymbol{x}, 0) = u_0(\boldsymbol{x}) \ge 0, \ \boldsymbol{\sigma}(\boldsymbol{x}, 0) = \nabla v_0(\boldsymbol{x}) & \text{in } \Omega,
\end{aligned}$$
(2.7)

where $(2.7)_2$ has been obtained applying the gradient operator to equation $(2.1)_2$ and adding the term rot(rot $\boldsymbol{\sigma}$) using the fact that rot $\boldsymbol{\sigma} = rot(\nabla v) = 0$. Once system (2.7) is solved, we can recover v from u^2 by solving

$$\begin{cases} \partial_t v - \Delta v + v = u^2 \text{ in } \Omega, \ t > 0, \\ \frac{\partial v}{\partial \mathbf{n}} = 0 \quad \text{on } \partial\Omega, \ t > 0, \\ v(\boldsymbol{x}, 0) = v_0(\boldsymbol{x}) > 0 \quad \text{in } \Omega. \end{cases}$$
(2.8)

This chapter is organized as follows: In Section 2.2, we give the notation and some preliminary results that will be used along this paper. In Section 2.3, we study the FE Backward Euler scheme corresponding to formulation (2.7)-(2.8), including mass-conservation, unconditional energy-stability, solvability, weak and strong estimates, convergence towards weak solutions, and optimal error estimates of the scheme. In Section 2.4, we propose two different linear iterative methods in order to approach the nonlinear scheme proposed in Section 2.3, which are an energy-stable Picard's method and the Newton's method. We prove the solvability and the convergence of these methods to the nonlinear scheme. Finally, in Section 2.5, we present some numerical results in agreement with the theoretical analysis about the error estimates.

2.2 Notations and preliminary results

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 $L^p(\Omega)$, $1 \le p \le \infty$, with norms $\|\cdot\|_m$ and $\|\cdot\|_{L^p}$, respectively. In particular, the $L^2(\Omega)$ -norm will be denoted by $\|\cdot\|_0$. We denote by $\boldsymbol{H}^1_{\sigma}(\Omega) := \{ \mathbf{u} \in \boldsymbol{H}^1(\Omega) : \mathbf{u} \cdot \mathbf{n} = 0 \text{ on } \partial\Omega \}$ and we will use the following equivalent norms in $H^1(\Omega)$ and $\mathbf{H}^1_{\sigma}(\Omega)$, respectively (see [7] and [1, Corollary 3.5], respectively):

$$\|u\|_{1}^{2} = \|\nabla u\|_{0}^{2} + \left(\int_{\Omega} u\right)^{2}, \quad \forall u \in H^{1}(\Omega),$$
$$\|\boldsymbol{\sigma}\|_{1}^{2} = \|\boldsymbol{\sigma}\|_{0}^{2} + \|\operatorname{rot} \,\boldsymbol{\sigma}\|_{0}^{2} + \|\nabla \cdot \boldsymbol{\sigma}\|_{0}^{2}, \quad \forall \boldsymbol{\sigma} \in \boldsymbol{H}_{\sigma}^{1}(\Omega)$$

If Z is a general Banach space, its topological dual will be denoted by Z'. Moreover, the letters C, K will denote different positive constants (independent of discrete parameters) which may change from line to line (or even within the same line).

We define the linear elliptic operators

$$Aw = g \quad \Leftrightarrow \quad \begin{cases} -\Delta w + w = g \text{ in } \Omega, \\ \frac{\partial w}{\partial \mathbf{n}} = 0 \text{ on } \partial \Omega, \end{cases}$$
(2.9)

and

$$B\boldsymbol{\sigma} = h \quad \Leftrightarrow \quad \begin{cases} -\nabla(\nabla \cdot \boldsymbol{\sigma}) + \operatorname{rot} (\operatorname{rot} \boldsymbol{\sigma}) + \boldsymbol{\sigma} = h \quad \text{in } \Omega, \\ \boldsymbol{\sigma} \cdot \mathbf{n} = 0, \quad [\operatorname{rot} \boldsymbol{\sigma} \times \mathbf{n}]_{tang} = 0 \quad \text{on } \partial\Omega, \end{cases}$$
(2.10)

which, in variational form, are given by $A : H^1(\Omega) \to H^1(\Omega)'$ and $B : \mathbf{H}^1_{\sigma}(\Omega) \to \mathbf{H}^1_{\sigma}(\Omega)'$ such that

$$\langle Aw, \bar{w} \rangle = (\nabla w, \nabla \bar{w}) + (w, \bar{w}), \quad \forall w, \bar{w} \in H^1(\Omega), \langle B\boldsymbol{\sigma}, \bar{\boldsymbol{\sigma}} \rangle = (\boldsymbol{\sigma}, \bar{\boldsymbol{\sigma}}) + (\nabla \cdot \boldsymbol{\sigma}, \nabla \cdot \bar{\boldsymbol{\sigma}}) + (\operatorname{rot} \boldsymbol{\sigma}, \operatorname{rot} \bar{\boldsymbol{\sigma}}), \quad \forall \boldsymbol{\sigma}, \bar{\boldsymbol{\sigma}} \in \boldsymbol{H}^1_{\sigma}(\Omega).$$

We assume the H^2 -regularity of problems (2.9) and (2.10). Consequently, we have the existence of some constants C > 0 such that

$$\|w\|_{2} \leq C \|Aw\|_{0}, \quad \forall w \in H^{2}(\Omega), \quad \text{and} \quad \|\boldsymbol{\sigma}\|_{2} \leq C \|B\boldsymbol{\sigma}\|_{0}, \quad \forall \boldsymbol{\sigma} \in \boldsymbol{H}^{2}(\Omega).$$
(2.11)

Along this paper, we will use repeatedly the classical 3D interpolation inequality

$$\|u\|_{L^3} \le C \|u\|_0^{1/2} \|u\|_1^{1/2} \quad \forall u \in H^1(\Omega).$$
(2.12)

Finally, we will use the following results (see [5] and [10]):

Lemma 2.2.1 Assume that $\delta, \beta, k > 0$ and $d^n \ge 0$ satisfy

$$\frac{d^{n+1}-d^n}{k}+\delta d^{n+1}\leq \beta, \quad \forall n\geq 0.$$

Then, for any $n_0 \ge 0$,

$$d^n \le (1+\delta k)^{-(n-n_0)} d^{n_0} + \delta^{-1}\beta, \ \forall n \ge n_0.$$

Lemma 2.2.2 (Uniform discrete Gronwall lemma) Let k > 0 and $d^n, g^n, h^n \ge 0$ such that

$$\frac{d^{n+1}-d^n}{k} \le g^n d^n + h^n, \ \forall n \ge 0.$$

If for any $r \in \mathbb{N}$, there exist $a_1(t_r)$, $a_2(t_r)$ and $a_3(t_r)$ depending on $t_r = kr$, such that

$$k\sum_{n=n_0}^{n_0+r-1} g^n \le a_1(t_r), \quad k\sum_{n=n_0}^{n_0+r-1} h^n \le a_2(t_r), \quad k\sum_{n=n_0}^{n_0+r-1} d^n \le a_3(t_r),$$

for any integer $n_0 \ge 0$, then

$$d^{n} \leq \left(a_{2}(t_{r}) + \frac{a_{3}(t_{r})}{t_{r}}\right) \exp\left\{a_{1}(t_{r})\right\}, \quad \forall n \geq r.$$

As consequence of Lemma 2.2.2 and Discrete Gronwall Lemma, we have the following result (see Corollary 1.2.4):

Corollary 2.2.3 Under hypothesis of Lemma 2.2.2. Let $k_0 > 0$ be fixed, then the following estimate holds for all $k \le k_0$

$$d^n \le C(d^0, k_0) \quad \forall n \ge 0.$$

2.3 Fully Discrete Backward Euler Scheme in variables (u, σ)

This section is devoted to design an unconditionally energy-stable scheme for model (2.1) (for a modified energy in variables $(u, \boldsymbol{\sigma})$), using a FE discretization in space and the backward Euler discretization in time (considered for simplicity on a uniform partition of [0, T] with time step k = T/N: $(t_n = nk)_{n=0}^{n=N}$). Concerning the space discretization, we consider $\{\mathcal{T}_h\}_{h>0}$ be a family of shape-regular and quasi-uniform triangulations of $\overline{\Omega}$ made up of simplexes K (triangles in two dimensions and tetrahedra in three dimensions), so that $\overline{\Omega} =$ $\bigcup_{K \in \mathfrak{T}_h} K$, where $h = \max_{K \in \mathfrak{T}_h} h_K$, with h_K being the diameter of K. Further, let $\mathfrak{N}_h = \{\mathbf{a}_i\}_{i \in \mathfrak{I}}$ denote the set of all the nodes of \mathfrak{T}_h . We choose the following continuous FE spaces for u, $\boldsymbol{\sigma}$ and v:

$$(U_h, \boldsymbol{\Sigma}_h, V_h) \subset H^1 \times \boldsymbol{H}^1_{\sigma} \times W^{1,6}, \text{ generated by } \mathbb{P}_k, \mathbb{P}_m, \mathbb{P}_r \text{ with } k, m, r \ge 1.$$

Now, let $A_h : U_h \to U_h$, $B_h : \Sigma_h \to \Sigma_h$ and $\widetilde{A}_h : V_h \to V_h$ be the linear operators defined, respectively, as follows:

$$(A_h u_h, \bar{u}_h) = (\nabla u_h, \nabla \bar{u}_h) + (u_h, \bar{u}_h), \quad \forall \bar{u}_h \in U_h, (B_h \boldsymbol{\sigma}_h, \bar{\boldsymbol{\sigma}}_h) = (\nabla \cdot \boldsymbol{\sigma}_h, \nabla \cdot \bar{\boldsymbol{\sigma}}_h) + (\operatorname{rot} \boldsymbol{\sigma}_h, \operatorname{rot} \bar{\boldsymbol{\sigma}}_h) + (\boldsymbol{\sigma}_h, \bar{\boldsymbol{\sigma}}_h), \quad \forall \bar{\boldsymbol{\sigma}}_h \in \boldsymbol{\Sigma}_h,$$

$$(\tilde{A}_h v_h, \bar{v}_h) = (\nabla v_h, \nabla \bar{v}_h) + (v_h, \bar{v}_h), \quad \forall \bar{v}_h \in V_h.$$

$$(2.13)$$

Moreover, we choose the following interpolation operators:

$$\mathfrak{R}_h^u: H^1(\Omega) \to U_h, \quad \mathfrak{R}_h^{\boldsymbol{\sigma}}: \boldsymbol{H}_{\sigma}^1(\Omega) \to \boldsymbol{\Sigma}_h, \quad \mathfrak{R}_h^v: H^1(\Omega) \to V_h$$

such that for all $u \in H^1(\Omega)$, $\boldsymbol{\sigma} \in \boldsymbol{H}^1_{\sigma}(\Omega)$ and $v \in H^1(\Omega)$, $\mathcal{R}^u_h u \in U_h$, $\mathcal{R}^{\boldsymbol{\sigma}}_h \boldsymbol{\sigma} \in \boldsymbol{\Sigma}_h$ and $\mathcal{R}^v_h v \in V_h$ satisfy

$$\left(\nabla(\mathfrak{R}_{h}^{u}u-u),\nabla\bar{u}_{h}\right)+\left(\mathfrak{R}_{h}^{u}u-u,\bar{u}_{h}\right)=0, \quad \forall\bar{u}_{h}\in U_{h},$$
(2.14)

$$(\nabla \cdot (\mathfrak{R}_{h}^{\sigma}\boldsymbol{\sigma} - \boldsymbol{\sigma}), \nabla \cdot \bar{\boldsymbol{\sigma}}_{h}) + (\operatorname{rot}(\mathfrak{R}_{h}^{\sigma}\boldsymbol{\sigma} - \boldsymbol{\sigma}), \operatorname{rot} \bar{\boldsymbol{\sigma}}_{h}) + (\mathfrak{R}_{h}^{\sigma}\boldsymbol{\sigma} - \boldsymbol{\sigma}, \bar{\boldsymbol{\sigma}}_{h}) = 0, \quad \forall \bar{\boldsymbol{\sigma}}_{h} \in \boldsymbol{\Sigma}_{h}, \quad (2.15)$$
$$(\nabla (\mathfrak{R}_{h}^{v}v - v), \nabla \bar{v}_{h}) + (\mathfrak{R}_{h}^{v}v - v, \bar{v}_{h}) = 0, \quad \forall \bar{v}_{h} \in V_{h}, \quad (2.16)$$

respectively. Observe that, from Lax-Milgram Theorem, the interpolation operators \mathcal{R}_h^u , \mathcal{R}_h^{σ} and \mathcal{R}_h^v are well defined. Moreover, the following interpolation errors hold

$$\frac{1}{h} \|\mathcal{R}_{h}^{u}u - u\|_{0} + \|\mathcal{R}_{h}^{u}u - u\|_{1} \le Ch^{k} \|u\|_{k+1} \quad \forall u \in H^{k+1}(\Omega),$$
(2.17)

$$\frac{1}{h} \| \mathcal{R}_{h}^{\boldsymbol{\sigma}} \boldsymbol{\sigma} - \boldsymbol{\sigma} \|_{0} + \| \mathcal{R}_{h}^{\boldsymbol{\sigma}} \boldsymbol{\sigma} - \boldsymbol{\sigma} \|_{1} \le Ch^{m} \| \boldsymbol{\sigma} \|_{m+1} \quad \forall \boldsymbol{\sigma} \in \boldsymbol{H}^{m+1}(\Omega),$$
(2.18)

$$\frac{1}{h} \|\mathcal{R}_{h}^{v}v - v\|_{0} + \|\mathcal{R}_{h}^{v}v - v\|_{1} \le Ch^{r} \|v\|_{r+1} \quad \forall v \in H^{r+1}(\Omega).$$
(2.19)

Also, the following stability properties will be used

$$\|(\mathcal{R}_{h}^{u}u,\mathcal{R}_{h}^{\boldsymbol{\sigma}}\boldsymbol{\sigma},\mathcal{R}_{h}^{v}v)\|_{W^{1,6}} \leq C\|(u,\boldsymbol{\sigma},v)\|_{2},$$
(2.20)

which can be obtained from (2.17)-(2.19), using the inverse inequality

$$\|(u_h, \boldsymbol{\sigma}_h, v_h)\|_{W^{1,6}} \le Ch^{-1} \|(u_h, \boldsymbol{\sigma}_h, v_h)\|_1 \text{ for all } (u_h, \boldsymbol{\sigma}_h, v_h) \in U_h \times \boldsymbol{\Sigma}_h \times V_h,$$

and comparing $\mathcal{R}_{h}^{u,\sigma,v}$ with an average interpolation of Clement or Scott-Zhang type (which is stable in $W^{1,6}$ -norm).

Lemma 2.3.1 Assume the H^2 -regularity for problems (2.9)-(2.10) given in (2.11). Then, the following estimates hold

$$\|u_h\|_{W^{1,6}} \le C \|A_h u_h\|_0 \quad \forall u_h \in U_h, \qquad \|v_h\|_{W^{1,6}} \le C \|\widetilde{A}_h v_h\|_0 \quad \forall v_h \in V_h,$$
(2.21)

$$\|\boldsymbol{\sigma}_h\|_{W^{1,6}} \le C \|B_h \boldsymbol{\sigma}_h\|_0 \quad \forall \boldsymbol{\sigma}_h \in \boldsymbol{\Sigma}_h.$$
(2.22)

Proof. First, we consider regular functions associated to the discrete functions $A_h u_h$, $\widetilde{A}_h v_h$ and $B_h \sigma_h$. We define $u(h), v(h) \in H^2(\Omega)$ and $\sigma(h) \in H^2(\Omega)$ as the solutions of problems

$$\begin{cases} -\Delta u(h) + u(h) = A_h u_h & \text{in } \Omega, \\ \frac{\partial u(h)}{\partial \mathbf{n}} = 0 & \text{on } \partial\Omega, \end{cases}$$
(2.23)

$$\begin{cases} -\Delta v(h) + v(h) = \widetilde{A}_h v_h & \text{in } \Omega, \\ \frac{\partial v(h)}{\partial \mathbf{n}} = 0 & \text{on } \partial\Omega, \end{cases}$$
(2.24)

and

$$\begin{cases} -\nabla(\nabla \cdot \boldsymbol{\sigma}(h)) + \operatorname{rot} (\operatorname{rot} \boldsymbol{\sigma}(h)) + \boldsymbol{\sigma}(h) = B_h \boldsymbol{\sigma}_h & \text{in } \Omega, \\ \boldsymbol{\sigma}(h) \cdot \mathbf{n} = 0, \quad [\operatorname{rot} \boldsymbol{\sigma}(h) \times \mathbf{n}]_{tang} = 0 & \text{on } \partial\Omega. \end{cases}$$
(2.25)

In particular, from (2.11),

$$||u(h)||_2 \le C ||A_h u_n||_0, ||v(h)||_2 \le C ||\widetilde{A}_h v_h||_0 \text{ and } ||\boldsymbol{\sigma}(h)||_2 \le C ||B_h \boldsymbol{\sigma}_h||_0.$$
 (2.26)

Now, we decompose the $W^{1,6}$ -norm as:

$$\begin{aligned} \|u_{h}\|_{W^{1,6}} &\leq \|u_{h} - \mathcal{R}_{h}^{u}u(h)\|_{W^{1,6}} + \|\mathcal{R}_{h}^{u}u(h) - u(h)\|_{W^{1,6}} + \|u(h)\|_{W^{1,6}} := I_{1} + I_{2} + I_{3}, \quad (2.27) \\ \|v_{h}\|_{W^{1,6}} &\leq \|v_{h} - \mathcal{R}_{h}^{v}v(h)\|_{W^{1,6}} + \|\mathcal{R}_{h}^{v}v(h) - v(h)\|_{W^{1,6}} + \|v(h)\|_{W^{1,6}} := H_{1} + H_{2} + H_{3}, \quad (2.28) \\ \|\boldsymbol{\sigma}_{h}\|_{W^{1,6}} &\leq \|\boldsymbol{\sigma}_{h} - \mathcal{R}_{h}^{\boldsymbol{\sigma}}\boldsymbol{\sigma}(h)\|_{W^{1,6}} + \|\mathcal{R}_{h}^{\boldsymbol{\sigma}}\boldsymbol{\sigma}(h) - \boldsymbol{\sigma}(h)\|_{W^{1,6}} + \|\boldsymbol{\sigma}(h)\|_{W^{1,6}} := J_{1} + J_{2} + J_{3}. \quad (2.29) \end{aligned}$$

In order to bound J_i (i = 1, 2), we test $(2.25)_1$ by $\bar{\sigma}_h \in \Sigma_h$ and using $(2.13)_2$ we have

$$(\nabla \cdot \boldsymbol{\sigma}_h, \nabla \cdot \bar{\boldsymbol{\sigma}}_h) + (\operatorname{rot} \boldsymbol{\sigma}_h, \operatorname{rot} \bar{\boldsymbol{\sigma}}_h) + (\boldsymbol{\sigma}_h, \bar{\boldsymbol{\sigma}}_h)$$

= $(\nabla \cdot \boldsymbol{\sigma}(h), \nabla \cdot \bar{\boldsymbol{\sigma}}_h) + (\operatorname{rot} \boldsymbol{\sigma}(h), \operatorname{rot} \bar{\boldsymbol{\sigma}}_h) + (\boldsymbol{\sigma}(h), \bar{\boldsymbol{\sigma}}_h), \quad \forall \bar{\boldsymbol{\sigma}}_h \in \Sigma_{\mathbf{A}}.30)$

By subtracting at both sides of equality (2.30) the terms $(\nabla \cdot \mathcal{R}_h^{\sigma} \boldsymbol{\sigma}(h), \nabla \cdot \bar{\boldsymbol{\sigma}}_h)$, $(\operatorname{rot} \mathcal{R}_h^{\sigma} \boldsymbol{\sigma}(h), \operatorname{rot} \bar{\boldsymbol{\sigma}}_h)$ and $(\mathcal{R}_h^{\sigma} \boldsymbol{\sigma}(h), \bar{\boldsymbol{\sigma}}_h)$, testing by $\bar{\boldsymbol{\sigma}}_h = \boldsymbol{\sigma}_h - \mathcal{R}_h^{\sigma} \boldsymbol{\sigma}(h) \in \boldsymbol{\Sigma}_h$ and using the Hölder and Young inequalities, we deduce

$$\|\boldsymbol{\sigma}_{h} - \mathcal{R}_{h}^{\boldsymbol{\sigma}}\boldsymbol{\sigma}(h)\|_{1} \leq C \|\mathcal{R}_{h}^{\boldsymbol{\sigma}}\boldsymbol{\sigma}(h) - \boldsymbol{\sigma}(h)\|_{1} \leq Ch \|\boldsymbol{\sigma}(h)\|_{2},$$
(2.31)

where in the last inequality interpolation error (2.18) was used. Then, using in (2.31) the inverse inequality $\|\boldsymbol{\sigma}_h\|_{W^{1,6}} \leq Ch^{-1} \|\boldsymbol{\sigma}_h\|_1$ for all $\boldsymbol{\sigma}_h \in \boldsymbol{\Sigma}_h$, we conclude that for i = 1, 2

$$J_i \le Ch^{-1} \|\mathcal{R}_h^{\boldsymbol{\sigma}} \boldsymbol{\sigma}(h) - \boldsymbol{\sigma}(h)\|_1 \le C \|\boldsymbol{\sigma}(h)\|_2.$$
(2.32)

Finally,

$$J_3 = \|\boldsymbol{\sigma}(h)\|_{W^{1,6}} \le C \|\boldsymbol{\sigma}(h)\|_2.$$
(2.33)

Therefore, using (2.32)-(2.33) in (2.29), and taking into account (2.26), we deduce (2.22). Proceeding analogously for I_i and H_i (i = 1, 2, 3), we deduce (2.21).

2.3.1 Definition of the scheme

By taking into account the reformulation (2.7), we consider the following FE Backward Euler Scheme in variables (u, σ) (*Scheme* **US**, from now on) which is a first order in time, nonlinear and coupled scheme:

• Initialization: We fix $(u_h^0, \boldsymbol{\sigma}_h^0) = (\mathcal{R}_h^u u_0, \mathcal{R}_h^{\boldsymbol{\sigma}} \boldsymbol{\sigma}_0) \in U_h \times \boldsymbol{\Sigma}_h$ and $v_h^0 = \mathcal{R}_h^v v_0 \in V_h$. Then, $\int_{\Omega} u_h^0 = \int_{\Omega} u_0 = m_0$.

Time step n: Given $(u_h^{n-1}, \boldsymbol{\sigma}_h^{n-1}) \in U_h \times \boldsymbol{\Sigma}_h$, compute $(u_h^n, \boldsymbol{\sigma}_h^n) \in U_h \times \boldsymbol{\Sigma}_h$ solving

$$\begin{cases} (\delta_t u_h^n, \bar{u}_h) + (\nabla u_h^n, \nabla \bar{u}_h) + (u_h^n \boldsymbol{\sigma}_h^n, \nabla \bar{u}_h) = 0, \quad \forall \bar{u}_h \in U_h, \\ (\delta_t \boldsymbol{\sigma}_h^n, \bar{\boldsymbol{\sigma}}_h) + (B_h \boldsymbol{\sigma}_h^n, \bar{\boldsymbol{\sigma}}_h) - 2(u_h^n \nabla u_h^n, \bar{\boldsymbol{\sigma}}_h) = 0, \quad \forall \bar{\boldsymbol{\sigma}}_h \in \boldsymbol{\Sigma}_h, \end{cases}$$
(2.34)

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

Once the scheme **US** is solved, given $v_h^{n-1} \in V_h$, we can recover $v_h^n = v_h^n((u_h^n)^2) \in V_h$ solving:

$$(\delta_t v_h^n, \bar{v}_h) + (\bar{A}_h v_h^n, \bar{v}_h) = ((u_h^n)^2, \bar{v}_h), \quad \forall \bar{v}_h \in V_h.$$
(2.35)

Given $u_h^n \in U_h$ and $v_h^{n-1} \in V_h$, Lax-Milgram theorem implies that there exists a unique $v_h^n \in V_h$ solution of (2.35).

Remark 2.3.2 By using the mass-lumping technique in all terms of (2.35) excepting the self-diffusion term $(\nabla v_h^n, \nabla \bar{v}_h)$, approximating by \mathbb{P}_1 -continuous FE and imposing a condition based on a geometrical property of the triangulation, related to the fact that the interior angles of the triangles or tetrahedra must be at most $\pi/2$, we can prove that if $v_h^{n-1} \geq 0$ then $v_h^n \geq 0$. However, in all numerical simulations that we have made without using mass-lumping, we have not found any example in which, beginning with $v_h^0 \geq 0$ we obtain $v_h^n(\mathbf{a}_i) < 0$, for some n > 0 and \mathbf{a}_i .

2.3.2 Solvability, Energy-Stability and Convergence

Assuming that the functions $\bar{u}_h = 1 \in U_h$ and $\bar{v}_h = 1 \in V_h$, we deduce that the scheme **US** conserves in time the total mass $\int_{\Omega} u_h^n$, that is,

$$\int_{\Omega} u_h^n = \int_{\Omega} u_h^{n-1} = \dots = \int_{\Omega} u_h^0,$$

and we have the following behavior for $\int_{\Omega} v_h^n$:

$$\delta_t \left(\int_{\Omega} v_h^n \right) = \int_{\Omega} (u_h^n)^2 - \int_{\Omega} v_h^n.$$

Now, we establish some results concerning to the solvability and energy-stability of scheme **US**, but we will omit their proofs because those follow the same ideas given in Chapter 1 (Theorem 1.4.3, Lemma 1.4.6 and Theorem 1.4.8, respectively).

Theorem 2.3.3 (Unconditional existence and conditional uniqueness) There exists $(u_h^n, \sigma_h^n) \in U_h \times \Sigma_h$ solution of the scheme **US**. Moreover, if

$$k \| (u_h^n, \boldsymbol{\sigma}_h^n) \|_1^4 \quad is \ small \ enough, \tag{2.36}$$

then the solution is unique.

Remark 2.3.4 In the case of 2D domains, from estimate (2.54) below, the uniqueness restriction (2.36) can be relaxed to kK_0^2 small enough, where K_0 is a constant depending on data (Ω, u_0, σ_0) , but independent of (k, h) and n.

Remark 2.3.5 In 3D domains, using the inverse inequality $||u_h||_1 \leq \frac{C}{h} ||u_h||_0$ (see Lemma 4.5.3 in [2], p. 111) and estimate (2.41) below, we have that

$$\|(u_h^n, \boldsymbol{\sigma}_h^n)\|_1^4 \le \frac{C}{h^4} \|(u_h^n, \boldsymbol{\sigma}_h^n)\|_0^4 \le \frac{C}{h^4} C_0^2$$

and therefore, the uniqueness restriction (2.36) can be rewrite as

$$\frac{kC_1}{h^4} \quad small \ enough, \tag{2.37}$$

where C_1 is a positive constant depending on data $(\Omega, u_0, \boldsymbol{\sigma}_0)$, but independent of n.
Definition 2.3.6 A numerical scheme with solution (u_n, σ_n) is called energy-stable with respect to the energy

$$\mathcal{E}(u, \boldsymbol{\sigma}) = \frac{1}{2} \|u\|_0^2 + \frac{1}{4} \|\boldsymbol{\sigma}\|_0^2, \qquad (2.38)$$

if this energy is time decreasing, that is

$$\mathcal{E}(u_h^n, \boldsymbol{\sigma}_h^n) \le \mathcal{E}(u_h^{n-1}, \boldsymbol{\sigma}_h^{n-1}), \quad \forall n.$$
(2.39)

Lemma 2.3.7 (Unconditional stability) The scheme **US** is unconditionally energy-stable with respect to $\mathcal{E}(u, \boldsymbol{\sigma})$. In fact, if $(u_h^n, \boldsymbol{\sigma}_h^n)$ is a solution of the scheme **US**, then the following discrete energy law holds

$$\delta_t \mathcal{E}(u_h^n, \boldsymbol{\sigma}_h^n) + \frac{k}{2} \|\delta_t u_h^n\|_0^2 + \frac{k}{4} \|\delta_t \boldsymbol{\sigma}_h^n\|_0^2 + \|\nabla u_h^n\|_0^2 + \frac{1}{2} \|\boldsymbol{\sigma}_h^n\|_1^2 = 0.$$
(2.40)

Remark 2.3.8 Looking at (2.40), we can say that the scheme **US** introduces the following two first order "numerical dissipation terms":

$$\frac{k}{2} \|\delta_t u_h^n\|_0^2 \quad and \quad \frac{k}{4} \|\delta_t \boldsymbol{\sigma}_h^n\|_0^2.$$

From the (local in time) discrete energy law (2.40), we deduce the following global in time estimates for (u_h^n, σ_h^n) solution of scheme **US**:

Theorem 2.3.9 (Uniform Weak estimates of scheme US) Let (u_h^n, σ_h^n) be a solution of scheme **US**. Then, the following estimates hold

$$\|(u_h^n, \boldsymbol{\sigma}_h^n)\|_0^2 + k^2 \sum_{m=1}^n \|(\delta_t u_h^m, \delta_t \boldsymbol{\sigma}_h^m)\|_0^2 + k \sum_{m=1}^n \|(\nabla u_h^m, \boldsymbol{\sigma}_h^m)\|_{L^2 \times H^1}^2 \le C_0, \quad \forall n \ge 1, \quad (2.41)$$

$$k \sum_{m=n_0+1}^{n+n_0} \|(u_h^m, \boldsymbol{\sigma}_h^m)\|_1^2 \le C_0 + C_1(nk), \quad \forall n \ge 1,$$
(2.42)

where the integer $n_0 \ge 0$ is arbitrary, with positive constants C_0, C_1 depending on the data $(\Omega, u_0, \boldsymbol{\sigma}_0)$, but independent of (k, h) and (n, n_0) .

Weak estimates of v_h^n in 3D domains

In this fully discrete scheme **US** it is not clear how to quantify the relation $\sigma_h^n \simeq \nabla v_h^n$, and therefore, the uniform estimates for v_n cannot be obtained directly from estimates for σ_h^n . Thus, in this subsection we will obtain directly uniform weak estimates for v_h^n .

Lemma 2.3.10 (Estimate of $\left|\int_{\Omega} v_h^n\right|$) Let v_h^n be the solution of (2.35). Then, it holds

$$\left| \int_{\Omega} v_h^n \right| \le K_0, \quad \forall n \ge 0, \tag{2.43}$$

where K_0 is a positive constant depending on the data u_0, σ_0, v_0 , but independent of k, h and n.

Proof. The proof follows as in Corollary 1.4.10.

Lemma 2.3.11 (Discrete duality estimates for v_h^n) Let v_h^n be the solution of (2.35). Then, the following estimates hold

$$\|\widetilde{A}_{h}^{-1}v_{h}^{n}\|_{1}^{2} \le K_{0}, \quad \forall n \ge 0,$$
(2.44)

$$k \sum_{m=n_0+1}^{n_0+n} \|v_h^m\|_0^2 \le K_0 + K_1(nk), \quad \forall n \ge 1,$$
(2.45)

with positive constants K_0, K_1 depending on the data $\Omega, u_0, \sigma_0, v_0$, but independent of (k, h)and (n, n_0) .

Proof. Testing (2.35) by $\bar{v} = \tilde{A}_h^{-1} v_h^n$, and using (2.21)₂ and (2.41), it is not difficult to deduce

$$\delta_t \left(\frac{1}{2} \| \widetilde{A}_h^{-1} v_h^n \|_1^2 \right) + \| v_h^n \|_0^2 \le \| u_h^n \|_0^2 \| \widetilde{A}_h^{-1} v_h^n \|_{L^{\infty}} \le C \| \widetilde{A}_h^{-1} v_h^n \|_{W^{1,6}} \le C \| v_h^n \|_0 \le \frac{1}{2} \| v_h^n \|_0^2 + C,$$

which implies that

$$\delta_t \left(\| \widetilde{A}_h^{-1} v_h^n \|_1^2 \right) + \| v_h^n \|_0^2 \le C,$$
(2.46)

where C is a constant independent of (k, h) and n. Then, using that $||v_h^n||_0^2 \ge C ||\widetilde{A}_h^{-1}v_h^n||_1^2$ (owing to $(2.21)_2$) in (2.46), we deduce

$$(1+Ck)\|\widetilde{A}_{h}^{-1}v_{h}^{n}\|_{1}^{2} - \|\widetilde{A}_{h}^{-1}v_{h}^{n-1}\|_{1}^{2} \le Ck, \qquad (2.47)$$

and therefore, using Lemma 2.2.1 in (2.47), we obtain (2.44). Finally, multiplying (2.46) by k and adding from $m = n_0 + 1$ to $m = n + n_0$, using (2.44), we conclude (2.45).

Lemma 2.3.12 (Weak estimates for v_n^h) Under hypothesis of Lemma 2.3.11, the following estimates hold

$$||v_h^n||_0^2 \le C_2, \quad \forall n \ge 0,$$
 (2.48)

$$k \sum_{m=n_0+1}^{n+n_0} \|v_h^m\|_1^2 \le C_2 + C_3(nk), \quad \forall n \ge 1,$$
(2.49)

with positive constants C_2, C_3 depending on the data $\Omega, u_0, \sigma_0, v_0$, but independent of (k, h)and (n, n_0) .

Proof. Testing (2.35) by $\bar{v} = v_h^n$ we obtain

$$\delta_t \left(\frac{1}{2} \| v_h^n \|_0^2 \right) + \frac{1}{2k} \| v_h^n - v_h^{n-1} \|_0^2 + \| v_h^n \|_1^2 = ((u_h^n)^2, v_h^n - v_h^{n-1}) + ((u_h^n)^2, v_h^{n-1}) \\ \leq \frac{1}{4k} \| v_h^n - v_h^{n-1} \|_0^2 + Ck \| u_h^n \|_{L^4}^4 + \frac{1}{2} \| u_h^n \|_{L^4}^2 \| v_h^{n-1} \|_0^2 + \frac{1}{2} \| u_h^n \|_{L^4}^2,$$

which implies that

$$\|v_h^n\|_0^2 - \|v_h^{n-1}\|_0^2 + k\|v_h^n\|_1^2 \le Ck^2 \|u_h^n\|_{L^4}^4 + k\|u_h^n\|_{L^4}^2 \|v_h^{n-1}\|_0^2 + k\|u_h^n\|_{L^4}^2.$$
(2.50)

Moreover, taking into account that $k \|u_h^n\|_{L^4}^2 \leq kC \|u_h^n\|_1^2$, from estimate (2.42) we deduce

$$k \|u_h^n\|_{L^4}^2 \le C_0 + C_1 k. \tag{2.51}$$

Then, from (2.50) and (2.51), we have

$$\|v_h^n\|_0^2 - \|v_h^{n-1}\|_0^2 + k\|v_h^n\|_1^2 \le (CC_0 + CC_1k + 1)k\|u_h^n\|_{L^4}^2 + k\|u_h^n\|_{L^4}^2\|v_h^{n-1}\|_0^2,$$
(2.52)

which, in particular implies

$$\|v_h^n\|_0^2 - \|v_h^{n-1}\|_0^2 \le C \, k \|u_h^n\|_{L^4}^2 + k \|u_h^n\|_{L^4}^2 \|v_h^{n-1}\|_0^2.$$
(2.53)

Therefore, taking into account estimates (2.42) and (2.45), applying Corollary 2.2.3 in (2.53), we conclude (2.48). Finally, summing for m from $n_0 + 1$ to $n + n_0$ in (2.52), and using (2.42) and (2.48), we deduce (2.49).

Convergence

Starting from the previous stability estimates, proceeding as in Theorem 1.4.11 we can prove the convergence towards weak solutions as $(k, h) \rightarrow 0$. Concretely, by introducing the functions:

- $(\widetilde{u}_{h,k}, \widetilde{\boldsymbol{\sigma}}_{h,k})$ are continuous functions on $[0, +\infty)$, linear on each interval (t_{n-1}, t_n) and equal to $(u_h^n, \boldsymbol{\sigma}_h^n)$ at $t = t_n, n \ge 0$;
- $(u_{h,k}^r, \boldsymbol{\sigma}_{h,k}^r)$ as the piecewise constant functions taking values $(u_h^n, \boldsymbol{\sigma}_h^n)$ on $(t_{n-1}, t_n]$, $n \ge 1$,

then, we have the following result:

Theorem 2.3.13 (Convergence) There exists a subsequence (k', h') of (k, h), with $k', h' \downarrow 0$, and a weak solution (u, σ) of (2.7) in $(0, +\infty)$, such that $(\tilde{u}_{h',k'}, \tilde{\sigma}_{h',k'})$ and $(u_{h',k'}^r, \sigma_{h',k'}^r)$ converge to (u, σ) weakly-* in $L^{\infty}(0, +\infty; L^2(\Omega) \times L^2(\Omega))$, weakly in $L^2(0, T; H^1(\Omega) \times H^1(\Omega))$ and strongly in $L^2(0, T; L^2(\Omega) \times L^2(\Omega))$, for any T > 0.

Note that, since the positivity of u_h^n cannot be assured, then the positivity of the limit function u cannot be proven. Moreover, if we introduce the functions:

- $\widetilde{v}_{h,k}$ are continuous functions on $[0, +\infty)$, linear on each interval (t_{n-1}, t_n) and equal to v_h^n , at $t = t_n$, $n \ge 0$;
- $v_{h,k}^r$ as the piecewise constant functions taking values v_h^n on $(t_{n-1}, t_n], n \ge 1$,

proceeding as in Lemma 1.4.12, and taking into account the estimates (2.48)-(2.49), the following result can be proved:

Corollary 2.3.14 There exists a subsequence (k', h') of (k, h), with $k', h' \downarrow 0$, and a weak solution v of (2.8) in $(0, +\infty)$, such that $\tilde{v}_{h',k'}$ and $v^r_{h',k'}$ converge to v weakly-* in $L^{\infty}(0, +\infty; L^2(\Omega))$, weakly in $L^2(0, T; H^1(\Omega))$ and strongly in $L^2(0, T; L^2(\Omega))$, for any T > 0.

Remark 2.3.15 From the equivalence of problems (2.1) and (2.7)-(2.8) stablished in Chapter 1, and taking into account Theorem 2.3.13 and Corollary 2.3.14, we deduce that the limit pair (u, v) is a weak-strong solution of problem (2.1).

2.3.3 Uniform Strong Estimates

In this subsection, we are going to establish a priori estimates in strong norms for any solution $(u_n, \boldsymbol{\sigma}_n)$ of the scheme **US** and v_h^n of (2.35). We will assume the estimate

$$\|(u_h^n, \boldsymbol{\sigma}_h^n)\|_1^2 \le K_0, \quad \forall n \ge 0, \tag{2.54}$$

with $K_0 > 0$ a constant depending on the initial data, but independent of (k, h) and n. Note that estimate (2.54) can be proven in 2D domains, following line to line the proof of Theorem 1.4.20.

Uniform Strong Estimates of the scheme US

Theorem 2.3.16 (Strong estimates) Let (u_h^n, σ_h^n) be a solution of the scheme **US** satisfying the assumption (2.54). Then, the following estimate holds

$$k \sum_{m=n_0+1}^{n+n_0} (\|(\delta_t u_h^m, \delta_t \boldsymbol{\sigma}_h^m)\|_0^2 + \|(u_h^m, \boldsymbol{\sigma}_h^m)\|_{W^{1,6}}^2) \le K_1 + K_2(nk), \quad \forall n \ge 1,$$
(2.55)

for any integer $n_0 \ge 0$, with positive constants K_1, K_2 depending on (Ω, u_0, σ_0) , but independent of (k, h) and (n, n_0) .

Proof. The proof follows as in Theorem 1.4.14, but in this case it is necessary to use the estimate

$$\|(u_h^n, \boldsymbol{\sigma}_h^n)\|_{W^{1,6}} \le C(\|(\delta_t u_h^n, \delta_t \boldsymbol{\sigma}_h^n)\|_0 + \|(u_h^n, \boldsymbol{\sigma}_h^n)\|_1^3 + \|u_h^n\|_0),$$
(2.56)

which is deduced from (2.21) and (2.22).

Theorem 2.3.17 (More regular estimates) Assume that $(u_0, \sigma_0) \in H^2(\Omega) \times H^2(\Omega)$. Under the hypothesis of Theorem 2.3.16, the following estimates hold

$$\|(\delta_t u_h^n, \delta_t \boldsymbol{\sigma}_h^n)\|_0^2 \le K_3, \quad \forall n \ge 1,$$

$$(2.57)$$

$$k \sum_{m=n_0+1}^{n+n_0} \| (\delta_t u_h^m, \delta_t \boldsymbol{\sigma}_h^m) \|_1^2 \le K_4 + K_5(nk), \quad \forall n \ge 1,$$
(2.58)

 $\|(u_h^n, \boldsymbol{\sigma}_h^n)\|_{W^{1,6}}^2 \le K_6, \quad \forall n \ge 0,$ (2.59)

for any integer $n_0 \ge 0$, with positive constants K_3, K_4, K_5, K_6 depending on data $(\Omega, u_0, \boldsymbol{\sigma}_0)$, but independent of (k, h) and (n, n_0) .

Proof. The proof follows as in Theorem 1.4.16, but in this case, in order to obtain (2.59) it is necessary to use (2.56).

Remark 2.3.18 In particular, from (2.59) one has $||(u_h^n, \boldsymbol{\sigma}_h^n)||_{L^{\infty}} \leq K_7$ for all $n \geq 0$, with $K_7 > 0$ a constant independent of (k, h) and n.

Uniform Strong estimates of v_h^n

Theorem 2.3.19 (Strong estimates for v_n^h) Assume (2.54) and let v_h^n be the solution of (2.35). Then, the following estimates hold

$$\|v_h^n\|_1^2 \le C_1, \quad \forall n \ge 0,$$
 (2.60)

$$k \sum_{m=n_0+1}^{n+n_0} (\|\delta_t v_h^m\|_0^2 + \|\widetilde{A}_h v_h^m\|_0^2) \le C_1 + C_2(nk), \quad \forall n \ge 1,$$
(2.61)

for any integer $n_0 \ge 0$, with positive constants C_1, C_2 depending on $\Omega, u_0, \sigma_0, v_0$, but independent of (k, h) and (n, n_0) .

Proof. Testing (2.35) by $\widetilde{A}_h v_h^n$ and $\delta_t v_h^n$, and using the Hölder and Young inequalities, we obtain

$$\delta_t \left(\|v_h^n\|_1^2 \right) + \frac{1}{2} \|\widetilde{A}_h v_h^n\|_0^2 + \frac{1}{2} \|\delta_t v_h^n\|_0^2 \le \|u_h^n\|_{L^4}^4,$$
(2.62)

which, taking into account $(2.21)_2$ and (2.54), in particular implies

$$(1+Ck)\|v_h^n\|_1^2 - \|v_h^{n-1}\|_1^2 \le kK_0^2.$$

Thus, from Lemma 2.2.1, we deduce

$$\|v_h^n\|_1^2 \le (1+Ck)^{-n} \|v_h^0\|_1^2 + CK_0^2 \le \|v_h^0\|_1^2 + CK_0^2, \quad \forall n \ge 0,$$

which implies (2.60). Moreover, multiplying (2.62) by k and adding from $m = n_0 + 1$ to $m = n + n_0$, using (2.54) and (2.60), we deduce (2.61).

Theorem 2.3.20 (More regular estimates for v_n^h) Assume that $v_0 \in H^2(\Omega)$. Under hypothesis of Theorems 2.3.17 and 2.3.19, the following estimates hold

$$\|\delta_t v_h^n\|_0^2 \le C_3, \quad \forall n \ge 1,$$
 (2.63)

$$k \sum_{m=n_0+1}^{n+n_0} \|\delta_t v_h^m\|_1^2 \le C_4 + C_5(nk), \quad \forall n \ge 1,$$
(2.64)

$$\|v_h^n\|_{W^{1,6}}^2 \le C_6, \quad \forall n \ge 0, \tag{2.65}$$

for any integer $n_0 \ge 0$, with positive constants C_3, C_4, C_5, C_6 depending on data $\Omega, u_0, \sigma_0, v_0$, but independent of (k, h) and (n, n_0) . *Proof.* Denote by $\tilde{v}_h^n = \delta_t v_h^n$. Then, making the time discrete derivative of (2.35) (using $\delta_t (u_h^n)^2 = (u_h^n + u_h^{n-1}) \delta_t u_h^n$), testing by \tilde{v}_h^n and using (2.54) and (2.57), we obtain

$$\frac{1}{2}\delta_t\left(\|\widetilde{v}_h^n\|_0^2\right) + \frac{1}{2}\|\widetilde{v}_h^n\|_1^2 \le C\|u_h^n + u_h^{n-1}\|_{L^3}^2\|\delta_t u_h^n\|_0^2 \le C.$$
(2.66)

In particular,

$$(1+k)\|\widetilde{v}_h^n\|_0^2 - \|\widetilde{v}_h^n\|_0^2 \le kC.$$

Then, from Lemma 2.2.1, we deduce

$$\|\widetilde{v}_{h}^{n}\|_{0}^{2} \leq (1+k)^{-(n-1)} \|\widetilde{v}_{h}^{1}\|_{0}^{2} + C, \quad \forall n \geq 1.$$
(2.67)

Observe that from (2.35) we have

$$(\delta_t v_h^1, \bar{v}_h) + (\widetilde{A}_h (v_h^1 - v_h^0), \bar{v}_h) + (\widetilde{A}_h v_h^0, \bar{v}_h) = ((u_h^1)^2, \bar{v}_h), \quad \forall \bar{v}_h \in V_h.$$
(2.68)

Then, testing (2.68) by $\bar{v}_h = \delta_t v_h^1$ and using the Hölder and Young inequalities and (2.54), we can obtain

$$\|\delta_t v_h^1\|_0^2 \le C \|\widetilde{A}_h v_h^0\|_0^2 + C \|u_h^1\|_{L^4}^4.$$
(2.69)

Moreover, considering the linear and continuous operator $\widetilde{A}_h^e: H^1(\Omega) \to V_h$ defined as

$$(\widetilde{A}_h^e v, \overline{v}_h) = (\nabla v, \nabla \overline{v}_h) + (v, \overline{v}_h), \quad \forall \overline{v}_h \in V_h,$$

(which is an extension of \widetilde{A}_h to $H^1(\Omega)$), using the inverse inequality $||v_h||_1 \leq \frac{1}{h} ||v_h||_0$ for all $v_h \in V_h$, and the interpolation error (2.19), we have

$$\begin{aligned} \|\widetilde{A}_{h}v_{h}^{0}\|_{0} &\leq \|\widetilde{A}_{h}^{e}(\mathcal{R}_{h}^{v}v_{0}-v_{0})\|_{0} + \|\widetilde{A}_{h}^{e}v_{0}\|_{0} \\ &\leq C\frac{1}{h}\|\nabla(\mathcal{R}_{h}^{v}v_{0}-v_{0})\|_{0} + C\|\mathcal{R}_{h}^{v}v_{0}-v_{0}\|_{0} + \|v_{0}\|_{2} \leq C\|v_{0}\|_{2}. \end{aligned}$$
(2.70)

Thus, using (2.54) and (2.70) in (2.69), we conclude that $\|\tilde{v}_h^1\|_0^2 \leq C$, where the constant C is independent of (k, h). Therefore, using this fact in (2.67), we conclude (2.63). Moreover, multiplying (2.66) by k and adding from $m = n_0 + 1$ to $m = n + n_0$, using (2.63), we deduce (2.64). Finally, taking into account (2.21)₂, we have

$$\|v_h^n\|_{W^{1,6}} \le \|\widetilde{A}_h v_h^n\|_0 \le \|\delta_t v_h^n\|_0 + \|u_h^n\|_{L^4}^2,$$

which, taking into account that from (2.20) we have $\|v_h^0\|_{W^{1,6}} = \|\mathcal{R}_h^v v_0\|_{W^{1,6}} \le C \|v_0\|_2$, and using (2.54) and (2.63), implies (2.65).

2.3.4 Error estimates at finite time

In this subsection, we will obtain error estimates for any solution $(u_h^n, \boldsymbol{\sigma}_h^n)$ of the scheme **US** and v_h^n of (2.35), with respect to sufficiently regular solutions $(u, \boldsymbol{\sigma})$ of (2.7) and v of (2.8) respectively. In our analysis, in order to obtain optimal error estimates we need to assume that both spaces $U_h, \boldsymbol{\Sigma}_h$ are generated by \mathbb{P}_m -continuous FE and V_h is generated by \mathbb{P}_{m+1} -continuous FE, with $m \geq 1$. This is a natural assumption taking into account that the energy norm for v in the continuous model has one order greater than the energy norms for $u, \boldsymbol{\sigma}$.

Error estimates for scheme US

We start introducing the following notations for the errors at $t = t_n$: $e_u^n = u(t_n) - u_h^n$ and $e_{\sigma}^n = \sigma(t_n) - \sigma_h^n$, and for the discrete in time derivative of these errors: $\delta_t e_u^n = \frac{e_u^n - e_u^{n-1}}{k}$ and $\delta_t e_{\sigma}^n = \frac{e_{\sigma}^n - e_{\sigma}^{n-1}}{k}$. Then, subtracting (2.7) at $t = t_n$ and the scheme **US**, we have that (e_u^n, e_{σ}^n) satisfies

$$(\delta_t e_u^n, \bar{u}_h) + (\nabla e_u^n, \nabla \bar{u}_h) + (e_u^n \boldsymbol{\sigma}(t_n) + u_h^n e_{\boldsymbol{\sigma}}^n, \nabla \bar{u}_h) = (\xi_1^n, \bar{u}_h), \quad \forall \bar{u}_h \in U_h,$$
(2.71)

$$(\delta_t e^n_{\boldsymbol{\sigma}}, \bar{\boldsymbol{\sigma}}_h) + \langle B e^n_{\boldsymbol{\sigma}}, \bar{\boldsymbol{\sigma}}_h \rangle = 2(e^n_u \nabla u(t_n) + u^n_h \nabla e^n_u, \bar{\boldsymbol{\sigma}}_h) + (\xi^n_2, \bar{\boldsymbol{\sigma}}_h), \quad \forall \bar{\boldsymbol{\sigma}}_h \in \boldsymbol{\Sigma}_h,$$
(2.72)

where ξ_1^n, ξ_2^n are the consistency errors associated to the scheme **US**, that is, $\xi_1^n = \delta_t(u(t_n)) - u_t(t_n)$ and $\xi_2^n = \delta_t(\boldsymbol{\sigma}(t_n)) - \boldsymbol{\sigma}_t(t_n)$. Now, considering the interpolation operators \mathcal{R}_h^u and $\mathcal{R}_h^{\boldsymbol{\sigma}}$ defined in (2.14)-(2.15), we decompose e_u^n and $e_{\boldsymbol{\sigma}}^n$ as follows

$$e_u^n = (\mathcal{I} - \mathcal{R}_h^u)u(t_n) + \mathcal{R}_h^u u(t_n) - u_h^n = e_{u,i}^n + e_{u,h}^n,$$
(2.73)

$$e_{\boldsymbol{\sigma}}^{n} = (\mathfrak{I} - \mathfrak{R}_{h}^{\boldsymbol{\sigma}})\boldsymbol{\sigma}(t_{n}) + \mathfrak{R}_{h}^{\boldsymbol{\sigma}}\boldsymbol{\sigma}(t_{n}) - \boldsymbol{\sigma}_{h}^{n} = e_{\boldsymbol{\sigma},i}^{n} + e_{\boldsymbol{\sigma},h}^{n}, \qquad (2.74)$$

where $e_{u,i}^n$ is the interpolation error and $e_{u,h}^n$ is the discrete error of u. Then, taking into account (2.14)-(2.15), from (2.71)-(2.74) we have

$$\left(\delta_t e_{u,h}^n, \bar{u}_h \right) + \left(\nabla e_{u,h}^n, \nabla \bar{u}_h \right) + \left(e_{u,h}^n \boldsymbol{\sigma}(t_n) + u_h^n e_{\boldsymbol{\sigma},h}^n, \nabla \bar{u}_h \right) = \left(\xi_1^n, \bar{u}_h \right) - \left(\delta_t e_{u,i}^n, \bar{u}_h \right) - \left(e_{u,i}^n \boldsymbol{\sigma}(t_n) + u_h^n e_{\boldsymbol{\sigma},i}^n, \nabla \bar{u}_h \right) + \left(e_{u,i}^n, \bar{u}_h \right), \quad \forall \bar{u}_h \in U_h, \quad (2.75)$$

$$(\delta_t e^n_{\boldsymbol{\sigma},h}, \bar{\boldsymbol{\sigma}}_h) + (B_h e^n_{\boldsymbol{\sigma},h}, \bar{\boldsymbol{\sigma}}_h) = (\xi_2^n, \bar{\boldsymbol{\sigma}}_h) + 2(e^n_{u,h} \nabla u(t_n) + u^n_h \nabla e^n_{u,h}, \bar{\boldsymbol{\sigma}}_h) + 2(e^n_{u,i} \nabla u(t_n) + u^n_h \nabla e^n_{u,i}, \bar{\boldsymbol{\sigma}}_h) - (\delta_t e^n_{\boldsymbol{\sigma},i}, \bar{\boldsymbol{\sigma}}_h), \quad \forall \bar{\boldsymbol{\sigma}}_h \in \boldsymbol{\Sigma}_h.$$
(2.76)

Notice that $\int_{\Omega} e_{u,h}^n = 0$ (since $u_h^0 = \mathcal{R}_h^u u_0$ and from (2.14) $\int_{\Omega} \mathcal{R}_h^u u(t_n) = \int_{\Omega} u(t_n) = m_0$), hence the following norms are equivalents: $\|\nabla e_{u,h}^n\|_0 \simeq \|e_{u,h}^n\|_1$.

Theorem 2.3.21 We assume that there exists (u, σ) an exact solution of (2.7) with the following regularity:

$$\begin{cases}
(u, \boldsymbol{\sigma}) \in L^{\infty}(0, T; H^{m+1}(\Omega) \times \boldsymbol{H}^{m+1}(\Omega)), & (u_t, \boldsymbol{\sigma}_t) \in L^2(0, T; H^{m+1}(\Omega) \times \boldsymbol{H}^{m+1}(\Omega)), \\
(u_{tt}, \boldsymbol{\sigma}_{tt}) \in L^2(0, T; H^1(\Omega)' \times \boldsymbol{H}^1_{\sigma}(\Omega)').
\end{cases}$$
(2.77)

Let $(u_h^n, \boldsymbol{\sigma}_h^n)$ be a solution of the scheme **US**. Then, if

$$k(\|(u,\boldsymbol{\sigma})\|_{L^{\infty}(H^{1})}^{4} + \|(u,\boldsymbol{\sigma})\|_{L^{\infty}(H^{2})}^{2}) \quad is \ small \ enough,$$
(2.78)

the following a priori error estimate holds

$$\|(e_{u,h}^{n}, e_{\sigma,h}^{n})\|_{l^{\infty}L^{2}\cap l^{2}H^{1}} \leq C(T)(k+h^{m+1})$$
(2.79)

where $C(T) = K_1 T exp(K_2T)$, with $K_1, K_2 > 0$ independent of (k, h).

Recall that $u, \boldsymbol{\sigma}$ are approximated by \mathbb{P}_m -continuous FE. *Proof.* Taking $\bar{u}_h = e_{u,h}^n \operatorname{n}(2.75), \, \bar{\boldsymbol{\sigma}}_h = \frac{1}{2} e_{\boldsymbol{\sigma},h}^n \operatorname{in}(2.76)$ and adding, the terms $(u_h^n \nabla e_{u,h}^n, e_{\boldsymbol{\sigma},h}^n)$ cancel, and we obtain

$$\delta_t \left(\frac{1}{2} \| e_{u,h}^n \|_0^2 + \frac{1}{4} \| e_{\sigma,h}^n \|_0^2 \right) + \frac{1}{2} \| (e_{u,h}^n, e_{\sigma,h}^n) \|_1^2 = (\xi_1^n, e_{u,h}^n) + \frac{1}{2} (\xi_2^n, e_{\sigma,h}^n) - (\delta_t e_{u,i}^n, e_{u,h}^n) \\ - \frac{1}{2} \left(\delta_t e_{\sigma,i}^n, e_{\sigma,h}^n \right) - (e_{u,h}^n, \boldsymbol{\sigma}(t_n) \cdot \nabla e_{u,h}^n - \nabla u(t_n) \cdot e_{\sigma,h}^n) - (e_{u,i}^n, \boldsymbol{\sigma}(t_n) \cdot \nabla e_{u,h}^n - \nabla u(t_n) \cdot e_{\sigma,h}^n) \\ - (u_h^n, e_{\sigma,i}^n \cdot \nabla e_{u,h}^n - \nabla e_{u,i}^n \cdot e_{\sigma,h}^n) + (e_{u,i}^n, e_{u,h}^n) = \sum_{i=1}^8 I_m.$$
(2.80)

Then, using the Hölder and Young inequalities, the 3D interpolation inequality (2.12), the interpolation errors (2.17)-(2.18), the stability property (2.20) and the hypothesis (2.77), we control the terms on the right hand side of (2.80) as follows

$$I_{1} + I_{2} \leq \varepsilon \| (e_{u,h}^{n}, e_{\sigma,h}^{n}) \|_{1}^{2} + C_{\varepsilon} \| (\xi_{1}^{n}, \xi_{2}^{n}) \|_{(H^{1})' \times (H^{1}_{\sigma})'}^{2} \\ \leq \varepsilon \| (e_{u,h}^{n}, e_{\sigma,h}^{n}) \|_{1}^{2} + Ck \int_{t_{n-1}}^{t_{n}} \| (u_{tt}(t), \boldsymbol{\sigma}_{tt}(t)) \|_{(H^{1})' \times (H^{1}_{\sigma})'}^{2} dt,$$

$$(2.81)$$

m=1

$$I_{5} \leq \|e_{u,h}^{n}\|_{L^{3}}(\|\nabla u(t_{n})\|_{0}\|e_{\sigma,h}^{n}\|_{L^{6}} + \|\nabla \cdot \boldsymbol{\sigma}(t_{n})\|_{0}\|e_{u,h}^{n}\|_{L^{6}}) \\ \leq \varepsilon \|(e_{u,h}^{n}, e_{\sigma,h}^{n})\|_{1}^{2} + C_{\varepsilon} \|(\nabla u(t_{n}), \nabla \cdot \boldsymbol{\sigma}(t_{n}))\|_{0}^{4}\|e_{u,h}^{n}\|_{0}^{2},$$
(2.82)

$$I_{6} \leq \|e_{u,i}^{n}\|_{0}(\|\nabla e_{u,h}^{n}\|_{0}\|\boldsymbol{\sigma}(t_{n})\|_{L^{\infty}} + \|\nabla u(t_{n})\|_{L^{3}}\|e_{\boldsymbol{\sigma},h}^{n}\|_{L^{6}})$$

$$\leq \varepsilon \|(e_{u,h}^{n}, e_{\boldsymbol{\sigma},h}^{n})\|_{1}^{2} + C_{\varepsilon}\|(\nabla u(t_{n}), \boldsymbol{\sigma}(t_{n}))\|_{L^{3} \times L^{\infty}}^{2}\|e_{u,i}^{n}\|_{0}^{2}$$

$$\leq \varepsilon \|(e_{u,h}^{n}, e_{\boldsymbol{\sigma},h}^{n})\|_{1}^{2} + Ch^{2(m+1)}\|u(t_{n})\|_{m+1}^{2} \leq \varepsilon \|(e_{u,h}^{n}, e_{\boldsymbol{\sigma},h}^{n})\|_{1}^{2} + Ch^{2(m+1)}, \quad (2.83)$$

$$I_{7} \leq |(e_{u,h}^{n}, e_{\sigma,i}^{n} \cdot \nabla e_{u,h}^{n} - \nabla e_{u,i}^{n} \cdot e_{\sigma,h}^{n})| + |(\mathcal{R}_{h}^{u}u(t_{n}), e_{\sigma,i}^{n} \cdot \nabla e_{u,h}^{n} - \nabla e_{u,i}^{n} \cdot e_{\sigma,h}^{n})| \\ \leq \varepsilon ||(e_{u,h}^{n}, e_{\sigma,h}^{n})||_{1}^{2} + C_{\varepsilon} ||e_{u,h}^{n}||_{0}^{2} ||(e_{u,i}^{n}, e_{\sigma,i}^{n})||_{W^{1,3} \times L^{\infty}}^{2} + C_{\varepsilon} ||\mathcal{R}_{h}^{u}u(t_{n})||_{W^{1,3} \cap L^{\infty}}^{2} ||(e_{u,i}^{n}, e_{\sigma,i}^{n})||_{0}^{2} \\ \leq \varepsilon ||(e_{u,h}^{n}, e_{\sigma,h}^{n})||_{1}^{2} + C ||(u(t_{n}), \sigma(t_{n}))||_{2}^{2} ||e_{u,h}^{n}||_{0}^{2} + Ch^{2(m+1)} ||(u(t_{n}), \sigma(t_{n}))||_{m+1}^{2} ||u(t_{n})||_{2}^{2} \\ \leq \varepsilon ||(e_{u,h}^{n}, e_{\sigma,h}^{n})||_{1}^{2} + C ||(u(t_{n}), \sigma(t_{n}))||_{2}^{2} ||e_{u,h}^{n}||_{0}^{2} + Ch^{2(m+1)}, \qquad (2.84)$$

 $I_8 \le \|e_{u,i}^n\|_0 \|e_{u,h}^n\|_0 \le \varepsilon \|e_{u,h}^n\|_1^2 + Ch^{2(m+1)},$ (2.85)

$$I_{3} + I_{4} \leq \|(e_{u,h}^{n}, e_{\sigma,h}^{n})\|_{0}\|((\Im - \mathcal{R}_{h}^{u})\delta_{t}u(t_{n}), (\Im - \mathcal{R}_{h}^{\sigma})\delta_{t}\sigma(t_{n}))\|_{0}$$

$$\leq \varepsilon \|(e_{u,h}^{n}, e_{\sigma,h}^{n})\|_{1}^{2} + Ch^{2(m+1)}\|(\delta_{t}u(t_{n}), \delta_{t}\sigma(t_{n}))\|_{m+1}^{2}$$

$$\leq \varepsilon \|(e_{u,h}^{n}, e_{\sigma,h}^{n})\|_{1}^{2} + \frac{Ch^{2(m+1)}}{k} \int_{t_{n-1}}^{t_{n}} \|(u_{t}, \sigma_{t})\|_{m+1}^{2} dt, \qquad (2.86)$$

where in the last inequality was used that $(\delta_t u(t_n), \delta_t \boldsymbol{\sigma}(t_n)) = \frac{1}{k} \int_{t_{n-1}}^{t_n} (u_t, \boldsymbol{\sigma}_t)$. Therefore, taking ε small enough, from (2.80)-(2.86) we obtain

$$\delta_{t} \left(\frac{1}{2} \| e_{u,h}^{n} \|_{0}^{2} + \frac{1}{4} \| e_{\sigma,h}^{n} \|_{0}^{2} \right) + \| (e_{u,h}^{n}, e_{\sigma,h}^{n}) \|_{1}^{2} \\ \leq Ck \int_{t_{n-1}}^{t_{n}} \| (u_{tt}(t), \boldsymbol{\sigma}_{tt}(t)) \|_{(H^{1})' \times (H_{\sigma}^{1})'}^{2} dt + \frac{Ch^{2(m+1)}}{k} \int_{t_{n-1}}^{t_{n}} \| (u_{t}, \boldsymbol{\sigma}_{t}) \|_{m+1}^{2} dt + Ch^{2(m+1)} \\ + C(\| (u(t_{n}), \boldsymbol{\sigma}(t_{n})) \|_{1}^{4} + \| (u(t_{n}), \boldsymbol{\sigma}(t_{n})) \|_{2}^{2}) \| e_{u,h}^{n} \|_{0}^{2}.$$

$$(2.87)$$

Then, multiplying (2.87) by k, adding from n = 1 to n = r, recalling that $e_{u,h}^0 = e_{\sigma,h}^0 = 0$, taking into account (2.77), we obtain

$$\left[\frac{1}{4} - kC\right] \|(e_{u,h}^r, e_{\sigma,h}^r)\|_0^2 + k\sum_{n=1}^r \|(e_{u,h}^n, e_{\sigma,h}^n)\|_1^2 \le Ck^2 + Ch^{2(m+1)} + Ck\sum_{n=0}^{r-1} \|e_{u,h}^n\|_0^2.$$

Therefore, assuming hypothesis (2.78) and using the Discrete Gronwall Lemma, we conclude (2.79).

Remark 2.3.22 Under hypothesis of Theorem 2.3.21, one has in particular

$$\|(u_h^n, \boldsymbol{\sigma}_h^n)\|_1^2 \le C + C(T) \left(k + \frac{h^{2(m+1)}}{k}\right).$$

Therefore, under the hypothesis

$$\frac{h^{2(m+1)}}{k} \le C,$$
(2.88)

we have the estimate

$$\|(u_h^n, \boldsymbol{\sigma}_h^n)\|_1^2 \le C,\tag{2.89}$$

hence the hypothesis (2.36) providing uniqueness of the scheme is equivalent to k small enough. Finally, since for any choice of (k, h) either (2.37) (see Remark 2.3.5) or (2.88) holds, one has the uniqueness of (u_h^n, σ_h^n) solution of (2.34) only imposing k small enough.

Error estimates for v_h^n solution of (2.35)

We introduce the following notation for the errors in $t = t_n$: $e_v^n = v(t_n) - v_h^n$, and for the discrete in time derivative of this error: $\delta_t e_v^n = \frac{e_v^n - e_v^{n-1}}{k}$. Then, subtracting (2.8) at $t = t_n$ and (2.35), we have that e_v^n satisfies

$$(\delta_t e_v^n, \bar{v}_h) + \langle A e_v^n, \bar{v}_h \rangle = ((u(t_n) + u_h^n) e_u^n, \bar{v}_h) + (\xi_3^n, \bar{v}_h), \quad \forall \bar{v}_h \in V_h,$$
(2.90)

where ξ_3^n is the consistency error associated to (2.35), that is, $\xi_3^n = \delta_t(v(t_n)) - v_t(t_n)$. Now, considering the interpolation operator \mathcal{R}_h^v defined in (2.16), we decompose e_v^n as follows

$$e_v^n = (\mathcal{I} - \mathcal{R}_h^v)v(t_n) + \mathcal{R}_h^v v(t_n) - v_h^n = e_{v,i}^n + e_{v,h}^n,$$
(2.91)

where $e_{v,i}^n$ is the interpolation error and $e_{v,h}^n$ is the discrete error of v. Then, taking into account (2.16), from (2.90)-(2.91) we have

$$\left(\delta_t e_{v,h}^n, \bar{v}_h\right) + \left(\tilde{A}_h e_{v,h}^n, \bar{v}_h\right) = \left(\xi_3^n, \bar{v}_h\right) + \left(\left(u(t_n) + u_h^n\right)(e_{u,h}^n + e_{u,i}^n), \bar{v}_h\right) - \left(\delta_t e_{v,i}^n, \bar{v}_h\right), \ \forall \bar{v}_h \notin 2W_2$$

Theorem 2.3.23 Under hypothesis of Theorem 2.3.21. Let v_h^n be the solution of (2.35), and assume the following regularity for v exact solution of (2.8):

$$(v_t, v_{tt}) \in L^2(0, T; H^{m+2}(\Omega) \times H^1(\Omega)').$$
 (2.93)

Then, the a priori error estimate holds

$$\|e_{v,h}^n\|_{l^{\infty}L^2 \cap l^2 H^1} \le C(T)(k+h^{m+1}), \tag{2.94}$$

where $C(T) = K_1 Texp(K_2T)$, with $K_1, K_2 > 0$ independent of (k, h).

Proof. Taking $\bar{v}_h = e_{v,h}^n$ in (2.92) and using the Hölder and Young inequalities, we obtain

$$\delta_t \left(\frac{1}{2} \| e_{v,h}^n \|_0^2 \right) + \frac{k}{2} \| \delta_t e_{v,h}^n \|_0^2 + \frac{1}{2} \| e_{v,h}^n \|_1^2 \le C \| \xi_3^n \|_{(H^1)'}^2 + C \| u(t_n) + u_h^n \|_{L^3}^2 (\| e_{u,h}^n \|_0^2 + \| e_{u,i}^n \|_0^2) + C \| (\mathfrak{I} - \mathcal{R}_h^v) \delta_t v(t_n) \|_0^2.$$
(2.95)

Using (2.17), (2.19) and proceeding as in (2.81) and (2.86), we bound the terms on the right hand side in (2.95) and we deduce

$$\delta_t \left(\|e_{v,h}^n\|_0^2 \right) + \|e_{v,h}^n\|_1^2 \le Ck \int_{t_{n-1}}^{t_n} \|v_{tt}(t)\|_{(H^1)'}^2 dt + C\|u(t_n) + u_h^n\|_{L^3}^2 \|e_{u,h}^n\|_0^2 + C\|u(t_n) + u_h^n\|_{L^3}^2 h^{2(m+1)} \|u(t_n)\|_{m+1}^2 + \frac{Ch^{2(m+2)}}{k} \int_{t_{n-1}}^{t_n} \|v_t\|_{m+2}^2 dt.$$
(2.96)

Then, multiplying (2.96) by k, adding from n = 1 to n = r, we obtain (recall $e_{v,h}^0 = 0$):

$$\begin{aligned} \|e_{v,h}^{r}\|_{0}^{2} + k\sum_{n=1}^{r} \|e_{v,h}^{n}\|_{1}^{2} &\leq Ck^{2} \int_{0}^{t_{r}} \|v_{tt}(t)\|_{(H^{1})'}^{2} dt + C \|e_{u,h}^{n}\|_{l^{\infty}L^{2}}^{2} k\sum_{n=1}^{r} \|u(t_{n}) + u_{h}^{n}\|_{L^{3}}^{2} \\ &+ Ch^{2(m+1)} k\sum_{n=1}^{r} \|u(t_{n}) + u_{h}^{n}\|_{L^{3}}^{2} + Ch^{2(m+2)} \int_{0}^{t_{r}} \|v_{t}\|_{m+2}^{2} dt. \end{aligned}$$

Then, using (2.42), (2.77), (2.93) and (2.79), we conclude (2.94).

Theorem 2.3.24 Under hypothesis of Theorem 2.3.23, but assuming the regularity:

$$v_{tt} \in L^2(0, T; L^2(\Omega)),$$
 (2.97)

the a priori error estimate

$$\|e_{v,h}^n\|_{l^{\infty}H^1 \cap l^2 W^{1,6}} \le C(T)(k+h^{m+1})$$
(2.98)

holds, where $C(T) = K_1 Texp(K_2T)$, with $K_1, K_2 > 0$ independent of (k, h).

Proof. Taking $\bar{v}_h = \tilde{A}_h e_{v,h}^n$ in (2.92) and using the Hölder and Young inequalities, we obtain

$$\delta_t \left(\frac{1}{2} \| e_{v,h}^n \|_1^2 \right) + \frac{k}{2} \| \delta_t e_{v,h}^n \|_1^2 + \frac{1}{2} \| \widetilde{A}_h e_{v,h}^n \|_0^2 \le C \| \xi_3^n \|_0^2 + C \| u(t_n) + u_h^n \|_{L^3}^2 \| e_{u,h}^n \|_{L^6}^2 + C \| (u(t_n) + u_h^n) e_{u,i}^n \|_0^2 + C \| (\mathfrak{I} - \mathfrak{R}_h^v) \delta_t v(t_n) \|_0^2.$$
(2.99)

Using the Hölder inequality, the interpolation error (2.17), the stability property (2.20) and the hypothesis (2.77), we have

$$\begin{aligned} \|(u(t_n) + u_h^n)e_{u,i}^n\|_0^2 &\leq C \|u(t_n) + \mathcal{R}_h^u u(t_n)\|_{L^{\infty}}^2 \|e_{u,i}^n\|_0^2 + C \|e_{u,h}^n\|_{L^6}^2 \|e_{u,i}^n\|_{L^3}^2 \\ &\leq Ch^{2(m+1)} + C \|e_{u,h}^n\|_{L^6}^2. \end{aligned}$$
(2.100)

Therefore, from (2.99), proceeding as in (2.81) and (2.86) and using (2.100), we deduce

$$\delta_t \left(\|e_{v,h}^n\|_1^2 \right) + \|\widetilde{A}_h e_{v,h}^n\|_0^2 \le Ck \int_{t_{n-1}}^{t_n} \|v_{tt}(t)\|_0^2 dt \\ + (C\|u(t_n) + u_h^n\|_{L^3}^2 + C) \|e_{u,h}^n\|_{L^6}^2 + Ch^{2(m+1)} + \frac{Ch^{2(m+2)}}{k} \int_{t_{n-1}}^{t_n} \|v_t\|_{m+2}^2 dt.$$

Now, in order to bound the term $||u(t_n) + u_h^n||_{L^3}^2$, we split the argument into two cases:

1. Estimates assuming $h \ll f(k)$ (h small enough with respect to k): From (2.79) we have that $k \sum_{n=1}^{r} ||e_{u,h}^{n}||_{1}^{2} \leq C(T)(k^{2} + h^{2(m+1)})$, which implies that

$$\|e_{u,h}^n\|_1 \le C(T)(k^{1/2} + \frac{h^{m+1}}{k^{1/2}}).$$
(2.101)

Moreover, using the interpolation inequality (2.12), (2.79), (2.20), (2.77) and (2.101), we obtain

$$\|u(t_n) + u_h^n\|_{L^3}^2 \le C \|u(t_n)\|_{L^3}^2 + C \|\mathcal{R}_h^u u(t_n)\|_{L^3}^2 + C \|e_{u,h}^n\|_{L^3}^2 \le C + C \|e_{u,h}^n\|_0 \|e_{u,h}^n\|_1 \le C + C(T)(k+h^{m+1})(k^{1/2} + \frac{h^{m+1}}{k^{1/2}}) \le C$$
(2.102)

under he hypothesis

$$\frac{h^{2(m+1)}}{k^{1/2}} \le C. \tag{2.103}$$

2. Estimates assuming $k \ll g(k)$ (k small enough with respect to h): Using the inverse inequality $||u_h||_{L^3} \leq \frac{C}{h^{1/2}} ||u_h||_0$ for all $u_h \in U_h$, (2.20), (2.77) and (2.79), we have that

$$\begin{aligned} \|u(t_n) + u_h^n\|_{L^3}^2 &\leq C \|u(t_n)\|_{L^3}^2 + C \|\mathcal{R}_h^u u(t_n)\|_{L^3}^2 + C \|e_{u,h}^n\|_{L^3}^2 \\ &\leq \frac{C}{h} \|e_{u,h}^n\|_0^2 + C \leq \frac{C(T)}{h} (k^2 + h^{2(m+1)}) + C \leq C \end{aligned}$$

under the hypothesis

$$\frac{k^2}{h} < C. \tag{2.104}$$

Therefore, since for any choice of (k, h) either (2.103) or (2.104) holds, we arrive at

$$\delta_t \left(\|e_{v,h}^n\|_1^2 \right) + \|\widetilde{A}_h e_{v,h}^n\|_0^2 \le Ck \int_{t_{n-1}}^{t_n} \|v_{tt}(t)\|_0^2 dt + C \|e_{u,h}^n\|_{L^6}^2 + Ch^{2(m+1)} + \frac{Ch^{2(m+2)}}{k} \int_{t_{n-1}}^{t_n} \|v_t\|_{m+2}^2 dt.$$
(2.105)

Multiplying (2.105) by k, adding from n = 1 to n = r, recalling that $e_{v,h}^0 = 0$ and using (2.77), (2.93), (2.97) and (2.79), we conclude (2.98).

2.4 Linear iterative methods to approach the Backward Euler scheme

In this section, we propose two different linear iterative methods to approach the Backward Euler scheme **US**, which are an energy-stable Picard's method and the Newton's method. We prove the solvability and the convergence of these methods to the nonlinear scheme.

2.4.1 Picard Method

In order to approximate the solution $(u_h^n, \boldsymbol{\sigma}_h^n)$ of the nonlinear scheme **US**, we consider the following Picard method: Let $(u_h^{n-1}, \boldsymbol{\sigma}_h^{n-1}) \in U_h \times \boldsymbol{\Sigma}_h$ be fixed. Given $u_h^{l-1} \in U_h$ (assuming $u_h^0 = u_h^{n-1}$ at the first iteration step), find $(u_h^l, \boldsymbol{\sigma}_h^l) \in U_h \times \boldsymbol{\Sigma}_h$ solving the linear coupled problem:

$$\begin{pmatrix}
\frac{1}{k}(u_h^l, \bar{u}_h) + (\nabla u_h^l, \nabla \bar{u}_h) + (u_h^{l-1}\boldsymbol{\sigma}_h^l, \nabla \bar{u}_h) = \frac{1}{k}(u_h^{n-1}, \bar{u}_h), \forall \bar{u}_h \in U_h, \\
\frac{1}{k}(\boldsymbol{\sigma}_h^l, \bar{\boldsymbol{\sigma}}_h) + (B_h\boldsymbol{\sigma}_h^l, \bar{\boldsymbol{\sigma}}_h) - 2(u_h^{l-1}\nabla u_h^l, \bar{\boldsymbol{\sigma}}_h) = \frac{1}{k}(\boldsymbol{\sigma}_h^{n-1}, \bar{\boldsymbol{\sigma}}_h), \forall \bar{\boldsymbol{\sigma}}_h \in \boldsymbol{\Sigma}_h,
\end{cases}$$
(2.106)

until the stopping criteria max $\left\{\frac{\|u_h^l - u_h^{l-1}\|_0}{\|u_h^{l-1}\|_0}, \frac{\|\boldsymbol{\sigma}_h^l - \boldsymbol{\sigma}_h^{l-1}\|_0}{\|\boldsymbol{\sigma}_h^{l-1}\|_0}\right\} \leq tol \text{ (with } tol > 0 \text{ being a tolerance parameter).}$

Theorem 2.4.1 (Unconditional Unique Solvability) There exists a unique (u_h^l, σ_h^l) solution of (2.106).

Proof. Since (2.106) can be rewritten as a square linear algebraic system, it is sufficient to prove uniqueness. Suppose that there exist $(u_{h,1}^l, \boldsymbol{\sigma}_{h,1}^l), (u_{h,2}^l, \boldsymbol{\sigma}_{h,2}^l) \in U_h \times \boldsymbol{\Sigma}_h$ two possible solutions of (2.106). Then defining $u_h^l = u_{h,1}^l - u_{h,2}^l$ and $\boldsymbol{\sigma}_h^l = \boldsymbol{\sigma}_{h,1}^l - \boldsymbol{\sigma}_{h,2}^l$, we have that $(u_h^l, \boldsymbol{\sigma}_h^l) \in U_h \times \boldsymbol{\Sigma}_h$ satisfies

$$\frac{1}{k}(u_h^l, \bar{u}_h) + (\nabla u_h^l, \nabla \bar{u}_h) + (u_h^{l-1} \boldsymbol{\sigma}_h^l, \nabla \bar{u}_h) = 0, \ \forall \bar{u}_h \in U_h,$$
(2.107)

$$\frac{1}{k}(\boldsymbol{\sigma}_{h}^{l}, \bar{\boldsymbol{\sigma}}_{h}) + (B_{h}\boldsymbol{\sigma}_{h}^{l}, \bar{\boldsymbol{\sigma}}_{h}) - 2(u_{h}^{l-1}\nabla u_{h}^{l}, \bar{\boldsymbol{\sigma}}_{h}) = 0, \ \forall \bar{\boldsymbol{\sigma}}_{h} \in \boldsymbol{\Sigma}_{h}.$$
(2.108)

Taking $\bar{u}_h = u_h^l$ and $\bar{\sigma}_h = \frac{1}{2} \sigma_h^l$ in (2.107)-(2.108) and adding, the terms $(u_h^{l-1} \nabla u_h^l, \sigma_h^l)$ cancel, and we obtain

$$\frac{1}{2k} \| (\boldsymbol{u}_h^l, \boldsymbol{\sigma}_h^l) \|_0^2 + \frac{1}{2} \| (\nabla \boldsymbol{u}_h^l, \boldsymbol{\sigma}_h^l) \|_{L^2 \times H^1}^2 \le 0,$$

and thus we conclude that $\|(u_h^l, \boldsymbol{\sigma}_h^l)\|_1 = 0$, which implies $u_{h,1}^l = u_{h,2}^l$ and $\boldsymbol{\sigma}_{h,1}^l = \boldsymbol{\sigma}_{h,2}^l$.

Theorem 2.4.2 (Local uniqueness of solution of scheme US and Convergence of Picard's method) Given $(u_h^{n-1}, \sigma_h^{n-1})$, there exists r > 0 (large enough) such that if

$$k \| (u_h^{n-1}, \boldsymbol{\sigma}_h^{n-1}) \|_1^4 \quad and \quad kr^4 \quad are \ small \ enough, \tag{2.109}$$

then the scheme **US** has a unique solution $(u_h^n, \boldsymbol{\sigma}_h^n)$ in $\overline{B}_r((u_h^{n-1}, \boldsymbol{\sigma}_h^{n-1})) := \{(u, \boldsymbol{\sigma}) \in U_h \times \Sigma_h : \|(u - u_h^{n-1}, \boldsymbol{\sigma} - \boldsymbol{\sigma}_h^{n-1})\|_1 \leq r\}$. Moreover, the sequence of solutions $\{u_h^l, \boldsymbol{\sigma}_h^l\}_{l\geq 0}$ of the iterative algorithm (2.106) (assuming $(u_h^0, \boldsymbol{\sigma}_h^0) = (u_h^{n-1}, \boldsymbol{\sigma}_h^{n-1})$ at the first iteration step), converges to $(u_h^n, \boldsymbol{\sigma}_h^n)$ strongly in $H^1(\Omega)$.

Proof. We consider the operator $R: U_h \to U_h$, given by $R(\tilde{u}) = u$, where $(u, \boldsymbol{\sigma})$ satisfies (2.106) with $u_h^{l-1} = \tilde{u}$ and $(u_h^l, \boldsymbol{\sigma}_h^l) = (u, \boldsymbol{\sigma})$, that is,

$$\frac{1}{k}(u,\bar{u}_h) + (\nabla u,\nabla\bar{u}_h) + (\tilde{u}\boldsymbol{\sigma},\nabla\bar{u}_h) = \frac{1}{k}(u_h^{n-1},\bar{u}_h), \ \forall \bar{u}_h \in U_h,$$
(2.110)

$$\frac{1}{k}(\boldsymbol{\sigma},\bar{\boldsymbol{\sigma}}_h) + (B_h\boldsymbol{\sigma},\bar{\boldsymbol{\sigma}}_h) - 2(\widetilde{u}\nabla u,\bar{\boldsymbol{\sigma}}_h) = \frac{1}{k}(\boldsymbol{\sigma}_h^{n-1},\bar{\boldsymbol{\sigma}}_h), \ \forall \bar{\boldsymbol{\sigma}}_h \in \boldsymbol{\Sigma}_h.$$
(2.111)

Observe that from Theorem 2.4.1, we have that for any $\tilde{u} \in U_h$ there exists a unique $(u, \boldsymbol{\sigma}) \in U_h \times \boldsymbol{\Sigma}_h$ solution of (2.110)-(2.111). Thus, R is well defined. Now, before to prove that R is contractive, we will construct a ball $\overline{B}_r(u_h^{n-1}) = \{u \in U_h : ||u - u_h^{n-1}||_1 \leq r\} \subset U_h$

such that $R(\overline{B}_r(u_h^{n-1})) \subseteq \overline{B}_r(u_h^{n-1})$. In order to define r, we consider $w = u - u_h^{n-1}$ and $\boldsymbol{\tau} = \boldsymbol{\sigma} - \boldsymbol{\sigma}_h^{n-1}$. Then, from (2.110)-(2.111) we have that $(w, \boldsymbol{\tau})$ verifies

$$\frac{1}{k}(w,\bar{u}_h) + (\nabla w,\nabla\bar{u}_h) = -(\tilde{u}\boldsymbol{\tau},\nabla\bar{u}_h) - (\nabla u_h^{n-1},\nabla\bar{u}_h) - (\tilde{u}\boldsymbol{\sigma}_h^{n-1},\nabla\bar{u}_h), \ \forall \bar{u}_h \in U_h, \ (2.112)$$
$$\frac{1}{k}(\boldsymbol{\tau},\bar{\boldsymbol{\sigma}}_h) + (B_h\boldsymbol{\tau},\bar{\boldsymbol{\sigma}}_h) = 2(\tilde{u}\nabla w,\bar{\boldsymbol{\sigma}}_h) - (B_h\boldsymbol{\sigma}_h^{n-1},\bar{\boldsymbol{\sigma}}_h) + 2(\tilde{u}\nabla u_h^{n-1},\bar{\boldsymbol{\sigma}}_h), \ \forall \bar{\boldsymbol{\sigma}}_h \in \boldsymbol{\Sigma}_h. \ (2.113)$$

Testing by $\bar{u}_h = w$ and $\bar{\sigma}_h = \frac{1}{2}\tau$ in (2.112)-(2.113) and adding, the terms $(\tilde{u}\nabla w, \tau)$ cancel, and using the fact that $\int_{\Omega} w = 0$ as well as the 3D interpolation inequality (2.12), we obtain

$$\begin{aligned} \frac{1}{2k} \|(w,\boldsymbol{\tau})\|_{0}^{2} + \frac{1}{2} \|(w,\boldsymbol{\tau})\|_{1}^{2} &\leq \frac{1}{8} \|(w,\boldsymbol{\tau})\|_{1}^{2} + C \|(u_{h}^{n-1},\boldsymbol{\sigma}_{h}^{n-1})\|_{1}^{2} \\ &+ \frac{1}{8} \|\widetilde{u} - u_{h}^{n-1}\|_{1}^{2} + \frac{1}{8} \|u_{h}^{n-1}\|_{1}^{2} + \frac{1}{8} \|(w,\boldsymbol{\tau})\|_{1}^{2} + C \|(u_{h}^{n-1},\boldsymbol{\sigma}_{h}^{n-1})\|_{1}^{4} \|(w,\boldsymbol{\tau})\|_{\theta}^{2}.114) \end{aligned}$$

Therefore, from (2.114) we deduce

$$\left[\frac{1}{2k} - C \|(u_h^{n-1}, \boldsymbol{\sigma}_h^{n-1})\|_1^4\right] \|(w, \boldsymbol{\tau})\|_0^2 + \frac{1}{4} \|(w, \boldsymbol{\tau})\|_1^2 \le C \|(u_h^{n-1}, \boldsymbol{\sigma}_h^{n-1})\|_1^2 + \frac{1}{8} \|\widetilde{u} - u_h^{n-1}\|_1^2.115)$$

Thus, if $k < \frac{1}{2C \| (u_h^{n-1}, \boldsymbol{\sigma}_h^{n-1}) \|_1^4}$, from (2.115) we conclude

$$\|(w,\boldsymbol{\tau})\|_{1}^{2} \leq C \|(u_{h}^{n-1},\boldsymbol{\sigma}_{h}^{n-1})\|_{1}^{2} + \frac{1}{2} \|\widetilde{u} - u_{h}^{n-1}\|_{1}^{2}.$$
(2.116)

Then, choosing r > 0 large enough such that

$$C \| (u_h^{n-1}, \boldsymbol{\sigma}_h^{n-1}) \|_1^2 \le \frac{1}{2} r^2,$$
 (2.117)

from (2.116) we deduce that $R(\overline{B}_r(u_h^{n-1})) \subseteq \overline{B}_r(u_h^{n-1})$. Then, we take the restriction of R to $\overline{B}_r(u_h^{n-1})$, that is, $R_r : \overline{B}_r(u_h^{n-1}) \to \overline{B}_r(u_h^{n-1})$. Let's prove that R_r is contractive. Let $\widetilde{u}_1, \widetilde{u}_2 \in \overline{B}_r(u_h^{n-1})$, and (u_1, σ_1) and (u_2, σ_2) solutions of (2.110)-(2.111) corresponding to \widetilde{u}_1 and \widetilde{u}_2 respectively (i.e., $R_r(\widetilde{u}_1) = u_1$ and $R_r(\widetilde{u}_2) = u_2$). Then, from (2.110)-(2.111) we have that $(u_1 - u_2, \sigma_1 - \sigma_2) \in U_h \times \Sigma_h$ satisfies

$$\frac{1}{k}(u_1-u_2,\bar{u}_h) + (\nabla(u_1-u_2),\nabla\bar{u}_h) + (\widetilde{u}_1(\boldsymbol{\sigma}_1-\boldsymbol{\sigma}_2),\nabla\bar{u}_h) + ((\widetilde{u}_1-\widetilde{u}_2)\boldsymbol{\sigma}_2,\nabla\bar{u}_h) = 0, \ \forall \bar{u}_h \in U_h,$$

$$\frac{1}{k}(\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2, \bar{\boldsymbol{\sigma}}_h) + (B_h(\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2), \bar{\boldsymbol{\sigma}}_h) - 2(\tilde{u}_1 \nabla (u_1 - u_2), \bar{\boldsymbol{\sigma}}_h) - 2((\tilde{u}_1 - \tilde{u}_2) \nabla u_2, \bar{\boldsymbol{\sigma}}_h) = 0, \ \forall \bar{\boldsymbol{\sigma}}_h \in \boldsymbol{\Sigma}_h.$$

Testing by $\bar{u}_h = u_1 - u_2$, $\bar{\boldsymbol{\sigma}}_h = \frac{1}{2}(\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2)$ and adding, the terms $(\tilde{u}_1(\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2), \nabla(u_1 - u_2))$ cancel, and using the Hölder and Young inequalities, the 3D interpolation inequality (2.12) and taking into account that $\int_{\Omega} u_1 - u_2 = 0$, we obtain

$$\frac{1}{2k} \|(u_1 - u_2, \boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2)\|_0^2 + \|u_1 - u_2\|_1^2 + \frac{1}{2}\|\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2\|_1^2 \\
\leq C\|\widetilde{u}_1 - \widetilde{u}_2\|_1(\|\boldsymbol{\sigma}_2\|_1\|u_1 - u_2\|_{L^3} + \|u_2\|_1\|\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2\|_{L^3}) \\
\leq \frac{1}{4}\|\widetilde{u}_1 - \widetilde{u}_2\|_1^2 + \frac{1}{2}\|u_1 - u_2\|_1^2 + \frac{1}{4}\|\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2\|_1^2 + C\|(u_1 - u_2, \boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2)\|_0^2\|(u_2, \boldsymbol{\sigma}_2)\|_1^4$$

and thus, we deduce that

$$\frac{1}{k} \| (u_1 - u_2, \boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2) \|_0^2 + \| u_1 - u_2 \|_1^2 + \frac{1}{2} \| \boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2 \|_1^2
\leq \frac{1}{2} \| \widetilde{u}_1 - \widetilde{u}_2 \|_1^2 + C \| (u_1 - u_2, \boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2) \|_0^2 \| (u_2, \boldsymbol{\sigma}_2) \|_1^4.$$
(2.118)

Therefore, since from (2.116) and (2.117) we have $||(u_2, \sigma_2)||_1^4 \leq C(r^4 + ||(u_h^{n-1}, \sigma_h^{n-1})||_1^4)$, if $\frac{1}{2k} > Cr^4$ and $\frac{1}{2k} > C||(u_h^{n-1}, \sigma_h^{n-1})||_1^4)$, from (2.118) we have

$$||R_r(\widetilde{u}_1) - R_r(\widetilde{u}_2)||_1^2 \le \frac{1}{2} ||\widetilde{u}_1 - \widetilde{u}_2||_1^2,$$

which implies that R_r is contractive. Then, as a consequence of the Banach fixed point theorem, we conclude that there exists a unique fixed point of R_r , $R_r(u) = u$. Thus, $(u, \boldsymbol{\sigma})$ is the unique solution of the scheme **US** in $\overline{B}_r(u_h^{n-1})$. Additionally, we conclude that the sequence of solutions $\{u_h^l, \boldsymbol{\sigma}_h^l\}_{l\geq 0}$ of the iterative algorithm (2.106), where $(u_h^0, \boldsymbol{\sigma}_h^0) = (u_h^{n-1}, \boldsymbol{\sigma}_h^{n-1})$, converges to the solution $(u_h^n, \boldsymbol{\sigma}_h^n)$.

Remark 2.4.3 In the case of 2D Domains, from estimate (2.54), the restriction $(2.109)_1$ can be relaxed to $k \leq K_0$, where K_0 is a constant depending on data (Ω, u_0, σ_0) , but independent of (k, h) and n.

Remark 2.4.4 We have that the restriction $(2.109)_1$ is equivalent to (2.36). Therefore, under hypothesis of Theorem 2.3.21 and arguing as in Remark 2.3.22, the conclusion of Theorem 2.4.2 remains true only assuming k small enough.

2.4.2 Newton's Method

In this subsection, in order to approximate the solution $(u_h^n, \boldsymbol{\sigma}_h^n)$ of the nonlinear scheme **US**, we consider Newton's algorithm: Let $(u_h^{n-1}, \boldsymbol{\sigma}_h^{n-1}) \in U_h \times \boldsymbol{\Sigma}_h$ be fixed. Given $(u_h^{l-1}, \boldsymbol{\sigma}_h^{l-1}) \in U_h \times \boldsymbol{\Sigma}_h$ (assuming $(u_h^0, \boldsymbol{\sigma}_h^0) = (u_h^{n-1}, \boldsymbol{\sigma}_h^{n-1})$ at the first iteration step), find $(u_h^l, \boldsymbol{\sigma}_h^l) \in U_h \times \boldsymbol{\Sigma}_h$ such that

$$\begin{cases} \frac{1}{k}(u_{h}^{l},\bar{u}_{h}) + (\nabla u_{h}^{l},\nabla\bar{u}_{h}) + (u_{h}^{l-1}\boldsymbol{\sigma}_{h}^{l},\nabla\bar{u}_{h}) + (u_{h}^{l}\boldsymbol{\sigma}_{h}^{l-1},\nabla\bar{u}_{h}) = \frac{1}{k}(u_{h}^{n-1},\bar{u}_{h}) + (u_{h}^{l-1}\boldsymbol{\sigma}_{h}^{l-1},\nabla\bar{u}_{h}), \\ \frac{1}{k}(\boldsymbol{\sigma}_{h}^{l},\bar{\boldsymbol{\sigma}}_{h}) + (B_{h}\boldsymbol{\sigma}_{h}^{l},\bar{\boldsymbol{\sigma}}_{h}) - 2(u_{h}^{l-1}\nabla u_{h}^{l},\bar{\boldsymbol{\sigma}}_{h}) \\ -2(u_{h}^{l}\nabla u_{h}^{l-1},\bar{\boldsymbol{\sigma}}_{h}) = \frac{1}{k}(\boldsymbol{\sigma}_{h}^{n-1},\bar{\boldsymbol{\sigma}}_{h}) - 2(u_{h}^{l-1}\nabla u_{h}^{l-1},\bar{\boldsymbol{\sigma}}_{h}), \end{cases}$$

$$(2.119)$$

for all $(\bar{u}_h, \bar{\boldsymbol{\sigma}}_h) \in U_h \times \boldsymbol{\Sigma}_h$; until the stopping criteria max $\left\{ \frac{\|u_h^l - u_h^{l-1}\|_0}{\|u_h^{l-1}\|_0}, \frac{\|\boldsymbol{\sigma}_h^l - \boldsymbol{\sigma}_h^{l-1}\|_0}{\|\boldsymbol{\sigma}_h^{l-1}\|_0} \right\} \leq tol.$

The following lemma will be necessary to obtain the convergence of Newton's method.

Lemma 2.4.5 Let X be a Banach space and consider a sequence $\{e_l\}_{l\geq 0} \subseteq X$, such that

 $||e_l||_X^2 \le C \left(||e_{l-1}||_X^2 \right)^2, \quad \forall l \ge 1 \quad and \quad ||e_0||_X^2 \text{ is small enough.}$

Then, e_l converges to 0 as $l \to +\infty$ in the X-norm.

In the following theorem, we will use this lemma to prove the convergence $(u_h^l, \boldsymbol{\sigma}_h^l) \rightarrow (u_h^n, \boldsymbol{\sigma}_h^n)$ in the $H^1(\Omega)$ -norm.

Theorem 2.4.6 (Conditional convergence of Newton's Method) Let (u_h^n, σ_h^n) be a fixed solution of the scheme **US** and let (u_h^l, σ_h^l) be any solution of (2.119). There exists $\delta_0 > 0$ small enough such that if

$$\|(e_u^0, e_{\sigma}^0)\|_1^2 \le \delta_0, \quad k\|(u_h^n, \sigma_h^n)\|_1^4 \quad and \quad k(\delta_0)^2 \quad are \ small \ enough,$$
 (2.120)

then $\{u_h^l, \boldsymbol{\sigma}_h^l\}_{l\geq 0}$ converges to $(u_h^n, \boldsymbol{\sigma}_h^n)$ in the $H^1(\Omega)$ -norm as $l \to +\infty$.

Proof. We can define problem (2.34) in a vectorial way,

$$(0,0) = \langle \mathbf{F}(u_h^n, \boldsymbol{\sigma}_h^n), (\bar{u}_h, \bar{\boldsymbol{\sigma}}_h) \rangle = (\langle F_1(u_h^n, \boldsymbol{\sigma}_h^n), \bar{u}_h \rangle, \langle F_2(u_h^n, \boldsymbol{\sigma}_h^n), \bar{\boldsymbol{\sigma}}_h \rangle), \qquad (2.121)$$

where each $F_i(u_h^n, \boldsymbol{\sigma}_h^n)$ corresponds with the equation $(2.34)_i$ (i = 1, 2). Therefore, Newton's method (2.119) reads

$$\langle \mathbf{F}'(u_h^{l-1},\boldsymbol{\sigma}_h^{l-1})(u_h^l-u_h^{l-1},\boldsymbol{\sigma}_h^l-\boldsymbol{\sigma}_h^{l-1}),(\bar{u}_h,\bar{\boldsymbol{\sigma}}_h)\rangle = -\langle \mathbf{F}(u_h^{l-1},\boldsymbol{\sigma}_h^{l-1}),(\bar{u}_h,\bar{\boldsymbol{\sigma}}_h)\rangle,$$

which can be rewritten as

$$(0,0) = (\langle F_1(u_h^{l-1}, \boldsymbol{\sigma}_h^{l-1}), \bar{u}_h \rangle, \langle F_2(u_h^{l-1}, \boldsymbol{\sigma}_h^{l-1}), \bar{\boldsymbol{\sigma}}_h \rangle) + (\langle F_1'(u_h^{l-1}, \boldsymbol{\sigma}_h^{l-1})(u_h^l - u_h^{l-1}, \boldsymbol{\sigma}_h^l - \boldsymbol{\sigma}_h^{l-1}), \bar{u}_h \rangle, \langle F_2'(u_h^{l-1}, \boldsymbol{\sigma}_h^{l-1})(u_h^l - u_h^{l-1}, \boldsymbol{\sigma}_h^l - \boldsymbol{\sigma}_h^{l-1}), \bar{\boldsymbol{\sigma}}_h \rangle)$$
(2.122)

Moreover, from a vectorial Taylor's formula of $\mathbf{F}(u_h^n, \boldsymbol{\sigma}_h^n)$ with center at $(u_h^{l-1}, \boldsymbol{\sigma}_h^{l-1})$, and using (2.121), we have that

$$\begin{aligned} (0,0) &= (\langle F_1(u_h^n, \boldsymbol{\sigma}_h^n), \bar{u}_h \rangle, \langle F_2(u_h^n, \boldsymbol{\sigma}_h^n), \bar{\boldsymbol{\sigma}}_h \rangle) \\ &= (\langle F_1(u_h^{l-1}, \boldsymbol{\sigma}_h^{l-1}), \bar{u}_h \rangle, \langle F_2(u_h^{l-1}, \boldsymbol{\sigma}_h^{l-1}), \bar{\boldsymbol{\sigma}}_h \rangle) \\ &+ (\langle F_1'(u_h^{l-1}, \boldsymbol{\sigma}_h^{l-1})(u_h^n - u_h^{l-1}, \boldsymbol{\sigma}_h^n - \boldsymbol{\sigma}_h^{l-1}), \bar{u}_h \rangle, \langle F_2'(u_h^{l-1}, \boldsymbol{\sigma}_h^{l-1})(u_h^n - u_h^{l-1}, \boldsymbol{\sigma}_h^n - \boldsymbol{\sigma}_h^{l-1}), \bar{\boldsymbol{\sigma}}_h \rangle) \\ &+ \frac{1}{2} \Big(\langle (u_h^n - u_h^{l-1}, \boldsymbol{\sigma}_h^n - \boldsymbol{\sigma}_h^{l-1})^t F_1''(u^{n+\varepsilon}, \boldsymbol{\sigma}^{n+\varepsilon})(u_h^n - u_h^{l-1}, \boldsymbol{\sigma}_h^n - \boldsymbol{\sigma}_h^{l-1}), \bar{\boldsymbol{u}}_h \rangle, \\ &\quad \langle (u_h^n - u_h^{l-1}, \boldsymbol{\sigma}_h^n - \boldsymbol{\sigma}_h^{l-1})^t F_2''(u^{n+\varepsilon}, \boldsymbol{\sigma}^{n+\varepsilon})(u_h^n - u_h^{l-1}, \boldsymbol{\sigma}_h^n - \boldsymbol{\sigma}_h^{l-1}), \bar{\boldsymbol{\sigma}}_h \rangle \Big), \end{aligned}$$

where $u^{n+\varepsilon} = \varepsilon u_h^n + (1-\varepsilon)u_h^{l-1}$, $\boldsymbol{\sigma}^{n+\varepsilon} = \varepsilon \boldsymbol{\sigma}_h^n + (1-\varepsilon)\boldsymbol{\sigma}_h^{l-1}$, and F'_i and F''_i denote the Jacobian and the Hessian of F_i (i = 1, 2), respectively. Therefore, denoting by $e_u^l = u_h^n - u_h^l$ and $e_{\boldsymbol{\sigma}}^l = \boldsymbol{\sigma}_h^n - \boldsymbol{\sigma}_h^l$, from (2.122)-(2.123), we deduce

$$\left\langle \frac{\partial F_1}{\partial u} (u_h^{l-1}, \boldsymbol{\sigma}_h^{l-1}) (e_u^l) + \frac{\partial F_1}{\partial \boldsymbol{\sigma}} (u_h^{l-1}, \boldsymbol{\sigma}_h^{l-1}) (e_{\boldsymbol{\sigma}}^l), \bar{u}_h \right\rangle$$
$$= -\frac{1}{2} \langle (e_u^{l-1}, e_{\boldsymbol{\sigma}}^{l-1})^t F_1'' (u^{n+\varepsilon}, \boldsymbol{\sigma}^{n+\varepsilon}) (e_u^{l-1}, e_{\boldsymbol{\sigma}}^{l-1}), \bar{u}_h \rangle, \quad (2.124)$$

$$\left\langle \frac{\partial F_2}{\partial u} (u_h^{l-1}, \boldsymbol{\sigma}_h^{l-1}) (e_u^l) + \frac{\partial F_2}{\partial \boldsymbol{\sigma}} (u_h^{l-1}, \boldsymbol{\sigma}_h^{l-1}) (e_{\boldsymbol{\sigma}}^l), \bar{\boldsymbol{\sigma}}_h \right\rangle$$
$$= -\frac{1}{2} \langle (e_u^{l-1}, e_{\boldsymbol{\sigma}}^{l-1})^t F_2'' (u^{n+\varepsilon}, \boldsymbol{\sigma}^{n+\varepsilon}) (e_u^{l-1}, e_{\boldsymbol{\sigma}}^{l-1}), \bar{\boldsymbol{\sigma}}_h \rangle. \quad (2.125)$$

Thus, from (2.124)-(2.125) and taking into account that F_i'' are constant matrices, we arrive at

$$\frac{1}{k}(e_{u}^{l},\bar{u}_{h}) + (\nabla e_{u}^{l},\nabla \bar{u}_{h}) + (e_{u}^{l}\boldsymbol{\sigma}_{h}^{l-1},\nabla \bar{u}_{h}) + (u_{h}^{l-1}e_{\boldsymbol{\sigma}}^{l},\nabla \bar{u}_{h}) = -(e_{u}^{l-1}e_{\boldsymbol{\sigma}}^{l-1},\nabla \bar{u}_{h}), \quad \forall \bar{u}_{h} \in U_{h},$$
(2.126)

$$\frac{1}{k}(e^{l}_{\boldsymbol{\sigma}},\bar{\boldsymbol{\sigma}}_{h}) + (B_{h}e^{l}_{\boldsymbol{\sigma}},\bar{\boldsymbol{\sigma}}_{h}) + 2(u^{l-1}_{h}e^{l}_{u},\nabla\cdot\bar{\boldsymbol{\sigma}}_{h}) = -(|e^{l-1}_{u}|^{2},\nabla\cdot\bar{\boldsymbol{\sigma}}_{h}), \quad \forall \bar{\boldsymbol{\sigma}}_{h} \in \boldsymbol{\Sigma}_{h}.$$
(2.127)

Testing by $\bar{u}_h = e_u^l$ and $\bar{\sigma}_h = e_{\sigma}^l$ in (2.126) and (2.127) respectively, taking into account that $\int_{\Omega} e_u^l = 0$ and using the Hölder and Young inequalities as well as the 3D interpolation inequality (2.12), we obtain

$$\frac{1}{k} \|(e_u^l, e_{\sigma}^l)\|_0^2 + \|(e_u^l, e_{\sigma}^l)\|_1^2 \le \frac{1}{2} \|(e_u^l, e_{\sigma}^l)\|_1^2 + C \|(e_u^l, e_{\sigma}^l)\|_0^2 \|(u_h^{l-1}, \sigma_h^{l-1})\|_1^4 + C \|(e_u^{l-1}, e_{\sigma}^{l-1})\|_1^4$$
(2.128)

In order to use an induction strategy, we can assume the hypothesis

$$\|(e_u^{l-1}, e_{\sigma}^{l-1})\|_1^2 \le \delta_0$$

which implies that

$$\|(u_h^{l-1}, \boldsymbol{\sigma}_h^{l-1})\|_1 \le \|(u_h^n, \boldsymbol{\sigma}_h^n)\|_1 + \sqrt{\delta_0},$$
(2.129)

where $\delta_0 > 0$ is a small enough constant. Therefore, from (2.128)-(2.129) we have

$$\left(\frac{1}{k} - C(\|(u_h^n, \boldsymbol{\sigma}_h^n)\|_1^4 + (\delta_0)^2)\right) \|(e_u^l, e_{\boldsymbol{\sigma}}^l)\|_0^2 + \frac{1}{2}\|(e_u^l, e_{\boldsymbol{\sigma}}^l)\|_1^2 \le C\left(\|(e_u^{l-1}, e_{\boldsymbol{\sigma}}^{l-1})\|_1^2\right)^2.$$
(2.130)

Thus, if $\frac{1}{2k} > C \| (u_h^n, \boldsymbol{\sigma}_h^n) \|_1^4$ and $\frac{1}{2k} > C(\delta_0)^2$ (which is possible owing to (2.120)₂ and (2.120)₃), from (2.130) we obtain

$$\|(e_u^l, e_{\sigma}^l)\|_1^2 \le C\left(\|(e_u^{l-1}, e_{\sigma}^{l-1})\|_1^2\right)^2.$$
(2.131)

Therefore, choosing δ_0 small enough such that $\delta_0 C \leq 1$, the inequality $||(e_u^l, e_{\sigma}^l)||_1^2 \leq \delta_0$ holds. Indeed, if we assume $||(e_u^0, e_{\sigma}^0)||_1^2 \leq \delta_0$, we obtain the following recurrence expression

$$\|(e_u^l, e_{\sigma}^l)\|_1^2 \le \|(e_u^{l-1}, e_{\sigma}^{l-1})\|_1^2 \le \dots \le \|(e_u^0, e_{\sigma}^0)\|_1^2 \le \delta_0.$$
(2.132)

Hence, from (2.131) the hypothesis of Lemma 2.4.5 are satisfied, and we conclude the convergence of $(u_h^l, \boldsymbol{\sigma}_h^l)$ to $(u_h^n, \boldsymbol{\sigma}_h^n)$ in the $H^1(\Omega)$ -norm.

Remark 2.4.7 If (2.54) is satisfied (recall that this estimate holds, at least, in 2D Domains), we can determine δ_0 in terms of k. Indeed, from (2.58), we have that

$$||(e_u^0, e_{\sigma}^0)||_1^2 = ||(u_h^n - u_h^{n-1}, \sigma_h^n - \sigma_h^{n-1})||_1^2 \le k(K_4 + K_5k),$$

and thus, we consider $\delta_0 := k(K_4 + K_5k)$. Then, hypothesis (2.120) in Theorem 2.4.6 are only imposed on k, and (2.120)₂ is reduced to $k \leq K_0$, where K_0 is a constant depending on data $(\Omega, u_0, \boldsymbol{\sigma}_0)$, but independent of (k, h) and n. **Remark 2.4.8** Since restriction $(2.120)_2$ is equivalent to (2.36), analogously as in Remark 2.3.5, under the hypothesis of Theorem 2.3.21, we have that the conclusion of Theorem 2.4.6 remains true assuming k small enough, $(2.120)_1$ and $(2.120)_3$.

Now, observe that from (2.132), we have the following uniform estimate for $(u_h^l, \boldsymbol{\sigma}_h^l)$ solution of (2.119):

$$\|(u_h^l, \boldsymbol{\sigma}_h^l)\|_1 \le \|(u_h^n, \boldsymbol{\sigma}_h^n)\|_1 + \sqrt{\delta_0}, \quad \forall l \ge 0.$$

$$(2.133)$$

Then, using the above estimate, we will prove the conditional unique solvability of (2.119).

Theorem 2.4.9 (Conditional Unique Solvability) Assume (2.120). Then there exists a unique (u_h^l, σ_h^l) solution of (2.119).

Proof. By linearity, it suffices to prove uniqueness of solution of (2.119). Suppose that there exist $(u_{h,1}^l, \boldsymbol{\sigma}_{h,1}^l), (u_{h,2}^l, \boldsymbol{\sigma}_{h,2}^l) \in U_h \times \boldsymbol{\Sigma}_h$ two solutions of (2.119). Then, denoting $u_h^l = u_{h,1}^l - u_{h,2}^l$ and $\boldsymbol{\sigma}_h^l = \boldsymbol{\sigma}_{h,1}^l - \boldsymbol{\sigma}_{h,2}^l$, we arrive at

$$\frac{1}{k}(u_h^l, \bar{u}_h) + (\nabla u_h^l, \nabla \bar{u}_h) + (u_h^{l-1} \boldsymbol{\sigma}_h^l, \nabla \bar{u}_h) + (u_h^l \boldsymbol{\sigma}_h^{l-1}, \nabla \bar{u}_h) = 0, \ \forall \bar{u}_h \in U_h,$$
(2.134)

$$\frac{1}{k}(\boldsymbol{\sigma}_{h}^{l},\bar{\boldsymbol{\sigma}}_{h}) + (B_{h}\boldsymbol{\sigma}_{h}^{l},\bar{\boldsymbol{\sigma}}_{h}) - 2(u_{h}^{l-1}\nabla u_{h}^{l},\bar{\boldsymbol{\sigma}}_{h}) - 2(u_{h}^{l}\nabla u_{h}^{l-1},\bar{\boldsymbol{\sigma}}_{h}) = 0, \ \forall \bar{\boldsymbol{\sigma}}_{h} \in \boldsymbol{\Sigma}_{h}.$$
 (2.135)

Taking $\bar{u}_h = u_h^l$ and $\bar{\sigma}_h = \frac{1}{2} \sigma_h^l$ in (2.134)-(2.135), taking into account that $\int_{\Omega} u_h^l = 0$ and using the Hölder and Young inequalities as well as the interpolation inequality (2.12), we obtain

$$\frac{1}{2k} \|(u_h^l, \boldsymbol{\sigma}_h^l)\|_0^2 + \frac{1}{2} \|(u_h^l, \boldsymbol{\sigma}_h^l)\|_1^2 \le \frac{1}{4} \|(u_h^l, \boldsymbol{\sigma}_h^l)\|_1^2 + C \|(u_h^{l-1}, \boldsymbol{\sigma}_h^{l-1})\|_1^4 \|(u_h^l, \boldsymbol{\sigma}_h^l)\|_0^2,$$

which, using (2.133) (recall that (2.133) holds assuming (2.120)), implies that

$$\left[\frac{1}{k} - C(\|(u_h^n, \boldsymbol{\sigma}_h^n)\|_1^4 + (\delta_0)^2)\right] \|(u_h^l, \boldsymbol{\sigma}_h^l)\|_0^2 + \frac{1}{2}\|(u_h^l, \boldsymbol{\sigma}_h^l)\|_1^2 \le 0.$$
(2.136)

Therefore, assuming $(2.120)_{2-3}$, from (2.136) we conclude that $||(u_h^l, \boldsymbol{\sigma}_h^l)||_1 = 0$, and therefore, $u_{h,1}^l = u_{h,2}^l$ and $\boldsymbol{\sigma}_{h,1}^l = \boldsymbol{\sigma}_{h,2}^l$. Thus, there exists a unique $(u_h^l, \boldsymbol{\sigma}_h^l)$ solution of (2.119).

2.5 Numerical results

In this section, we consider the nonlinear scheme **US** with right hand sides $f(\mathbf{x}, t)$, $\mathbf{g}(\mathbf{x}, t)$ and $h(\mathbf{x}, t)$ in (2.34) and (2.35) respectively, where these right hand sides are chosen corresponding to the exact solutions $u = e^{-t}(\cos(2\pi x)\cos(2\pi y)+2)$, $v = (1+\sin(t))(\cos(2\pi x)\cos(2\pi y)+2)$ and $\boldsymbol{\sigma} = \nabla v = (1+\sin(t))(-2\pi\sin(2\pi x)\cos(2\pi y), -2\pi\sin(2\pi y)\cos(2\pi x))$. In our computation, we take $\Omega = [0,1] \times [0,1]$, and we use a uniform partition with m + 1 nodes in each direction. We choose the spaces for $u, \boldsymbol{\sigma}$ and v, generated by $\mathbb{P}_1, \mathbb{P}_1, \mathbb{P}_2$ -continuous FE, respectively. The linear iterative method used to approach the nonlinear scheme **US** is the Newton Method, and in all the cases, the iterative method stops when the relative error in L^2 -norm is less than $\varepsilon = 10^{-6}$.

In order to check numerically the error estimates obtained in our theoretical analysis, we choose $k = 10^{-5}$ and the numerical results with respect to time T = 0.001 are listed in Tables 2.1-2.3. We can see that when $h \to 0$, $||u(t_n) - u_h^n||_{L^2H^1}$ is convergent in optimal rate $\mathcal{O}(h)$, and $||u_h^n - \mathcal{R}_h^u u_h^n||_{L^2H^1}$, $||u(t_n) - u_h^n||_{L^{\infty}L^2}$, $||u_h^n - \mathcal{R}_h^u u_h^n||_{L^{\infty}L^2}$, $||v(t_n) - v_h^n||_{L^{\infty}H^1}$ and $||v_h^n - \mathcal{R}_h^v v_h^n||_{L^{\infty}H^1}$ are convergent in optimal rate $\mathcal{O}(h^2)$.

$m \times m$	$ u(t_n) - u_h^n _{L^{\infty}L^2}$	Order	$\ u_h^n - \mathcal{R}_h^u u_h^n\ _{L^\infty L^2}$	Order
40×40	$2.5 imes 10^{-3}$	-	$1.5 imes 10^{-3}$	-
50×50	$1.6 imes 10^{-3}$	1.9970	9×10^{-4}	1.9846
60×60	1.1×10^{-3}	1.9980	7×10^{-4}	1.9896
70×70	8×10^{-4}	1.9985	5×10^{-4}	1.9923
80×80	6×10^{-4}	1.9989	4×10^{-4}	1.9938

Table 2.1: Error orders for $||u(t_n) - u_h^n||_{L^{\infty}L^2}$ and $||u_h^n - \mathcal{R}_h^u u_h^n||_{L^{\infty}L^2}$.

$m \times m$	$ u(t_n) - u_h^n _{L^2H^1}$	Order	$\ u_h^n - \mathcal{R}_h^u u_h^n\ _{L^2 H^1}$	Order
40×40	1.11×10^{-2}	-	5.219×10^{-4}	-
50×50	8.9×10^{-3}	0.9978	3.348×10^{-4}	1.9896
60×60	7.4×10^{-3}	0.9985	2.328×10^{-4}	1.9937
70×70	6.3×10^{-3}	0.9989	1.711×10^{-4}	1.9966
80×80	5.5×10^{-3}	0.9992	1.310×10^{-4}	1.9988

Table 2.2: Error orders for $||u(t_n) - u_h^n||_{L^2H^1}$ and $||u_h^n - \mathcal{R}_h^u u_h^n||_{L^2H^1}$.

$m \times m$	$ v(t_n) - v_h^n _{L^{\infty}H^1}$	Order	$\ v_h^n - \mathcal{R}_h^v v_h^n\ _{L^\infty H^1}$	Order
40×40	1.08×10^{-2}	-	9.875×10^{-4}	-
50×50	$6.9 imes 10^{-3}$	1.9985	5.526×10^{-4}	2.6014
60×60	$4.8 imes 10^{-3}$	1.9990	3.448×10^{-4}	2.5874
70×70	$3.5 imes 10^{-3}$	1.9993	2.318×10^{-4}	2.5768
80×80	$2.7 imes 10^{-3}$	1.9995	1.645×10^{-4}	2.5684

Table 2.3: Error orders for $||v(t_n) - v_h^n||_{L^{\infty}H^1}$ and $||v_h^n - \mathcal{R}_h^v v_h^n||_{L^{\infty}H^1}$.

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Chapter 3 Asymptotic behaviour for a chemo-repulsion system with quadratic production: The continuous problem and fully discrete numerical schemes

3.1 Introduction

The directed movement of cells in response to a chemical stimulus is known in biology as chemotaxis. More specifically, if the cells move towards regions of high chemical concentration, the motion is called chemoattraction, while if the cells move towards regions of lower chemical concentration, the motion is called chemorepulsion. Models for chemoattraction and chemorepulsion motion has been studied in literature (see [4, 9, 7, 10] and references therein). One of the most important characteristics of chemoattractant models is that the finite blow up of solutions can happen in space dimension greater or equal to 2; while in chemorepulsion models this phenomenon is not expected. Many works have been devoted to study in what cases and how this phenomenon takes place.

In those cases in which blow-up phenomenon does not happen, it is interesting to study the asymptotic behaviour of the solutions of the model. In fact, in [14], Osaki and Yagi studied the convergence of the solution of the Keller-Segel model to a stationary solution in the one-dimensional case. In [8], the convergence of the solution of the Keller-Segel model with an additional term of cross-diffusion to a steady state was shown. In [4] the authors proved the convergence to constant state for a chemorepulsion model with linear production. Therefore, taking into account the results above, the aim of this paper is to study the asymptotic behaviour of the following parabolic-parabolic repulsive-productive chemotaxis model (with quadratic production term):

$$\begin{cases} \partial_t u - \Delta u = \nabla \cdot (u \nabla v) \text{ in } \Omega, \ t > 0, \\ \partial_t v - \Delta v + v = u^2 \text{ in } \Omega, \ t > 0, \\ \frac{\partial u}{\partial \mathbf{n}} = \frac{\partial v}{\partial \mathbf{n}} = 0 \text{ on } \partial \Omega, \ t > 0, \\ u(\boldsymbol{x}, 0) = u_0(\boldsymbol{x}) \ge 0, \ v(\boldsymbol{x}, 0) = v_0(\boldsymbol{x}) \ge 0 \text{ in } \Omega, \end{cases}$$
(3.1)

where Ω is a *n*-dimensional open bounded domain, n = 2, 3, with boundary $\partial\Omega$; and the unknowns are $u(\boldsymbol{x}, t) \geq 0$, the cell density, and $v(\boldsymbol{x}, t) \geq 0$, the chemical concentration. This model has been studied in Chapter 1, and it was proved that model (3.1) is well-posed: there exists global in time weak-strong solution in the sense of Definition 3.2.1 (below), and, for 2D domains, there exists a unique global in time strong solution.

On the other hand, another interesting topic is to study the asymptotic behaviour of fully discrete numerical schemes approximating (3.1). In fact, in [5] Guillén-González and Samsidy studied and proved asymptotic convergence for a fully discrete finite element scheme for a Ginzburg-Landau model for nematic liquid crystal flow. In [12] Merlet and Pierre studied the asymptotic behaviour of the Backward Euler scheme applied to gradient flows. It is important to notice that, in chemotaxis models, there are few works studying large-time behaviour for fully discrete schemes. We refer to [2], where the authors shown convergence at infinite time of a finite volume scheme for a Keller-Segel model with an additional term of cross-diffusion. Meanwhile, the behavior at infinite time of a fully discrete scheme for at infinite time of a fully discrete scheme for the study the large-time behavior for two fully discrete numerical schemes associated to model (3.1).

This chapter is organized as follows: In Section 3.2, we study the asymptotic behavior of the global weak-strong solutions for the model (3.1), and we prove the exponential convergence as time goes to infinity to a constant state. In Section 3.3, we analyze this same behavior for two fully discrete numerical schemes associated to system (3.1): the nonlinear backward Euler in the variables (u, v), and the nonlinear scheme defined in Chapter 2 by introducing the auxiliary variable $\boldsymbol{\sigma} = \nabla v$. Moreover, in order to analyze the asymptotic behaviour for the backward Euler scheme, we study its solvability and unconditional energystability. Finally, in Section 3.4, we compare the numerical schemes throughout several numerical simulations.

3.1.1 Notation

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 $L^p(\Omega)$, $1 \le p \le \infty$, with norms $\|\cdot\|_m$ and $\|\cdot\|_{L^p}$, respectively. In particular, the $L^2(\Omega)$ -norm will be denoted by $\|\cdot\|_0$. We denote by $\boldsymbol{H}^1_{\sigma}(\Omega) := \{ \mathbf{u} \in \boldsymbol{H}^1(\Omega) : \mathbf{u} \cdot \mathbf{n} = 0 \text{ on } \partial\Omega \}$ and we will use the following equivalent norms in $H^1(\Omega)$ and $\mathbf{H}^1_{\sigma}(\Omega)$, respectively (see [13] and [1, Corollary 3.5], respectively):

$$||u||_{1}^{2} = ||\nabla u||_{0}^{2} + \left(\int_{\Omega} u\right)^{2}, \quad \forall u \in H^{1}(\Omega),$$
(3.2)

$$\|\boldsymbol{\sigma}\|_{1}^{2} = \|\boldsymbol{\sigma}\|_{0}^{2} + \|\operatorname{rot}\,\boldsymbol{\sigma}\|_{0}^{2} + \|\nabla\cdot\boldsymbol{\sigma}\|_{0}^{2}, \quad \forall \boldsymbol{\sigma} \in \boldsymbol{H}_{\sigma}^{1}(\Omega).$$
(3.3)

In particular, (3.3) implies that

$$\|\nabla v\|_1^2 = \|\nabla v\|_0^2 + \|\Delta v\|_0^2, \quad \forall v : \nabla v \in \boldsymbol{H}^1_{\sigma}(\Omega).$$

If Z is a general Banach space, its topological dual will be denoted by Z'. Moreover, the letters C, K will denote different positive constants (independent of discrete parameters) which may change from line to line (or even within the same line).

3.2 Continuous problem

First we give the following definition of weak-strong solutions for problem (3.1).

Definition 3.2.1 (Weak-strong solutions) Given $(u_0, v_0) \in L^2(\Omega) \times H^1(\Omega)$ with $u_0, v_0 \geq 0$ a.e. $\boldsymbol{x} \in \Omega$, a pair (u, v) is called weak-strong solution of problem (3.1) in $(0, +\infty)$, if $u \geq 0, v \geq 0$ a.e. $(t, \boldsymbol{x}) \in (0, +\infty) \times \Omega$,

$$(u,v) \in L^{\infty}(0,+\infty; L^{2}(\Omega) \times H^{1}(\Omega)) \cap L^{2}(0,T; H^{1}(\Omega) \times H^{2}(\Omega)), \quad \forall T > 0,$$

$$\partial_{t}u \in L^{q'}(0,T; (H^{1}(\Omega))') \quad and \quad \partial_{t}v \in L^{q'}(0,T; L^{2}(\Omega)), \quad \forall T > 0,$$

$$(3.4)$$

where q' = 2 in 2D and q' = 4/3 in 3D (q' is the conjugate exponent of q = 2 in 2D and q = 4 in 3D); the following variational formulation holds

$$\int_0^T \langle \partial_t u, \bar{u} \rangle + \int_0^T (\nabla u, \nabla \bar{u}) + \int_0^T (u \nabla v, \nabla \bar{u}) = 0, \quad \forall \bar{u} \in L^q(0, T; H^1(\Omega)), \quad \forall T > 0, \quad (3.5)$$

the following equation holds pointwisely

$$\partial_t v - \Delta v + v = u^2, \quad a.e. \ (t, \mathbf{x}) \in (0, +\infty) \times \Omega,$$
(3.6)

the initial conditions $(3.1)_4$ are satisfied and the following energy inequality (in integral version) holds for a.e. $t_0, t_1 : t_1 \ge t_0 \ge 0$:

$$\mathcal{E}(u(t_1), v(t_1)) - \mathcal{E}(u(t_0), v(t_0)) + \int_{t_0}^{t_1} \left(\|\nabla u(s)\|_0^2 + \frac{1}{2} \|\nabla v(s)\|_1^2 \right) \, ds \le 0, \tag{3.7}$$

where $\mathcal{E}(u(t), v(t)) = \frac{1}{2} \|u(t)\|_0^2 + \frac{1}{4} \|\nabla v(t)\|_0^2$.

Remark 3.2.2 In particular, the energy inequality (3.7) is valid for $t_0 = 0$. Moreover, (3.7) shows the dissipative character of the model with respect to the total energy $\mathcal{E}(u(t), v(t))$.

Remark 3.2.3 (Positivity) $u \ge 0$ in 2D domains and $v \ge 0$ in any (2D or 3D) dimension are a consequence of (3.4)-(3.6). Indeed, this follows from the fact that in these cases we can test (3.5) by $u_{-} := \min\{u, 0\} \in L^{2}(0, T; H^{1}(\Omega))$ and (3.6) by $v_{-} := \min\{v, 0\} \in L^{2}(0, T; H^{2}(\Omega)) \hookrightarrow L^{2}(0, T; L^{2}(\Omega))$.

Observe that the problem (3.1) conserves in time the total mass $\int_{\Omega} u$, because taking $\bar{u} = 1$ in (3.5),

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

Moreover, integrating (3.6) in Ω we deduce the following behavior of $\int_{\Omega} v$:

$$\frac{d}{dt}\left(\int_{\Omega} v\right) + \int_{\Omega} v = \int_{\Omega} u^2.$$

We recall that in Chapter 1 it was proved the existence of weak-strong solutions of problem (3.1) (satisfying in particular the energy inequality (3.7)), through convergence of a time-discrete numerical scheme associated to model (3.1).

3.2.1 Convergence at infinite time

In this subsection, we will prove the exponential convergence of any weak-strong solution (u, v) of problem (3.1) obtained by Galerkin approximations. First, we will prove exponential bounds for weak-strong norms a.e. $t \ge 0$.

Theorem 3.2.4 Let (u, v) be any weak-strong solution of problem (3.1) obtained by Galerkin approximations. Then, the following estimates hold

$$\|(u(t) - m_0, \nabla v(t))\|_0^2 \le C_0 e^{-2t}, \quad a.e. \quad t \ge 0.$$
(3.8)

$$\|v(t) - (m_0)^2\|_0^2 \le C_0 e^{-t}, \quad \forall t \ge 0,$$
(3.9)

where $m_0 := \frac{1}{|\Omega|} \int_{\Omega} u_0$ and C_0 is a positive constant depending on the data (u_0, v_0) , but independent of t.

Proof. For each $m \ge 1$, we say that (u^m, v^m) is a Galerkin solution if $u^m : [0, +\infty) \to U_m$ and $v^m : [0, +\infty) \to V_m$ are \mathcal{C}^1 functions and satisfy

$$\begin{cases} (\partial_t u^m, \bar{u}) + (\nabla u^m, \nabla \bar{u}) + (u^m \nabla v^m, \nabla \bar{u}) = 0, & \forall \bar{u} \in U_m, \ t \ge 0\\ (\partial_t v^m, \bar{v}) + (\nabla v^m, \nabla \bar{v}) + (v^m, \bar{v}) - ((u^m)^2, \bar{v}) = 0, & \forall \bar{v} \in V_m, \ t \ge 0, \\ u^m(0) = u_0^m := P_m(u_0), \qquad v^m(0) = v_0^m := Q_m(v_0), \end{cases}$$
(3.10)

where U_m and V_m are finite dimensional spaces generated by orthonormal eigenfunctions of the operator $(-\Delta + \mathcal{I})$, with Δ and \mathcal{I} being the laplacian and identity operators; $P_m : L^2(\Omega) \to U_m$ denotes the projection from $L^2(\Omega)$ onto U_m , and $Q_m : H^1(\Omega) \to V_m$ the projection from $H^1(\Omega)$ onto V_m . Then, (3.10) can be regarded as a Cauchy problem for a first order ordinary differential system in time, and the classical existence and uniqueness theory for ordinary differential systems implies that, for every $m \geq 1$, there exist $T_m > 0$ and unique functions $u^m : [0, T_m) \to U_m$ and $V_m : [0, T_m) \to V_m$ that solve (3.10), with either $T_m = +\infty$ or $\lim_{t\to T_m} \|(u^m(t), v^m(t))\|_0 = +\infty$. Now, we are going to deduce some estimates for (u^m, v^m) showing that only $T_m = +\infty$ can be true.

We define $\widetilde{u}^m := u^m - m_0$ and taking $\overline{u} = \widetilde{u}^m$ and $\overline{v} = -\frac{1}{2}\Delta v^m$ in (3.10), we arrive at

$$\frac{1}{2}\frac{d}{dt}\left(\|\widetilde{u}^m(t)\|_0^2 + \frac{1}{2}\|\nabla v^m(t)\|_0^2\right) + \|\widetilde{u}^m(t)\|_1^2 + \frac{1}{2}\|\nabla v^m(t)\|_1^2 = 0,$$
(3.11)

from which we deduce that

$$\begin{cases} (u^m, \nabla v^m) \text{ is bounded in } L^{\infty}(0, +\infty; L^2(\Omega) \times \boldsymbol{L}^2(\Omega)), \\ (\nabla u^m, \nabla v^m) \text{ is bounded in } L^2(0, +\infty; \boldsymbol{L}^2(\Omega) \times \boldsymbol{H}^1(\Omega)). \end{cases}$$
(3.12)

Moreover, Moreover, we observe that the function $y^m(t) = \left(\int_{\Omega} v^m(\boldsymbol{x}, t) d\boldsymbol{x}\right)^2$ satisfies $(y^m)'(t) + y^m(t) \leq w^m(t)$, with $w^m(t) = ||u^m(t)||_0^4$. In fact, it follows by taking $\bar{v} = 1$ in (3.10), multiplying the resulting equation by $\int_{\Omega} v^m(\boldsymbol{x}, t) d\boldsymbol{x}$ and using the Young inequality. Therefore, $y^m(t) = y^m(0) e^{-t} + \int_0^t e^{-(t-s)} w^m(s) ds$, which implies that

$$\left(\int_{\Omega} v^m(\boldsymbol{x},t) \, d\boldsymbol{x}\right)^2 \le \left(\int_{\Omega} v_0^m(\boldsymbol{x}) \, d\boldsymbol{x}\right)^2 + \|u^m\|_{L^{\infty}(0,+\infty;L^2)}^4, \quad \forall t \ge 0.$$
(3.13)

Then, from (3.12) and (3.13), we deduce that

$$v^m$$
 is bounded in $L^{\infty}(0, +\infty; H^1(\Omega)) \cap L^2(0, T; H^2(\Omega)), \quad \forall T > 0.$ (3.14)

Taking into account (3.12) and (3.14), we can deduce $(\partial_t u^m, \partial_t \nabla v^m)$ is bounded in $L^{4/3}(0,T; H^1(\Omega)' \times \mathbf{H}^1(\Omega)')$. Therefore, proceeding as in Theorem 1.4.11, we obtain that there exists a subsequence m' of m, and (u,v) weak-strong solution of (3.1), such that $(u^{m'}, v^{m'})$ converges to (u, v) weakly-* in $L^{\infty}(0, +\infty; L^2(\Omega) \times H^1(\Omega))$, weakly in $L^2(0, T; H^1(\Omega) \times H^2(\Omega))$ and strongly in $L^2(0, T; L^2(\Omega) \times H^1(\Omega)) \cap C([0, T]; H^1(\Omega)' \times L^p(\Omega))$, for any T > 0, $1 \le p < 6$. Therefore, in particular

$$\|(\widetilde{u}^{m'}(t), \nabla v^{m'}(t))\|_{0}^{2} \to \|(\widetilde{u}(t), \nabla v(t))\|_{0}^{2}, \text{ a.e. } t \ge 0.$$
(3.15)

Moreover, from the equality (3.11), we deduce

$$\|\widetilde{u}^{m'}(t)\|_{0}^{2} + \frac{1}{2} \|\nabla v^{m'}(t)\|_{0}^{2} \le \|(u_{0}^{m'} - m_{0}, \nabla v_{0}^{m'})\|_{0}^{2} e^{-2t}, \quad \forall t \ge 0.$$
(3.16)

Thus, from (3.15)-(3.16), we arrive at (3.8). Finally, testing (3.6) by $\tilde{v} := v - (m_0)^2$, one can obtain

$$\frac{1}{2}\frac{d}{dt}\|\widetilde{v}(t)\|_0^2 + \|\widetilde{v}(t)\|_1^2 = \int_{\Omega} ((u(\boldsymbol{x},t))^2 - (m_0)^2)\widetilde{v}(\boldsymbol{x},t)d\boldsymbol{x},$$

which, using the Hölder and Young inequalities, implies that

$$\frac{d}{dt} \|\widetilde{v}(t)\|_0^2 + \|\widetilde{v}(t)\|_1^2 \le \|u(t) + m_0\|_{L^3}^2 \|u(t) - m_0\|_0^2.$$
(3.17)

Therefore, from (3.17) and (3.8), we can deduce for all $t \ge 0$,

$$\begin{aligned} \|\widetilde{v}(t)\|_{0}^{2} &\leq \|v_{0} - (m_{0})^{2}\|_{0}^{2}e^{-t} + e^{-t}\int_{0}^{t}\|u(s) - m_{0}\|_{0}^{2}\|u(s) + m_{0}\|_{L^{3}}^{2}e^{s}ds \\ &\leq C_{0}e^{-t} + C_{0}e^{-t}\int_{0}^{t}\|u(s) + m_{0}\|_{L^{3}}^{2}e^{-2s}e^{s}ds \\ &\leq C_{0}e^{-t} + C_{0}e^{-t}\int_{0}^{t}\|\nabla u(s)\|_{0}^{2}e^{-s}ds + C_{0}e^{-t}\int_{0}^{t}\|u(s) + m_{0}\|_{0}^{2}e^{-s}ds \end{aligned}$$

from which, using (3.12), we conclude (3.9).

In next theorem, we will show, for large times, exponential bounds for more regular norms.

Theorem 3.2.5 Let $\varepsilon > 0$. Under hypothesis of Theorem 3.2.4, there exists a constant $C_1 > 0$ such that if $\varepsilon^2 \leq \frac{1}{2C_1}$ it holds

$$\|(u(t) - m_0, \nabla v(t))\|_1^2 \le 2\varepsilon e^{-\frac{1}{2}(t - t_2)}, \quad a.e. \ t \ge t_2(\varepsilon),$$
(3.18)

with $t_2 := t_2(\varepsilon) \ge 0$ a large enough time that will be obtained in the proof.

Proof. We define $F_m(t) := \|\widetilde{u}^m(t)\|_1^2 + \frac{1}{2} \|\nabla v^m(t)\|_1^2$. Then, from (3.8) and (3.11), we have that $t^{+\infty}$

$$\int_{t}^{+\infty} F_m(s)ds \le \|(u^m(t) - m_0, \nabla v^m(t))\|_0^2 \le C_0 e^{-2t},$$

which, in particular, implies that for all $\delta > 0$, there exists a large enough time $t_0 = t_0(\delta) \ge 0$ such that

$$\int_{t_0}^{+\infty} F_m(s) ds \le \delta. \tag{3.19}$$

Then, taking into account that $F_m(t)$ satisfies (3.19), proceeding as in [3, Lemma 2.1], we have that for all $\delta > 0$, $t \ge t_0(\delta)$ and $\tau > 0$, there exists a time $\bar{t} \in [t, t + \tau]$ such that

$$F_m(\bar{t}) \le \frac{2\delta}{\tau}.\tag{3.20}$$

Indeed, the set of points $\bar{t} \in [t, t + \tau]$ satisfying (3.20) has measure greater than $\tau/2$. Now, in order to obtain strong estimates, we take $\bar{u} = -\Delta u^m$ and $\bar{v} = \frac{1}{2}\Delta^2 v^m$ in (3.10), and proceeding as in (1.33), we arrive at

$$\frac{d}{dt} \Big(\|\nabla \widetilde{u}^m(t)\|_0^2 + \frac{1}{2} \|\Delta v^m(t)\|_0^2 \Big) + \|\Delta \widetilde{u}^m(t)\|_0^2 + \|\Delta v^m(t)\|_1^2 \le C \|\widetilde{u}^m(t)\|_1^6 + C \|\nabla v^m(t)\|_1^6.$$
(3.21)

Then, adding (3.11) and (3.21), we have

$$\frac{d}{dt} \Big(\|\widetilde{u}^m(t)\|_1^2 + \frac{1}{2} \|\nabla v^m(t)\|_1^2 \Big) + \|\widetilde{u}^m(t)\|_2^2 + \|\nabla v^m(t)\|_2^2 \le C_1 \Big(\|\widetilde{u}^m(t)\|_1^2 + \frac{1}{2} \|\nabla v^m(t)\|_1^2 \Big)^3,$$

or equivalently, $F_m(t)$ satisfies

$$F'_m(t) + G_m(t) \le C_1 F_m(t)^3,$$
(3.22)

with $G_m(t) = \|\widetilde{u}^m(t)\|_2^2 + \|\nabla v^m(t)\|_2^2$. Therefore, taking into account that $F_m(t)$ satisfies (3.22), proceeding as in [3, Lemma 2.2], we can deduce that for any $\varepsilon > 0$ and $t_1 \ge 0$,

$$F_m(t_1) \le \varepsilon/2 \qquad \Rightarrow \qquad F_m(t) \le \varepsilon, \quad \forall t \in \left[t_1, t_1 + \frac{1}{2C_1\varepsilon^2}\right].$$
 (3.23)

Thus, as consequence of (3.20) and (3.23), following the proof of [3, Theorem 2.3], we conclude that for any $\varepsilon > 0$, taking $\tau = \frac{1}{4C_1\varepsilon^2}$, $\delta = \frac{1}{16C_1\varepsilon}$ and $t_0 = t_0(\delta)$ such that $F_m(t)$ satisfies (3.19), where C_1 is the constant in the estimate (3.22), it holds

$$F_m(t) \le \varepsilon, \quad \forall t \ge t_2(\varepsilon) := t_0(\delta) + \frac{1}{4C_1\varepsilon^2}.$$
 (3.24)

Therefore, from (3.22) and (3.24), using the fact that $G_m(t) \ge F_m(t)$ and taking ε such that $\varepsilon^2 \le \frac{1}{2C_1}$, we deduce

$$F'_{m}(t) + \frac{1}{2}G_{m}(t) \leq 0, \quad \forall t \geq t_{2} := t_{2}(\varepsilon)$$

$$F_{m}(t) \leq F_{m}(t_{2})e^{-\frac{1}{2}(t-t_{2})} \leq \varepsilon e^{-\frac{1}{2}(t-t_{2})}, \quad \forall t \geq t_{2}.$$
(3.25)

and

Moreover, from (3.24), (3.22) and (3.19) we have that $(\tilde{u}^m, \nabla v^m)$ is bounded in $L^{\infty}(t_2, +\infty; H^1(\Omega) \times H^1(\Omega)) \cap L^2(t_2, +\infty; H^2(\Omega) \times H^2(\Omega))$. Then, using the fact that $(\partial_t \tilde{u}^m, \partial_t \nabla v^m)$ is bounded in $L^2(t_2, +\infty; L^2(\Omega) \times L^2(\Omega))$, a compactness result of Aubin-Lions type implies that $(\tilde{u}^m, \nabla v^m)$ is relatively compact in $L^2(t_2, t_3; H^1(\Omega) \times H^1(\Omega))$ for all $t_3 \geq t_2$. Therefore, in particular for some subsequence m' of m, we have

$$\|(\widetilde{u}^{m'}(t), \nabla v^{m'}(t))\|_{1}^{2} \to \|(\widetilde{u}(t), \nabla v(t))\|_{1}^{2}, \text{ a.e. } t \ge t_{2},$$

and using (3.25) we arrive at (3.18).

3.3 Fully Discrete Schemes associated to system (3.1)

In this section, we study the large-time behavior for two fully discrete schemes associated to model (3.1): the nonlinear backward Euler for model (3.1), and the nonlinear scheme defined in Chapter 2 by introducing the auxiliary variable $\boldsymbol{\sigma} = \nabla v$. Along this section we will use repeatedly the following result (see[6, Lemma 4.1]):

Lemma 3.3.1 Assume that $\delta, k > 0$ and $\beta, d^n \ge 0$ satisfy

$$(1+\delta k)d^{n+1} - d^n \le \beta k, \qquad \forall n \ge 0.$$

Then,

$$d^{n} \leq (1+\delta k)^{-(n-n_{0})} d^{n_{0}} + \delta^{-1}\beta, \qquad \forall n \geq n_{0} \geq 0.$$

3.3.1 Scheme UV

The first scheme that will be studied in this paper is obtained by using FE backward Euler for the system (3.1) (considered for simplicity 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 $\{\mathcal{T}_h\}_{h>0}$ be a family of shape-regular and quasi-uniform triangulations of $\overline{\Omega}$ made up of simplexes (triangles in two dimensions and tetrahedra in three dimensions), so that $\overline{\Omega} = \bigcup_{K \in \mathfrak{T}_h} K$, where $h = \max_{K \in \mathfrak{T}_h} h_K$, with h_K being the diameter of K. Further, let $\mathcal{N}_h = \{a_i\}_{i \in \mathcal{I}}$ denote the set of all the nodes of \mathfrak{T}_h . We choose finite element spaces for u and v, which we denote by $(U_h, V_h) \subset H^1 \times W^{1,6}$ generated by $(\mathbb{P}_m, \mathbb{P}_{2m})$ -continuous FE, with $m \geq 1$. Then, we consider the following first order in time, nonlinear and coupled scheme (Scheme **UV**, from now on):

Initialization: Let $(u_h^0, v_h^0) \in U_h \times V_h$ be a suitable approximation of $(u_0, v_0) \in L^2(\Omega) \times H^1(\Omega)$, as $h \to 0$, with $\frac{1}{|\Omega|} \int_{\Omega} u_h^0 = \frac{1}{|\Omega|} \int_{\Omega} u_0 = m_0$, and satisfying (3.27) below. **Time step** n: Given $(u_h^{n-1}, v_h^{n-1}) \in U_h \times V_h$, compute $(u_h^n, v_h^n) \in U_h \times V_h$ solving $\int (\delta_t u_h^n, \bar{u}_h) + (\nabla u_h^n, \nabla \bar{u}_h) + (u_h^n \nabla v_h^n, \nabla \bar{u}_h) = 0, \quad \forall \bar{u}_h \in U_h,$ (2.26)

$$\begin{cases} (\delta_{t}u_{h}^{n}, u_{h}) + (\nabla u_{h}^{n}, \nabla u_{h}) + (u_{h}^{n} \nabla v_{h}^{n}, \nabla u_{h}) = 0, \quad \forall u_{h} \in U_{h}, \\ (\delta_{t}v_{h}^{n}, \bar{v}_{h}) + (\nabla v_{h}^{n}, \nabla \bar{v}_{h}) + (v_{h}^{n}, \bar{v}_{h}) - ((u_{h}^{n})^{2}, \bar{v}_{h}) = 0, \quad \forall \bar{v}_{h} \in V_{h}, \end{cases}$$
(3.26)

where we denote in general $\delta_t a^n = \frac{a^n - a^{n-1}}{k}$. For the initial approximation $(u_h^0, v_h^0) \in U_h \times V_h$ we assume that there exists a positive constant C independent of (k, h) such that

$$\|(u_h^0, v_h^0)\|_{L^2 \times H^1} \le C \|(u_0, v_0)\|_{L^2 \times H^1}.$$
(3.27)

Existence, energy-stability and convergence

Assuming that the functions $\bar{u}_h = 1 \in U_h$ and $\bar{v}_h = 1 \in V_h$, we deduce that the scheme **UV** conserves the total mass $\int_{\Omega} u_h^n$, that is,

$$\int_{\Omega} u_h^n = \int_{\Omega} u_h^{n-1} = \dots = \int_{\Omega} u_h^0, \qquad (3.28)$$

and we have the following behavior for $\int_{\Omega} v_h^n$

$$\delta_t \left(\int_{\Omega} v_h^n \right) = \int_{\Omega} (u_h^n)^2 - \int_{\Omega} v_h^n.$$
(3.29)

Theorem 3.3.2 (Unconditional existence) There exists $(u_h^n, v_h^n) \in U_h \times V_h$ solution of the scheme UV.

Proof. The proof follows the argument of Theorem 1.4.3, by using the Leray-Schauder fixed point theorem. \blacksquare

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

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

$$(3.30)$$

Then, the discrete chemical equation $(3.26)_2$ can be rewritten as

$$(\delta_t v_h^n, \bar{v}_h) + (A_h v_h^n, \bar{v}_h) - ((u_h^n)^2, \bar{v}_h) = 0, \quad \forall \bar{v}_h \in V_h.$$
(3.31)

Moreover, the following estimate holds (see for instance, Lemma 2.3.1):

$$\|v_h\|_{W^{1,6}} \le C \|A_h v_h\|_0, \quad \forall v_h \in V_h,.$$
(3.32)

Lemma 3.3.3 (Unconditional stability) The scheme UV is unconditionally energystable. In fact, if (u_n, v_n) is any solution of UV, then the following discrete energy law holds

$$\delta_t \mathcal{E}(u_h^n, v_h^n) + \frac{k}{2} \|\delta_t u_h^n\|_0^2 + \frac{k}{4} \|\delta_t \nabla v_h^n\|_0^2 + \|\nabla u_h^n\|_0^2 + \frac{1}{2} \|(A_h - I)v_h^n\|_0^2 + \frac{1}{2} \|\nabla v_h^n\|_0^2 = \emptyset 3.33)$$

where $\mathcal{E}(u_h^n, v_h^n) = \frac{1}{2} \|u_h^n\|_0^2 + \frac{1}{4} \|\nabla v_h^n\|_0^2.$

Proof. Taking $\bar{u}_h = u_h^n$ in $(3.26)_1$, $\bar{v}_h = \frac{1}{2}(A_h - I)v_h^n$ in (3.31) and using (3.30), we obtain

$$\int_{\Omega} u_h^n \cdot \delta_t u_h^n + \|\nabla u_h^n\|_0^2 + \frac{1}{2} \int_{\Omega} \nabla v_h^n \cdot \delta_t \nabla v_h^n + \frac{1}{2} \|(A_h - I)v_h^n\|_0^2 + \frac{1}{2} \|\nabla v_h^n\|_0^2 = 0.$$
(3.34)

To get (3.34), the fact that $(u_h^n)^2 \in V_h$ is essential (which holds from the choice $(\mathbb{P}_m, \mathbb{P}_{2m})$ approximation for (U_h, V_h)) in order to cancel the terms $(u_h^n \nabla v_h^n, \nabla u_h^n)$ and

 $-\frac{1}{2}((u_h^n)^2, (A_h - I)v_h^n)$. Moreover, using the formula $a(a - b) = \frac{1}{2}(a^2 - b^2) + \frac{1}{2}(a - b)^2$ we deduce that

$$\int_{\Omega} u_h^n \cdot \delta_t u_h^n + \frac{1}{2} \int_{\Omega} \nabla v_h^n \cdot \delta_t \nabla v_h^n = \delta_t \left(\frac{1}{2} \| u_h^n \|_0^2 + \frac{1}{4} \| \nabla v_h^n \|_0^2 \right) + \frac{k}{2} \| \delta_t u_h^n \|_0^2 + \frac{k}{4} \| \delta_t \nabla v_h^n \|_0^2.$$
(3.35)

Thus, from (3.34)-(3.35), we deduce (3.33).

From the (local in time) discrete energy law (3.33), we deduce the following global in time estimates for (u_h^n, v_h^n) solution of the scheme **UV**:

Lemma 3.3.4 (Uniform Weak estimates) Let (u_h^n, v_h^n) be a solution of the scheme **UV**. Then, the following estimates hold

$$\begin{aligned} \|(u_h^n, \nabla v_h^n)\|_0^2 + k^2 \sum_{m=1}^n \|(\delta_t u_h^m, \delta_t \nabla v_h^m)\|_0^2 \\ + k \sum_{m=1}^n \left(\|\nabla u_h^m\|_0^2 + \|\nabla v_h^m\|_0^2 + \|(A_h - I)v_h^m\|_0^2 \right) \le C_0, \quad \forall n \ge 1, \quad (3.36) \end{aligned}$$

$$\left| \int_{\Omega} v_h^n \right| \le C_0, \quad \forall n \ge 0, \tag{3.37}$$

$$k \sum_{m=n_0+1}^{n_0+n} \|(u_h^m, v_h^m)\|_{H^1 \times W^{1,6}}^2 \le C_0 + C_1(nk), \quad \forall n \ge 1,$$
(3.38)

where $n_0 \ge 0$ is any integer and C_0, C_1 are positive constants depending on the data (u_0, v_0) and (Ω, u_0, v_0) respectively, but independent of (k, h) and (n, n_0) .

Proof. Multiplying (3.33) by k, summing for $m = 1, \dots, n$ and using (3.27), we obtain (3.36). On the other hand, from (3.29) and using (3.36), we have

$$(1+k)\left|\int_{\Omega} v_h^n\right| - \left|\int_{\Omega} v_h^{n-1}\right| \le k\left|\int_{\Omega} (u_h^n)^2\right| = k\|u_h^n\|_0^2 \le kC_0.$$
(3.39)

Then, using Lemma 3.3.1 in (3.39), we deduce

$$\left|\int_{\Omega} v_h^n\right| \le (1+k)^{-n} \left|\int_{\Omega} v_h^0\right| + C_0 \le \left|\int_{\Omega} v_h^0\right| + C_0, \quad \forall n \ge 0,$$

which implies (3.37). Finally, from (3.33), summing for m from $n_0 + 1$ to $n + n_0$, using (3.32), (3.36), (3.37) and the Poincaré inequality for the zero-mean value function $u_h^m - m_0$, where $m_0 = \frac{1}{|\Omega|} \int_{\Omega} u_0 = \frac{1}{|\Omega|} \int_{\Omega} u_h^m$, we have $n_0 + n$

$$k \sum_{m=n_0+1}^{n_0+n} \|(u_h^m - m_0, v_h^m)\|_{H^1 \times W^{1,6}}^2 \le C_0 + C_1(nk),$$

and thus, we deduce (3.38).

Starting from the previous stability estimates, we can prove the convergence towards weak solutions of (3.1). Concretely, by introducing the functions:

- $(\widetilde{u}_{h,k}, \widetilde{v}_{h,k})$ are continuous functions on $[0, +\infty)$, linear on each interval (t_n, t_{n+1}) and equal to (u_h^n, v_h^n) at $t = t_n, n \ge 0$;
- $(u_{h,k}^r, v_{h,k}^r)$ as the piecewise constant functions taking values (u_h^n, v_h^n) on $(t_{n-1}, t_n], n \ge 1$,

we have the following result:

Theorem 3.3.5 (Convergence) There exist subsequences (k') of (k) and (h') of (h), with $k', h' \downarrow 0$, and a weak-strong solution (u, v) of (3.1) in $(0, +\infty)$, such that $(\tilde{u}_{h',k'}, \tilde{v}_{h',k'})$ and $(u_{h',k'}^r, v_{h',k'}^r)$ converge to (u, v) weakly-* in $L^{\infty}(0, +\infty; L^2(\Omega) \times H^1(\Omega))$, weakly in $L^2(0, T; H^1(\Omega) \times W^{1,6}(\Omega))$ and strongly in $L^2(0, T; L^2(\Omega) \times L^p(\Omega)) \cap C([0, T]; H^1(\Omega)' \times L^q(\Omega))$, for any T > 0, $1 \le p < +\infty$ and $1 \le q < 6$.

Remark 3.3.6 Note that, since the positivity of u_h^n cannot be assured, then the positivity of the limit function u cannot be proven in the 3D case (see Remark 3.2.3).

Proof. Proceeding as in Theorem 1.4.11 (whose proof follows the arguments of [11]), we can prove that there exist subsequences (k') of (k) and (h') of (h), with $k', h' \downarrow 0$, and (u, v) satisfying (3.5), (3.6) and the initial conditions $(3.1)_4$, such that $(\tilde{u}_{h',k'}, \tilde{v}_{h',k'})$ and $(u_{h',k'}^r, v_{h',k'}^r)$ converge to (u, v) weakly-* in $L^{\infty}(0, +\infty; L^2(\Omega) \times H^1(\Omega))$, weakly in $L^2(0, T; H^1(\Omega) \times W^{1,6}(\Omega))$ and strongly in $L^2(0, T; L^2(\Omega) \times L^p(\Omega)) \cap C([0, T]; H^1(\Omega)' \times L^q(\Omega))$, for any T > 0, $1 \le p < +\infty$ and $1 \le q < 6$. Moreover, it holds

$$\frac{d}{dt} \left(\frac{1}{2} \| \widetilde{u}_{k',h'}(t) \|_{0}^{2} + \frac{1}{4} \| \nabla \widetilde{v}_{k',h'}(t) \|_{0}^{2} \right) + \frac{(t_{n}-t)}{2} \| (\delta_{t}u_{n}, \delta_{t}\nabla v_{n}) \|_{0}^{2} \\ + \| \nabla u_{k',h'}^{r}(t) \|_{0}^{2} + \frac{1}{2} \| (A_{h}-I)v_{k',h'}^{r}(t) \|_{0}^{2} + \frac{1}{2} \| \nabla v_{k',h'}^{r}(t) \|_{0}^{2} = 0.$$

In order to obtain that (u, v) satisfies the energy inequality (3.7), we need to prove that

$$\liminf_{(k',h')\to(0,0)} \int_{t_0}^{t_1} \|(A_h - I)v_{k',h'}^r(t)\|_0^2 \ge \int_{t_0}^{t_1} \|\Delta v(t)\|_0^2.$$
(3.40)

Taking into account that $\{(A_h - I)v_{k',h'}^r\}$ is bounded in $L^2(0,T;L^2(\Omega))$, we have that there exists $w \in L^2(0,T;L^2(\Omega))$ such that for some subsequence of (k',h'), still denoted by (k',h'),

$$(A_h - I)v_{k',h'}^r \to w \quad \text{weakly in} \quad L^2(0,T;L^2(\Omega).$$
 (3.41)

Therefore, on the one hand, since $u^2 \in L^2(0,T;L^{3/2}(\Omega)) \hookrightarrow L^2(0,T;H^1(\Omega)')$, we have

$$\partial_t v - \Delta v + v = u^2 \quad \text{in } L^2(H^1)', \tag{3.42}$$
and, on the other hand, using (3.41), we can deduce

$$\partial_t v + w + v = u^2 \quad \text{in } L^2(H^1)'.$$
 (3.43)

Thus, from (3.42)-(3.43), we deduce that $w = -\Delta v$ in $\mathcal{D}'(\Omega)$, which implies $-\Delta v \in L^2(0,T;L^2(\Omega))$ because of $w \in L^2(0,T;L^2(\Omega))$. Therefore, (u,v) satisfies the regularity (3.4) and taking into account (3.41), we conclude (3.40). Finally, using (3.40) and arguing as in the last part of the proof of Theorem 1.4.11, we deduce that (u,v) satisfies the energy inequality (3.7), and therefore, (u,v) is a weak-strong solution of (3.1).

Large-time behavior of the scheme UV

In this subsection, we will prove exponential bounds for any solution (u_h^n, v_h^n) of the scheme **UV** in weak-strong norms. In fact, the next result is the discrete version of Theorem 3.2.4.

Theorem 3.3.7 Let (u_h^n, v_h^n) be a solution of the scheme UV associated to an initial data $(u_h^0, v_h^0) \in U_h \times V_h$ which is a suitable approximation of $(u_0, v_0) \in L^2(\Omega) \times H^1(\Omega)$, as $h \to 0$, with $\frac{1}{|\Omega|} \int_{\Omega} u_h^0 = \frac{1}{|\Omega|} \int_{\Omega} u_0 = m_0$. Then,

$$\|(u_h^n - m_0, \nabla v_h^n)\|_0^2 \le C_0 e^{-\frac{2}{1+2k}kn}, \quad \forall n \ge 0,$$
(3.44)

$$\|v_h^n - (m_0)^2\|_0^2 \le C_0 e^{-\frac{1}{1+k}kn}, \quad \forall n \ge 0,$$
(3.45)

$$k\sum_{m>n} \left(\|\widetilde{u}_h^m\|_1^2 + \frac{1}{2} \|(A_h - I)v_h^n\|_0^2 + \frac{1}{2} \|\nabla v_h^n\|_0^2 \right) \le C_0 e^{-\frac{2}{1+2k}kn}, \quad \forall n \ge 0,$$
(3.46)

where C_0 is a positive constant depending on the data (u_0, v_0) , but independent of (k, h) and n.

Proof. Taking $\bar{u}_h = \tilde{u}_h^n := u_h^n - m_0$ in $(3.26)_1$, $\bar{v}_h = \frac{1}{2}(A_h - I)v_h^n$ in (3.31) and using (3.28) and (3.30), we obtain

$$\delta_t \left(\frac{1}{2} \| \widetilde{u}_h^n \|_0^2 + \frac{1}{4} \| \nabla v_h^n \|_0^2 \right) + \frac{k}{2} \| \delta_t \widetilde{u}_h^n \|_0^2 + \frac{k}{4} \| \delta_t \nabla v_h^n \|_0^2 + \| \widetilde{u}_h^n \|_1^2 + \frac{1}{2} \| (A_h - I) v_h^n \|_0^2 + \frac{1}{2} \| \nabla v_h^n \|_0^2 = 0.$$
(3.47)

Again, to get (3.47), the fact that $(u_h^n)^2 \in V_h$ is essential (which comes from the choice $(\mathbb{P}_m, \mathbb{P}_{2m})$ approximation for (U_h, V_h)) in order to cancel the terms $(u_h^n \nabla v_h^n, \nabla \widetilde{u}_h^n)$ and $-\frac{1}{2}((u_h^n)^2, (A_h - I)v_h^n)$. Then, from (3.47) we can obtain

$$(1+2k)\left(\|\widetilde{u}_{h}^{n}\|_{0}^{2}+\frac{1}{2}\|\nabla v_{h}^{n}\|_{0}^{2}\right)-\left(\|\widetilde{u}_{h}^{n-1}\|_{0}^{2}+\frac{1}{2}\|\nabla v_{h}^{n-1}\|_{0}^{2}\right)\leq0.$$
(3.48)

Then, applying Lemma 3.3.1 to (3.48), using the inequality $1 - x \le e^{-x}$ for all $x \ge 0$ as well as (3.36), we have for all $n \ge 0$,

$$\|\widetilde{u}_{h}^{n}\|_{0}^{2} + \frac{1}{2}\|\nabla v_{h}^{n}\|_{0}^{2} \leq (1+2k)^{-n} \left(\|\widetilde{u}_{h}^{0}\|_{0}^{2} + \frac{1}{2}\|\nabla v_{h}^{0}\|_{0}^{2}\right) \leq C_{0} \left(1 - \frac{2}{1+2k}k\right)^{n} \leq C_{0}e^{-\frac{2}{1+2k}kn},$$
(3.49)

which implies (3.44). Moreover, taking $\bar{v}_h = \tilde{v}_h^n := v_h^n - (m_0)^2$ in (3.31), we can deduce

$$\frac{1}{2}\delta_t \|\widetilde{v}_h^n\|_0^2 + \|\widetilde{v}_h^n\|_1^2 = \int_{\Omega} ((u_h^n)^2 - (m_0)^2)\widetilde{v}_h^n,$$

which, using the Hölder and Young inequalities, implies that

$$(1+k)\|\widetilde{v}_{h}^{n}\|_{0}^{2} - \|\widetilde{v}_{h}^{n-1}\|_{0}^{2} \le k\|u_{h}^{n} + m_{0}\|_{L^{3}}^{2}\|u_{h}^{n} - m_{0}\|_{0}^{2}.$$
(3.50)

Then, multiplying (3.50) by $(1+k)^{n-1}$, summing from n = 1 to n = m and using (3.36) and (3.49), we deduce

$$\begin{split} \|\widetilde{v}_{h}^{m}\|_{0}^{2} &\leq (1+k)^{-m} \|\widetilde{v}_{h}^{0}\|_{0}^{2} + k(1+k)^{-m} \sum_{n=1}^{m} (1+k)^{n-1} \|u_{h}^{n} - m_{0}\|_{0}^{2} \|u_{h}^{n} + m_{0}\|_{L^{3}}^{2} \\ &\leq C_{0}(1+k)^{-m} + C_{0}k(1+k)^{-m} \sum_{n=1}^{m} (1+k)^{n-1}(1+2k)^{-n} \|u_{h}^{n} + m_{0}\|_{L^{3}}^{2} \\ &\leq C_{0}(1+k)^{-m} \left[1 + k \sum_{n=1}^{m} \|\nabla u_{h}^{n}\|_{0}^{2} + \frac{k}{1+2k} \sum_{n=1}^{m} \left(\frac{1+k}{1+2k}\right)^{n-1} \|u_{h}^{n} + m_{0}\|_{0}^{2} \right] \\ &\leq C_{0}e^{-\frac{1}{1+k}km} \left[1 + C_{0} + C_{0}\frac{k}{1+2k} \sum_{n=1}^{m} \left(\frac{1+k}{1+2k}\right)^{n-1} \right] \\ &\leq C_{0}e^{-\frac{1}{1+k}km} \left[1 + C_{0} + C_{0}\left(1 - \left(\frac{1+k}{1+2k}\right)^{m}\right) \right], \quad \forall m \geq 0, \end{split}$$

from which we arrive at (3.45). Finally, from (3.44) and (3.47), we have that for all $n \ge 0$,

$$k\sum_{m>n} \left(\|\widetilde{u}_h^m\|_1^2 + \frac{1}{2} \|(A_h - I)v_h^n\|_0^2 + \frac{1}{2} \|\nabla v_h^n\|_0^2 \right) \le \|(u_h^n - m_0, \nabla v_h^n)\|_0^2 \le C_0 e^{-\frac{2}{1+2k}kn}.$$

3.3.2 Scheme US

The second scheme which will be analyzed has been defined and studied in Chapter 2, where the auxiliary variable $\boldsymbol{\sigma} = \nabla v$ is introduced, and the model (3.1) is rewritten as follows:

$$\begin{aligned}
& (\partial_t u - \nabla \cdot (\nabla u) = \nabla \cdot (u\sigma) & \text{in } \Omega, \ t > 0, \\
& (\partial_t \sigma - \nabla (\nabla \cdot \sigma) + \sigma + \text{rot}(\text{rot } \sigma) = \nabla (u^2) & \text{in } \Omega, \ t > 0, \\
& (\partial_t \sigma - \nabla (\nabla \cdot \sigma) + \sigma + \text{rot}(\text{rot } \sigma) = \nabla (u^2) & \text{in } \Omega, \ t > 0, \\
& (\partial_t \sigma - \nabla (\nabla \cdot \sigma) + \sigma + \text{rot}(\text{rot } \sigma) = \nabla (u^2) & \text{in } \Omega, \ t > 0, \\
& (\mathbf{a}, \mathbf{b}) = 0 & \text{on } \partial\Omega, \ t > 0, \\
& (\mathbf{a}, \mathbf{b}) = u_0(\mathbf{x}) > 0, \ \sigma(\mathbf{x}, 0) = \nabla v_0(\mathbf{x}) & \text{in } \Omega.
\end{aligned}$$
(3.51)

In fact, $(3.51)_2$ was obtained applying the gradient to equation $(3.1)_2$ and adding the term $rot(rot \boldsymbol{\sigma})$ using the fact that $rot \boldsymbol{\sigma} = rot(\nabla v) = 0$. Once solved (3.51), it is possible to recover v from u^2 solving

$$\begin{cases} \frac{\partial_t v - \Delta v + v = u^2 \text{ in } \Omega, \ t > 0, \\ \frac{\partial v}{\partial \mathbf{n}} = 0 \quad \text{on } \partial\Omega, \ t > 0, \\ v(\mathbf{x}, 0) = v_0(\mathbf{x}) > 0 \quad \text{in } \Omega. \end{cases}$$
(3.52)

Based on the above decomposition, the scheme is obtained by using FE backward Euler for the system (3.51)-(3.52) (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**. We choose finite element spaces for u, σ and v, which we denote by $(U_h, \Sigma_h, V_h) \subset H^1 \times \mathbf{H}_{\sigma}^1 \times W^{1,6}$ generated by $\mathbb{P}_k, \mathbb{P}_m, \mathbb{P}_r$ -continuous FE, with $k, m, r \geq 1$. Then, we consider the following first order in time, nonlinear and coupled scheme (Scheme **US**, from now on):

Initialization: Let $(u_h^0, \boldsymbol{\sigma}_h^0, v_h^0) \in U_h \times \boldsymbol{\Sigma}_h \times V_h$ be a suitable approximation of $(u_0, \boldsymbol{\sigma}_0, v_0)$, as $h \to 0$, with $\frac{1}{|\Omega|} \int_{\Omega} u_h^0 = \frac{1}{|\Omega|} \int_{\Omega} u_0 = m_0$. Time step w Given $(u_h^{n-1}, \boldsymbol{\sigma}^{n-1}) \in U_h \times \boldsymbol{\Sigma}_h$ compute $(u_h^n, \boldsymbol{\sigma}^n) \in U_h \times \boldsymbol{\Sigma}_h$ solving

Time step n: Given $(u_h^{n-1}, \boldsymbol{\sigma}_h^{n-1}) \in U_h \times \boldsymbol{\Sigma}_h$, compute $(u_h^n, \boldsymbol{\sigma}_h^n) \in U_h \times \boldsymbol{\Sigma}_h$ solving

$$\begin{cases} (\delta_t u_h^n, \bar{u}_h) + (\nabla u_h^n, \nabla \bar{u}_h) + (u_h^n \boldsymbol{\sigma}_h^n, \nabla \bar{u}_h) = 0, \quad \forall \bar{u}_h \in U_h, \\ (\delta_t \boldsymbol{\sigma}_h^n, \bar{\boldsymbol{\sigma}}_h) + (\boldsymbol{\sigma}_h^n, \bar{\boldsymbol{\sigma}}) + (\nabla \cdot \boldsymbol{\sigma}_h^n, \nabla \cdot \bar{\boldsymbol{\sigma}}) + (\operatorname{rot} \boldsymbol{\sigma}_h^n, \operatorname{rot} \bar{\boldsymbol{\sigma}}) - 2(u_h^n \nabla u_h^n, \bar{\boldsymbol{\sigma}}_h) = 0, \quad \forall \bar{\boldsymbol{\sigma}}_h \in \boldsymbol{\Sigma}_h \end{cases}$$

$$(3.53)$$

Once solved (3.53), given $v_h^{n-1} \in V_h$ we can recover $v_h^n = v_h^n((u_h^n)^2)$ solving:

$$(\delta_t v_h^n, \bar{v}_h) + (\nabla v_h^n, \nabla \bar{v}_h) + (v_h^n, \bar{v}_h) - ((u_h^n)^2, \bar{v}_h) = 0, \quad \forall \bar{v}_h \in V_h.$$
(3.54)

Known results

The scheme **US** also conserves the total mass $\int_{\Omega} u_h^n$ (satisfying (3.28)), and also has the behaviour for $\int_{\Omega} v_h^n$ given in (3.29). The existence of $(u_h^n, \boldsymbol{\sigma}_h^n) \in U_h \times \boldsymbol{\Sigma}_h$ solution of the scheme **US**, v_h^n solution of (3.54), and the unconditional energy-stability of the scheme **US** was proved in Chapter 2. In fact, the following discrete energy law holds

$$\delta_t \mathcal{E}(u_h^n, \boldsymbol{\sigma}_h^n) + \frac{k}{2} \|\delta_t u_h^n\|_0^2 + \frac{k}{4} \|\delta_t \boldsymbol{\sigma}_h^n\|_0^2 + \|\nabla u_h^n\|_0^2 + \frac{1}{2} \|\boldsymbol{\sigma}_h^n\|_1^2 = 0, \qquad (3.55)$$

where $\mathcal{E}(u_h^n, \boldsymbol{\sigma}_h^n) = \frac{1}{2} \|u_h^n\|_0^2 + \frac{1}{4} \|\boldsymbol{\sigma}_h^n\|_0^2$.

From the (local in time) discrete energy law (3.55), the following global in time weak estimates for $(u_h^n, \boldsymbol{\sigma}_h^n)$ are deduced (see Theorem 2.3.9):

$$\begin{split} \|(u_h^n, \boldsymbol{\sigma}_h^n)\|_0^2 + k^2 \sum_{m=1}^n \|(\delta_t u_h^m, \delta_t \boldsymbol{\sigma}_h^m)\|_0^2 + k \sum_{m=1}^n \|(\nabla u_h^m, \boldsymbol{\sigma}_h^m)\|_{L^2 \times H^1}^2 \le C_0, \quad \forall n \ge 1, \\ k \sum_{m=n_0+1}^{n_0+n} \|u_h^m\|_1^2 \le C_0 + C_1(nk), \quad \forall n \ge 1, \end{split}$$

where $n_0 \geq 0$ is any integer and C_0, C_1 are positive constants depending on the data $(\Omega, u_0, \boldsymbol{\sigma}_0)$, but independent of (k, h) and (n, n_0) .

Large-time behavior of scheme US

Theorem 3.3.8 Let $(u_h^n, \boldsymbol{\sigma}_h^n)$ be a solution of the scheme \boldsymbol{US} associated to an initial data $(u_h^0, \boldsymbol{\sigma}_h^0) \in U_h \times \boldsymbol{\Sigma}_h$ which is a suitable approximation of $(u_0, \boldsymbol{\sigma}_0) \in L^2(\Omega) \times \boldsymbol{L}^2(\Omega)$, as $h \to 0$, with $\frac{1}{|\Omega|} \int_{\Omega} u_h^0 = \frac{1}{|\Omega|} \int_{\Omega} u_0 = m_0$. Then,

$$\|(u_h^n - m_0, \boldsymbol{\sigma}_h^n)\|_0^2 \le C_0 e^{-\frac{2}{1+2k}kn}, \quad \forall n \ge 0,$$
(3.56)

$$k\sum_{m>n} \left(\|\widetilde{u}_h^m\|_1^2 + \frac{1}{2} \|\boldsymbol{\sigma}_h^m\|_1^2 \right) \le C_0 e^{-\frac{2}{1+2k}kn}, \quad \forall n \ge 0,$$
(3.57)

where C_0 is a positive constant depending on the data $(u_0, \boldsymbol{\sigma}_0)$, but independent of (k, h) and n.

Proof. Taking $\bar{u}_h = \tilde{u}_h^n := u_h^n - m_0$ in $(3.53)_1$, $\bar{\sigma}_h = \frac{1}{2}\sigma_h^n$ in (3.54) and using (3.28), we obtain

$$\delta_t \left(\frac{1}{2} \| \widetilde{u}_h^n \|_0^2 + \frac{1}{4} \| \boldsymbol{\sigma}_h^n \|_0^2 \right) + \frac{k}{2} \| \delta_t \widetilde{u}_h^n \|_0^2 + \frac{k}{4} \| \delta_t \boldsymbol{\sigma}_h^n \|_0^2 + \| \widetilde{u}_h^n \|_1^2 + \frac{1}{2} \| \boldsymbol{\sigma}_h^n \|_1^2 = 0.$$
(3.58)

Then, from (3.58) we can obtain

$$(1+2k)\left(\|\widetilde{u}_{h}^{n}\|_{0}^{2}+\frac{1}{2}\|\boldsymbol{\sigma}_{h}^{n}\|_{0}^{2}\right)-\left(\|\widetilde{u}_{h}^{n-1}\|_{0}^{2}+\frac{1}{2}\|\boldsymbol{\sigma}_{h}^{n-1}\|_{0}^{2}\right)\leq0.$$
(3.59)

Then, applying Lemma 3.3.1 to (3.59), and proceeding as in (3.49), we arrive at (3.56). Finally, from (3.56) and (3.58), we have that for all $n \ge 0$,

$$k \sum_{m>n} \left(\|\widetilde{u}_h^m\|_1^2 + \frac{1}{2} \|\boldsymbol{\sigma}_h^m\|_1^2 \right) \le \|(u_h^n - m_0, \boldsymbol{\sigma}_h^n)\|_0^2 \le C_0 e^{-\frac{2}{1+2k}kn}$$

Corollary 3.3.9 Let $v_h^n = v_h^n((u_h^n)^2)$ be a solution of (3.54) associated to an initial data $v_h^0 \in V_h$ which is a suitable approximation of $v_0 \in H^1(\Omega)$, as $h \to 0$. Then (3.45) holds.

Proof. The proof follows as in Theorem 3.3.7.

Now, in order to obtain more regular estimates, we consider the linear operators \widetilde{A}_h : $U_h \to U_h$ and $B_h : \Sigma_h \to \Sigma_h$ defined as follows

$$\begin{cases} (\widetilde{A}_h u_h, \bar{u}_h) = (\nabla u_h, \nabla \bar{u}_h) + (u_h, \bar{u}_h), & \forall \bar{u}_h \in U_h, \\ (B_h \boldsymbol{\sigma}_h, \bar{\boldsymbol{\sigma}}_h) = (\nabla \cdot \boldsymbol{\sigma}_h, \nabla \cdot \bar{\boldsymbol{\sigma}}_h) + (\operatorname{rot} \boldsymbol{\sigma}_h, \operatorname{rot} \bar{\boldsymbol{\sigma}}_h) + (\boldsymbol{\sigma}_h, \bar{\boldsymbol{\sigma}}_h), & \forall \bar{\boldsymbol{\sigma}}_h \in \boldsymbol{\Sigma}_h. \end{cases}$$

Then, we rewrite (3.53) as

$$\begin{cases} (\delta_t u_h^n, \bar{u}_h) + (\widetilde{A}_h u_h^n, \bar{u}_h) - (u_h^n, \bar{u}_h) + (u_h^n \boldsymbol{\sigma}_h^n, \nabla \bar{u}_h) = 0, \quad \forall \bar{u}_h \in U_h, \\ (\delta_t \boldsymbol{\sigma}_h^n, \bar{\boldsymbol{\sigma}}_h) + (B_h \boldsymbol{\sigma}_h^n, \bar{\boldsymbol{\sigma}}_h) - 2(u_h^n \nabla u_h^n, \bar{\boldsymbol{\sigma}}_h) = 0, \quad \forall \bar{\boldsymbol{\sigma}}_h \in \boldsymbol{\Sigma}_h. \end{cases}$$
(3.60)

Moreover, the following estimates hold (see for instance, Lemma 2.3.1):

$$\|u_h\|_{W^{1,6}} \le C \|A_h u_h\|_0 \quad \forall u_h \in U_h, \qquad \|\boldsymbol{\sigma}_h\|_{W^{1,6}} \le C \|B_h \boldsymbol{\sigma}_h\|_0 \quad \forall \boldsymbol{\sigma}_h \in \boldsymbol{\Sigma}_h.$$

Theorem 3.3.10 Under hypothesis of Theorem 3.3.8, the following estimate holds

$$k \sum_{m>n} \| (\widetilde{A}_h \widetilde{u}_h^m, B_h \boldsymbol{\sigma}_h^m) \|_0^2 \le C \left(\frac{1}{k} e^{-\frac{2}{1+2k}k(n-1)} + \left(\frac{1}{k^2} e^{-\frac{4}{1+2k}k(n-1)} + 1 \right) e^{-\frac{2}{1+2k}kn} \right), \ \forall n \ge 1,$$
(3.61)

where C is a positive constant independent of (k, h) and n.

Proof. We define $F_n := \|\widetilde{u}_h^n\|_1^2 + \frac{1}{2} \|\boldsymbol{\sigma}_h^n\|_1^2$. Then, from (3.57) we have that

$$\sum_{m>n} F_m \le \frac{1}{k} C_0 e^{-\frac{2}{1+2k}kn}, \quad \forall n \ge 0,$$

which, taking into account that $F_m \ge 0$ for all $m \in \mathbb{N}$, implies that

$$F_n \le \frac{1}{k} C_0 e^{-\frac{2}{1+2k}k(n-1)}, \quad \forall n \ge 1.$$
 (3.62)

Now, taking $\bar{u}_h = \tilde{A}_h \tilde{u}_h^n$ and $\bar{\sigma}_h = B_h \sigma_h^n$ in (3.60), we have

$$\frac{1}{2}\delta_{t}\Big(\|(\widetilde{u}_{h}^{n},\boldsymbol{\sigma}_{h}^{n})\|_{1}^{2}\Big) + \frac{k}{2}\|(\delta_{t}\widetilde{u}_{h}^{n},\delta_{t}\boldsymbol{\sigma}_{h}^{n})\|_{1}^{2} + \|(\widetilde{A}_{h}\widetilde{u}_{h}^{n},B_{h}\boldsymbol{\sigma}_{h}^{n})\|_{0}^{2} \leq \|\widetilde{u}_{h}^{n}\|_{1}^{2} + \tau\|(\widetilde{A}_{h}\widetilde{u}_{h}^{n},B_{h}\boldsymbol{\sigma}_{h}^{n})\|_{0}^{2} \\
+ C_{\tau}\|\nabla\widetilde{u}_{h}^{n}\|_{L^{3}}^{2}\|\boldsymbol{\sigma}_{h}^{n}\|_{L^{6}}^{2} + C_{\tau}\|\widetilde{u}_{h}^{n}\|_{L^{6}}^{2}\|\nabla\cdot\boldsymbol{\sigma}_{h}^{n}\|_{L^{3}}^{2} + C_{\tau}\|\nabla\widetilde{u}_{h}^{n}\|_{L^{3}}^{2}\|\widetilde{u}_{h}^{n}\|_{L^{6}}^{2} + C_{\tau}(m_{0})^{2}\|(\nabla\widetilde{u}_{h}^{n},\nabla\cdot\boldsymbol{\sigma}_{h}^{n})\|_{0}^{2} \\
\leq \|\widetilde{u}_{h}^{n}\|_{1}^{2} + \tau\|(\widetilde{A}_{h}\widetilde{u}_{h}^{n},B_{h}\boldsymbol{\sigma}_{h}^{n})\|_{0}^{2} + \tau\|(\nabla\widetilde{u}_{h}^{n},\nabla\cdot\boldsymbol{\sigma}_{h}^{n})\|_{L^{6}}^{2} + C_{\tau}\|\widetilde{u}_{h}^{n}\|_{1}^{2}\|\boldsymbol{\sigma}_{h}^{n}\|_{1}^{4} + C_{\tau}\|\widetilde{u}_{h}^{n}\|_{1}^{6} \\
+ C_{\tau}\|\boldsymbol{\sigma}_{h}^{n}\|_{1}^{2}\|\widetilde{u}_{h}^{n}\|_{1}^{4} + C_{\tau}(m_{0})^{2}\|(\widetilde{u}_{h}^{n},\boldsymbol{\sigma}_{h}^{n})\|_{1}^{2}.$$
(3.63)

Therefore, taking into account that $||(u_h, \boldsymbol{\sigma}_h)||_{W^{1,6}}^2 \leq C ||(\widetilde{A}_h u_h, B_h \boldsymbol{\sigma}_h)||_0^2$ for all $(u_h, \boldsymbol{\sigma}_h) \in U_h \times \boldsymbol{\Sigma}_h$ (see Lemma 2.3.1), from (3.63) (choosing τ small enough) we deduce

$$\delta_t \Big(\| (\widetilde{u}_h^n, \boldsymbol{\sigma}_h^n) \|_1^2 \Big) + \| (\widetilde{A}_h \widetilde{u}_h^n, B_h \boldsymbol{\sigma}_h^n) \|_0^2 \le C_1 \Big(\| (\widetilde{u}_h^n, \boldsymbol{\sigma}_h^n) \|_1^2 \Big)^3 + C_2 \| (\widetilde{u}_h^n, \boldsymbol{\sigma}_h^n) \|_1^2.$$
(3.64)

Then, from (3.64), taking into account (3.62) and (3.57), we deduce for all $n \ge 1$,

$$\begin{split} k \sum_{m>n} \| (\widetilde{A}_h \widetilde{u}_h^m, B_h \boldsymbol{\sigma}_h^m) \|_0^2 &\leq \| (\widetilde{u}_h^n, \boldsymbol{\sigma}_h^n) \|_1^2 + (\frac{1}{k^2} C_0^2 C_1 e^{-\frac{4}{1+2k}k(n-1)} + C_2) k \sum_{m>n} \| (\widetilde{u}_h^m, \boldsymbol{\sigma}_h^m) \|_1^2 \\ &\leq \frac{1}{k} C_0 e^{-\frac{2}{1+2k}k(n-1)} + \left(C_3 \frac{1}{k^2} e^{-\frac{4}{1+2k}k(n-1)} + C_4 \right) e^{-\frac{2}{1+2k}kn}, \end{split}$$

from which we conclude (3.61).

Remark 3.3.11 In the case of the scheme UV it is not clear how to obtain one more regular estimate equivalent to the obtained in Theorem 3.3.10 for the scheme US. In fact, a key step in the proof of Theorem 3.3.10, is to integrate by parts in the term $(u_h^n \sigma_h^n, \nabla(\widetilde{A}_h \widetilde{u}_h^n))$ arriving at $(\nabla u_h^n \cdot \sigma_h^n, \widetilde{A}_h \widetilde{u}_h^n) + (u_h^n \nabla \cdot \sigma_h^n, \widetilde{A}_h \widetilde{u}_h^n)$, which it is not possible for the scheme UV in the term $(u_h^n \nabla v_h^n, \nabla(\widetilde{A}_h \widetilde{u}_h^n))$, because $u_h^n \nabla v_h^n$ does not have a derivative in $L^2(\Omega)$.

3.4 Numerical Simulations

In this section we will compare the results of several numerical simulations that we have carried out using the schemes studied in the paper. We are considering \mathcal{P}_1 -continuous approximation for u_h^n , σ_h^n and \mathcal{P}_2 -continuous approximation for v_h^n . Moreover, we have chosen the 2D domain $\Omega = [0, 2]^2$ using a structured mesh, and all the simulations are carried out using **FreeFem++** software. The linear iterative method used to approach the nonlinear schemes **US** and **UV** is the Newton Method, and in all the cases, the iterative method stops when the relative error in L^2 -norm is less than $\varepsilon = 10^{-6}$.

3.4.1 Positivity

The aim of this subsection is to compare the fully discrete schemes **UV** and **US** in terms of positivity. Theoretically, for both schemes, is not clear the positivity of the variables u_h^n and v_h^n . In fact, in some simulations, we obtain numerical results in which u_h^n is negative. For example, choosing $k = 10^{-5}$, the initial conditions (see Figure 3.1):

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

and

$$v_0 = 200xy(2-x)(2-y)exp(-30(y-1)^2 - 30(x-1)^2) + 0.0001,$$

and taking meshes in space increasingly thinner $(h = \frac{1}{10}, h = \frac{1}{20}, h = \frac{1}{35}$ and $h = \frac{1}{75})$, we



Figure 3.1: Initial conditions.

obtain that in both schemes, the discrete cell density u_h^n takes negative values for some $x \in \Omega$ in some times $t_n > 0$ (see Figures 3.2-3.5). Moreover, as h tends to 0, (a) the behaviour of both schemes is increasingly similar, and (b) the negative values taken for u_h^n in both schemes are closer to 0. This is in accordance with the results obtained in Chapter 1, where it was proved that the only time-discrete schemes corresponding to the schemes **UV** and **US** are equivalents and have nonnegative solution (u_n, v_n) .



Figure 3.2: Minimum values of u_h^n , with $h = \frac{1}{10}$.

Remark 3.4.1 In the computations, the execution time for the scheme UV is smaller than the execution time for the scheme US. In fact, the scheme UV is twice faster than the scheme US.

On the other hand, with respect to the discrete chemical concentration v_h^n , we observe that the same behavior is obtained for the minimum of v_h^n in both schemes. In fact, independently of h, if v_0 is positive, then v_h also is positive (we show this behavior in Figure 3.6 for the case $h = \frac{1}{35}$, but the same holds for the cases $h = \frac{1}{10}$, $h = \frac{1}{20}$ and $h = \frac{1}{75}$).

3.4.2 Energy-Stability

In Lemma 3.3.3, the unconditional energy-stability for the scheme **UV** with respect to the energy $\mathcal{E}(u, v)$ was proved. In fact, if (u_h^n, v_h^n) is any solution of the scheme **UV**, the following relation holds

$$\delta_t \mathcal{E}(u_h^n, v_h^n) + \|\nabla u_h^n\|_0^2 + \frac{1}{2} \|(A_h - I)v_h^n\|_0^2 + \frac{1}{2} \|\nabla v_h^n\|_0^2 \le 0, \quad \forall n.$$



Figure 3.3: Minimum values of u_h^n , with $h = \frac{1}{20}$.

On the other hand, in Chapter 2 it was proved the unconditional energy-stability for the scheme **US** with respect to the modified energy $\mathcal{E}(u, \boldsymbol{\sigma})$. Even more, if $(u_h^n, \boldsymbol{\sigma}_h^n)$ is any solution of the scheme **US**, it holds

$$\delta_t \mathcal{E}(u_h^n, \boldsymbol{\sigma}_h^n) + \|\nabla u_h^n\|_0^2 + \frac{1}{2} \|\boldsymbol{\sigma}_h^n\|_1^2 \le 0, \quad \forall n$$

Then, the aim of this subsection is to compare numerically the energy-stability of the schemes **UV** and **US** with respect to the energy $\mathcal{E}(u, v)$. Indeed, if we take $k = 10^{-6}$, $h = \frac{1}{25}$ and the initial conditions

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

and

$$v_0 = 20xy(2-x)(2-y)exp(-30(y-1)^2 - 30(x-1)^2) + 0.0001,$$

we obtain that:

- (a) The schemes **UV** and **US** satisfy the energy decreasing in time property for the energy $\mathcal{E}(u, v)$, that is, $\mathcal{E}(u_h^n, v_h^n) \leq \mathcal{E}(u_h^{n-1}, v_h^{n-1})$ for all n, see Figure 3.7.
- (b) The schemes **UV** and **US** satisfy (see Figure 3.8)

$$RE(u_h^n, v_h^n) := \delta_t \mathcal{E}(u_h^n, v_h^n) + \|\nabla u_h^n\|_0^2 + \frac{1}{2} \|(A_h - I)v_h^n\|_0^2 + \frac{1}{2} \|\nabla v_h^n\|_0^2 \le 0, \quad \forall n.$$



Figure 3.4: Minimum values of u_h^n , with $h = \frac{1}{35}$.



Figure 3.5: Minimum values of u_h^n , with $h = \frac{1}{75}$.



Figure 3.6: Minimum values of v_h^n , with $h = \frac{1}{35}$.



Figure 3.7: Energy $\mathcal{E}(u_h^n, v_h^n)$ of schemes **UV** and **US**.



Figure 3.8: Residue $RE(u_h^n, v_h^n)$ of schemes **UV** and **US**.

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Chapter 4 Energy stable fully discrete schemes for a chemo-repulsion model with linear production

4.1 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):

$$\begin{cases} \partial_t u - \Delta u = \nabla \cdot (u \nabla v) & \text{in } \Omega, \ t > 0, \\ \partial_t v - \Delta v + v = u & \text{in } \Omega, \ t > 0, \\ \frac{\partial u}{\partial \mathbf{n}} = \frac{\partial v}{\partial \mathbf{n}} = 0 & \text{on } \partial \Omega, \ t > 0, \\ u(\boldsymbol{x}, 0) = u_0(\boldsymbol{x}) \ge 0, \ v(\boldsymbol{x}, 0) = v_0(\boldsymbol{x}) \ge 0 & \text{in } \Omega, \end{cases}$$
(4.1)

in a bounded domain $\Omega \subseteq \mathbb{R}^d$, d = 2, 3, with boundary $\partial\Omega$. The unknowns for this model are $u(\boldsymbol{x}, t) \geq 0$, the cell density, and $v(\boldsymbol{x}, t) \geq 0$, the chemical concentration. Problem (4.1) is conservative in u, because the total mass $\int_{\Omega} u(\cdot, t)$ remains constant in time, as we can check integrating equation (4.1)₁ in Ω ,

$$\frac{d}{dt}\left(\int_{\Omega} u(\cdot,t)\right) = 0, \quad \text{i.e.} \quad \int_{\Omega} u(\cdot,t) = \int_{\Omega} u_0 := m_0, \quad \forall t > 0.$$
(4.2)

Problem (4.1) is well-posed [7]: In 3D domains, there exist global in time nonnegative

weak solutions of model (4.1) in the following sense:

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

satisfying the following 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

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

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

$$F(s) := s(lns - 1) + 1 \ge 0 \implies F'(s) = lns \implies F''(s) = s^{-1}, \quad \forall s > 0,$$

then multiplying $(4.1)_1$ by F'(u), $(4.1)_2$ by $-\Delta v$, integrating over Ω , using $(4.1)_3$ and adding, the chemotactic and production terms cancel, and we obtain

$$\frac{d}{dt}\int_{\Omega} \left(F(u) + \frac{1}{2}|\nabla v|^2\right) d\boldsymbol{x} + \int_{\Omega} \left(4|\nabla(\sqrt{u})|^2 + |\Delta v|^2 + |\nabla v|^2\right) d\boldsymbol{x} = 0.$$
(4.3)

The aim of this work is to design numerical methods for model (4.1) conserving, at the discrete level, the mass-conservation and energy-stability properties of the continuous model (see (4.2)-(4.3), 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 [14, 15], proved error estimates for a conservative Finite Element (FE) approximation. A mixed FE approximation is studied in [12]. 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-stablity 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 Chapters 1 and 2 of this PhD thesis, respectively. However, as far as we know, for the chemo-repulsion model with linear production (4.1) there are not 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 (see Chapters 1 and 2). 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 multiplying the *u*-equation by the nonlinear function $F'(u) = \ln u$.

In this paper, we propose three unconditional energy stable fully discrete schemes, in which, in order to obtain rigorously a discrete version of the energy law (4.3), 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 $(4.1)_1$ 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 $(4.1)_1$ 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], it is obtained $\int_{\Omega} |\nabla u|^2$ which gives directly an estimate for ∇u in $L^2(\Omega)$.

This chapter is organized as follows: In Section 4.2, we give the notation and define the regularized functions that will be used in the fully discrete approximations. In Section 4.3, we study a nonlinear fully discrete FE approximation of (4.1) 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 (**H**) below). In Section 4.4, 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 4.5, we study a linear fully discrete FE approximation constructed by mixing the regularization procedure with the Energy Quadratization (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, 19], phase fields [18] (and references therein) and molecular beam epitaxial growth [16] models, among others. Finally, in Section 4.6, we compare the behavior of the schemes throughout several numerical simulations, and

provide some conclusions in Section 4.7.

4.2 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 by $H^1_{\sigma}(\Omega) := \{ \boldsymbol{\sigma} \in H^1(\Omega) : \boldsymbol{\sigma} \cdot \mathbf{n} = 0 \text{ on } \partial \Omega \}$ and we will use the following equivalent norms in $H^1(\Omega)$ and $\mathbf{H}^1_{\sigma}(\Omega)$, respectively (see [13] and [1, Corollary 3.5], respectively):

$$\|u\|_{1}^{2} = \|\nabla u\|_{0}^{2} + \left(\int_{\Omega} u\right)^{2}, \quad \forall u \in H^{1}(\Omega),$$
$$\|\boldsymbol{\sigma}\|_{1}^{2} = \|\boldsymbol{\sigma}\|_{0}^{2} + \|\operatorname{rot} \,\boldsymbol{\sigma}\|_{0}^{2} + \|\nabla \cdot \boldsymbol{\sigma}\|_{0}^{2}, \quad \forall \boldsymbol{\sigma} \in \boldsymbol{H}_{\sigma}^{1}(\Omega)$$

where rot σ 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 (4.1), 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 $\lambda_{\varepsilon} : \mathbb{R} \to [\varepsilon, \varepsilon^{-1}]$ given by

$$\lambda_{\varepsilon}(s) := \begin{cases} \varepsilon & \text{if } s \leq \varepsilon, \\ s & \text{if } \varepsilon \leq s \leq \varepsilon^{-1}, \\ \varepsilon^{-1} & \text{if } s \geq \varepsilon^{-1}. \end{cases}$$
(4.4)

If we define

$$F_{\varepsilon}''(s) := \frac{1}{\lambda_{\varepsilon}(s)},\tag{4.5}$$

then, we can integrate twice in (4.5), imposing the conditions $F'_{\varepsilon}(1) = F_{\varepsilon}(1) = 0$, and we obtain a convex function $F_{\varepsilon} : \mathbb{R} \to [0, +\infty)$, such that $F_{\varepsilon} \in C^{2,1}(\mathbb{R})$ (see Figure 4.1). Even more, for $\varepsilon \in (0, e^{-2})$, it holds [3]

$$F_{\varepsilon}(s) \ge \frac{\varepsilon}{2}s^2 - 2 \quad \forall s \ge 0 \quad \text{and} \quad F_{\varepsilon}(s) \ge \frac{s^2}{2\varepsilon} \quad \forall s \le 0.$$
 (4.6)

Finally, we will use the following result to get large time estimates [11]:



Figure 4.1: Functions λ_{ε} and F_{ε} and its derivatives.

Lemma 4.2.1 Assume that $\delta, \beta, k > 0$ and $d^n \ge 0$ satisfy

 $(1+\delta k)d^{n+1} \le d^n + k\beta, \quad \forall n \ge 0.$

Then, for any $n_0 \ge 0$,

$$d^n \le (1+\delta k)^{-(n-n_0)} d^{n_0} + \delta^{-1} \beta, \quad \forall n \ge n_0.$$

4.3 Scheme UV

In this section, we propose an energy-stable nonlinear fully discrete scheme (in the variables (u, v)) associated to model (4.1). With this aim, taking into account the functions λ_{ε} and F_{ε} and its derivatives, we consider the following regularized version of problem (4.1): Find $u_{\varepsilon}, v_{\varepsilon} : \Omega \times [0, T] \to \mathbb{R}$ such that

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

$$(4.7)$$

Remark 4.3.1 The idea is to define a fully discrete scheme associated to (4.7), taking in general $\varepsilon = \varepsilon(k, h)$, such that $\varepsilon(k, h) \to 0$ as $(k, h) \to 0$, where k is the time step and h the mesh size.

Observe that multiplying $(4.7)_1$ by $F'_{\varepsilon}(u_{\varepsilon})$, $(4.7)_2$ by $-\Delta v_{\varepsilon}$, integrating over Ω and adding, again the chemotactic and production terms cancel, and we obtain the following energy law

$$\frac{d}{dt}\int_{\Omega} \left(F_{\varepsilon}(u_{\varepsilon}) + \frac{1}{2}|\nabla v_{\varepsilon}|^{2}\right) d\boldsymbol{x} + \int_{\Omega} \left(F_{\varepsilon}''(u_{\varepsilon})|\nabla u_{\varepsilon}|^{2} + |\Delta v_{\varepsilon}|^{2} + |\nabla v_{\varepsilon}|^{2}\right) d\boldsymbol{x} = 0.$$

In particular, the modified energy

$$\mathcal{E}_{\varepsilon}(u,v) = \int_{\Omega} \Big(F_{\varepsilon}(u) + \frac{1}{2} |\nabla v|^2 \Big) d\boldsymbol{x}$$

is decreasing in time. 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 shaperegular and quasi-uniform family of triangulations of Ω , denoted by $\{\mathcal{T}_h\}_{h>0}$, with simplices $K, h_K = diam(K)$ 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:

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

Remark 4.3.2 The right angled requirement and the choice of \mathbb{P}_1 -continuous FE for U_h are necessary in order to obtain the relation (4.10) below, which is essential in order to prove the energy-stability of the scheme **UV** (see Theorem 4.3.7 below).

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

$$(u_1, u_2)^h := \int_{\Omega} \Pi^h(u_1 u_2), \quad |u|_h = \sqrt{(u, u)^h}.$$
 (4.8)

Remark 4.3.3 In U_h , the norms $|\cdot|_h$ and $||\cdot||_0$ are equivalents uniformly with respect to h (see [4]).

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

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

$$(4.9)$$

and the standard H^1 -projection $\mathbb{R}^h : H^1(\Omega) \to V_h$. Moreover, for each $\varepsilon \in (0, 1)$ we consider the construction of the operator $\Lambda_{\varepsilon} : U_h \to L^{\infty}(\Omega)^{d \times d}$ 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. \boldsymbol{x} in Ω , and the following relation holds

$$(\Lambda_{\varepsilon}u^{h})\nabla\Pi^{h}(F_{\varepsilon}'(u^{h})) = \nabla u^{h} \quad \text{in } \Omega.$$
(4.10)

Basically, $\Lambda_{\varepsilon} u^h$ is a constant by elements matrix such that (4.10) holds by elements. We highlight that (4.10) is satisfied due to the right angled constraint (**H**) and the choice of \mathbb{P}_1 -continuous FE for U_h . Moreover, the following stability estimate holds [3, 10]

$$\|\Lambda_{\varepsilon}(u^{h})\|_{L^{r}}^{r} \leq C(1+\|u^{h}\|_{1}^{2}), \quad \forall u^{h} \in U_{h} \quad (\text{for } r=2(d+1)/d),$$
(4.11)

where the constant C > 0 is independent of ε and h.

We recall the result below concerning to $\Lambda_{\varepsilon}(\cdot)$ (see [3, Lemma 2.1]).

Lemma 4.3.4 Let $\|\cdot\|$ denote the spectral norm on $\mathbb{R}^{d \times d}$. Then for any given $\varepsilon \in (0,1)$ the function $\Lambda_{\varepsilon} : U_h \to [L^{\infty}(\Omega)]^{d \times d}$ is continuous and satisfies

$$\varepsilon \xi^T \xi \le \xi^T \Lambda_{\varepsilon}(u^h) \xi \le \varepsilon^{-1} \xi^T \xi, \quad \forall \xi \in \mathbb{R}^d, \ \forall u^h \in U_h.$$
 (4.12)

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

$$\|(\Lambda_{\varepsilon}(u_{1}^{h}) - \Lambda_{\varepsilon}(u_{2}^{h}))|_{K}\| \leq \varepsilon^{-2} \max_{l=1,\dots,d} \{ |u_{1}^{h}(\mathbf{a}_{l}^{K}) - u_{2}^{h}(\mathbf{a}_{l}^{K}))| + |u_{1}^{h}(\mathbf{a}_{0}^{K}) - u_{2}^{h}(\mathbf{a}_{0}^{K}))| \}, \quad (4.13)$$

where \mathbf{a}_0^K is the right-angled vertex.

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

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

Then, the following estimate holds (see for instance, Lemma 2.3.1):

$$\|v^{h}\|_{W^{1,6}} \le C \|A_{h}v^{h}\|_{0}, \quad \forall v^{h} \in V_{h}.$$
(4.14)

Taking into account the regularized problem (4.7), 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 $\begin{cases} (\delta_t u_{\varepsilon}^n, \bar{u})^h + (\nabla u_{\varepsilon}^n, \nabla \bar{u}) + (\Lambda_{\varepsilon}(u_{\varepsilon}^n) \nabla v_{\varepsilon}^n, \nabla \bar{u}) = 0, \quad \forall \bar{u} \in U_h, \\ (\delta_t v_{\varepsilon}^n, \bar{v}) + (A_h v_{\varepsilon}^n, \bar{v}) - (u^n \ \bar{v}) = 0 \quad \forall \bar{u} \in V. \end{cases}$

$$(\delta_t v_{\varepsilon}^n, \bar{v}) + (A_h v_{\varepsilon}^n, \bar{v}) - (u_{\varepsilon}^n, \bar{v}) = 0, \quad \forall \bar{v} \in V_h,$$

$$(4.15)$$

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

Mass conservation and Energy-stability 4.3.1

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,

$$(u_{\varepsilon}^{n},1) = (u_{\varepsilon}^{n},1)^{h} = (u_{\varepsilon}^{n-1},1)^{h} = \dots = (u_{h}^{0},1)^{h} = (u_{h}^{0},1) = (Q^{h}u_{0},1) = (u_{0},1) := m_{0}, \quad (4.16)$$

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

$$\delta_t \left(\int_{\Omega} v_{\varepsilon}^n \right) + \int_{\Omega} v_{\varepsilon}^n = \int_{\Omega} u_{\varepsilon}^n = m_0.$$
(4.17)

Lemma 4.3.5 (Estimate of $\left|\int_{\Omega} v_{\varepsilon}^{n}\right|$) The following estimate holds

$$\left| \int_{\Omega} v_{\varepsilon}^{n} \right| \le (1+k)^{-n} \left| \int_{\Omega} v_{0} \right| + m_{0}, \quad \forall n \ge 0.$$

$$(4.18)$$

Proof. From (4.17) we have $(1+k) \left| \int_{\Omega} v_{\varepsilon}^{n} \right| - \left| \int_{\Omega} v_{\varepsilon}^{n-1} \right| \le k m_{0}$, and therefore, applying Lemma 4.2.1 (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 (4.18).

Definition 4.3.6 A numerical scheme with solution $(u_{\varepsilon}^n, v_{\varepsilon}^n)$ is called energy-stable with respect to the energy

$$\mathcal{E}^{h}_{\varepsilon}(u,v) = (F_{\varepsilon}(u),1)^{h} + \frac{1}{2} \|\nabla v\|_{0}^{2}$$
(4.19)

if this energy is time decreasing, that is, $\mathcal{E}^h_{\varepsilon}(u^n_{\varepsilon}, v^n_{\varepsilon}) \leq \mathcal{E}^h_{\varepsilon}(u^{n-1}_{\varepsilon}, v^{n-1}_{\varepsilon})$ for all $n \geq 1$.

Theorem 4.3.7 (Unconditional stability) The scheme UV is unconditional energy stable with respect to $\mathcal{E}^h_{\varepsilon}(u, v)$. In fact, if $(u^n_{\varepsilon}, v^n_{\varepsilon})$ is a solution of UV, then the following discrete energy law holds

$$\delta_t \mathcal{E}^h_{\varepsilon}(u^n_{\varepsilon}, v^n_{\varepsilon}) + \varepsilon \frac{k}{2} \|\delta_t u^n_{\varepsilon}\|^2_0 + \frac{k}{2} \|\delta_t \nabla v^n_{\varepsilon}\|^2_0 + \varepsilon \|\nabla u^n_{\varepsilon}\|^2_0 + \|(A_h - I)v^n_{\varepsilon}\|^2_0 + \|\nabla v^n_{\varepsilon}\|^2_0 \le 0.$$
(4.20)

Proof. Testing $(4.15)_1$ by $\bar{u} = \Pi^h(F'_{\varepsilon}(u^n_{\varepsilon}))$ and $(4.15)_2$ by $\bar{v} = (A_h - I)v^n_{\varepsilon}$, adding and taking into account that $\Lambda_{\varepsilon}(u^n_{\varepsilon})$ is symmetric as well as (4.10) (which implies that $\nabla \Pi^h(F'_{\varepsilon}(u^n_{\varepsilon})) = \Lambda_{\varepsilon}^{-1}(u^n_{\varepsilon})\nabla u^n_{\varepsilon}$), the terms $-(\Lambda_{\varepsilon}(u^n_{\varepsilon})\nabla v^n_{\varepsilon}, \nabla \Pi^h(F'_{\varepsilon}(u^n_{\varepsilon}))) =$ $-(\nabla v^n_{\varepsilon}, \Lambda_{\varepsilon}(u^n_{\varepsilon})\nabla \Pi^h(F'_{\varepsilon}(u^n_{\varepsilon}))) = -(\nabla v^n_{\varepsilon}, \nabla u^n_{\varepsilon})$ and $(u^n_{\varepsilon}, (A_h - I)v^n_{\varepsilon}) = (\nabla u^n_{\varepsilon}, \nabla v^n_{\varepsilon})$ cancel, and we obtain

$$(\delta_t u_{\varepsilon}^n, F_{\varepsilon}'(u_{\varepsilon}^n))^h + \int_{\Omega} (\nabla u_{\varepsilon}^n)^T \cdot \Lambda_{\varepsilon}^{-1}(u_{\varepsilon}^n) \cdot \nabla u_{\varepsilon}^n d\boldsymbol{x} + \delta_t \left(\frac{1}{2} \|\nabla v_{\varepsilon}^n\|_0^2\right) + \frac{k}{2} \|\delta_t \nabla v_{\varepsilon}^n\|_0^2 + \|(A_h - I)v_{\varepsilon}^n\|_0^2 + \|\nabla v_{\varepsilon}^n\|_0^2 = 0.$$
(4.21)

Moreover, observe that from the Taylor formula we have

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

and therefore,

$$F_{\varepsilon}'(u_{\varepsilon}^{n})\delta_{t}u_{\varepsilon}^{n} = \delta_{t}\left(F_{\varepsilon}(u_{\varepsilon}^{n})\right) + \frac{k}{2}F_{\varepsilon}''(\theta u_{\varepsilon}^{n} + (1-\theta)u_{\varepsilon}^{n-1})(\delta_{t}u_{\varepsilon}^{n})^{2}.$$
(4.22)

Then, using (4.22) and taking into account that Π^h is linear and $F''_{\varepsilon}(s) \geq \varepsilon$ for all $s \in \mathbb{R}$, we have

$$(\delta_t u_{\varepsilon}^n, F_{\varepsilon}'(u_{\varepsilon}^n))^h = \int_{\Omega} \Pi^h(\delta_t u_{\varepsilon}^n \cdot F_{\varepsilon}'(u_{\varepsilon}^n)) = \delta_t \Big(\int_{\Omega} \Pi^h(F_{\varepsilon}(u_{\varepsilon}^n)) \Big) + \frac{k}{2} \int_{\Omega} \Pi^h(F_{\varepsilon}''(\theta u_{\varepsilon}^n + (1-\theta)u_{\varepsilon}^{n-1})(\delta_t u_{\varepsilon}^n)^2) \ge \delta_t(F_{\varepsilon}(u_{\varepsilon}^n), 1)^h + \varepsilon \frac{k}{2} |\delta_t u_{\varepsilon}^n|_h^2.$$

$$(4.23)$$

Thus, from (4.12), (4.21), (4.23) and Remark 4.3.3, we arrive at (4.20).

Corollary 4.3.8 (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

$$(F_{\varepsilon}(u_{\varepsilon}^{n}),1)^{h} + \frac{1}{2} \|v_{\varepsilon}^{n}\|_{1}^{2} + k \sum_{m=1}^{n} \left(\varepsilon \|\nabla u_{\varepsilon}^{m}\|_{0}^{2} + \|(A_{h} - I)v_{\varepsilon}^{m}\|_{0}^{2} + \|\nabla v_{\varepsilon}^{m}\|_{0}^{2}\right) \le C_{0}, \quad \forall n \ge 1, \quad (4.24)$$

$$k \sum_{m=n_0+1}^{n+n_0} \|v_{\varepsilon}^m\|_{W^{1,6}}^2 \le C_1(1+kn), \quad \forall n \ge 1,$$
(4.25)

where the integer $n_0 \ge 0$ is arbitrary, 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

$$\int_{\Omega} (\Pi^{h}(u_{\varepsilon^{-}}^{n}))^{2} \leq C_{0}\varepsilon, \quad and \quad \int_{\Omega} |u_{\varepsilon}^{n}| \leq m_{0} + C\sqrt{\varepsilon}, \quad \forall n \geq 1,$$
(4.26)

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

$$\begin{aligned} \mathcal{E}^{h}_{\varepsilon}(u^{0}_{h}, v^{0}_{h}) &= \int_{\Omega} \Pi^{h}(F_{\varepsilon}(u^{0}_{h})) + \frac{1}{2} \|\nabla v^{0}_{h}\|^{2}_{0} \leq C \int_{\Omega} \Pi^{h}((u^{0}_{h})^{2} + 1) + \frac{1}{2} \|\nabla v^{0}_{h}\|^{2}_{0} \\ &\leq C(\|u^{0}_{h}\|^{2}_{0} + \|\nabla v^{0}_{h}\|^{2}_{0} + 1) \leq C(\|u_{0}\|^{2}_{0} + \|v_{0}\|^{2}_{1} + 1) \leq C_{0}, \end{aligned}$$
(4.27)

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 (4.20) and (4.27), we have

$$\mathcal{E}^{h}_{\varepsilon}(u^{n}_{\varepsilon}, v^{n}_{\varepsilon}) + k \sum_{m=1}^{n} \left(\varepsilon \|\nabla u^{m}_{\varepsilon}\|^{2}_{0} + \|(A_{h} - I)v^{m}_{\varepsilon}\|^{2}_{0} + \|\nabla v^{m}_{\varepsilon}\|^{2}_{0} \right) \leq \mathcal{E}^{h}_{\varepsilon}(u^{0}_{h}, v^{0}_{h}) \leq C_{0}.$$
(4.28)

Thus, from (4.18) and (4.28) we conclude (4.24). Moreover, adding (4.20) from $m = n_0 + 1$ to $m = n + n_0$, and using (4.14) and (4.24), we deduce (4.25). By other hand, if $\varepsilon \in (0, e^{-2})$, from (4.6)₂ and taking into account that $F_{\varepsilon}(s) \geq 0$ for all $s \in \mathbb{R}$, we have $\frac{1}{2\varepsilon}(u_{\varepsilon}^n(\boldsymbol{x}))^2 \leq F_{\varepsilon}(u_{\varepsilon}^n(\boldsymbol{x}))$ for all $u_{\varepsilon}^n \in U_h$; and therefore, using that $(\Pi^h(u))^2 \leq \Pi^h(u^2)$ for all $u \in C(\overline{\Omega})$, we have

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

where in the last inequality (4.24) was used. Thus, we obtain $(4.26)_1$. Finally, considering $u_{\varepsilon+}^n := \max\{u_{\varepsilon}^n, 0\} \ge 0$, taking into account that $u_{\varepsilon}^n = u_{\varepsilon+}^n + u_{\varepsilon-}^n$ and $|u_{\varepsilon}^n| = u_{\varepsilon+}^n - u_{\varepsilon-}^n = u_{\varepsilon}^n - 2u_{\varepsilon-}^n$, using the Hölder and Young inequalities as well as (4.16) and (4.26)₁, we have

$$\int_{\Omega} |u_{\varepsilon}^{n}| \leq \int_{\Omega} \Pi^{h} |u_{\varepsilon}^{n}| = \int_{\Omega} u_{\varepsilon}^{n} - 2 \int_{\Omega} \Pi^{h} (u_{\varepsilon-}^{n}) \leq m_{0} + C \Big(\int_{\Omega} (\Pi^{h} (u_{\varepsilon-}^{n}))^{2} \Big)^{1/2} \leq m_{0} + C \sqrt{\varepsilon},$$

which implies $(4.26)_2$.

Remark 4.3.9 The $l^{\infty}(L^1)$ -norm is the only norm in which u_{ε}^n is bounded independently of (k, h) and ε (see $(4.26)_2$). However, we can also obtain ε -dependent bounds for u_{ε}^n . In fact, from (4.6) 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 (4.24), implies that $(\sqrt{\varepsilon} u_{\varepsilon}^n)$ is bounded in $l^{\infty}(L^2) \cap l^2(H^1)$.

Remark 4.3.10 (Approximated positivity)

1. From $(4.26)_1$, the following estimate holds

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

2. Assuming V_h furnished by \mathbb{P}_1 -continuous FE and considering the following approximation for the v-equation:

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

$$(4.29)$$

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

$$\max_{n\geq 0} \|\Pi^h(v_{\varepsilon-}^n)\|_0^2 \le C\varepsilon \quad and \quad k\sum_{m=1}^n \|\Pi^h(v_{\varepsilon-}^n)\|_1^2 \le C\varepsilon(kn), \tag{4.30}$$

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 (4.29), taking into account that $(\nabla \Pi^h(v_{\varepsilon^+}^n), \nabla \Pi^h(v_{\varepsilon^-}^n)) \ge 0$ (owing to the interior angles of the triangles or tetrahedra are less than or equal to $\pi/2$), and using again that $(\Pi^h(v))^2 \le \Pi^h(v^2)$ for all $v \in C(\overline{\Omega})$, we have

$$\begin{split} \left(\frac{1}{k}+1\right) \|\Pi^{h}(v_{\varepsilon^{-}}^{n})\|_{0}^{2} + \|\nabla\Pi^{h}(v_{\varepsilon^{-}}^{n})\|_{0}^{2} &\leq \int_{\Omega} \Pi^{h} \left[\left(u_{\varepsilon}^{n}+\frac{1}{k}v_{\varepsilon}^{n-1}\right)v_{\varepsilon^{-}}^{n} \right] \\ &\leq \int_{\Omega} \Pi^{h} \left[\left(u_{\varepsilon^{-}}^{n}+\frac{1}{k}v_{\varepsilon^{-}}^{n-1}\right)v_{\varepsilon^{-}}^{n} \right] \\ &\leq \frac{1}{2} \left(\frac{1}{k}+1\right) \|\Pi^{h}(v_{\varepsilon^{-}}^{n})\|_{0}^{2} + \frac{1}{2} \|\Pi^{h}(u_{\varepsilon^{-}}^{n})\|_{0}^{2} + \frac{1}{2k} \|\Pi^{h}(v_{\varepsilon^{-}}^{n-1})\|_{0}^{2}, \end{split}$$

from which, using $(4.26)_1$, we arrive at

$$\frac{1}{2} \left(\frac{1}{k} + 1\right) \|\Pi^{h}(v_{\varepsilon^{-}}^{n})\|_{0}^{2} + \|\nabla\Pi^{h}(v_{\varepsilon^{-}}^{n})\|_{0}^{2} \le \frac{1}{2} C_{0}\varepsilon + \frac{1}{2k} \|\Pi^{h}(v_{\varepsilon^{-}}^{n-1})\|_{0}^{2}.$$
(4.31)

Therefore, if $v_h^0 \geq 0$ (which holds for instance by considering $v_h^0 = \widetilde{R}^h v_0$, where \widetilde{R}^h is an average interpolator of Clement or Scott-Zhang type, and using that $v_0 \geq 0$), using Lemma 4.2.1 in (4.31), we conclude (4.30)₁. Finally, multiplying (4.31) by k and adding from m = 1 to m = n, and using again that $v_h^0 \geq 0$, we arrive at (4.30)₂.

4.3.2 Well-posedness

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

Theorem 4.3.11 (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 $R: U_h \times V_h \to U_h \times V_h$ by $R(\tilde{u}, \tilde{v}) = (u, v)$, such that $(u, v) \in U_h \times V_h$ solves the following linear decoupled problem

$$u \in U_h \quad \text{s.t.} \quad \frac{1}{k} (u, \bar{u})^h + (\nabla u, \nabla \bar{u}) = \frac{1}{k} (u_{\varepsilon}^{n-1}, \bar{u})^h - (\Lambda_{\varepsilon}(\tilde{u}) \nabla \tilde{v}, \nabla \bar{u}), \quad \forall \bar{u} \in U_h,$$
(4.32)

$$v \in V_h$$
 s.t. $\frac{1}{k}(v,\bar{v}) + (A_h v,\bar{v}) = \frac{1}{k}(v_{\varepsilon}^{n-1},\bar{v}) + (\tilde{u},\bar{v}), \quad \forall \bar{v} \in V_h.$ (4.33)

- 1. *R* is well defined. Applying the Lax-Milgram theorem to (4.32) and (4.33), 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 (4.32)-(4.33).
- 2. Let us now prove that all possible fixed points of λR (with $\lambda \in (0, 1]$) are bounded. In fact, observe that if (u, v) is a fixed point of λR , then $R(u, v) = (\frac{1}{\lambda}u, \frac{1}{\lambda}v)$, and therefore (u, v) satisfies the coupled system

$$\begin{cases}
\frac{1}{k}(u,\bar{u})^{h} + (\nabla u,\nabla\bar{u}) + \lambda(\Lambda_{\varepsilon}(u)\nabla v,\nabla\bar{u}) = \frac{\lambda}{k}(u_{\varepsilon}^{n-1},\bar{u})^{h}, \quad \forall \bar{u} \in U_{h}, \\
\frac{1}{k}(v,\bar{v}) + (A_{h}v,\bar{v}) - \lambda(u,\bar{v}) = \frac{\lambda}{k}(v_{\varepsilon}^{n-1},\bar{v}), \quad \forall \bar{v} \in V_{h}.
\end{cases}$$
(4.34)

Then, testing $(4.34)_1$ and $(4.34)_2$ by $\bar{u} = \Pi^h(F'_{\varepsilon}(u))$ and $\bar{v} = (A_h - I)v$ respectively, proceeding as in Theorem 4.3.7 and taking into account that $\lambda \in (0, 1]$, we obtain

$$(F_{\varepsilon}(u),1)^{h} + \frac{1}{2} \|\nabla v\|_{0}^{2} + k \left(\varepsilon \|\nabla u\|_{0}^{2} + \|(A_{h} - I)v\|_{0}^{2} + \|\nabla v\|_{0}^{2}\right)$$

$$\leq (F_{\varepsilon}(\lambda u_{\varepsilon}^{n-1}),1)^{h} + \frac{\lambda^{2}}{2} \|\nabla v_{\varepsilon}^{n-1}\|_{0}^{2} \leq C(u_{\varepsilon}^{n-1},v_{\varepsilon}^{n-1}),(4.35)$$

where the last estimate is λ -independent (arguing as in (4.27)). Moreover, proceeding as in Lemma 4.3.5 and Corollary 4.3.8 (taking into account (4.35)), 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 λ and h.

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

 $(\widetilde{u}^l, \widetilde{v}^l) \to (\widetilde{u}, \widetilde{v}) \text{ in } U_h \times V_h \text{ as } l \to +\infty.$ (4.36)

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

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

where in the first inequality (4.11) 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 $\{R(\tilde{u}^l, \tilde{\boldsymbol{\sigma}}^l)\}_{l \in \mathbb{N}}$, still denoted by $\{R(\tilde{u}^l, \tilde{\boldsymbol{\sigma}}^l)\}_{l \in \mathbb{N}}$, such that

$$R(\widetilde{u}^l, \widetilde{v}^l) \to (u', v') \quad \text{in } W^{1,\infty}(\Omega)^2, \quad \text{as } l \to +\infty.$$
 (4.37)

Then, from (4.36)-(4.37) and using Lemma 4.3.4, a standard procedure allows us to pass to the limit, as l goes to $+\infty$, in (4.32)-(4.33) (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 $R(\tilde{u}^l, \tilde{v}^l) \to R(\tilde{u}, \tilde{v})$ 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**.

Lemma 4.3.12 (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 $(\bar{u}, \bar{v}) \in U_h \times V_h$,

$$\frac{1}{k}(u,\bar{u})^{h} + (\nabla u,\nabla\bar{u}) + (\Lambda_{\varepsilon}(u_{\varepsilon}^{n,1})\nabla v,\nabla\bar{u}) + ((\Lambda_{\varepsilon}(u_{\varepsilon}^{n,1}) - \Lambda_{\varepsilon}(u_{\varepsilon}^{n,2}))\nabla v_{\varepsilon}^{n,2},\nabla\bar{u}) = 0, \quad (4.38)$$

$$\frac{1}{k}(v,\bar{v}) + (A_h v,\bar{v}) = (u,\bar{v}).$$
(4.39)

Taking $\bar{u} = u$, $\bar{v} = A_h v$ in (4.38)-(4.39), 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 4.3.3, we obtain

$$\frac{1}{k} \|(u, \nabla v)\|_{0}^{2} + \|(u, A_{h}v)\|_{H^{1} \times L^{2}}^{2} \leq \|u\|_{0} \|A_{h}v\|_{0} \\
+ \|\Lambda_{\varepsilon}(u_{\varepsilon}^{n,1})\|_{L^{6}} \|\nabla v\|_{L^{3}} \|\nabla u\|_{0} + \|\Lambda_{\varepsilon}(u_{\varepsilon}^{n,1}) - \Lambda_{\varepsilon}(u_{\varepsilon}^{n,2})\|_{L^{\infty}} \|\nabla v_{\varepsilon}^{n,2}\|_{0} \|\nabla u\|_{0} \\
\leq \frac{1}{4} \|A_{h}v\|_{0} + \|u\|_{0}^{2} + \frac{1}{4} \|\nabla u\|_{0}^{2} + \frac{1}{4} \|A_{h}v\|_{0}^{2} + C \|\Lambda_{\varepsilon}(u_{\varepsilon}^{n,1})\|_{L^{6}}^{4} \|\nabla v\|_{0}^{2} \\
+ \frac{1}{4} \|\nabla u\|_{0}^{2} + \|\Lambda_{\varepsilon}(u_{\varepsilon}^{n,1}) - \Lambda_{\varepsilon}(u_{\varepsilon}^{n,2})\|_{L^{\infty}}^{2} \|\nabla v_{\varepsilon}^{n,2}\|_{0}^{2}.$$

Then, taking into account (4.11), (4.13), (4.24), (4.26)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

$$\begin{aligned} \|(u,\nabla v)\|_{0}^{2} &+ \frac{k}{2} \|(u,A_{h}v)\|_{H^{1}\times L^{2}}^{2} \leq k \left(1 + C \|\Lambda_{\varepsilon}(u_{\varepsilon}^{n,1})\|_{L^{6}}^{4}\right) \|(u,\nabla v)\|_{0}^{2} + kC_{0}C\varepsilon^{-2}\|u\|_{L^{\infty}}^{2} \\ &\leq k \left(1 + C_{1}(h)^{2}(1 + C_{2}(h))^{4/r} + kC_{0}C_{3}(h)\varepsilon^{-2}\right) \|(u,\nabla v)\|_{0}^{2} := k g(h,\varepsilon) \|(u,\nabla v)\|_{0}^{2}. \end{aligned}$$

Therefore, if $k g(h, \varepsilon) < 1$, we conclude that u = 0, and therefore (from (4.39)) v = 0.

4.4 Scheme US

In this section, we propose another energy-stable nonlinear fully discrete scheme associated to model (4.1), which is obtained by introducing the auxiliary variable $\boldsymbol{\sigma} = \nabla v$. In fact, taking into account the functions λ_{ε} and F_{ε} and its derivatives (given in (4.4)-(4.5)), another regularized version of problem (4.1) reads: Find $u_{\varepsilon} : \Omega \times [0, T] \to \mathbb{R}$ and $\boldsymbol{\sigma}_{\varepsilon} : \Omega \times [0, T] \to \mathbb{R}^d$ such that

$$\begin{cases} \partial_t u_{\varepsilon} - \nabla \cdot (\lambda_{\varepsilon}(u_{\varepsilon})\nabla(F'_{\varepsilon}(u_{\varepsilon}))) - \nabla \cdot (u_{\varepsilon}\boldsymbol{\sigma}_{\varepsilon}) = 0 \text{ in } \Omega, \ t > 0, \\ \partial_t \boldsymbol{\sigma}_{\varepsilon} + \operatorname{rot}(\operatorname{rot} \boldsymbol{\sigma}_{\varepsilon}) - \nabla(\nabla \cdot \boldsymbol{\sigma}_{\varepsilon}) + \boldsymbol{\sigma}_{\varepsilon} = u_{\varepsilon}\nabla(F'_{\varepsilon}(u_{\varepsilon})) \text{ in } \Omega, \ t > 0, \\ \frac{\partial u_{\varepsilon}}{\partial \mathbf{n}} = 0 \text{ on } \partial\Omega, \ t > 0, \\ \boldsymbol{\sigma}_{\varepsilon} \cdot \mathbf{n} = 0, \ [\operatorname{rot} \boldsymbol{\sigma}_{\varepsilon} \times \mathbf{n}]_{tang} = 0 \text{ on } \partial\Omega, \ t > 0, \\ u_{\varepsilon}(\boldsymbol{x}, 0) = u_0(\boldsymbol{x}) \ge 0, \ \boldsymbol{\sigma}_{\varepsilon}(\boldsymbol{x}, 0) = \nabla v_0(\boldsymbol{x}), \quad \operatorname{in } \Omega. \end{cases}$$
(4.40)

This kind of formulation considering $\boldsymbol{\sigma} = \nabla v$ as auxiliary variable has been used in the construction of numerical schemes for other chemotaxis models (see for instance [17] and

Chapter 2 of this PhD thesis). Once problem (4.40) is solved, we can recover v_{ε} from u_{ε} solving

$$\begin{cases} \partial_t v_{\varepsilon} - \Delta v_{\varepsilon} + v_{\varepsilon} = u_{\varepsilon} & \text{in } \Omega, \ t > 0, \\ \frac{\partial v_{\varepsilon}}{\partial \mathbf{n}} = 0 & \text{on } \partial \Omega, \ t > 0, \\ v_{\varepsilon}(\boldsymbol{x}, 0) = v_0(\boldsymbol{x}) \ge 0 & \text{in } \Omega. \end{cases}$$
(4.41)

Observe that multiplying $(4.40)_1$ by $F'_{\varepsilon}(u_{\varepsilon})$, $(4.40)_2$ by $\boldsymbol{\sigma}_{\varepsilon}$, and integrating over Ω , we obtain the following energy law

$$\frac{d}{dt}\int_{\Omega}\left(F_{\varepsilon}(u_{\varepsilon})+\frac{1}{2}|\boldsymbol{\sigma}_{\varepsilon}|^{2}\right)d\boldsymbol{x}+\int_{\Omega}\lambda_{\varepsilon}(u_{\varepsilon})|\nabla(F_{\varepsilon}'(u_{\varepsilon}))|^{2}d\boldsymbol{x}+\|\boldsymbol{\sigma}_{\varepsilon}\|_{1}^{2}=0.$$

In particular, the modified energy

$$\mathcal{E}_{\varepsilon}(u, \boldsymbol{\sigma}) = \int_{\Omega} \Big(F_{\varepsilon}(u) + \frac{1}{2} |\boldsymbol{\sigma}|^2 \Big) d\boldsymbol{x}$$

is decreasing in time. Then, we consider a fully discrete approximation of the regularized problem (4.40) using a 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-angles simplices. We choose the following continuous FE spaces for u_{ε} , $\boldsymbol{\sigma}_{\varepsilon}$, and v_{ε} :

$$(U_h, \Sigma_h, V_h) \subset H^1(\Omega)^3$$
, generated by $\mathbb{P}_1, \mathbb{P}_m, \mathbb{P}_r$ with $m, r \geq 1$.

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

• <u>Scheme</u> **US**:

Initialization: Let $(u_h^0, \boldsymbol{\sigma}_h^0) = (Q^h u_0, \widetilde{Q}^h(\nabla v_0)) \in U_h \times \boldsymbol{\Sigma}_h$. **Time step** n: Given $(u_{\varepsilon}^{n-1}, \boldsymbol{\sigma}_{\varepsilon}^{n-1}) \in U_h \times \boldsymbol{\Sigma}_h$, compute $(u_{\varepsilon}^n, \boldsymbol{\sigma}_{\varepsilon}^n) \in U_h \times \boldsymbol{\Sigma}_h$ solving

$$\begin{cases} (\delta_t u_{\varepsilon}^n, \bar{u})^h + (\lambda_{\varepsilon}(u_{\varepsilon}^n) \nabla \Pi^h(F_{\varepsilon}'(u_{\varepsilon}^n)), \nabla \bar{u}) = -(\lambda_{\varepsilon}(u_{\varepsilon}^n) \boldsymbol{\sigma}_{\varepsilon}^n, \nabla \bar{u}), & \forall \bar{u} \in U_h, \\ (\delta_t \boldsymbol{\sigma}_{\varepsilon}^n, \bar{\boldsymbol{\sigma}}) + (B_h \boldsymbol{\sigma}_{\varepsilon}^n, \bar{\boldsymbol{\sigma}}) = (\lambda_{\varepsilon}(u_{\varepsilon}^n) \nabla \Pi^h(F_{\varepsilon}'(u_{\varepsilon}^n)), \bar{\boldsymbol{\sigma}}), & \forall \bar{\boldsymbol{\sigma}} \in \Sigma_h, \end{cases}$$
(4.42)

where Q^h is the L^2 -projection on U_h defined in (4.9), \tilde{Q}^h is the standard L^2 -projection on Σ_h , and the operator B_h is defined as

$$(B_h\boldsymbol{\sigma}_{\varepsilon}^n,\bar{\boldsymbol{\sigma}})=(\operatorname{rot}\,\boldsymbol{\sigma}_{\varepsilon}^n,\operatorname{rot}\,\bar{\boldsymbol{\sigma}})+(\nabla\cdot\boldsymbol{\sigma}_{\varepsilon}^n,\nabla\cdot\bar{\boldsymbol{\sigma}})+(\boldsymbol{\sigma}_{\varepsilon}^n,\bar{\boldsymbol{\sigma}}).$$

We recall that $\Pi^h : C(\overline{\Omega}) \to U_h$ is the Lagrange interpolation operator, and the discrete semiinner product $(\cdot, \cdot)^h$ was defined in (4.8). 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:

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

$$(4.43)$$

Given $u_{\varepsilon}^{n} \in U_{h}$ and $v_{\varepsilon}^{n-1} \in V_{h}$, Lax-Milgram theorem implies that there exists a unique $v_{\varepsilon}^{n} \in V_{h}$ solution of (4.43). The solvability of (4.42) will be proved in Subsection 4.4.2.

4.4.1 Mass conservation and Energy-stability

Observe that the scheme **US** is also conservative in u (satisfying (4.16)) and also has the behavior for $\int_{\Omega} v_n$ given in (4.17).

Definition 4.4.1 A numerical scheme with solution $(u_{\varepsilon}^n, \sigma_{\varepsilon}^n)$ is called energy-stable with respect to the energy

$$\mathcal{E}^{h}_{\varepsilon}(u,\boldsymbol{\sigma}) = (F_{\varepsilon}(u),1)^{h} + \frac{1}{2} \|\boldsymbol{\sigma}\|_{0}^{2}$$
(4.44)

if this energy is time decreasing, that is, $\mathcal{E}^h_{\varepsilon}(u^n_{\varepsilon}, \boldsymbol{\sigma}^n_{\varepsilon}) \leq \mathcal{E}^h_{\varepsilon}(u^{n-1}_{\varepsilon}, \boldsymbol{\sigma}^{n-1}_{\varepsilon})$ for all $n \geq 1$.

Theorem 4.4.2 (Unconditional stability) The scheme **US** is unconditional energy stable with respect to $\mathcal{E}^h_{\varepsilon}(u, \boldsymbol{\sigma})$. In fact, if $(u^n_{\varepsilon}, \boldsymbol{\sigma}^n_{\varepsilon})$ is a solution of **US**, then the following discrete energy law holds

$$\delta_t \mathcal{E}^h_{\varepsilon}(u^n_{\varepsilon}, \boldsymbol{\sigma}^n_{\varepsilon}) + \varepsilon \frac{k}{2} \|\delta_t u^n_{\varepsilon}\|_0^2 + \frac{k}{2} \|\delta_t \boldsymbol{\sigma}^n_{\varepsilon}\|_0^2 + \int_{\Omega} \lambda_{\varepsilon}(u^n_{\varepsilon}) |\nabla \Pi^h(F'_{\varepsilon}(u^n_{\varepsilon}))|^2 d\boldsymbol{x} + \|\boldsymbol{\sigma}^n_{\varepsilon}\|_1^2 \le 0.$$
(4.45)

Proof. Testing $(4.42)_1$ by $\bar{u} = \Pi^h(F'_{\varepsilon}(u^n_{\varepsilon}))$, $(4.42)_2$ by $\bar{\boldsymbol{\sigma}} = \boldsymbol{\sigma}^n_{\varepsilon}$ and adding, the terms $(\lambda_{\varepsilon}(u^n_{\varepsilon})\nabla\Pi^h(F'_{\varepsilon}(u_{\varepsilon})), \boldsymbol{\sigma}^n_{\varepsilon})$ cancel, and we obtain

$$(\delta_t u_{\varepsilon}^n, \Pi^h(F_{\varepsilon}'(u_{\varepsilon}^n)))^h + \int_{\Omega} \lambda_{\varepsilon}(u_{\varepsilon}^n) |\nabla \Pi^h(F_{\varepsilon}'(u_{\varepsilon}^n))|^2 d\boldsymbol{x} + \delta_t \left(\frac{1}{2} \|\boldsymbol{\sigma}_{\varepsilon}^n\|_0^2\right) + \frac{k}{2} \|\delta_t \boldsymbol{\sigma}_{\varepsilon}^n\|_0^2 + \|\boldsymbol{\sigma}_{\varepsilon}^n\|_1^2 = 0,$$

which, proceeding as in (4.22)-(4.23) and using Remark 4.3.3, implies (4.45).

Corollary 4.4.3 (Uniform estimates) Assume that $(u_0, v_0) \in L^2(\Omega) \times H^1(\Omega)$. Let $(u_{\varepsilon}^n, \boldsymbol{\sigma}_{\varepsilon}^n)$ be a solution of scheme **US**. Then, it holds

$$(F_{\varepsilon}(u_{\varepsilon}^{n}),1)^{h} + \|\boldsymbol{\sigma}_{\varepsilon}^{n}\|_{0}^{2} + k \sum_{m=1}^{n} \left(\varepsilon \|\nabla \Pi^{h}(F_{\varepsilon}'(u_{\varepsilon}^{m}))\|_{0}^{2} + \|\boldsymbol{\sigma}_{\varepsilon}^{m}\|_{1}^{2}\right) \le C_{0}, \quad \forall n \ge 1,$$

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 (4.26) hold. *Proof.* Proceeding as in (4.27) (using the fact that $(u_h^0, \boldsymbol{\sigma}_h^0) = (Q^h u_0, \widetilde{Q}^h(\nabla v_0)))$, we can deduce that

$$(F_{\varepsilon}(u_h^0), 1)^h + \|\boldsymbol{\sigma}_h^0\|_0^2 \le C_0, \tag{4.46}$$

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 (4.45) and estimate (4.46), we have

$$(F_{\varepsilon}(u_{\varepsilon}^{n}),1)^{h} + \|\boldsymbol{\sigma}_{\varepsilon}^{n}\|_{0}^{2} + k\sum_{m=1}^{n} \left(\varepsilon \|\nabla\Pi^{h}(F_{\varepsilon}'(u_{\varepsilon}^{m}))\|_{0}^{2} + \|\boldsymbol{\sigma}_{\varepsilon}^{m}\|_{1}^{2}\right) \leq (F_{\varepsilon}(u_{h}^{0}),1)^{h} + \|\boldsymbol{\sigma}_{h}^{0}\|_{0}^{2} \leq C_{0}.$$

Finally, the estimates given in (4.26) are proved as in Corollary 4.3.8.

Remark 4.4.4 The conclusions obtained in Remark 4.3.9 and the approximated positivity results established in Remark 4.3.10 remain true for the scheme US.

4.4.2 Well-posedness

Theorem 4.4.5 (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 $(u_{\varepsilon}^{n-1}, \boldsymbol{\sigma}_{\varepsilon}^{n-1}) \in U_h \times \boldsymbol{\Sigma}_h$, we define the operator $R: U_h \times \boldsymbol{\Sigma}_h \to U_h \times \boldsymbol{\Sigma}_h$ by $R(\tilde{u}, \tilde{\boldsymbol{\sigma}}) = (u, \boldsymbol{\sigma})$, such that $(u, \boldsymbol{\sigma}) \in U_h \times \boldsymbol{\Sigma}_h$ solves the following linear decoupled problem

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

$$(4.47)$$

$$\boldsymbol{\sigma} \in \boldsymbol{\Sigma}_h \text{ s.t. } \frac{1}{k} (\boldsymbol{\sigma}, \bar{\boldsymbol{\sigma}}) + (B_h \boldsymbol{\sigma}, \bar{\boldsymbol{\sigma}}) = \frac{1}{k} (\boldsymbol{\sigma}_{\varepsilon}^{n-1}, \bar{\boldsymbol{\sigma}}) + (\lambda_{\varepsilon}(\tilde{u}) \nabla \Pi^h(F_{\varepsilon}'(\tilde{u})), \bar{\boldsymbol{\sigma}}), \quad \forall \bar{\boldsymbol{\sigma}} \in \boldsymbol{\Sigma}_h.$$
(4.48)

- 1. *R* is well defined. Applying the Lax-Milgram theorem to (4.47) and (4.48), 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 (4.47)-(4.48).
- 2. Let us now prove that all possible fixed points of λR (with $\lambda \in (0, 1]$) are bounded. In fact, observe that if (u, σ) is a fixed point of λR , then (u, σ) satisfies the coupled system

$$\begin{cases} \frac{1}{k}(u,\bar{u})^{h} + \lambda(\lambda_{\varepsilon}(u)\nabla\Pi^{h}(F_{\varepsilon}'(u)),\nabla\bar{u}) + \lambda(\lambda_{\varepsilon}(u)\boldsymbol{\sigma},\nabla\bar{u}) = \frac{\lambda}{k}(u_{\varepsilon}^{n-1},\bar{u})^{h}, \quad \forall\bar{u}\in U_{h},\\ \frac{1}{k}(\boldsymbol{\sigma},\bar{\boldsymbol{\sigma}}) + (B_{h}\boldsymbol{\sigma},\bar{\boldsymbol{\sigma}}) - \lambda(\lambda_{\varepsilon}(u)\nabla\Pi^{h}(F_{\varepsilon}'(u)),\bar{\boldsymbol{\sigma}}) = \frac{\lambda}{k}(\boldsymbol{\sigma}_{\varepsilon}^{n-1},\bar{\boldsymbol{\sigma}}), \quad \forall\bar{\boldsymbol{\sigma}}\in\boldsymbol{\Sigma}_{h}. \end{cases}$$

$$(4.49)$$

Then, testing $(4.49)_1$ and $(4.49)_2$ by $\bar{u} = \Pi^h(F'_{\varepsilon}(u)) \in U_h$ and $\bar{\sigma} = \sigma \in \Sigma_h$ respectively, proceeding as in Theorem 4.4.2 and taking into account that $\lambda \in (0, 1]$, we obtain

$$(F_{\varepsilon}(u),1)^{h} + \frac{1}{2} \|\boldsymbol{\sigma}\|_{0}^{2} + k \left(\varepsilon \lambda \|\nabla \Pi^{h}(F_{\varepsilon}'(u))\|_{0}^{2} + \|\boldsymbol{\sigma}\|_{1}^{2}\right)$$

$$\leq (F_{\varepsilon}(\lambda u_{\varepsilon}^{n-1}),1)^{h} + \frac{\lambda^{2}}{2} \|\boldsymbol{\sigma}_{\varepsilon}^{n-1}\|_{0}^{2} \leq C(u_{\varepsilon}^{n-1},\boldsymbol{\sigma}_{\varepsilon}^{n-1}), \quad (4.50)$$

which implies $\|\boldsymbol{\sigma}\|_1 \leq C$ (with the constant C > 0 independent of λ). Moreover, proceeding as in the proof of (4.26) (using (4.50)) we deduce $\|u\|_{L^1} \leq C$, where the constant C depends on data $(\Omega, u_{\varepsilon}^{n-1}, \boldsymbol{\sigma}_{\varepsilon}^{n-1}, \varepsilon)$.

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

$$(\widetilde{u}^l, \widetilde{\boldsymbol{\sigma}}^l) \to (\widetilde{u}, \widetilde{\boldsymbol{\sigma}}) \text{ in } U_h \times \boldsymbol{\Sigma}_h \text{ as } l \to +\infty.$$
 (4.51)

In particular, $\{(\widetilde{u}^l, \widetilde{\boldsymbol{\sigma}}^l)\}_{l \in \mathbb{N}}$ is bounded in $W^{1,\infty}(\Omega) \times \boldsymbol{W}^{1,\infty}(\Omega)$. Observe that from (4.51), we have that for h fixed, $\widetilde{u}^l \to \widetilde{u}$ in $C(\overline{\Omega})$; and thus, $F'_{\varepsilon}(\widetilde{u}^l) \to F'_{\varepsilon}(\widetilde{u})$ in $C(\overline{\Omega})$ since F'_{ε} is a Lipschitz continuous function. Then, the linearity and continuity of Π^h with respect to $C^0(\overline{\Omega})$ -norm imply that $\Pi^h(F'_{\varepsilon}(\widetilde{u}^l)) \to \Pi^h(F'_{\varepsilon}(\widetilde{u}))$ in $C(\overline{\Omega})$. Moreover, if we denote $(u^l, \boldsymbol{\sigma}^l) = R(\widetilde{u}^l, \widetilde{\boldsymbol{\sigma}}^l)$, we can deduce (recall that $\varepsilon \leq \lambda_{\varepsilon}(s) \leq \varepsilon^{-1}$ for all $s \in \mathbb{R}$)

$$\frac{1}{2k} \| (u^l, \boldsymbol{\sigma}^l) \|_0^2 + \frac{1}{2} \| \boldsymbol{\sigma}^l \|_1^2 \le \frac{1}{2k} \| (u_{\varepsilon}^{n-1}, \boldsymbol{\sigma}_{\varepsilon}^{n-1}) \|_0^2 + C(h, k) \varepsilon^{-2} \| \widetilde{\boldsymbol{\sigma}}^l \|_{L^6}^2 + C \varepsilon^{-2} \| \nabla \Pi^h (F'_{\varepsilon}(\widetilde{u}^l)) \|_0^2 + C(h, k) \varepsilon^{-2} \| \nabla \Pi^h (F'_{\varepsilon}(\widetilde{u}^l)) \|_0^2 \le C,$$

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

$$R(\widetilde{u}^l, \widetilde{\boldsymbol{\sigma}}^l) \to (u', \boldsymbol{\sigma}') \quad \text{in } W^{1,\infty}(\Omega) \times \boldsymbol{W}^{1,\infty}(\Omega).$$
 (4.52)

Then, from (4.51)-(4.52), a standard procedure allows us to pass to the limit, as l goes to $+\infty$, in (4.47)-(4.48) (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 $R(\tilde{u}^l, \tilde{\sigma}^l) \to R(\tilde{u}, \tilde{\sigma})$ 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 \mathbf{US} .

Lemma 4.4.6 (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

$$\frac{1}{k}(u,\bar{u})^{h} + (\lambda_{\varepsilon}(u_{\varepsilon}^{n,1})\nabla\Pi^{h}(F_{\varepsilon}'(u_{\varepsilon}^{n,1}) - F_{\varepsilon}'(u_{\varepsilon}^{n,2})),\nabla\bar{u}) + ((\lambda_{\varepsilon}(u_{\varepsilon}^{n,1}) - \lambda_{\varepsilon}(u_{\varepsilon}^{n,2}))\nabla\Pi^{h}F_{\varepsilon}'(u_{\varepsilon}^{n,2}),\nabla\bar{u}) + (\lambda_{\varepsilon}(u_{\varepsilon}^{n,1}) - \lambda_{\varepsilon}(u_{\varepsilon}^{n,2}))\boldsymbol{\sigma}_{\varepsilon}^{n,2},\nabla\bar{u}) = 0, \ \forall\bar{u} \in U_{h},$$
(4.53)

$$\frac{1}{k}(\boldsymbol{\sigma}, \bar{\boldsymbol{\sigma}}) + (B_h \boldsymbol{\sigma}, \bar{\boldsymbol{\sigma}}) = (\lambda_{\varepsilon}(u_{\varepsilon}^{n,1}) \nabla \Pi^h(F_{\varepsilon}'(u_{\varepsilon}^{n,1}) - F_{\varepsilon}'(u_{\varepsilon}^{n,2})), \bar{\boldsymbol{\sigma}}) \\
+ ((\lambda_{\varepsilon}(u_{\varepsilon}^{n,1}) - \lambda_{\varepsilon}(u_{\varepsilon}^{n,2})) \nabla \Pi^h F_{\varepsilon}'(u_{\varepsilon}^{n,2}), \bar{\boldsymbol{\sigma}}), \quad \forall \bar{\boldsymbol{\sigma}} \in \boldsymbol{\Sigma}_h.$$
(4.54)

Taking $\bar{u} = u$, $\bar{\sigma} = \sigma$ in (4.53)-(4.54), adding the resulting expressions and using the fact that $\int_{\Omega} u = 0$ as well as Remark 4.3.3, estimates in Corollary 4.4.3 and some inverse inequalities, we obtain

$$\begin{aligned} \frac{1}{k} \|(u, \boldsymbol{\sigma})\|_{0}^{2} + \|\boldsymbol{\sigma}\|_{1}^{2} &\leq \|\lambda_{\varepsilon}(u_{\varepsilon}^{n,1})\|_{L^{\infty}} \|\nabla\Pi^{h}(F_{\varepsilon}'(u_{\varepsilon}^{n,1}) - F_{\varepsilon}'(u_{\varepsilon}^{n,2}))\|_{0} \|\nabla u\|_{0} \\ &+ \|\lambda_{\varepsilon}(u_{\varepsilon}^{n,1}) - \lambda_{\varepsilon}(u_{\varepsilon}^{n,2})\|_{L^{\infty}} \|\nabla\Pi^{h}F_{\varepsilon}'(u_{\varepsilon}^{n,2})\|_{0} \|\nabla u\|_{0} + \|\lambda_{\varepsilon}(u_{\varepsilon}^{n,1})\|_{L^{\infty}} \|\boldsymbol{\sigma}\|_{0} \|\nabla u\|_{0} \\ &+ \|\lambda_{\varepsilon}(u_{\varepsilon}^{n,1}) - \lambda_{\varepsilon}(u_{\varepsilon}^{n,2})\|_{L^{\infty}} \|\boldsymbol{\sigma}_{\varepsilon}^{n,2}\|_{0} \|\nabla u\|_{0} + \|\lambda_{\varepsilon}(u_{\varepsilon}^{n,1})\|_{L^{\infty}} \|\nabla\Pi^{h}(F_{\varepsilon}'(u_{\varepsilon}^{n,1}) - F_{\varepsilon}'(u_{\varepsilon}^{n,2}))\|_{0} \|\boldsymbol{\sigma}\|_{0} \\ &+ \|\lambda_{\varepsilon}(u_{\varepsilon}^{n,1}) - \lambda_{\varepsilon}(u_{\varepsilon}^{n,2})\|_{L^{3}} \|\nabla\Pi^{h}F_{\varepsilon}'(u_{\varepsilon}^{n,2})\|_{0} \|\boldsymbol{\sigma}\|_{L^{6}} \\ &\leq \varepsilon^{-2}C(h)\|u\|_{0}^{2} + \varepsilon^{-1}C(h)\|u\|_{0}^{2} + \frac{1}{6}\|\boldsymbol{\sigma}\|_{0} + \varepsilon^{-2}C(h)\|u\|_{0}^{2} + C_{0}C(h)\|u\|_{0}^{2} \\ &+ \frac{1}{6}\|\boldsymbol{\sigma}\|_{0} + \varepsilon^{-4}C(h)\|u\|_{0}^{2} + \frac{1}{6}\|\boldsymbol{\sigma}\|_{1} + \varepsilon^{-2}C(h)\|u\|_{0}^{2}, \end{aligned}$$

and therefore,

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

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

4.5 Scheme UZSW

In this section, we propose an energy-stable linear fully discrete scheme associated to model (4.1). With this aim, we introduce the new variables

$$z_{\varepsilon} = F'_{\varepsilon}(u_{\varepsilon}), \ \boldsymbol{\sigma}_{\varepsilon} = \nabla v_{\varepsilon} \text{ and } w_{\varepsilon} = \sqrt{F_{\varepsilon}(u_{\varepsilon}) + A}, \text{ with } (A > 0).$$

Then, a regularized version of problem (4.1) in the variables $(u_{\varepsilon}, z_{\varepsilon}, \boldsymbol{\sigma}_{\varepsilon}, w_{\varepsilon})$ is the following:

$$\begin{aligned}
& (\partial_t u_{\varepsilon} - \nabla \cdot (\lambda_{\varepsilon}(u_{\varepsilon}) \nabla z_{\varepsilon}) - \nabla \cdot (u_{\varepsilon} \boldsymbol{\sigma}_{\varepsilon}) = 0 \text{ in } \Omega, \ t > 0, \\
& (\partial_t \boldsymbol{\sigma}_{\varepsilon} + \operatorname{rot}(\operatorname{rot} \boldsymbol{\sigma}_{\varepsilon}) - \nabla (\nabla \cdot \boldsymbol{\sigma}_{\varepsilon}) + \boldsymbol{\sigma}_{\varepsilon} = u_{\varepsilon} \nabla z_{\varepsilon} \quad \text{in } \Omega, \ t > 0, \\
& (\partial_t w_{\varepsilon} = \frac{1}{2\sqrt{F_{\varepsilon}(u_{\varepsilon}) + A}} F_{\varepsilon}'(u_{\varepsilon}) \partial_t u_{\varepsilon} \quad \text{in } \Omega, \ t > 0, \\
& z_{\varepsilon} = \frac{1}{\sqrt{F_{\varepsilon}(u_{\varepsilon}) + A}} F_{\varepsilon}'(u_{\varepsilon}) w_{\varepsilon} \quad \text{in } \Omega, \ t > 0, \\
& \frac{\partial z_{\varepsilon}}{\partial \mathbf{n}} = 0 \quad \text{on } \partial\Omega, \ t > 0, \\
& \boldsymbol{\sigma}_{\varepsilon} \cdot \mathbf{n} = 0, \quad [\operatorname{rot} \boldsymbol{\sigma}_{\varepsilon} \times \mathbf{n}]_{tang} = 0 \quad \text{on } \partial\Omega, \ t > 0, \\
& u_{\varepsilon}(\boldsymbol{x}, 0) = u_{0}(\boldsymbol{x}) \ge 0, \ \boldsymbol{\sigma}_{\varepsilon}(\boldsymbol{x}, 0) = \nabla v_{0}(\boldsymbol{x}), \ w_{\varepsilon}(\boldsymbol{x}, 0) = \sqrt{F_{\varepsilon}(u_{0}(\boldsymbol{x})) + A} \quad \text{in } \Omega,
\end{aligned}$$
(4.55)

for all constant A > 0.

Remark 4.5.1 Notice that problems (4.40) and (4.55) are equivalents for all A > 0. In fact, if $(u_{\varepsilon}, \sigma_{\varepsilon})$ is a solution of the scheme **US**, then defining $z_{\varepsilon} = F'_{\varepsilon}(u_{\varepsilon})$ and $w_{\varepsilon} = \sqrt{F_{\varepsilon}(u_{\varepsilon}) + A}$, 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

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

and $(4.55)_4$, we deduce that $z_{\varepsilon} = F'_{\varepsilon}(u_{\varepsilon})$, and therefore, $(u_{\varepsilon}, \boldsymbol{\sigma}_{\varepsilon})$ is a solution of (4.40).

As in the previous section, once solved (4.55), we can recover v_{ε} from u_{ε} solving (4.41). Observe that multiplying (4.55)₁ by z_{ε} , (4.55)₂ by σ_{ε} , (4.55)₃ by $2w_{\varepsilon}$, (4.55)₄ by $\partial_t u_{\varepsilon}$, integrating over Ω and using the boundary conditions of (4.55), we obtain the following energy law

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

In particular, the modified energy

$$\mathcal{E}(w, \boldsymbol{\sigma}) = \int_{\Omega} \left(|w|^2 + \frac{1}{2} |\boldsymbol{\sigma}|^2 \right) d\boldsymbol{x}$$

is decreasing in time. Then, we consider a fully discrete approximation of the regularized problem (4.55) using a 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-angles simplices is not imposed), and we choose the following continuous FE spaces for $u_{\varepsilon}, z_{\varepsilon}, \sigma_{\varepsilon}, w_{\varepsilon}$ and v_{ε} :

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

Remark 4.5.2 The constraint $k \leq l$ implies $U_h \subseteq Z_h$ which will be used to prove the wellposedness of the scheme **UZSW** (see Theorem 4.5.6 below).

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

• <u>Scheme UZSW:</u>

Initialization: Let $(u_h^0, \boldsymbol{\sigma}_h^0, w_{h,\varepsilon}^0) = (Q^h u_0, \widetilde{Q}^h(\nabla v_0), \widehat{Q}^h(\sqrt{F_{\varepsilon}(u_0) + A})) \in U_h \times \Sigma_h \times W_h.$

Time step n: Given $(u_{\varepsilon}^{n-1}, \boldsymbol{\sigma}_{\varepsilon}^{n-1}, w_{\varepsilon}^{n-1}) \in U_h \times \boldsymbol{\Sigma}_h \times W_h$, compute $(u_{\varepsilon}^n, z_{\varepsilon}^n, \boldsymbol{\sigma}_{\varepsilon}^n, w_{\varepsilon}^n) \in U_h \times Z_h \times \boldsymbol{\Sigma}_h \times W_h$ solving

$$\begin{cases} (\delta_t u_{\varepsilon}^n, \bar{z}) + (\lambda_{\varepsilon} (u_{\varepsilon}^{n-1}) \nabla z_{\varepsilon}^n, \nabla \bar{z}) = -(u_{\varepsilon}^{n-1} \sigma_{\varepsilon}^n, \nabla \bar{z}), & \forall \bar{z} \in Z_h, \\ (\delta_t \sigma_{\varepsilon}^n, \bar{\sigma}) + (B_h \sigma_{\varepsilon}^n, \bar{\sigma}) = (u_{\varepsilon}^{n-1} \nabla z_{\varepsilon}^n, \bar{\sigma}), & \forall \bar{\sigma} \in \Sigma_h, \\ (\delta_t w_{\varepsilon}^n, \bar{w}) = \left(\frac{1}{2\sqrt{F_{\varepsilon}(u_{\varepsilon}^{n-1}) + A}} F_{\varepsilon}'(u_{\varepsilon}^{n-1}) \delta_t u_{\varepsilon}^n, \bar{w}\right), & \forall \bar{w} \in W_h, \\ (z_{\varepsilon}^n, \bar{u}) = \left(\frac{1}{\sqrt{F_{\varepsilon}(u_{\varepsilon}^{n-1}) + A}} F_{\varepsilon}'(u_{\varepsilon}^{n-1}) w_{\varepsilon}^n, \bar{u}\right), & \forall \bar{u} \in U_h. \end{cases}$$
(4.56)

Recall that $(B_h \boldsymbol{\sigma}_{\varepsilon}^n, \bar{\boldsymbol{\sigma}}) := (\operatorname{rot} \boldsymbol{\sigma}_{\varepsilon}^n, \operatorname{rot} \bar{\boldsymbol{\sigma}}) + (\nabla \cdot \boldsymbol{\sigma}_{\varepsilon}^n, \nabla \cdot \bar{\boldsymbol{\sigma}}) + (\boldsymbol{\sigma}_{\varepsilon}^n, \bar{\boldsymbol{\sigma}})$ for all $\bar{\boldsymbol{\sigma}} \in \Sigma_h$, Q^h is the L^2 -projection on U_h defined in (4.9), and \widetilde{Q}^h and \widehat{Q}^h are the standard L^2 -projections on $\boldsymbol{\Sigma}_h$ 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 (4.43).

4.5.1 Mass conservation and Energy-stability

Observe that the scheme **UZSW** is also conservative in u (satisfying (4.16)) and also has the behavior for $\int_{\Omega} v_n$ given in (4.17).

Definition 4.5.3 A numerical scheme with solution $(u_{\varepsilon}^n, z_{\varepsilon}^n, \boldsymbol{\sigma}_{\varepsilon}^n, w_{\varepsilon}^n)$ is called energy-stable with respect to the energy

$$\mathcal{E}(w,\boldsymbol{\sigma}) = \|w\|_0^2 + \frac{1}{2}\|\boldsymbol{\sigma}\|_0^2$$
(4.57)

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

Theorem 4.5.4 (Unconditional stability) The scheme UZSW is unconditional energy stable with respect to $\mathcal{E}(w, \boldsymbol{\sigma})$. In fact, if $(u_{\varepsilon}^n, z_{\varepsilon}^n, \boldsymbol{\sigma}_{\varepsilon}^n, w_{\varepsilon}^n)$ is a solution of UZSW, then the following discrete energy law holds

$$\delta_t \mathcal{E}(w_{\varepsilon}^n, \boldsymbol{\sigma}_{\varepsilon}^n) + k \|\delta_t w_{\varepsilon}^n\|_0^2 + \frac{k}{2} \|\delta_t \boldsymbol{\sigma}_{\varepsilon}^n\|_0^2 + \int_{\Omega} \lambda_{\varepsilon}(u_{\varepsilon}^{n-1}) |\nabla z_{\varepsilon}^n|^2 + \|\boldsymbol{\sigma}_{\varepsilon}^n\|_1^2 = 0.$$
(4.58)

Proof. The proof follows taking $(\bar{z}, \bar{\sigma}, \bar{w}, \bar{u}) = (z_{\varepsilon}^n, \sigma_{\varepsilon}^n, 2w_{\varepsilon}^n, \delta_t u_{\varepsilon}^n)$ in (4.56).

From the (local in time) discrete energy law (4.58), we deduce the following global in time estimates for $(u_{\varepsilon}^{n}, z_{\varepsilon}^{n}, \boldsymbol{\sigma}_{\varepsilon}^{n}, w_{\varepsilon}^{n})$ solution of the scheme **UZSW**:

Corollary 4.5.5 (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

$$\|w_{\varepsilon}^{n}\|_{0}^{2} + \|\boldsymbol{\sigma}_{\varepsilon}^{n}\|_{0}^{2} + k\sum_{m=1}^{n} \left(\int_{\Omega} \lambda_{\varepsilon}(u_{\varepsilon}^{m-1}) |\nabla z_{\varepsilon}^{m}|^{2} + \|\boldsymbol{\sigma}_{\varepsilon}^{m}\|_{1}^{2} \right) \le C_{0}, \quad \forall n \ge 1,$$

$$(4.59)$$

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 (4.27) and taking into account that $u_0 \ge 0$ and $(u_h^0, \boldsymbol{\sigma}_h^0, w_{h,\varepsilon}^0) = (Q^h u_0, \widetilde{Q}^h(\nabla v_0), \widehat{Q}^h(\sqrt{F_{\varepsilon}(u_0(\boldsymbol{x})) + A}))$, we have that

$$\|w_{h,\varepsilon}^{0}\|_{0}^{2} + \frac{1}{2}\|\boldsymbol{\sigma}_{h}^{0}\|_{0}^{2} = \|\widehat{Q}^{h}(\sqrt{F_{\varepsilon}(u_{0}) + A})\|_{0}^{2} + \frac{1}{2}\|\widetilde{Q}^{h}(\nabla v_{0})\|_{0}^{2} \le \int_{\Omega} (F_{\varepsilon}(u_{0}) + A) + \frac{1}{2}\|\nabla v_{0}\|_{0}^{2} \le C \int_{\Omega} ((u_{0})^{2} + 1) + \frac{1}{2}\|\nabla v_{0}\|_{0}^{2} \le C(\|u_{0}\|_{0}^{2} + \|v_{0}\|_{1}^{2} + 1) \le C_{0}, \quad (4.60)$$

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 (4.58) by k, adding from m = 1 to m = n and using (4.60), we arrive at (4.59).
4.5.2 Well-posedness

Theorem 4.5.6 (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 $(u_{\varepsilon,1}^n, z_{\varepsilon,1}^n, \boldsymbol{\sigma}_{\varepsilon,1}^n, w_{\varepsilon,1}^n), (u_{\varepsilon,2}^n, z_{\varepsilon,2}^n, \boldsymbol{\sigma}_{\varepsilon,2}^n, w_{\varepsilon,2}^n) \in U_h \times Z_h \times \Sigma_h \times W_h$ two possible solutions of **UZSW**. Then defining $u = u_{\varepsilon,1}^n - u_{\varepsilon,2}^n, z = z_{\varepsilon,1}^n - z_{\varepsilon,2}^n, \boldsymbol{\sigma} = \boldsymbol{\sigma}_{\varepsilon,1}^n - \boldsymbol{\sigma}_{\varepsilon,2}^n$ and $w = w_{\varepsilon,1}^n - w_{\varepsilon,2}^n$, we have that $(u, z, \boldsymbol{\sigma}, w) \in U_h \times Z_h \times \Sigma_h \times W_h$ satisfies

$$\begin{cases}
\frac{1}{k}(u,\bar{z}) + (\lambda_{\varepsilon}(u_{\varepsilon}^{n-1})\nabla z, \nabla \bar{z}) = -(u_{\varepsilon}^{n-1}\boldsymbol{\sigma}, \nabla \bar{z}), \quad \forall \bar{z} \in Z_{h}, \\
\frac{1}{k}(\boldsymbol{\sigma}, \bar{\boldsymbol{\sigma}}) + (B_{h}\boldsymbol{\sigma}, \bar{\boldsymbol{\sigma}}) = (u_{\varepsilon}^{n-1}\nabla z, \bar{\boldsymbol{\sigma}}), \quad \forall \bar{\boldsymbol{\sigma}} \in \Sigma_{h}, \\
\frac{1}{k}(w,\bar{w}) = \frac{1}{2k} \left(\frac{1}{\sqrt{F_{\varepsilon}(u_{\varepsilon}^{n-1}) + A}} F_{\varepsilon}'(u_{\varepsilon}^{n-1}) u, \bar{w}\right), \quad \forall \bar{w} \in W_{h}, \\
(z,\bar{u}) = \left(\frac{1}{\sqrt{F_{\varepsilon}(u_{\varepsilon}^{n-1}) + A}} F_{\varepsilon}'(u_{\varepsilon}^{n-1}) w, \bar{u}\right), \quad \forall \bar{u} \in U_{h}.
\end{cases}$$
(4.61)

Taking $(\bar{z}, \bar{\sigma}, \bar{w}, \bar{u}) = (z, \sigma, 2w, \frac{1}{k}u)$ in (4.61) and adding, we obtain

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

Taking into account that $\lambda_{\varepsilon}(u_{\varepsilon}^{n-1}) \geq \varepsilon$, we deduce that $(\nabla z, \boldsymbol{\sigma}, w) = (\mathbf{0}, \mathbf{0}, 0)$, hence z = C := cte. Moreover, using the fact that w = 0 and z = C, from $(4.61)_4$ we conclude that z = 0. Finally, taking $\bar{z} = u$ in $(4.61)_1$ (which is possible thanks to the choice $U_h \subseteq Z_h$), since $(\nabla z, \boldsymbol{\sigma}) = (\mathbf{0}, \mathbf{0})$ we conclude u = 0.

4.6 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) 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 comparison, we will also consider the classical Backward Euler scheme for model (4.1), 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

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

Remark 4.6.1 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 regularized functions F_{ε} , F'_{ε} and F''_{ε} (see (4.5) and Figure 4.1) 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 $(u_{\varepsilon}^n, v_{\varepsilon}^n, \boldsymbol{\sigma}_{\varepsilon}^n) := (u^n, v^n, \boldsymbol{\sigma}^n)$.

(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

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

until the stopping criteria max $\left\{ \frac{\|u^{l+1} - u^{l}\|_{0}}{\|u^{l}\|_{0}}, \frac{\|v^{l+1} - v^{l}\|_{0}}{\|v^{l}\|_{0}} \right\} \le tol.$

(ii) Picard method to approach a solution (uⁿ, σⁿ) of the scheme US
Initialization (l = 0): Set (u⁰, σ⁰) = (uⁿ⁻¹, σⁿ⁻¹) ∈ U_h × Σ_h.
Algorithm: Given (u^l, σ^l) ∈ U_h × Σ_h, compute (u^{l+1}, σ^{l+1}) ∈ U_h × Σ_h such that

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

until the stopping criteria max $\left\{ \frac{\|u^{l+1} - u^l\|_0}{\|u^l\|_0}, \frac{\|\boldsymbol{\sigma}^{l+1} - \boldsymbol{\sigma}^l\|_0}{\|\boldsymbol{\sigma}^l\|_0} \right\} \leq tol.$ Note that a residual term $(\nabla(u^{l+1} - u^l), \nabla \bar{u})$ is considered.

(iii) Picard method to approach a solution (uⁿ, vⁿ) of the scheme BEUV
Initialization (l = 0): Set (u⁰, v⁰) = (uⁿ⁻¹, vⁿ⁻¹) ∈ U_h × V_h.
Algorithm: Given (u^l, v^l) ∈ U_h × V_h, compute (u^{l+1}, v^{l+1}) ∈ U_h × V_h such that

$$\begin{cases} \frac{1}{k}(u^{l+1},\bar{u}) + (\nabla u^{l+1},\nabla\bar{u}) = \frac{1}{k}(u^{n-1},\bar{u}) - (u^{l}\nabla v^{l+1},\nabla\bar{u}), & \forall \bar{u} \in U_{h} \\ \frac{1}{k}(v^{l+1},\bar{v}) + (A_{h}v^{l+1},\bar{v}) = \frac{1}{k}(v^{n-1},\bar{v}) + (u^{l},\bar{v}), & \forall \bar{v} \in V_{h}, \end{cases}$$

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

Remark 4.6.2 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 u-equation, we compute u^{l+1} .

4.6.1 Positivity of u^n

In this subsection, we compare the positivity of the variable $u^n \in U_h$ in the four schemes. Here, we choose the space V_h generated by \mathbb{P}_2 -continuous FE. We recall that for the three schemes studied in this paper, namely schemes **UV**, **UZSW** and **US**, it is not clear the positivity of the variable u^n . Moreover, for the schemes **UV** and **US**, it was proved that $\Pi^h(u_{\varepsilon^-}^n) \to 0$ in $L^2(\Omega)$ as $\varepsilon \to 0$ (see Remarks 4.3.10 and 4.4.4); while for the scheme **UZSW** this fact is not clear. For this reason, in Figures 4.3-4.5 we compare the positivity of the variable u_{ε}^n in the schemes, taking $\varepsilon = 10^{-3}$, $\varepsilon = 10^{-5}$ and $\varepsilon = 10^{-8}$. In the scheme **UZSW** we fix A = 1 (and thus, $F_{\varepsilon}(s) + A \ge 1$ for all $s \in \mathbb{R}$). We consider the time step $k = 10^{-5}$, the tolerance parameter for the linear iterative methods $tol = 10^{-4}$ and the initial conditions (see Figure 4.2)

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

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

Note that $u_0, v_0 > 0$ in Ω , $\min(u_0) = u_0(1, 1) = 0.0001$ and $\max(v_0) = v_0(1, 1) = 100.0001$. Moreover, 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 thicker meshes we had convergence problems of the iterative method.

In the case of the schemes **UV** and **US**, we observe that although u_{ε}^{n} is negative for some $x \in \Omega$ in some times $t_{n} > 0$, when $\varepsilon \to 0$ these values are closer to 0; while in the case of



Figure 4.2: Initial conditions.

the scheme **UZSW**, this same behavior is not observed (see Figures 4.3-4.5). Finally, in the case of the scheme **BEUV** (see Figure 4.6), we have also observed negative values for the minimum of u^n in some times $t_n > 0$, with more negative values than in the schemes **UV** and **US**.

Remark 4.6.3 In Figures 4.3 and 4.5 there are also negative values of minimum of u_{ε}^{n} for $\varepsilon = 10^{-5}$ and $\varepsilon = 10^{-8}$, but those are of order 10^{-4} and 10^{-7} respectively in both figures.

4.6.2 Energy stability

In this subsection, we compare numerically the stability of the schemes UV, UZSW, US and BEUV with respect to the "exact" energy

$$\mathcal{E}_e(u,v) = \int_{\Omega} F_0(u(\boldsymbol{x})) d\boldsymbol{x} + \frac{1}{2} \|\nabla v\|_0^2, \qquad (4.62)$$

where

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

It was proved that the schemes **UV**, **UZSW** and **US** are unconditionally energy-stables with respect to modified energies obtained in terms of the variables of each scheme. Even more, some energy inequalities are satisfied (see Theorems 4.3.7, 4.4.2 and 4.5.4). However,



Figure 4.3: Minimum values of u_{ε}^{n} computed using the scheme **UV**.

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 (4.62), which comes from the continuous problem (4.1) (see (4.3)). Therefore, it is interesting to compare numerically the schemes with respect to this energy $\mathcal{E}_e(u^n, v^n)$, and to study the behaviour of the corresponding discrete residual of the energy law (4.3):

$$RE_e(u^n, v^n) := \delta_t \mathcal{E}_e(u^n, v^n) + 4 \int_{\Omega} |\nabla \sqrt{u_+^n}|^2 d\boldsymbol{x} + \|(A_h - I)v^n\|_0^2 + \|\nabla v^n\|_0^2.$$
(4.63)

1. First test: We consider $k = 10^{-3}$, $h = \frac{1}{40}$, $tol = 10^{-4}$ and the initial conditions (see Figure 4.7)

 $u_0 = 7w + 7.0001$ and $v_0 = -7w + 7.0001$,

where $w := cos(2\pi x)cos(2\pi y)$. We choose V_h generated by \mathbb{P}_2 -continuous FE. Then, we obtain that:

(i) The scheme **BEUV** satisfies the energy decreasing in time property for the exact energy $\mathcal{E}_e(u, v)$, that is,

$$\mathcal{E}_e(u^n, v^n) \le \mathcal{E}_e(u^{n-1}, v^{n-1}) \quad \forall n.$$

$$(4.64)$$

Its behaviour can be observed in Figure 4.8. The same behaviour is obtained for the schemes **UV** and **US** independently of the choice of ε . In the case of the scheme



Figure 4.4: Minimum values of u_{ε}^{n} computed using the scheme **UZSW**.

UZSW, this property (4.64) is not satisfied for any value of ε . Indeed, increasing energies are obtained for different values of ε (see Figure 4.9).

- (ii) The scheme **BEUV** satisfies the discrete energy inequality $RE_e(u^n, v^n) \leq 0$ for $RE_e(u^n, v^n)$ defined in (4.63) (see Figure 4.10). The same is observed for the schemes **UV** and **US** independently of the choice of ε . 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 $RE_e(u^n_{\varepsilon}, v^n_{\varepsilon})$ obtained for each ε reaches very large positive values (see Figure 4.11).
 - 2. Second test: We consider $k = 10^{-5}$, $h = \frac{1}{20}$, $tol = 10^{-4}$ and the initial conditions $u_0 = 14w + 14.0001$ and $v_0 = -14w + 14.0001$,

with the function w as before. Now, we choose the space V_h generated by \mathbb{P}_1 -continuous FE. Then, we obtain that:

- (i) The schemes **BEUV**, **UV** and **US** satisfy the energy decreasing in time property (4.64), independently of the choice of ε .
- (ii) The schemes **UV** and **US** satisfy the discrete energy inequality $RE_e(u_{\varepsilon}^n, v_{\varepsilon}^n) \leq 0$, independently of the choice of ε ; while the scheme **BEUV** have $RE(u^n, v^n) > 0$ for some $n \geq 0$ (see Figure 4.12).



Figure 4.5: Minimum values of u_{ε}^{n} computed using the scheme **US**.

4.7 Conclusions

In this paper we have developed three new mass-conservative and unconditionally energystable fully discrete FE schemes for the chemorepulsion production model (4.1), namely UV, US and UZSW. From the theoretical point of view we have obtained:

- (i) The well-posedness of the numerical schemes (with conditional uniqueness for the nonlinear schemes **UV** and **US**).
- (ii) The nonlinear scheme **UV** is unconditional energy-stable with respect to the energy $\mathcal{E}^{h}_{\varepsilon}(u, v)$ given in (4.19), 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 energystables with respect to the modified energies $\mathcal{E}^h_{\varepsilon}(u, \sigma)$ (given in (4.44)) and $\mathcal{E}(w, \sigma)$ (given in (4.57)) respectively, without the constraint on the triangulation related with the right-angles 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 (4.62)) or some modified energy (see Remark 4.6.1).



Figure 4.6: Minimum values of u^n computed using the scheme **BEUV**.

(v) In the schemes **UV** and **US** there is a control for $\Pi^h(u_{\varepsilon^-}^n)$ in L^2 -norm, which tends to 0 as $\varepsilon \to 0$. This allows to conclude the nonnegativity of the solution u_{ε}^n in the limit when $\varepsilon \to 0$. This property is not clear for the linear scheme **UZSW**.

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

- (i) There are initial conditions for which the scheme **UZSW** is not energy stable with respect to the energy $\mathcal{E}_e(u, v)$, that is, the decreasing in time property (4.64) is not satisfied for any value of ε . Indeed, time increasing energies are obtained for different values of ε .
- (ii) 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 overcomed considering thinner meshes.
- (iii) The schemes **UV** and **US** have decreasing in time energy $\mathcal{E}_e(u, v)$, independently of the choice of ε . In fact, the discrete energy inequality $RE_e(u_{\varepsilon}^n, v_{\varepsilon}^n) \leq 0$ is satisfied in all cases, for $RE_e(u_{\varepsilon}^n, v_{\varepsilon}^n)$ defined in (4.63).
- (iv) The scheme **BEUV** has decreasing in time energy $\mathcal{E}_e(u, v)$, but the discrete energy inequality $RE_e(u^n, v^n) \leq 0$ is not satisfied for some $n \geq 0$.



(a) Initial cell density u_0



(b) Initial chemical concentration v_0



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



Figure 4.8: Energy $\mathcal{E}_e(u^n, v^n)$ of the scheme **BEUV**.



Figure 4.9: Energy $\mathcal{E}_e(u_{\varepsilon}^n, v_{\varepsilon}^n)$ of the scheme **UZSW** for different values of ε .



Figure 4.10: $RE_e(u^n, v^n)$ of the scheme **BEUV** (with approximation \mathbb{P}_2 -continuous for V_h).



Figure 4.11: $RE_e(u_{\varepsilon}^n, v_{\varepsilon}^n)$ of the scheme **UZSW** for different values of ε .



Figure 4.12: $RE_e(u^n, v^n)$ of the schemes **BEUV**, **UV**, and **US** (with approximation \mathbb{P}_1 continuous for V_h)

.

In the previous figure: on the bottom, scheme **US** (for $\varepsilon = 10^{-3}, 10^{-5}, 10^{-8}$); in the middle, scheme **UV** (for $\varepsilon = 10^{-3}, 10^{-5}, 10^{-8}$); and on the top, scheme **BEUV**.

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Chapter 5 On a chemo-repulsion model with nonlinear production: The continuous problem and unconditionally energy stable fully discrete schemes

5.1 Introduction

Chemotaxis is the biological process of the movement of living organisms in response to a chemical stimulus, which can be given towards a higher (chemo-attraction) or lower (chemo-repulsion) concentration of a chemical substance. At the same time, the presence of living organisms can produce or consume chemical substance. A repulsive-productive chemotaxis model can be given by the following parabolic PDE's system:

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

where $\Omega \subseteq \mathbb{R}^d$, d = 2,3, is a bounded domain with boundary $\partial\Omega$. The unknowns for this model are $u(\boldsymbol{x},t) \geq 0$, the cell density, and $v(\boldsymbol{x},t) \geq 0$, the chemical concentration. Moreover, $f(u) \geq 0$ (if $u \geq 0$) is the production term. In this paper, we consider the particular case in which $f(u) = u^p$, with 1 , and then we focus on the followinginitial-boundary problem:

$$\begin{cases} \partial_t u - \Delta u = \nabla \cdot (u \nabla v) \text{ in } \Omega, \ t > 0, \\ \partial_t v - \Delta v + v = u^p \text{ in } \Omega, \ t > 0, \\ \frac{\partial u}{\partial \mathbf{n}} = \frac{\partial v}{\partial \mathbf{n}} = 0 \text{ on } \partial\Omega, \ t > 0, \\ u(\boldsymbol{x}, 0) = u_0(\boldsymbol{x}) > 0, \ v(\boldsymbol{x}, 0) = v_0(\boldsymbol{x}) > 0 \text{ in } \Omega. \end{cases}$$
(5.1)

In the case of linear (p = 1) and quadratic (p = 2) production terms, the problem (5.1) is well-posed (see [7] and Chapter 1 of this PhD thesis, respectively) in the following sense: there exist global in time weak solutions (based on an energy inequality) and, for 2D domains, there exists a unique global in time strong solution. However, as far as we know, there are not works studying problem (5.1) with production u^p , with 1 .

Problem (5.1) is conservative in u, because the total mass $\int_{\Omega} u(\cdot, t)$ remains constant in time, as we can check integrating equation $(5.1)_1$ in Ω ,

$$\frac{d}{dt}\left(\int_{\Omega} u(\cdot, t)\right) = 0, \quad \text{i.e.} \quad \int_{\Omega} u(\cdot, t) = \int_{\Omega} u_0 := m_0, \quad \forall t > 0.$$
(5.2)

The first aim of this work is to study the existence of weak-strong solutions for problem (5.1) (in the sense of Definition 5.3.1 below), satisfying in particular the energy inequality (5.8) below. The second aim of this work is to design numerical methods for model (5.1) conserving, at the discrete level, the mass-conservation and energy-stability properties of the continuous model (see (5.2) and (5.8), 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), in [9] Filbet proved the existence of discrete solutions and the convergence of a finite volume scheme. Saito, in [16, 17], studied error estimates for a conservative Finite Element (FE) approximation. In [8], some error estimates are proved for a fully discrete discontinuous FE method, and a mixed FE approximation is studied in [14].

Energy stable numerical schemes have been also studied in the chemotaxis framework. An energy-stable finite volume scheme for a Keller-Segel model with an additional cross-diffusion term has been studied in [6]. In Chapters 1 and 2 of this PhD thesis, unconditionally energy stable time-discrete numerical schemes and fully discrete FE schemes for a chemo-repulsion model with quadratic production have been analyzed. Unconditionally energy stable fully discrete FE schemes for a chemo-repulsion model with linear production has been studied in Chapter 4. However, as far as we know, for the chemo-repulsion model with production term u^p (5.1) there are not works studying energy-stable numerical schemes.

This chapter is organized as follows: In Section 5.2, we give the notation and some preliminary results that will be used throughout the paper. In Section 5.3, we prove the existence of weak-strong solutions of model (5.1) (in the sense of Definition 5.3.1 below) by using a regularization technique. In Section 5.4, we propose three fully discrete FE nonlinear approximations of problem (5.1), where the first one is defined in the variables (u, v), and the second and third ones introduce $\boldsymbol{\sigma} = \nabla v$ as an auxiliary variable. We prove some unconditional properties such as mass-conservation, energy-stability and solvability of the schemes. In Section 5.5, we compare the behavior of the schemes throughout several

numerical simulations; and in Section 5.6, the main conclusions obtained in this paper are sumarized.

5.2 Notation and preliminary results

We recall some functional spaces which will be used throughout this paper. We will consider the usual Lebesgue spaces $L^q(\Omega)$, $1 \leq q \leq \infty$, with norm $\|\cdot\|_{L^q}$. In particular, the $L^2(\Omega)$ norm will be denoted by $\|\cdot\|_0$. From now on, (\cdot, \cdot) will denote the standard L^2 -inner product over Ω . We also consider the usual Sobolev spaces $W^{m,p}(\Omega) = \{u \in L^p(\Omega) : \|\partial^{\alpha}u\|_{L^p} < +\infty, \forall |\alpha| < m\}$, for a multi-index α and $m \in \mathbb{N}$, with norm denoted by $\|\cdot\|_{W^{m,p}}$. In the case when p = 2, we denote $H^m(\Omega) := W^{m,2}(\Omega)$, with respective norm $\|\cdot\|_m$. Moreover, we denote by

$$\boldsymbol{H}_{\boldsymbol{\sigma}}^{1}(\Omega) := \{ \boldsymbol{\sigma} \in \boldsymbol{H}^{1}(\Omega) : \boldsymbol{\sigma} \cdot \mathbf{n} = 0 \text{ on } \partial\Omega \},\$$
$$W_{\mathbf{n}}^{m,p}(\Omega) := \left\{ u \in W^{m,p}(\Omega) : \frac{\partial u}{\partial \mathbf{n}} = 0 \text{ on } \partial\Omega \right\},\$$

and we will use the following equivalent norms in $H^1(\Omega)$ and $H^1_{\sigma}(\Omega)$, respectively (see [15] and [2, Corollary 3.5], respectively):

$$\|u\|_{1}^{2} = \|\nabla u\|_{0}^{2} + \left(\int_{\Omega} u\right)^{2}, \quad \forall u \in H^{1}(\Omega),$$
$$\|\boldsymbol{\sigma}\|_{1}^{2} = \|\boldsymbol{\sigma}\|_{0}^{2} + \|\operatorname{rot} \,\boldsymbol{\sigma}\|_{0}^{2} + \|\nabla \cdot \boldsymbol{\sigma}\|_{0}^{2}, \quad \forall \boldsymbol{\sigma} \in \boldsymbol{H}_{\sigma}^{1}(\Omega),$$
(5.3)

where rot $\boldsymbol{\sigma}$ denotes the well-known rotational operator (also called curl) which is scalar for 2D domains and vectorial for 3D ones. In particular, (5.3) implies that, for all $\boldsymbol{\sigma} = \nabla v \in \boldsymbol{H}_{\sigma}^{1}(\Omega)$,

$$\|\nabla v\|_1^2 = \|\nabla v\|_0^2 + \|\Delta v\|_0^2.$$
(5.4)

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.

We will use the following results:

Theorem 5.2.1 ([10]) Let $1 < q < +\infty$ and suppose that $f \in L^{q}(0,T;L^{q}(\Omega)), u_{0} \in \widehat{W}^{2-\frac{2}{q},q}(\Omega)$, where

$$\widehat{W}^{2-\frac{2}{q},q}(\Omega) \quad := \quad \left\{ \begin{array}{ll} W^{2-\frac{2}{q},q}(\Omega) & if \quad 1-\frac{2}{q}-\frac{1}{q}<0, \\ W^{2-\frac{2}{q},q}_{\mathbf{n}}(\Omega) & if \quad 1-\frac{2}{q}-\frac{1}{q}>0. \end{array} \right.$$

Then, the problem

$$\left\{ \begin{array}{ll} \partial_t u - \Delta u = f \quad in \ \Omega, \ t > 0, \\ \frac{\partial u}{\partial \mathbf{n}} = 0 \quad on \ \partial\Omega, \ t > 0, \\ u(\boldsymbol{x}, 0) = u_0(\boldsymbol{x}) \quad in \ \Omega, \end{array} \right.$$

admits a unique solution u in the class

$$u \in L^{q}(0,T; W^{2,q}(\Omega)) \cap C([0,T]; \widehat{W}^{2-\frac{2}{q},q}(\Omega)), \quad \partial_{t}u \in L^{q}(0,T; L^{q}(\Omega)).$$

Moreover, there exists a positive constant $C = C(q, \Omega, T)$ such that

$$\|u\|_{C(0,T;\widehat{W}^{2-\frac{2}{q},q}(\Omega))} + \|\partial_{t}u\|_{L^{q}(0,T;L^{q}(\Omega))} + \|u\|_{L^{q}(0,T;W^{2,q}(\Omega))} \le C(\|f\|_{L^{q}(0,T;L^{q}(\Omega))} + \|u_{0}\|_{\widehat{W}^{2-\frac{2}{q},q}(\Omega)}).$$

Proposition 5.2.2 ([1]) Let X be a Banach space, $\Omega \subseteq X$ an open subset, $U \subseteq \Omega$ a nonempty convex subset and $J: \Omega \to \mathbb{R}$ a functional. Suppose that J is G-differentiable in Ω . Then, J is convex over U if and only if the following relation holds

$$J(x_1) - J(x_2) \le \delta J(x_1, x_1 - x_2), \ \forall x_1, x_2 \in U, \ x_1 \neq x_2.$$
(5.5)

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

Lemma 5.2.3 Assume that $\delta, \beta, k > 0$ and $d^n \ge 0$ satisfy

$$(1+\delta k)d^{n+1} \le d^n + k\beta, \quad \forall n \ge 0.$$

Then, for any $n_0 \ge 0$,

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

5.3 Analysis of the continuous model

In this section, we will prove the existence of weak-strong solutions of problem (5.1) in the sense of the following definition.

Definition 5.3.1 (Weak-strong solutions of (5.1)) Let $1 . Given <math>(u_0, v_0) \in L^p(\Omega) \times H^1(\Omega)$ with $u_0 \ge 0$, $v_0 \ge 0$ a.e. in Ω , a pair (u, v) is called weak-strong solution of problem (5.1) in $(0, +\infty)$, if $u \ge 0$, $v \ge 0$ a.e. in $(0, +\infty) \times \Omega$,

$$\begin{aligned} u \in L^{\infty}(0, +\infty; L^{p}(\Omega)) \cap L^{\frac{5p}{p+3}}(0, T; W^{1, \frac{5p}{p+3}}(\Omega)), \quad \forall T > 0, \\ v \in L^{\infty}(0, +\infty; H^{1}(\Omega)) \cap L^{2}(0, T; H^{2}(\Omega)), \quad \forall T > 0, \\ \partial_{t}u \in L^{\frac{10p}{3p+6}}(0, T; W^{1, \frac{10p}{7p-6}}(\Omega)'), \quad \partial_{t}v \in L^{\frac{5}{3}}(0, T; L^{\frac{5}{3}}(\Omega)), \quad \forall T > 0, \end{aligned}$$

the following variational formulation for the u-equation holds

$$\int_{0}^{T} \langle \partial_{t} u, \bar{u} \rangle + \int_{0}^{T} (\nabla u, \nabla \bar{u}) + \int_{0}^{T} (u \nabla v, \nabla \bar{u}) = 0, \quad \forall \bar{u} \in L^{\frac{10p}{7p-6}}(0, T; W^{1, \frac{10p}{7p-6}}(\Omega)), \quad \forall T > 0,$$
(5.6)

the v-equation holds pointwisely

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

$$(5.7)$$

the boundary condition $\frac{\partial v}{\partial \mathbf{n}} = 0$ and the initial conditions $(5.1)_4$ are satisfied and the following energy inequality (in integral version) holds for a.e. t_0, t_1 with $t_1 \ge t_0 \ge 0$:

$$\mathcal{E}(u(t_1), v(t_1)) - \mathcal{E}(u(t_0), v(t_0)) + \int_{t_0}^{t_1} \left(\frac{4}{p} \|\nabla(u^{p/2}(s))\|_0^2 + \|\nabla v(s)\|_1^2\right) \, ds \le 0, \tag{5.8}$$

where

$$\mathcal{E}(u,v) = \frac{1}{p-1} \|u\|_p^p + \frac{1}{2} \|\nabla v\|_0^2.$$
(5.9)

Observe that any weak-strong solution of (5.1) is conservative in u (see (5.2)). In addition, integrating $(5.1)_2$ in Ω , we deduce

$$\frac{d}{dt}\left(\int_{\Omega} v\right) + \int_{\Omega} v = \int_{\Omega} u^{p}.$$
(5.10)

5.3.1 Regularized problem

In order to prove the existence of weak-strong solution of problem (5.1) in the sense of Definition 5.3.1, we introduce the following regularized problem associated to model (5.1): Let $\varepsilon \in (0, 1)$, find $(u^{\varepsilon}, z^{\varepsilon})$, with $u^{\varepsilon} \ge 0$ a.e. in $(0, +\infty) \times \Omega$, such that, for all T > 0,

$$u^{\varepsilon}, z^{\varepsilon} \in \widetilde{\mathfrak{X}} := \{ w \in L^{\infty}(0, T; W^{\frac{4}{5}, \frac{5}{3}}(\Omega)) \cap L^{\frac{5}{3}}(0, T; W^{2, \frac{5}{3}}(\Omega)) : \partial_{t}w \in L^{\frac{5}{3}}(0, T; L^{\frac{5}{3}}(\Omega)) \},$$
(5.11)

and

$$\begin{aligned} \partial_t u^{\varepsilon} &- \Delta u^{\varepsilon} = \nabla \cdot (u^{\varepsilon} \nabla v^{\epsilon} (z^{\varepsilon})) & \text{in } \Omega, \ t > 0, \\ \partial_t z^{\varepsilon} &- \Delta z^{\varepsilon} + z^{\varepsilon} = (u^{\varepsilon})^p & \text{in } \Omega, \ t > 0, \\ \frac{\partial u^{\varepsilon}}{\partial \mathbf{n}} &= \frac{\partial z^{\varepsilon}}{\partial \mathbf{n}} = 0 & \text{on } \partial\Omega, \ t > 0, \\ u^{\varepsilon} (\boldsymbol{x}, 0) &= u_0^{\varepsilon} (\boldsymbol{x}) \ge 0, \ z^{\varepsilon} (\boldsymbol{x}, 0) = v_0^{\varepsilon} (\boldsymbol{x}) - \varepsilon \Delta v_0^{\varepsilon} (\boldsymbol{x}) & \text{in } \Omega, \end{aligned} \tag{5.12}$$

where $v^{\varepsilon} = v^{\varepsilon}(z^{\varepsilon})$ is the unique solution of the elliptic-Newman problem

$$\begin{cases} v^{\varepsilon} - \varepsilon \Delta v^{\varepsilon} = z^{\varepsilon} & \text{in } \Omega, \\ \frac{\partial v^{\varepsilon}}{\partial \mathbf{n}} = 0 & \text{on } \partial \Omega, \end{cases}$$
(5.13)

and $(u_0^{\varepsilon}, z_0^{\varepsilon}) \in W^{\frac{4}{5}, \frac{5}{3}}(\Omega)^2$ with

$$(u_0^{\varepsilon}, z_0^{\varepsilon}) \to (u_0, z_0) \quad \text{in } L^2(\Omega) \times L^2(\Omega), \quad \text{as } \varepsilon \to 0.$$
 (5.14)

From now on in this section, we will denote $v^{\varepsilon}(z^{\varepsilon})$ solution of (5.13) only by v^{ε} . Observe that if $(u^{\varepsilon}, z^{\varepsilon})$ is any solution of (5.12), then (5.2) and (5.10) are satisfied for $(u, v) = (u^{\varepsilon}, v^{\varepsilon})$.

Theorem 5.3.2 Let $\varepsilon \in (0, 1)$. Then, there exists at least one solution of problem (5.11)-(5.12).

Proof. We will use the Leray-Schauder fixed point theorem. With this aim, we denote

$$\mathfrak{X} := L^{\infty}(0,T;L^2(\Omega)) \cap L^2(0,T;H^1(\Omega)),$$

and we define the operator $R: \mathfrak{X} \times \mathfrak{X} \to \widetilde{\mathfrak{X}} \times \widetilde{\mathfrak{X}} \hookrightarrow \mathfrak{X} \times \mathfrak{X}$ by $R(\widetilde{u}^{\varepsilon}, \widetilde{z}^{\varepsilon}) = (u^{\varepsilon}, z^{\varepsilon})$, such that $(u^{\varepsilon}, z^{\varepsilon})$ solves the following linear decoupled problem

$$\begin{cases} \frac{\partial_t u^{\varepsilon} - \Delta u^{\varepsilon} = \nabla \cdot (\widetilde{u}_+^{\varepsilon} \nabla \widetilde{v}^{\varepsilon}) & \text{in } \Omega, \ t > 0, \\ \frac{\partial_t z^{\varepsilon} - \Delta z^{\varepsilon} = (\widetilde{u}^{\varepsilon})^p - \widetilde{z}^{\varepsilon} & \text{in } \Omega, \ t > 0, \\ \frac{\partial u^{\varepsilon}}{\partial \mathbf{n}} = \frac{\partial z^{\varepsilon}}{\partial \mathbf{n}} = 0 & \text{on } \partial\Omega, \ t > 0, \\ u^{\varepsilon}(\boldsymbol{x}, 0) = u_0^{\varepsilon}(\boldsymbol{x}) \ge 0, \ z^{\varepsilon}(\boldsymbol{x}, 0) = v_0^{\varepsilon}(\boldsymbol{x}) - \varepsilon \Delta v_0^{\varepsilon}(\boldsymbol{x}) & \text{in } \Omega, \end{cases}$$
(5.15)

where $\tilde{v}^{\varepsilon} = v^{\varepsilon}(\tilde{z}^{\varepsilon})$ and, in general, we denote $a_{+} := \max\{a, 0\}$.

- 1. *R* is well defined. Observe that if $\tilde{z}_{\varepsilon} \in \mathfrak{X}$, from the H^2 and H^3 -regularity of problem (5.13) (see [11, Theorems 2.4.2.7 and 2.5.1.1] respectively), we have that $\tilde{v}^{\varepsilon} \in L^{\infty}(0,T; H^2(\Omega)) \cap L^2(0,T; H^3(\Omega))$. Thus, we deduce that $\nabla \tilde{v}^{\varepsilon} \in L^{\infty}(0,T; H^1(\Omega)) \cap L^2(0,T; H^2(\Omega)) \hookrightarrow L^{10}(0,T; L^{10}(\Omega))$. Then, using this fact and taking into account that $(\tilde{u}^{\varepsilon}, \tilde{z}^{\varepsilon}) \in \mathfrak{X} \times \mathfrak{X}$, we obtain that $\nabla \cdot (\tilde{u}^{\varepsilon}_+ \nabla \tilde{v}^{\varepsilon}) \in L^{\frac{5}{3}}(0,T; L^{\frac{5}{3}}(\Omega))$ and $(\tilde{u}^{\varepsilon})^p + \tilde{z}^{\varepsilon} \in L^{\frac{5}{3}}(0,T; L^{\frac{5}{3}}(\Omega))$ for any $p \in (1,2)$. Thus, applying Theorem 5.2.1 to (5.15), we deduce that there exists a unique $(u^{\varepsilon}, z^{\varepsilon}) \in \tilde{\mathfrak{X}} \times \tilde{\mathfrak{X}}$ solution of (5.15).
- 2. Let us now prove that all possible fixed points of λR (with $\lambda \in (0, 1]$) are bounded in $\mathfrak{X} \times \mathfrak{X}$ and $u^{\varepsilon} \geq 0$. In fact, observe that if $(u^{\varepsilon}, z^{\varepsilon})$ is a fixed point of λR , then $(u^{\varepsilon}, z^{\varepsilon})$ satisfies

$$\begin{cases} \partial_t u^{\varepsilon} - \Delta u^{\varepsilon} = \lambda \nabla \cdot (u_+^{\varepsilon} \nabla v^{\varepsilon}) & \text{in } \Omega, \ t > 0, \\ \partial_t z^{\varepsilon} - \Delta z^{\varepsilon} = \lambda (u^{\varepsilon})^p - \lambda z^{\varepsilon} & \text{in } \Omega, \ t > 0, \\ \frac{\partial u^{\varepsilon}}{\partial \mathbf{n}} = \frac{\partial z^{\varepsilon}}{\partial \mathbf{n}} = 0 & \text{on } \partial \Omega, \ t > 0, \\ u^{\varepsilon}(\boldsymbol{x}, 0) = u_0^{\varepsilon}(\boldsymbol{x}) \ge 0, \ z^{\varepsilon}(\boldsymbol{x}, 0) = v_0^{\varepsilon}(\boldsymbol{x}) - \varepsilon \Delta v_0^{\varepsilon}(\boldsymbol{x}) & \text{in } \Omega, \end{cases}$$
(5.16)

Then, multiplying $(5.16)_1$ by $u_{-}^{\varepsilon} := \min\{u^{\varepsilon}, 0\}$ and integrating in Ω , we have

$$\frac{1}{2}\frac{d}{dt}\|u_{-}^{\varepsilon}\|_{0}^{2}+\|\nabla u_{-}^{\varepsilon}\|_{0}^{2}=\lambda(u_{+}^{\varepsilon}\nabla v^{\varepsilon},\nabla u_{-}^{\varepsilon})=0,$$

which, taking into account that $u_0^{\varepsilon}(\boldsymbol{x}) \geq 0$, implies that $u^{\varepsilon} \geq 0$ a.e. in $(0, +\infty) \times \Omega$. Thus, $u_+^{\varepsilon} = u^{\varepsilon}$. Now, testing $(5.16)_1$ and $(5.16)_2$ by $\frac{p}{p-1}(u^{\varepsilon})^{p-1}$ and $-\Delta v^{\varepsilon}$ respectively, and adding both equations, the terms $-\lambda \frac{p}{p-1}(u^{\varepsilon} \nabla v^{\varepsilon}, \nabla (u^{\varepsilon})^{p-1})$ and $\lambda(\nabla(u^{\varepsilon})^p, \nabla v^{\varepsilon})$ cancel, and taking into account (5.13), we obtain

$$\frac{d}{dt} \mathcal{E}_{\varepsilon}(u^{\varepsilon}, v^{\varepsilon}) + \frac{4}{p} \int_{\Omega} |\nabla((u^{\varepsilon})^{p/2})|^{2} \\
+ \varepsilon \|\nabla(\Delta v^{\varepsilon})\|_{0}^{2} + \|\Delta v^{\varepsilon}\|_{0}^{2} = -\lambda \|\nabla v^{\varepsilon}\|_{0}^{2} - \lambda \varepsilon \|\Delta v^{\varepsilon}\|_{0}^{2} \le 0,$$
(5.17)

where

$$\mathcal{E}_{\varepsilon}(u^{\varepsilon}, v^{\varepsilon}) := \frac{1}{p-1} \|u^{\varepsilon}\|_{L^{p}}^{p} + \frac{1}{2} \|\nabla v^{\varepsilon}\|_{0}^{2} + \frac{\varepsilon}{2} \|\Delta v^{\varepsilon}\|_{0}^{2}$$

Moreover, we observe that the function $y^{\varepsilon}(t) = \left(\int_{\Omega} v^{\varepsilon}(\boldsymbol{x},t) d\boldsymbol{x}\right)^2$ satisfies $(y^{\varepsilon})'(t) + y^{\varepsilon}(t) \leq w^{\varepsilon}(t)$, with $w^{\varepsilon}(t) = ||u^{\varepsilon}(t)||_{L^p}^{2p}$. In fact, it follows by multiplying (5.10) (for $(u,v) = (u^{\varepsilon},v^{\varepsilon})$) by $\int_{\Omega} v^{\varepsilon}(\boldsymbol{x},t) d\boldsymbol{x}$ and using the Young inequality. Therefore, $y^{\varepsilon}(t) =$

$$y^{\varepsilon}(0) e^{-t} + \int_{0}^{t} e^{-(t-s)} w^{\varepsilon}(s) ds, \text{ which implies that}$$
$$\left(\int_{\Omega} v^{\varepsilon}(\boldsymbol{x}, t) d\boldsymbol{x}\right)^{2} \le \left(\int_{\Omega} v_{0}^{\varepsilon}(\boldsymbol{x}) d\boldsymbol{x}\right)^{2} + \|u^{\varepsilon}\|_{L^{\infty}(0, +\infty; L^{p})}^{2p}, \quad \forall t \ge 0.$$
(5.18)

Then, from (5.17)-(5.18) and using (5.4), we deduce the following estimates with respect to λ :

$$\begin{cases} (u^{\varepsilon}, v^{\varepsilon}) \text{ is bounded in } L^{\infty}(0, +\infty; L^{p}(\Omega) \times \boldsymbol{H}^{2}(\Omega)), \\ u^{\varepsilon} \text{ is bounded in } L^{p}(0, T; L^{3p}(\Omega)) \text{ and } v^{\varepsilon} \text{ is bounded in } L^{2}(0, T; \boldsymbol{H}^{3}(\Omega)). \end{cases}$$

$$(5.19)$$

Then, from (5.19) we conclude that z^{ε} is bounded in \mathfrak{X} . Moreover, testing (5.16)₁ by u^{ε} , we have

$$\frac{1}{2}\frac{d}{dt}\|u^{\varepsilon}\|_{0}^{2} + \|u^{\varepsilon}\|_{1}^{2} = -\lambda(u^{\varepsilon}\nabla v^{\varepsilon}, \nabla u^{\varepsilon}) + \|u^{\varepsilon}\|_{0}^{2} \leq \frac{1}{2}\|u^{\varepsilon}\|_{1}^{2} + C\Big(\|\nabla v^{\varepsilon}\|_{1}^{4} + 1\Big)\|u^{\varepsilon}\|_{0}^{2},$$

from which, taking into account (5.19) and using the Gronwall Lemma, we deduce that u^{ε} is bounded in \mathfrak{X} .

- 3. *R* is compact. Let $\{(\widetilde{u}_n^{\varepsilon}, \widetilde{z}_n^{\varepsilon})\}_{n \in \mathbb{N}}$ be a bounded sequence in $\mathfrak{X} \times \mathfrak{X}$. Then $(u_n^{\varepsilon}, z_n^{\varepsilon}) = R(\widetilde{u}_n^{\varepsilon}, \widetilde{z}_n^{\varepsilon})$ solves (5.15) (with $(\widetilde{u}_n^{\varepsilon}, \widetilde{z}_n^{\varepsilon})$ and $(u_n^{\varepsilon}, z_n^{\varepsilon})$ instead of $(\widetilde{u}^{\varepsilon}, \widetilde{z}^{\varepsilon})$ and $(u^{\varepsilon}, z^{\varepsilon})$ respectively). Therefore, analogously as in item 1, we obtain that $\nabla \cdot ((\widetilde{u}_{n+}^{\varepsilon}) \nabla \widetilde{v}_n^{\varepsilon})$ is bounded $L^{\frac{5}{3}}(0, T; L^{\frac{5}{3}}(\Omega))$ and $(\widetilde{u}_n^{\varepsilon})^p + \widetilde{z}_n^{\varepsilon}$ is bounded $L^{\frac{5}{3}}(0, T; L^{\frac{5}{3}}(\Omega))$; and therefore, from Theorem 5.2.1 we conclude that $\{R(\widetilde{u}_n^{\varepsilon}, \widetilde{z}_n^{\varepsilon})\}_{n \in \mathbb{N}}$ is bounded in $\widetilde{\mathfrak{X}} \times \widetilde{\mathfrak{X}}$ which is compactly embedded in $\mathfrak{X} \times \mathfrak{X}$, and thus *R* is compact.
- 4. We prove that R is continuous. Let $\{(\widetilde{u}_n^{\varepsilon}, \widetilde{z}_n^{\varepsilon})\}_{n \in \mathbb{N}} \subset \mathfrak{X} \times \mathfrak{X}$ be a sequence such that

$$(\widetilde{u}_n^{\varepsilon}, \widetilde{z}_n^{\varepsilon}) \to (\widetilde{u}^{\varepsilon}, \widetilde{z}^{\varepsilon}) \text{ in } \mathfrak{X} \times \mathfrak{X}, \text{ as } n \to +\infty.$$
 (5.20)

Therefore, $\{(\widetilde{u}_n^{\varepsilon}, \widetilde{z}_n^{\varepsilon})\}_{n \in \mathbb{N}}$ is bounded in $\mathfrak{X} \times \mathfrak{X}$, and from item 3 we deduce that $\{(u_n^{\varepsilon}, z_n^{\varepsilon}) = R(\widetilde{u}_n^{\varepsilon}, \widetilde{z}_n^{\varepsilon})\}_{n \in \mathbb{N}}$ is bounded in $\widetilde{\mathfrak{X}} \times \widetilde{\mathfrak{X}}$. Then, there exist $(\hat{u}^{\varepsilon}, \hat{z}^{\varepsilon})$ and a subsequence of $\{R(\widetilde{u}_n^{\varepsilon}, \widetilde{z}_n^{\varepsilon})\}_{n \in \mathbb{N}}$ still denoted by $\{R(\widetilde{u}_n^{\varepsilon}, \widetilde{z}_n^{\varepsilon})\}_{n \in \mathbb{N}}$ such that

$$R(\widetilde{u}_n^{\varepsilon}, \widetilde{z}_n^{\varepsilon}) \to (\hat{u}^{\varepsilon}, \hat{z}^{\varepsilon}) \quad \text{weakly in } \widetilde{\mathfrak{X}} \times \widetilde{\mathfrak{X}} \text{ and strongly in } \mathfrak{X} \times \mathfrak{X}.$$
 (5.21)

Then, from (5.20)-(5.21), a standard procedure allows us to pass to the limit, as n goes to $+\infty$, in (5.15) (with $(\widetilde{u}_n^{\varepsilon}, \widetilde{z}_n^{\varepsilon})$ and $(u_n^{\varepsilon}, z_n^{\varepsilon})$ instead of $(\widetilde{u}^{\varepsilon}, \widetilde{z}^{\varepsilon})$ and $(u^{\varepsilon}, z^{\varepsilon})$ respectively), and we deduce that $R(\widetilde{u}^{\varepsilon}, \widetilde{z}^{\varepsilon}) = (\widehat{u}^{\varepsilon}, \widehat{z}^{\varepsilon})$. Therefore, we have proved that any convergent subsequence of $\{R(\widetilde{u}_n^{\varepsilon}, \widetilde{z}_n^{\varepsilon})\}_{n \in \mathbb{N}}$ converges to $R(\widetilde{u}^{\varepsilon}, \widetilde{z}^{\varepsilon})$ strong in $\mathfrak{X} \times \mathfrak{X}$, and from uniqueness of $R(\widetilde{u}^{\varepsilon}, \widetilde{z}^{\varepsilon})$, we conclude that the whole sequence $R(\widetilde{u}^{\varepsilon}_n, \widetilde{z}^{\varepsilon}_n) \to R(\widetilde{u}^{\varepsilon}, \widetilde{z}^{\varepsilon})$ in $\mathfrak{X} \times \mathfrak{X}$. Thus, R is continuous.

Therefore, the hypotheses of the Leray-Schauder fixed point theorem are satisfied and we conclude that the map $R(\widetilde{u}^{\varepsilon}, \widetilde{z}^{\varepsilon})$ has a fixed point $(u^{\varepsilon}, z^{\varepsilon})$, that is, $R(u^{\varepsilon}, z^{\varepsilon}) = (u^{\varepsilon}, z^{\varepsilon})$, which is a solution of problem (5.11)-(5.12).

Existence of weak-strong solutions of (5.1)5.3.2

Theorem 5.3.3 There exists at least one (u, v) weak-strong solution of problem (5.1).

Proof. Observe that a variational problem associated to (5.12) is:

$$\begin{cases} \int_{0}^{T} \langle \partial_{t} u^{\varepsilon}, \bar{u} \rangle + \int_{0}^{T} (\nabla u^{\varepsilon}, \nabla \bar{u}) + \int_{0}^{T} (u^{\varepsilon} \nabla v^{\varepsilon}, \nabla \bar{u}) = 0, \quad \forall \bar{u} \in L^{\frac{10p}{7p-6}}(0, T; W^{1, \frac{10p}{7p-6}}(\Omega)) \\ \int_{0}^{T} \langle \partial_{t} z^{\varepsilon}, \bar{z} \rangle + \int_{0}^{T} (\nabla z^{\varepsilon}, \nabla \bar{z}) + \int_{0}^{T} (z^{\varepsilon}, \bar{z}) = \int_{0}^{T} ((u^{\varepsilon})^{p}, \bar{z}), \quad \forall \bar{z} \in L^{\frac{5}{2}}(0, T; H^{1}(\Omega)). \end{cases}$$

$$(5.22)$$

Recall that $v^{\varepsilon} = v^{\varepsilon}(z^{\varepsilon})$ is the unique solution of problem (5.13). From (5.17) we have that $(u^{\varepsilon}, v^{\varepsilon})$ satisfies the following energy equality:

$$\frac{d}{dt}\mathcal{E}_{\varepsilon}(u^{\varepsilon}, v^{\varepsilon}) + \frac{4}{p} \|\nabla((u^{\varepsilon})^{p/2})\|_{0}^{2} + \varepsilon \|\Delta v^{\varepsilon}\|_{1}^{2} + \|\nabla v^{\varepsilon}\|_{1}^{2} = 0.$$
(5.23)

Then, from (5.23) and using (5.18) we deduce that

$$\{u^{\varepsilon}\} \text{ is bounded in } L^{\infty}(0, +\infty; L^{p}(\Omega)) \cap L^{p}(0, T; L^{3p}(\Omega)) \hookrightarrow L^{\frac{3p}{3}}(0, T; L^{\frac{3p}{3}}(\Omega)),$$

$$\{v^{\varepsilon}\} \text{ is bounded in } L^{\infty}(0, +\infty; H^{1}(\Omega)) \cap L^{2}(0, T; H^{2}(\Omega)),$$

$$\sqrt{\varepsilon}\Delta v^{\varepsilon} \text{ is bounded in } L^{\infty}(0, +\infty; L^{2}(\Omega)) \cap L^{2}(0, T; H^{1}(\Omega)),$$

$$(5.24)$$

and therefore,

$$z^{\varepsilon} \text{ is bounded in } L^{\infty}(0, +\infty; L^{2}(\Omega)) \cap L^{2}(0, T; H^{1}(\Omega)),$$

$$\{\partial_{t}u^{\varepsilon}\} \text{ is bounded in } L^{\frac{10p}{3p+6}}(0, T; W^{1, \frac{10p}{7p-6}}(\Omega)'), \qquad (5.25)$$

$$\{\partial_{t}z^{\varepsilon}\} \text{ is bounded in } L^{\frac{5}{3}}(0, T; H^{1}(\Omega)').$$

Moreover, taking into account that from (5.23) and (5.24)₁ we have that $\nabla((u^{\varepsilon})^{p/2})$ is bounded in $L^2(0,T;L^2(\Omega))$ and $u^{1-\frac{p}{2}}$ is bounded in $L^{\frac{10p}{6-3p}}(0,T;L^{\frac{10p}{6-3p}}(\Omega))$, we conclude that $\nabla u^{\varepsilon} = \frac{2}{p} u^{1-\frac{p}{2}} \nabla ((u^{\varepsilon})^{p/2}) \text{ is bounded in } L^{\frac{5p}{p+3}}(0,T;L^{\frac{5p}{p+3}}(\Omega)). \text{ Therefore, we deduce that}$ {

$$\{u^{\varepsilon}\}$$
 is bounded in $L^{\frac{op}{p+3}}(0,T;W^{1,\frac{op}{p+3}}(\Omega)).$ (5.26)

Notice that from (5.13) and (5.24), we can deduce that $||z^{\varepsilon} - v^{\varepsilon}||_0 \leq \varepsilon ||\Delta v^{\varepsilon}||_0 \to 0$ as $\varepsilon \to 0$. Moreover, taking into account (5.25)₂ and (5.26), the Aubin-Lions Lemma implies that $\{u^{\varepsilon}\}$ is relatively compact in $L^{\frac{5p}{p+3}}(0,T;L^2(\Omega))$. Then, using these facts as well as (5.24)-(5.26), we deduce that there exists (u,v), with $u \geq 0$ a.e. in $(0,+\infty) \times \Omega$, with

$$\begin{cases} u \in L^{\infty}(0, +\infty; L^{p}(\Omega)) \cap L^{\frac{5p}{3}}(0, T; L^{\frac{5p}{3}}(\Omega)) \cap L^{\frac{5p}{p+3}}(0, T; W^{1, \frac{5p}{p+3}}(\Omega)), \\ v \in L^{\infty}(0, +\infty; H^{1}(\Omega)) \cap L^{2}(0, T; H^{2}(\Omega)), \end{cases}$$

such that for some subsequence of $\{u^{\varepsilon}, z^{\varepsilon}, v^{\varepsilon}\}$ still denoted by $\{u^{\varepsilon}, z^{\varepsilon}, v^{\varepsilon}\}$, the following convergences hold when $\varepsilon \to 0$,

$$\begin{cases} u^{\varepsilon} \to u \quad \text{weakly in} \quad L^{\frac{5p}{3}}(0,T;L^{\frac{5p}{3}}(\Omega)) \cap L^{\frac{5p}{p+3}}(0,T;W^{1,\frac{5p}{p+3}}(\Omega)), \\ v^{\varepsilon} \to v \quad \text{weakly in} \quad L^{2}(0,T;H^{2}(\Omega)), \\ z^{\varepsilon} \to v \quad \text{weakly in} \quad L^{2}(0,T;H^{1}(\Omega)), \\ \partial_{t}u^{\varepsilon} \to \partial_{t}u \quad \text{weakly in} \quad L^{\frac{10p}{3p+6}}(0,T;W^{1,\frac{10p}{7p-6}}(\Omega)'), \\ \partial_{t}z^{\varepsilon} \to \partial_{t}v \quad \text{weakly in} \quad L^{\frac{5}{3}}(0,T;H^{1}(\Omega)'). \end{cases}$$
(5.27)

Taking into account that the embedding $L^{\infty}(0,T;L^2(\Omega)) \cap L^2(0,T;H^1(\Omega)) \hookrightarrow L^3(0,T;L^3(\Omega))$ is compact, from $(5.24)_2$ we deduce that

$$\nabla v^{\varepsilon} \to \nabla v \text{ strongly in } \boldsymbol{L}^{3}(0,T;\boldsymbol{L}^{3}(\Omega)).$$
 (5.28)

Thus, from $(5.27)_1$ and (5.28) we deduce

$$u^{\varepsilon} \nabla v^{\varepsilon} \to u \nabla v \text{ weakly in } L^{\frac{15p}{5p+9}}(0,T; L^{\frac{15p}{5p+9}}(\Omega)),$$

and therefore, using that $u^{\varepsilon} \nabla v^{\varepsilon}$ is bounded in $L^{\frac{10p}{3p+6}}(0,T;L^{\frac{10p}{3p+6}})$, we deduce that

$$u^{\varepsilon} \nabla v^{\varepsilon} \to u \nabla v \text{ weakly in } L^{\frac{10p}{3p+6}}(0,T;L^{\frac{10p}{3p+6}}).$$
 (5.29)

Thus, taking to the limit when $\varepsilon \to 0$ in (5.22), and using (5.27) and (5.29), we obtain that (u, v) satisfies

$$\int_{0}^{T} \langle \partial_{t} u, \bar{u} \rangle + \int_{0}^{T} (\nabla u, \nabla \bar{u}) + \int_{0}^{T} (u \nabla v, \nabla \bar{u}) = 0, \quad \forall \bar{u} \in L^{\frac{10p}{7p-6}}(0, T; W^{1, \frac{10p}{7p-6}}(\Omega)), \quad (5.30)$$

$$\int_{0}^{T} \langle \partial_{t} v, \bar{z} \rangle + \int_{0}^{T} (\nabla v, \nabla \bar{z}) + \int_{0}^{T} (v, \bar{z}) = \int_{0}^{T} (u^{p}, \bar{z}), \quad \forall \bar{z} \in L^{\frac{5}{2}}(0, T; H^{1}(\Omega)), \tag{5.31}$$

and therefore, integrating by parts in (5.31) and taking into account that $u^p \in L^{\frac{5}{3}}(0,T;L^{\frac{5}{3}}(\Omega))$ and $v \in L^2(0,T;H^2(\Omega))$, we arrive at

$$\partial_t v - \Delta v + v = u^p \text{ in } L^{\frac{5}{3}}(0, T; L^{\frac{5}{3}}(\Omega)),$$
 (5.32)

with $\frac{\partial v}{\partial \mathbf{n}} = 0$ on $\partial \Omega$. Notice that the limit function v is nonnegative. In fact, it follows by testing (5.32) by v_{-} and taking into account that $v_0 \geq 0$. Finally, we will prove that (u, v) satisfies the energy inequality (5.8). Indeed, integrating (5.23) in time from t_0 to t_1 , with $t_1 > t_0 \geq 0$, and taking into account that

$$\int_{t_0}^{t_1} \frac{d}{dt} \mathcal{E}_{\varepsilon}(u^{\varepsilon}, v^{\varepsilon}) = \mathcal{E}_{\varepsilon}(u^{\varepsilon}(t_1), v^{\varepsilon}(t_1)) - \mathcal{E}_{\varepsilon}(u^{\varepsilon}(t_0), v^{\varepsilon}(t_0)) \quad \forall t_0 < t_1,$$

since $\mathcal{E}_{\varepsilon}(u^{\varepsilon}(t), v^{\varepsilon}(t))$ is continuous in time, we deduce

$$\mathcal{E}_{\varepsilon}(u^{\varepsilon}(t_1), v^{\varepsilon}(t_1)) - \mathcal{E}_{\varepsilon}(u^{\varepsilon}(t_0), v^{\varepsilon}(t_0)) + \int_{t_0}^{t_1} \left(\frac{4}{p} \|\nabla((u^{\varepsilon}(t))^{p/2})\|_0^2 + \varepsilon \|\Delta v^{\varepsilon}(t)\|_1^2 + \|\nabla v^{\varepsilon}(t)\|_1^2\right) dt \le 0, \quad \forall t_0 < t_1.$$
(5.33)

Now, we will prove that

$$\mathcal{E}_{\varepsilon}(u^{\varepsilon}(t), v^{\varepsilon}(t)) \to \mathcal{E}(u(t), v(t)), \quad \text{a.e. } t \in [0, +\infty).$$
 (5.34)

From $(5.24)_1$ we can deduce that u^{ε} is relatively compact in $L^p(0,T;L^p(\Omega))$. Therefore,

$$u^{\varepsilon} \to u \text{ strongly in } L^p(0,T;L^p(\Omega)).$$
 (5.35)

Moreover, for any T > 0,

$$\begin{aligned} \|\mathcal{E}_{\varepsilon}(u^{\varepsilon}(t), v^{\varepsilon}(t)) - \mathcal{E}(u(t), v(t))\|_{L^{1}(0,T)} &= \int_{0}^{T} |\mathcal{E}_{\varepsilon}(u^{\varepsilon}(t), v^{\varepsilon}(t)) - \mathcal{E}(u(t), v(t))| dt \\ &\leq \int_{0}^{T} \left| \frac{1}{p-1} \left(\|u^{\varepsilon}(t)\|_{L^{p}}^{p} - \|u(t)\|_{L^{p}}^{p} \right) + \frac{1}{2} \left(\|\nabla v^{\varepsilon}(t)\|_{0}^{2} - \|\nabla v(t)\|_{0}^{2} \right) \right| dt + \frac{\varepsilon}{2} \|\Delta v^{\varepsilon}\|_{0}^{2} \\ &\leq C \frac{p}{p-1} \|u^{\varepsilon} - u\|_{L^{p}(0,T;L^{p})} \left(\|u^{\varepsilon}\|_{L^{p}(0,T;L^{p})}^{p} + \|u\|_{L^{p}(0,T;L^{p})}^{p} \right) \frac{p-1}{p} \\ &+ \frac{1}{2} \|\nabla v^{\varepsilon} - \nabla v\|_{L^{2}(0,T;L^{2})} \left(\|\nabla v^{\varepsilon}\|_{L^{2}(0,T;L^{2})} + \|\nabla v\|_{L^{2}(0,T;L^{2})} \right) + \frac{\varepsilon}{2} \|\Delta v^{\varepsilon}\|_{0}^{2}. \end{aligned}$$
(5.36)

Then, taking into account that $u^{\varepsilon} \to u$ strongly in $L^{p}(0,T;L^{p}(\Omega))$, $\nabla v^{\varepsilon} \to \nabla v$ strongly in $L^{2}(0,T;L^{2}(\Omega))$ for any T > 0, and Δv^{ε} is bounded in $L^{2}(0,T;L^{2}(\Omega))$, from (5.36) we conclude that $\mathcal{E}_{\varepsilon}(u^{\varepsilon}(t),v^{\varepsilon}(t)) \to \mathcal{E}(u(t),v(t))$ strongly in $L^{1}(0,T)$ for all T > 0, which implies in particular (5.34). Finally, observe that from (5.35) we have that $(u^{\varepsilon})^{p/2} \to u^{p/2}$ strongly in $L^2(0,T;L^2(\Omega))$; and since $\nabla((u^{\varepsilon})^{p/2}$ is bounded in $L^2(0,T;L^2(\Omega))$ we deduce that

$$\nabla((u^{\varepsilon})^{p/2}) \to \nabla(u^{p/2})$$
 weakly in $L^2(0,T;L^2(\Omega))$.

Then, on the one hand

$$\begin{aligned} \liminf_{\varepsilon \to 0} \int_{t_0}^{t_1} \left(\frac{4}{p} \| \nabla ((u^{\varepsilon}(t))^{p/2}) \|_0^2 + \varepsilon \| \Delta v^{\varepsilon}(t) \|_1^2 + \| \nabla v^{\varepsilon}(t) \|_1^2 \right) dt \\ \geq \int_{t_0}^{t_1} \left(\frac{4}{p} \| \nabla (u(t)^{p/2}) \|_0^2 + \| \nabla v(t) \|_1^2 \right) dt \quad \forall t_1 \ge t_0 \ge 0, \end{aligned}$$

and on the other hand, owing to (5.34),

$$\liminf_{\varepsilon \to 0} \left[\mathcal{E}_{\varepsilon}(u^{\varepsilon}(t_1), v^{\varepsilon}(t_1)) - \mathcal{E}_{\varepsilon}(u^{\varepsilon}(t_0), v^{\varepsilon}(t_0)) \right] = \mathcal{E}(u(t_1), v(t_1)) - \mathcal{E}(u(t_0), v(t_0)),$$

for a.e. $t_1, t_0 : t_1 \ge t_0 \ge 0$. Thus, taking limits as $\varepsilon \to 0$ in the inequality (5.33), we deduce the energy inequality (5.8) for a.e. $t_0, t_1 : t_1 \ge t_0 \ge 0$.

5.4 Fully discrete numerical schemes

In this section we will propose three fully discrete numerical schemes associated to model (5.1). We prove some unconditional properties such as mass-conservation, energy-stability and solvability of the schemes.

5.4.1 Scheme UV ε

In this section, in order to construct an energy-stable fully discrete scheme of model (5.1), we are going to make a regularization procedure, in which we will adapt the ideas of [3] (see also [12]). With this aim, given $\varepsilon \in (0, 1)$ we consider a function $F_{\varepsilon} : \mathbb{R} \to [0, +\infty)$, approximation of $f(s) = s^p$, such that $F_{\varepsilon} \in C^2(\mathbb{R})$ and

$$F_{\varepsilon}''(s) := \begin{cases} \varepsilon^{p-2} & \text{if } s \leq \varepsilon, \\ s^{p-2} & \text{if } \varepsilon \leq s \leq \varepsilon^{-1}, \\ \varepsilon^{2-p} & \text{if } s \geq \varepsilon^{-1}. \end{cases}$$
(5.37)

Then, F_{ε} is obtained integrating in (5.37) and imposing the conditions $F'_{\varepsilon}(1) = \frac{1}{p-1}$ and $F_{\varepsilon}(1) = \frac{1}{p(p-1)} + \frac{p^3 - 4p^2 + 3p + 2}{2p(p-1)^2} \varepsilon^p$ (see Figure 5.1); and

$$a_{\varepsilon}(s) := (p-1)\frac{F'_{\varepsilon}(s)}{F''_{\varepsilon}(s)} = \begin{cases} (p-1)s + (2-p)\varepsilon & \text{if } s \leq \varepsilon, \\ s & \text{if } \varepsilon \leq s \leq \varepsilon^{-1}, \\ (p-1)s + (2-p)\varepsilon^{-1} & \text{if } s \geq \varepsilon^{-1}. \end{cases}$$
(5.38)





(b) $F'_{\varepsilon}(s)$ vs $F'(s) := \frac{1}{p-1}s^{p-1}$

(a) $F_{\varepsilon}(s)$ vs $F(s) := \frac{1}{p(p-1)}s^p + \frac{p^3 - 4p^2 + 3p + 2}{2p(p-1)^2}\varepsilon^p$



(c) $F_{\varepsilon}''(s)$ vs $F''(s) := s^{p-2}$

Figure 5.1: The function F_{ε} and its derivatives.

Lemma 5.4.1 The function F_{ε} satisfies

$$F_{\varepsilon}(s) \ge \frac{\varepsilon^{p-2}s^2}{4} \qquad \forall s \le \varepsilon \quad and \quad F_{\varepsilon}(s) \ge Cs^p \qquad \forall s > \varepsilon,$$
 (5.39)

where the constant C > 0 is independent of ε .

Proof. Since $F_{\varepsilon} \in C^2(\mathbb{R})$, using the Taylor formula as well as the definition of F_{ε} and F'_{ε} , we have that, for some $s_0 \in \mathbb{R}$ between 0 and s,

$$F_{\varepsilon}(s) = F_{\varepsilon}(0) + F_{\varepsilon}'(0)s + \frac{1}{2}F_{\varepsilon}''(s_0)s^2 = \left(\frac{2-p}{p-1}\right)^2 \varepsilon^p + \frac{2-p}{p-1}\varepsilon^{p-1}s + \frac{1}{2}F_{\varepsilon}''(s_0)s^2.$$
(5.40)

Then, taking into account that $F_{\varepsilon}''(s) = \varepsilon^{p-2}$ for all $s \leq \varepsilon$, from (5.40) we have that: (a) if $s \in [0, \varepsilon], F_{\varepsilon}(s) \geq \frac{1}{2}\varepsilon^{p-2}s^2$; and (b) if s < 0, by using the Young inequality,

$$F_{\varepsilon}(s) \ge \left(\frac{2-p}{p-1}\right)^2 \varepsilon^p - \frac{1}{4} \varepsilon^{p-2} s^2 - \left(\frac{2-p}{p-1}\right)^2 \varepsilon^p + \frac{1}{2} \varepsilon^{p-2} s^2 = \frac{1}{4} \varepsilon^{p-2} s^2,$$

from which we deduce $(5.39)_1$. Finally, $(5.39)_2$ follows directly from the definition of F_{ε} for $s \geq \varepsilon$.

Remark 5.4.2 Notice that estimates in (5.39) imply that $|s|^p \leq K_1 F_{\varepsilon}(s) + K_2$ for all $s \in \mathbb{R}$, where the constants $K_1, K_2 > 0$ are independent of ε .

Then, taking into account the functions F_{ε} , its derivatives and a_{ε} , a regularized version of problem (5.1) reads: Find $u_{\varepsilon} : \Omega \times [0,T] \to \mathbb{R}$ and $v_{\varepsilon} : \Omega \times [0,T] \to \mathbb{R}$, with $u_{\varepsilon}, v_{\varepsilon} \ge 0$, such that

$$\begin{cases} \partial_t u_{\varepsilon} - \Delta u_{\varepsilon} - \nabla \cdot (a_{\varepsilon}(u_{\varepsilon})\nabla v_{\varepsilon}) = 0 \quad \text{in } \Omega, \ t > 0, \\ \partial_t v_{\varepsilon} - \Delta v_{\varepsilon} + v_{\varepsilon} = p(p-1)F_{\varepsilon}(u_{\varepsilon}) \quad \text{in } \Omega, \ t > 0, \\ \frac{\partial u_{\varepsilon}}{\partial \mathbf{n}} = \frac{\partial v_{\varepsilon}}{\partial \mathbf{n}} = 0 \quad \text{on } \partial\Omega, \ t > 0, \\ u_{\varepsilon}(\boldsymbol{x}, 0) = u_0(\boldsymbol{x}) \ge 0, \ v_{\varepsilon}(\boldsymbol{x}, 0) = v_0(\boldsymbol{x}) \ge 0 \quad \text{in } \Omega. \end{cases}$$
(5.41)

Remark 5.4.3 The idea is to define a fully discrete scheme associated to (5.41), taking in general $\varepsilon = \varepsilon(k, h)$, such that $\varepsilon(k, h) \to 0$ as $(k, h) \to 0$, where k is the time step and h the mesh size.

Observe that (formally) multiplying $(5.41)_1$ by $pF'_{\varepsilon}(u_{\varepsilon})$, $(5.41)_2$ by $-\Delta v_{\varepsilon}$, integrating over Ω and adding, the chemotaxis and production terms cancel and we obtain the following energy law

$$\frac{d}{dt} \int_{\Omega} \left(pF_{\varepsilon}(u_{\varepsilon}) + \frac{1}{2} |\nabla v_{\varepsilon}|^2 \right) d\boldsymbol{x} + \int_{\Omega} pF_{\varepsilon}''(u_{\varepsilon}) |\nabla u_{\varepsilon}|^2 d\boldsymbol{x} + \|\nabla v_{\varepsilon}\|_1^2 = 0.$$

In particular, the modified energy

$$\mathcal{E}_{\varepsilon}(u,v) = \int_{\Omega} \left(pF_{\varepsilon}(u) + \frac{1}{2} |\nabla v|^2 \right) d\boldsymbol{x}$$

is decreasing in time. Thus, we consider a fully discrete approximation of the regularized problem (5.41) using a FE discretization in space and the backward Euler discretization 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, $h_K = diam(K)$ and $h := \max_{K \in \mathcal{T}_h} h_K$, so that $\overline{\Omega} = \bigcup_{K \in \mathcal{T}_h} \overline{K}$. Further, let $\mathcal{N}_h = \{\mathbf{a}_i\}_{i \in \mathcal{I}}$ denote the set of all the vertices of \mathcal{T}_h , and 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_{ε} and v_{ε} :

$$(U_h, V_h) \subset H^1(\Omega)^2$$
, generated by $\mathbb{P}_1, \mathbb{P}_r$ with $r \ge 1$

Remark 5.4.4 The right-angled constraint (**H**) and the approximation of U_h by \mathbb{P}_1 -continuous FE are necessary to obtain the relations (5.44)-(5.45) below, which are essential in order to obtain the energy-stability of the scheme $UV\varepsilon$ (see Theorem 5.4.9 below).

We denote the Lagrange interpolation operator by $\Pi^h : C(\overline{\Omega}) \to U_h$, 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):

$$(u_1, u_2)^h := \int_{\Omega} \Pi^h(u_1 u_2), \quad |u|_h = \sqrt{(u, u)^h}.$$
 (5.42)

Remark 5.4.5 In U_h , the norms $|\cdot|_h$ and $||\cdot||_0$ are equivalents uniformly with respect to h (see [5]).

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

$$(Q^h u, \bar{u})^h = (u, \bar{u}), \quad \forall \bar{u} \in U_h, \tag{5.43}$$

and the standard H^1 -projection $\mathbb{R}^h : H^1(\Omega) \to V_h$. Moreover, owing to the right angled constraint (**H**) and the choice of \mathbb{P}_1 -continuous FE for U_h , following the ideas of [3] (see also [12]), for each $\varepsilon \in (0, 1)$, we can construct two operators $\Lambda^i_{\varepsilon} : U_h \to L^{\infty}(\Omega)^{d \times d}$ (i = 1, 2) such that $\Lambda^i_{\varepsilon} u^h$ are symmetric matrices and $\Lambda^1_{\varepsilon} u^h$ is positive definite, for all $u^h \in U_h$ and a.e. in Ω , and satisfy

$$(\Lambda^{1}_{\varepsilon}u^{h})\nabla\Pi^{h}(F'_{\varepsilon}(u^{h})) = \nabla u^{h} \quad \text{in } \Omega,$$
(5.44)

$$(\Lambda_{\varepsilon}^2 u^h) \nabla \Pi^h(F_{\varepsilon}'(u^h)) = (p-1) \nabla \Pi^h(F_{\varepsilon}(u^h)) \quad \text{in } \Omega.$$
(5.45)

Basically, $\Lambda_{\varepsilon}^{i} u^{h}$ (i = 1, 2) are constant by elements matrices such that (5.44) and (5.45) holds by elements. In the 1-dimensional case, $\Lambda_{\varepsilon}^{i}$ are constructed as follows: For all $u^{h} \in U_{h}$ and $K \in \mathcal{T}_{h}$ with vertices \mathbf{a}_{0}^{K} and \mathbf{a}_{1}^{K} , we set

$$\Lambda_{\varepsilon}^{1}(u^{h})|_{K} := \begin{cases} \frac{u^{h}(\mathbf{a}_{1}^{K}) - u^{h}(\mathbf{a}_{0}^{K})}{F_{\varepsilon}'(u^{h}(\mathbf{a}_{1}^{K})) - F_{\varepsilon}'(u^{h}(\mathbf{a}_{0}^{K}))} & \text{if } u^{h}(\mathbf{a}_{0}^{K}) \neq u^{h}(\mathbf{a}_{1}^{K}), \\ \frac{1}{F_{\varepsilon}''(u^{h}(\mathbf{a}_{0}^{K}))} & \text{if } u^{h}(\mathbf{a}_{0}^{K}) = u^{h}(\mathbf{a}_{1}^{K}), \end{cases}$$
(5.46)

for some $\xi \in K$, and

$$\Lambda_{\varepsilon}^{2}(u^{h})|_{K} := \begin{cases} (p-1)\frac{F_{\varepsilon}(u^{h}(\mathbf{a}_{1}^{K})) - F_{\varepsilon}(u^{h}(\mathbf{a}_{0}^{K}))}{F_{\varepsilon}'(u^{h}(\mathbf{a}_{1}^{K})) - F_{\varepsilon}'(u^{h}(\mathbf{a}_{0}^{K}))} = (p-1)\frac{F_{\varepsilon}'(u^{h}(\xi_{1}))}{F_{\varepsilon}''(u^{h}(\xi_{2}))} & \text{if } u^{h}(\mathbf{a}_{0}^{K}) \neq u^{h}(\mathbf{a}_{1}^{K}), \\ (p-1)\frac{F_{\varepsilon}'(u^{h}(\mathbf{a}_{0}^{K}))}{F_{\varepsilon}''(u^{h}(\mathbf{a}_{0}^{K}))} & \text{if } u^{h}(\mathbf{a}_{0}^{K}) = u^{h}(\mathbf{a}_{1}^{K}), \end{cases}$$
(5.47)

for some $\xi_1, \xi_2 \in K$. Following [3] (see also [12]), these constructions can be extended to dimensions 2 and 3, and from (5.46) the following estimate holds:

$$\varepsilon^{2-p}\xi^T\xi \le \xi^T\Lambda^1_{\varepsilon}(u^h)^{-1}\xi \le \varepsilon^{p-2}\xi^T\xi, \quad \forall \xi \in \mathbb{R}^d, \ u^h \in U_h.$$
(5.48)

Now, we prove the following result which will be used to proof the well-posedness of the scheme $\mathbf{UV}\varepsilon$.

Lemma 5.4.6 Let $\|\cdot\|$ denote the spectral norm on $\mathbb{R}^{d\times d}$. Then for any given $\varepsilon \in (0,1)$ the function $\Lambda^2_{\varepsilon}: U_h \to [L^{\infty}(\Omega)]^{d\times d}$ satisfies, for all $u_1^h, u_2^h \in U_h$ and $K \in \mathfrak{T}_h$ with vertices $\{\mathbf{a}_l^K\}_{l=0}^d$,

$$\begin{aligned} \| (\Lambda_{\varepsilon}^{2}(u_{1}^{h}) - \Lambda_{\varepsilon}^{2}(u_{2}^{h}))|_{K} \| \\ &\leq 3\varepsilon^{2(p-2)} \max\{1, (p-1)\varepsilon^{2(p-2)}\} \max_{l=1,\dots,d} \{ |u_{1}^{h}(\mathbf{a}_{l}^{K}) - u_{2}^{h}(\mathbf{a}_{l}^{K}))| + |u_{1}^{h}(\mathbf{a}_{0}^{K}) - u_{2}^{h}(\mathbf{a}_{0}^{K})| \} \\ \end{aligned}$$

where \mathbf{a}_0^K is the right-angled vertex.

Proof. The proof follows the ideas of [4, Lemma 2.1], with some modifications. For simplicity in the notation, we will prove (5.49) in the 1-dimensional case, but this proof can be extended to dimensions 2 and 3 as in [4, Lemma 2.1]. Observe that, from (5.47)

$$\| (\Lambda_{\varepsilon}^{2}(u_{1}^{h}) - \Lambda_{\varepsilon}^{2}(u_{2}^{h}))|_{K} \| \leq |(\Lambda_{\varepsilon}^{2}(u_{1}^{h}) - \Lambda_{\varepsilon}^{2}(u_{1,2}^{h}))|_{K}| + |(\Lambda_{\varepsilon}^{2}(u_{1,2}^{h}) - \Lambda_{\varepsilon}^{2}(u_{2}^{h}))|_{K}|$$

$$= (p-1) \left| \frac{F_{\varepsilon}'(\mu_{11})}{F_{\varepsilon}''(\mu_{12})} - \frac{F_{\varepsilon}'(\xi_{1})}{F_{\varepsilon}''(\xi_{2})} \right| + (p-1) \left| \frac{F_{\varepsilon}'(\xi_{1})}{F_{\varepsilon}''(\xi_{2})} - \frac{F_{\varepsilon}'(\mu_{21})}{F_{\varepsilon}''(\mu_{22})} \right|,$$
(5.50)

where $u_{1,2}^h \in \mathbb{P}_1(K)$ with $u_{1,2}^h(\mathbf{a}_0^K) = u_2^h(\mathbf{a}_0^K)$ and $u_{1,2}^h(\mathbf{a}_1^K) = u_1^h(\mathbf{a}_1^K)$, μ_{1i} (i = 1, 2) lie between $u_1^h(\mathbf{a}_0^K)$ and $u_1^h(\mathbf{a}_1^K)$, μ_{2i} (i = 1, 2) lie between $u_2^h(\mathbf{a}_0^K)$ and $u_2^h(\mathbf{a}_1^K)$, and ξ_i (i = 1, 2) lie between $u_1^h(\mathbf{a}_1^K)$ and $u_2^h(\mathbf{a}_1^K)$, and ξ_i (i = 1, 2) lie between $u_1^h(\mathbf{a}_1^K)$ and $u_2^h(\mathbf{a}_0^K)$. Then, first we will show that

$$(p-1)\left|\frac{F_{\varepsilon}'(\mu_{11})}{F_{\varepsilon}''(\mu_{12})} - \frac{F_{\varepsilon}'(\xi_1)}{F_{\varepsilon}''(\xi_2)}\right| \le 3\varepsilon^{2(p-2)} \max\{1, (p-1)\varepsilon^{2(p-2)}\}|u_1^h(\mathbf{a}_0^K) - u_2^h(\mathbf{a}_0^K)|, \quad (5.51)$$

for $u_1^h(\mathbf{a}_0^K) \neq u_2^h(\mathbf{a}_0^K)$, because the case $u_1^h(\mathbf{a}_0^K) = u_2^h(\mathbf{a}_0^K)$ is trivially true. With this aim, we consider γ_i (i = 1, 2) lying between $u_1^h(\mathbf{a}_0^K)$ and $u_2^h(\mathbf{a}_0^K)$ such that

$$F_{\varepsilon}'(\gamma_1) = \frac{F_{\varepsilon}(u_2^h(\mathbf{a}_0^K)) - F_{\varepsilon}(u_1^h(\mathbf{a}_0^K))}{u_2^h(\mathbf{a}_0^K) - u_1^h(\mathbf{a}_0^K)} \quad \text{and} \quad F_{\varepsilon}''(\gamma_2) = \frac{F_{\varepsilon}'(u_2^h(\mathbf{a}_0^K)) - F_{\varepsilon}'(u_1^h(\mathbf{a}_0^K))}{u_2^h(\mathbf{a}_0^K) - u_1^h(\mathbf{a}_0^K)}, \quad (5.52)$$

and therefore, from (5.50) and (5.52), we deduce

$$(u_2^h(\mathbf{a}_0^K) - u_1^h(\mathbf{a}_0^K))F_{\varepsilon}'(\gamma_1) = (u_2^h(\mathbf{a}_0^K) - u_1^h(\mathbf{a}_1^K))F_{\varepsilon}'(\xi_1) + (u_1^h(\mathbf{a}_1^K) - u_1^h(\mathbf{a}_0^K))F_{\varepsilon}'(\mu_{11}), \quad (5.53)$$

$$(u_2^h(\mathbf{a}_0^K) - u_1^h(\mathbf{a}_0^K))F_{\varepsilon}''(\gamma_2) = (u_2^h(\mathbf{a}_0^K) - u_1^h(\mathbf{a}_1^K))F_{\varepsilon}''(\xi_2) + (u_1^h(\mathbf{a}_1^K) - u_1^h(\mathbf{a}_0^K))F_{\varepsilon}''(\mu_{12}).$$
(5.54)

Then, for $u_2^h(\mathbf{a}_0^K)$, $u_1^h(\mathbf{a}_0^K)$ and $u_1^h(\mathbf{a}_1^K)$, there are only 3 options: (1) $u_1^h(\mathbf{a}_1^K)$ lies between $u_2^h(\mathbf{a}_0^K)$ and $u_1^h(\mathbf{a}_0^K)$; (ii) $u_2^h(\mathbf{a}_0^K)$ lies between $u_1^h(\mathbf{a}_1^K)$ and $u_1^h(\mathbf{a}_0^K)$; and (iii) $u_1^h(\mathbf{a}_0^K)$ lies between $u_1^h(\mathbf{a}_1^K)$ and $u_2^h(\mathbf{a}_0^K)$; and $(iii) u_1^h(\mathbf{a}_0^K)$ lies between $u_1^h(\mathbf{a}_1^K)$ and $u_2^h(\mathbf{a}_0^K)$.

Notice that from (5.37)-(5.38), we have that F'_{ε} and $(p-1)\frac{F'_{\varepsilon}}{F''_{\varepsilon}}$ are globally Lipschitz functions with constants ε^{p-2} and 1 respectively, and $\frac{1}{|F''_{\varepsilon}|} \leq \varepsilon^{p-2}$. Then, in case (i), taking into account that all intermediate values $\mu_{1i}, \gamma_i, \xi_i$ (i = 1, 2) lie between $u_2^h(\mathbf{a}_0^K)$ and $u_1^h(\mathbf{a}_0^K)$, we have

$$(p-1) \left| \frac{F_{\varepsilon}'(\mu_{11})}{F_{\varepsilon}''(\mu_{12})} - \frac{F_{\varepsilon}'(\xi_{1})}{F_{\varepsilon}''(\xi_{2})} \right| \leq (p-1) \left| \frac{F_{\varepsilon}'(\mu_{11}) - F_{\varepsilon}'(\mu_{12})}{F_{\varepsilon}''(\mu_{12})} \right| \\ + (p-1) \left| \frac{F_{\varepsilon}'(\mu_{12})}{F_{\varepsilon}''(\mu_{12})} - \frac{F_{\varepsilon}'(\xi_{2})}{F_{\varepsilon}''(\xi_{2})} \right| + (p-1) \left| \frac{F_{\varepsilon}'(\xi_{1}) - F_{\varepsilon}'(\xi_{2})}{F_{\varepsilon}''(\xi_{2})} \right| \\ \leq (p-1)\varepsilon^{2(p-2)} |\mu_{11} - \mu_{12}| + |\mu_{12} - \xi_{2}| + (p-1)\varepsilon^{2(p-2)} |\xi_{1} - \xi_{2}| \\ \leq 3 \max\{1, (p-1)\varepsilon^{2(p-2)}\} |u_{1}^{h}(\mathbf{a}_{0}^{K}) - u_{2}^{h}(\mathbf{a}_{0}^{K})|.$$
(5.55)

In case (ii), all intermediate values $\mu_{1i}, \gamma_i, \xi_i$ (i = 1, 2) lie between $u_1^h(\mathbf{a}_1^K)$ and $u_1^h(\mathbf{a}_0^K)$, and from (5.53)-(5.54) by eliminating the term $(u_2^h(\mathbf{a}_0^K) - u_1^h(\mathbf{a}_1^K))$, we have the equality

$$(u_1^h(\mathbf{a}_1^K) - u_1^h(\mathbf{a}_0^K)) \left[\frac{F_{\varepsilon}'(\xi_1)}{F_{\varepsilon}''(\xi_2)} - \frac{F_{\varepsilon}'(\mu_{11})}{F_{\varepsilon}''(\mu_{12})} \right] = (u_2^h(\mathbf{a}_0^K) - u_1^h(\mathbf{a}_0^K)) \frac{F_{\varepsilon}''(\gamma_2)}{F_{\varepsilon}''(\mu_{12})} \left[\frac{F_{\varepsilon}'(\xi_1)}{F_{\varepsilon}''(\xi_2)} - \frac{F_{\varepsilon}'(\gamma_1)}{F_{\varepsilon}''(\gamma_2)} \right],$$

from which, bounding the term $\left|\frac{F'_{\varepsilon}(\xi_1)}{F''_{\varepsilon}(\xi_2)} - \frac{F'_{\varepsilon}(\gamma_1)}{F''_{\varepsilon}(\gamma_2)}\right|$ as in (5.55), we obtain

$$(p-1) |u_1^h(\mathbf{a}_1^K) - u_1^h(\mathbf{a}_0^K))| \left| \frac{F_{\varepsilon}'(\mu_{11})}{F_{\varepsilon}''(\mu_{12})} - \frac{F_{\varepsilon}'(\xi_1)}{F_{\varepsilon}''(\xi_2)} \right| \\ \leq \varepsilon^{2(p-2)} 3 \max\{1, (p-1)\varepsilon^{2(p-2)}\} |u_1^h(\mathbf{a}_0^K) - u_2^h(\mathbf{a}_0^K)| |u_1^h(\mathbf{a}_1^K) - u_1^h(\mathbf{a}_0^K))|,$$

and therefore, dividing by $|u_1^h(\mathbf{a}_1^K) - u_1^h(\mathbf{a}_0^K))|$ we arrive at

$$(p-1)\left|\frac{F_{\varepsilon}'(\mu_{11})}{F_{\varepsilon}''(\mu_{12})} - \frac{F_{\varepsilon}'(\xi_1)}{F_{\varepsilon}''(\xi_2)}\right| \le 3\varepsilon^{2(p-2)}\max\{1, (p-1)\varepsilon^{2(p-2)}\}|u_1^h(\mathbf{a}_0^K) - u_2^h(\mathbf{a}_0^K)|.$$
(5.56)

In case (iii), by arguing analogously to case (ii), from (5.53)-(5.54) we have

$$(u_1^h(\mathbf{a}_1^K) - u_2^h(\mathbf{a}_0^K)) \left[\frac{F_{\varepsilon}'(\xi_1)}{F_{\varepsilon}''(\xi_2)} - \frac{F_{\varepsilon}'(\mu_{11})}{F_{\varepsilon}''(\mu_{12})} \right] = (u_2^h(\mathbf{a}_0^K) - u_1^h(\mathbf{a}_0^K)) \frac{F_{\varepsilon}''(\gamma_2)}{F_{\varepsilon}''(\xi_2)} \left[\frac{F_{\varepsilon}'(\gamma_1)}{F_{\varepsilon}''(\gamma_2)} - \frac{F_{\varepsilon}'(\mu_{11})}{F_{\varepsilon}''(\mu_{12})} \right],$$

which implies (5.56). Therefore, we have proved (5.51).

Analogously, we can prove that

$$(p-1)\left|\frac{F_{\varepsilon}'(\xi_1)}{F_{\varepsilon}''(\xi_2)} - \frac{F_{\varepsilon}'(\mu_{21})}{F_{\varepsilon}''(\mu_{22})}\right| \le 3\varepsilon^{2(p-2)} \max\{1, (p-1)\varepsilon^{2(p-2)}\}|u_1^h(\mathbf{a}_1^K) - u_2^h(\mathbf{a}_1^K)|.$$
(5.57)

Thus, from (5.50), (5.51) and (5.57) we conclude (5.49).

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

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

Then, the following estimate holds (see for instance, Lemma 2.3.1):

$$\|v^{h}\|_{W^{1,6}} \le C \|A_{h}v^{h}\|_{0}, \quad \forall v^{h} \in V_{h}.$$
(5.58)

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

• <u>Scheme</u> **UV**ε:

Initialization: Let $(u^0, v^0) = (Q^h u_0, R^h v_0) \in U_h \times V_h$. **Time step** n: Given $(u_{\varepsilon}^{n-1}, v_{\varepsilon}^{n-1}) \in U_h \times V_h$, compute $(u_{\varepsilon}^n, v_{\varepsilon}^n) \in U_h \times V_h$ solving

$$\begin{cases} (\delta_t u_{\varepsilon}^n, \bar{u})^h + (\nabla u_{\varepsilon}^n, \nabla \bar{u}) = -(\Lambda_{\varepsilon}^2(u_{\varepsilon}^n) \nabla v_{\varepsilon}^n, \nabla \bar{u}), & \forall \bar{u} \in U_h, \\ (\delta_t v_{\varepsilon}^n, \bar{v}) + (A_h v_{\varepsilon}^n, \bar{v}) = p(p-1)(\Pi^h(F_{\varepsilon}(u_{\varepsilon}^n)), \bar{v}), & \forall \bar{v} \in V_h, \end{cases}$$
(5.59)

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

Remark 5.4.7 (Positivity of v_{ε}^{n}) By using the mass-lumping technique in all terms of $(5.59)_{2}$ excepting the self-diffusion term $(\nabla v_{\varepsilon}^{n}, \nabla \bar{v})$, and approximating V_{h} by \mathbb{P}_{1} -continuous FE, we can prove that if $v_{\varepsilon}^{n-1} \geq 0$ then $v_{\varepsilon}^{n} \geq 0$. In fact, it follows testing $(5.59)_{2}$ by $\bar{v} = \Pi^{h}(v_{\varepsilon}^{n}) \in V_{h}$, where $v_{\varepsilon}^{n} := \min\{v_{\varepsilon}^{n}, 0\}$ (see Remark 4.3.10).

Mass-conservation, Energy-stability and Solvability

Since $\bar{u} = 1 \in U_h$ and $\bar{v} = 1 \in V_h$, we deduce that the scheme $\mathbf{UV}\varepsilon$ is conservative in u_{ε}^n , that is,

$$(u_{\varepsilon}^{n},1) = (u_{\varepsilon}^{n},1)^{h} = (u_{\varepsilon}^{n-1},1)^{h} = \dots = (u^{0},1)^{h} = (u^{0},1) = (Q^{h}u_{0},1) = (u_{0},1) := m_{0}, (5.60)$$

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

$$\delta_t \left(\int_{\Omega} v_{\varepsilon}^n \right) = p(p-1) \int_{\Omega} \Pi^h(F_{\varepsilon}(u_{\varepsilon}^n)) - \int_{\Omega} v_{\varepsilon}^n.$$
(5.61)

Definition 5.4.8 A numerical scheme with solution $(u_{\varepsilon}^n, v_{\varepsilon}^n)$ is called energy-stable with respect to the energy

$$\mathcal{E}^{h}_{\varepsilon}(u,v) = p(F_{\varepsilon}(u),1)^{h} + \frac{1}{2} \|\nabla v\|_{0}^{2}$$
(5.62)

if this energy is time decreasing, that is $\mathcal{E}^h_{\varepsilon}(u^n_{\varepsilon}, v^n_{\varepsilon}) \leq \mathcal{E}^h_{\varepsilon}(u^{n-1}_{\varepsilon}, v^{n-1}_{\varepsilon})$ for all $n \geq 1$.

Theorem 5.4.9 (Unconditional stability) The scheme $UV\varepsilon$ is unconditional energy stable with respect to $\mathcal{E}^h_{\varepsilon}(u, v)$. In fact, if $(u^n_{\varepsilon}, v^n_{\varepsilon})$ is a solution of $UV\varepsilon$, then the following discrete energy law holds

$$\delta_t \mathcal{E}^h_{\varepsilon}(u^n_{\varepsilon}, v^n_{\varepsilon}) + \frac{k\varepsilon^{2-p}p}{2} \|\delta_t u^n_{\varepsilon}\|^2_0 + \frac{k}{2} \|\delta_t \nabla v^n_{\varepsilon}\|^2_0 + p\varepsilon^{2-p} \|\nabla u^n_{\varepsilon}\|^2_0 + \|(A_h - I)\nabla v^n_{\varepsilon}\|^2_0 + \|\nabla v^n_{\varepsilon}\|^2_0 \le 0.$$

$$\tag{5.63}$$

Proof. Testing $(5.59)_1$ by $\bar{u} = p\Pi^h(F'_{\varepsilon}(u^n_{\varepsilon}))$ and $(5.59)_2$ by $\bar{v} = (A_h - I)v^n_{\varepsilon}$, adding and taking into account that $\Lambda^i_{\varepsilon}(u^n_{\varepsilon})$ are symmetric as well as (5.44)-(5.45), the terms $-p(\Lambda^2_{\varepsilon}(u^n_{\varepsilon})\nabla v^n_{\varepsilon}, \nabla\Pi^h(F'_{\varepsilon}(u^n_{\varepsilon}))) = -p(\nabla v^n_{\varepsilon}, \Lambda^2_{\varepsilon}(u^n_{\varepsilon})\nabla\Pi^h(F'_{\varepsilon}(u^n_{\varepsilon}))) = -p(p-1)(\nabla v^n_{\varepsilon}, \nabla\Pi^h(F_{\varepsilon}(u^n_{\varepsilon})))$

and $p(p-1)(\Pi^h(F_{\varepsilon}(u_{\varepsilon}^n)), (A_h-I)v_{\varepsilon}^n) = p(p-1)(\nabla\Pi^h(F_{\varepsilon}(u_{\varepsilon}^n)), \nabla v_{\varepsilon}^n)$ cancel, and using that $\nabla\Pi^h(F'_{\varepsilon}(u_{\varepsilon}^n)) = \Lambda^1_{\varepsilon}(u_{\varepsilon}^n)^{-1}\nabla u_{\varepsilon}^n$ we obtain

$$p(\delta_t u_{\varepsilon}^n, F_{\varepsilon}'(u_{\varepsilon}^n))^h + p \int_{\Omega} (\nabla u_{\varepsilon}^n)^T \cdot \Lambda_{\varepsilon}^1(u_{\varepsilon}^n)^{-1} \cdot \nabla u_{\varepsilon}^n d\boldsymbol{x} + \delta_t \left(\frac{1}{2} \|\nabla v_{\varepsilon}^n\|_0^2\right) + \frac{k}{2} \|\delta_t \nabla v_{\varepsilon}^n\|_0^2 + \|(A_h - I)v_{\varepsilon}^n\|_0^2 + \|\nabla v_{\varepsilon}^n\|_0^2 = 0.$$
(5.64)

Moreover, observe that from the Taylor formula we have

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

and therefore,

$$\delta_t u_{\varepsilon}^n \cdot F_{\varepsilon}'(u_{\varepsilon}^n) = \delta_t \Big(F_{\varepsilon}(u_{\varepsilon}^n) \Big) + \frac{k}{2} F_{\varepsilon}''(\theta u_{\varepsilon}^n + (1-\theta)u_{\varepsilon}^{n-1})(\delta_t u_{\varepsilon}^n)^2.$$
(5.65)

Then, using (5.65) and taking into account that Π^h is linear and $F_{\varepsilon}''(s) \ge \varepsilon^{2-p}$ for all $s \in \mathbb{R}$, we have

$$(\delta_t u_{\varepsilon}^n, F_{\varepsilon}'(u_{\varepsilon}^n))^h = \delta_t \Big(\int_{\Omega} \Pi^h(F_{\varepsilon}(u_{\varepsilon}^n)) \Big) + \frac{k}{2} \int_{\Omega} \Pi^h(F_{\varepsilon}''(\theta u_{\varepsilon}^n + (1-\theta)u_{\varepsilon}^{n-1})(\delta_t u_{\varepsilon}^n)^2) \\ \ge \delta_t \Big((F_{\varepsilon}(u_{\varepsilon}^n), 1)^h \Big) + \frac{k\varepsilon^{2-p}}{2} |\delta_t u_{\varepsilon}^n|_h^2.$$
(5.66)

Thus, from (5.64), (5.48), (5.66) and Remark 5.4.5, we arrive at (5.63).

Corollary 5.4.10 (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 $UV\varepsilon$. Then, it holds

$$p(F_{\varepsilon}(u_{\varepsilon}^{n}),1)^{h} + \frac{1}{2} \|v_{\varepsilon}^{n}\|_{1}^{2} + k \sum_{m=1}^{n} \left(p \varepsilon^{2-p} \|\nabla u_{\varepsilon}^{m}\|_{0}^{2} + \|(A_{h} - I)v_{\varepsilon}^{m}\|_{0}^{2} + \|\nabla v_{\varepsilon}^{m}\|_{0}^{2} \right) \leq \frac{C_{0}}{(p-1)^{2}}, \quad \forall n \geq 1.$$

$$(5.67)$$

$$k \sum_{m=n_0+1}^{n+n_0} \|v_{\varepsilon}^m\|_{W^{1,6}}^2 \le \frac{C_1}{(p-1)^2} (1+kn), \quad \forall n \ge 1,$$
(5.68)

where the integer $n_0 \ge 0$ is arbitrary, 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,

$$\|\Pi^{h}(u_{\varepsilon^{-}}^{n})\|_{0}^{2} \leq \frac{C_{0}}{(p-1)^{2}}\varepsilon^{2-p} \quad and \quad \|u_{\varepsilon}^{n}\|_{L^{p}}^{p} \leq \frac{C_{0}K}{(p-1)^{2}} + K, \quad \forall n \geq 1,$$
(5.69)

where $u_{\varepsilon-}^n := \min\{u_{\varepsilon}^n, 0\} \leq 0$ and the constant K > 0 is independent of k, h, n and ε .

Remark 5.4.11 (Approximated positivity of u_{ε}^{n}) From $(5.69)_{1}$, the following estimate holds

$$\max_{n \ge 0} \|\Pi^h(u_{\varepsilon-}^n)\|_0^2 \le \frac{C_0}{(p-1)^2} \varepsilon^{2-p}.$$

Proof. First, taking into account that $(u^0, v^0) = (Q^h u_0, R^h v_0), u_0 \ge 0$ (and therefore, $u^0 \ge 0$), as well as the definition of F_{ε} , we have that

$$\begin{aligned} \mathcal{E}_{\varepsilon}^{h}(u^{0}, v^{0}) &= p \int_{\Omega} \Pi^{h}(F_{\varepsilon}(u^{0})) + \frac{1}{2} \|\nabla v^{0}\|_{0}^{2} \leq \frac{C}{p-1} \int_{\Omega} \Pi^{h}\left((u^{0})^{2} + \frac{1}{p-1}\right) + \frac{1}{2} \|\nabla v^{0}\|_{0}^{2} \\ &\leq \frac{C}{p-1} \left(\|u^{0}\|_{0}^{2} + \|\nabla v^{0}\|_{0}^{2} + \frac{1}{p-1} \right) \leq \frac{C}{p-1} \left(\|u_{0}\|_{0}^{2} + \|v_{0}\|_{1}^{2} + \frac{1}{p-1} \right) \leq \frac{C_{0}}{(p-1)^{2}} (5.70) \end{aligned}$$

where the constant $C_0 > 0$ depends on the data (Ω, u_0, v_0) , but is independent of k, h, n and ε . Therefore, from the discrete energy law (5.63) and estimate (5.70), we have

$$\mathcal{E}^{h}_{\varepsilon}(u^{n}_{\varepsilon}, v^{n}_{\varepsilon}) + k \sum_{m=1}^{n} \left(p \varepsilon^{2-p} \| \nabla u^{m}_{\varepsilon} \|_{0}^{2} + \| (A_{h} - I) v^{m}_{\varepsilon} \|_{0}^{2} + \| \nabla v^{m}_{\varepsilon} \|_{0}^{2} \right) \leq \mathcal{E}^{h}_{\varepsilon}(u^{0}, v^{0}) \leq \frac{C_{0}}{(p-1)^{2}}.$$
(5.71)

Moreover, from (5.61), the definition of F_{ε} , Remark 5.4.2 and (5.71), we have

$$(1+k)\left|\int_{\Omega} v_{\varepsilon}^{n}\right| - \left|\int_{\Omega} v_{\varepsilon}^{n-1}\right| \le kp(p-1)\int_{\Omega} \Pi^{h}(F_{\varepsilon}(u_{\varepsilon}^{n})) \le k\frac{C}{p-1},$$
(5.72)

where the constant C > 0 is independent of k, h, n and ε . Then, applying Lemma 5.2.3 in (5.72) (for $\delta = 1$ and $\beta = \frac{C}{p-1}$), we arrive at

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

which, together with (5.71), imply (5.67). Moreover, adding (5.63) from $m = n_0 + 1$ to $m = n + n_0$, and using (5.58) and (5.67), we deduce (5.68).

On the other hand, from $(5.39)_1$, we have $\frac{1}{4}\varepsilon^{p-2}(u_{\varepsilon-}^n(\boldsymbol{x}))^2 \leq F_{\varepsilon}(u_{\varepsilon}^n(\boldsymbol{x}))$ for all $u_{\varepsilon}^n \in U_h$; and therefore, using that $(\Pi^h u)^2 \leq \Pi^h(u^2)$ for all $u \in C(\overline{\Omega})$, we have

$$\frac{1}{4}\varepsilon^{p-2}\int_{\Omega}(\Pi^{h}(u_{\varepsilon-}^{n}))^{2} \leq \frac{1}{4}\varepsilon^{p-2}\int_{\Omega}\Pi^{h}((u_{\varepsilon-}^{n})^{2}) \leq \int_{\Omega}\Pi^{h}(F_{\varepsilon}(u_{\varepsilon}^{n})) \leq \frac{C_{0}}{(p-1)^{2}},$$

where in the last inequality (5.67) was used. Thus, we obtain $(5.69)_1$. Finally, taking into account that $|\Pi^h u|^p \leq \Pi^h(|u|^p)$ for all $u \in C(\overline{\Omega})$, as well as Remark 5.4.2 and (5.67), we have

$$\|u_{\varepsilon}^{n}\|_{L^{p}}^{p} = \int_{\Omega} |\Pi^{h} u_{\varepsilon}^{n}|^{p} \leq \int_{\Omega} \Pi^{h} (|u_{\varepsilon}^{n}|^{p}) \leq \int_{\Omega} \Pi^{h} (K_{1} F_{\varepsilon}(u_{\varepsilon}^{n}) + K_{2}) \leq \frac{C_{0} K}{(p-1)^{2}} + K,$$

arriving at $(5.69)_2$.

Theorem 5.4.12 (Unconditional existence) There exists at least one solution $(u_{\varepsilon}^n, v_{\varepsilon}^n)$ of scheme $UV\varepsilon$.

Proof. The proof follows as in Theorem 4.3.11, by using the Leray-Schauder fixed point theorem. \blacksquare

5.4.2 Scheme $US\varepsilon$

In this section, in order to construct another energy-stable fully discrete scheme of (5.1), we are going to use the regularized functions F_{ε} , F'_{ε} and F''_{ε} defined in Section 5.4.1 and we will consider the auxiliary variable $\boldsymbol{\sigma} = \nabla v$. Then, another regularized version of problem (5.1) reads: Find $u_{\varepsilon} : \Omega \times [0, T] \to \mathbb{R}$ and $\boldsymbol{\sigma}_{\varepsilon} : \Omega \times [0, T] \to \mathbb{R}^d$, with $u_{\varepsilon} \ge 0$, such that

$$\begin{cases} \partial_t u_{\varepsilon} - \Delta u_{\varepsilon} - \nabla \cdot (u_{\varepsilon} \boldsymbol{\sigma}_{\varepsilon}) = 0 \quad \text{in } \Omega, \ t > 0, \\ \partial_t \boldsymbol{\sigma}_{\varepsilon} + \operatorname{rot}(\operatorname{rot} \boldsymbol{\sigma}_{\varepsilon}) - \nabla (\nabla \cdot \boldsymbol{\sigma}_{\varepsilon}) + \boldsymbol{\sigma}_{\varepsilon} = p \ u_{\varepsilon} \nabla (F'_{\varepsilon}(u_{\varepsilon})) \quad \text{in } \Omega, \ t > 0, \\ \frac{\partial u_{\varepsilon}}{\partial \mathbf{n}} = 0, \ \boldsymbol{\sigma}_{\varepsilon} \cdot \mathbf{n} = 0, \ [\operatorname{rot} \boldsymbol{\sigma}_{\varepsilon} \times \mathbf{n}]_{tang} = 0 \quad \text{on } \partial\Omega, \ t > 0, \\ u_{\varepsilon}(\boldsymbol{x}, 0) = u_0(\boldsymbol{x}) \ge 0, \ \boldsymbol{\sigma}_{\varepsilon}(\boldsymbol{x}, 0) = \nabla v_0(\boldsymbol{x}), \quad \text{in } \Omega. \end{cases}$$
(5.73)

This kind of formulation considering $\boldsymbol{\sigma} = \nabla v$ as auxiliary variable has been used in the construction of numerical schemes for other chemotaxis models (see for instance [18] and Chapters 2 and 4 of this PhD thesis). Once problem (5.73) is solved, we can recover v_{ε} from u_{ε} solving

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

Observe that (formally) multiplying $(5.73)_1$ by $pF'_{\varepsilon}(u_{\varepsilon})$, $(5.73)_2$ by $\boldsymbol{\sigma}_{\varepsilon}$, integrating over Ω and adding both equations, the terms $p(u_{\varepsilon}\nabla(F'_{\varepsilon}(u_{\varepsilon})), \boldsymbol{\sigma}_{\varepsilon})$ cancel, and we obtain the following energy law

$$\frac{d}{dt}\int_{\Omega}\left(pF_{\varepsilon}(u_{\varepsilon})+\frac{1}{2}|\boldsymbol{\sigma}_{\varepsilon}|^{2}\right)d\boldsymbol{x}+\int_{\Omega}pF_{\varepsilon}''(u_{\varepsilon})|\nabla u_{\varepsilon}|^{2}d\boldsymbol{x}+\|\boldsymbol{\sigma}_{\varepsilon}\|_{1}^{2}=0.$$

In particular, the modified energy

$$\mathcal{E}_{\varepsilon}(u, \boldsymbol{\sigma}) = \int_{\Omega} \left(pF_{\varepsilon}(u) + \frac{1}{2} |\boldsymbol{\sigma}|^2 \right) d\boldsymbol{x}$$
is decreasing in time. Then, we consider a fully discrete approximation of the regularized problem (5.73) using a FE discretization in space and the backward Euler discretization in time (considered for simplicity on a uniform partition of [0, T] with time step k = T/N: $(t_n = nk)_{n=0}^{n=N})$. Concerning the space discretization, we consider the triangulation as in the scheme $\mathbf{UV}\varepsilon$, imposing again the constraint (**H**) related with the right angled simplices. We choose the following continuous FE spaces for u_{ε} , $\boldsymbol{\sigma}_{\varepsilon}$, and v_{ε} :

$$(U_h, \Sigma_h, V_h) \subset H^1(\Omega)^3$$
, generated by $\mathbb{P}_1, \mathbb{P}_m, \mathbb{P}_r$ with $m, r \ge 1$.

Remark 5.4.13 The right-angled constraint (**H**) and the approximation of U_h by \mathbb{P}_1 -continuous FE are necessary again to obtain the relation (5.44) and the estimate (5.48) for Λ_{ε}^1 , which are essential in order to obtain the energy-stability of the scheme $US\varepsilon$ (see Theorem 5.4.17 below).

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

• <u>Scheme</u> $US\varepsilon$:

Initialization: Let $(u^0, \boldsymbol{\sigma}^0) = (Q^h u_0, \widetilde{Q}^h(\nabla v_0)) \in U_h \times \boldsymbol{\Sigma}_h$. **Time step** n: Given $(u_{\varepsilon}^{n-1}, \boldsymbol{\sigma}_{\varepsilon}^{n-1}) \in U_h \times \boldsymbol{\Sigma}_h$, compute $(u_{\varepsilon}^n, \boldsymbol{\sigma}_{\varepsilon}^n) \in U_h \times \boldsymbol{\Sigma}_h$ solving

$$\begin{cases} (\delta_t u_{\varepsilon}^n, \bar{u})^h + (\nabla u_{\varepsilon}^n, \nabla \bar{u}) = -(u_{\varepsilon}^n \boldsymbol{\sigma}_{\varepsilon}^n, \nabla \bar{u}), & \forall \bar{u} \in U_h, \\ (\delta_t \boldsymbol{\sigma}_{\varepsilon}^n, \bar{\boldsymbol{\sigma}}) + (B_h \boldsymbol{\sigma}_{\varepsilon}^n, \bar{\boldsymbol{\sigma}}) = p(u_{\varepsilon}^n \nabla \Pi^h(F_{\varepsilon}'(u_{\varepsilon}^n)), \bar{\boldsymbol{\sigma}}), & \forall \bar{\boldsymbol{\sigma}} \in \Sigma_h, \end{cases}$$
(5.74)

where Q^h is the L^2 -projection on U_h defined in (5.43), \tilde{Q}^h is the standard L^2 -projection on Σ_h , and the operator B_h is defined as

$$(B_h \boldsymbol{\sigma}_{\varepsilon}^n, \bar{\boldsymbol{\sigma}}) = (\text{rot } \boldsymbol{\sigma}_{\varepsilon}^n, \text{rot } \bar{\boldsymbol{\sigma}}) + (\nabla \cdot \boldsymbol{\sigma}_{\varepsilon}^n, \nabla \cdot \bar{\boldsymbol{\sigma}}) + (\boldsymbol{\sigma}_{\varepsilon}^n, \bar{\boldsymbol{\sigma}}), \quad \forall \bar{\boldsymbol{\sigma}} \in \boldsymbol{\Sigma}_h.$$

We recall that $\Pi^h : C(\overline{\Omega}) \to U_h$ is the Lagrange interpolation operator, and the discrete semi-inner product $(\cdot, \cdot)^h$ was defined in (5.42).

Remark 5.4.14 Notice that the right-angled constraint (**H**) is necessary in the implementation of the scheme $UV\varepsilon$ (in order to construct the matricial function $\Lambda^2_{\varepsilon}(u^n_{\varepsilon})$); while, for the implementation of the scheme $US\varepsilon$, this hypothesis (**H**) is not necessary. **Remark 5.4.15** Following the ideas of Chapter 4 (see Section 4.4), we can construct another unconditional energy-stable nonlinear scheme in the variables $(u_{\varepsilon}^n, \boldsymbol{\sigma}_{\varepsilon}^n)$ without imposing the right-angled constraint (**H**), replacing the self-diffusion term $(\nabla u_{\varepsilon}^n, \nabla \bar{u})$ by $\nabla \cdot (\frac{1}{F_{\varepsilon}'(u_{\varepsilon}^n)} \nabla \Pi^h(F_{\varepsilon}'(u_{\varepsilon}^n)))$. However, this scheme has convergence problems for the linear iterative method as $p \to 1$ and $\varepsilon \to 0$.

Once the scheme $\mathbf{US}\varepsilon$ 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:

$$(\delta_t v_{\varepsilon}^n, \bar{v}) + (\nabla v_{\varepsilon}^n, \nabla \bar{v}) + (v_{\varepsilon}^n, \bar{v}) = p(p-1)(F_{\varepsilon}(u_{\varepsilon}^n), \bar{v}), \quad \forall \bar{v} \in V_h.$$
(5.75)

Given $u_{\varepsilon}^{n} \in U_{h}$ and $v_{\varepsilon}^{n-1} \in V_{h}$, Lax-Milgram theorem implies that there exists a unique $v_{\varepsilon}^{n} \in V_{h}$ solution of (5.75). Moreover, notice that the result concerning to the positivity of v_{ε}^{n} solution of scheme $\mathbf{UV}_{\varepsilon}$ established in Remark 5.4.7 remains true for v_{ε}^{n} in the scheme $\mathbf{US}_{\varepsilon}$.

Mass-conservation and Energy-stability

Observe that the scheme **US** ε is also conservative in u (satisfying (5.60)), and we have the following behavior for $\int_{\Omega} v_{\varepsilon}^{n}$:

$$\delta_t \left(\int_{\Omega} v_{\varepsilon}^n \right) = p(p-1) \int_{\Omega} F_{\varepsilon}(u_{\varepsilon}^n) - \int_{\Omega} v_{\varepsilon}^n.$$

Definition 5.4.16 A numerical scheme with solution $(u_{\varepsilon}^n, \sigma_{\varepsilon}^n)$ is called energy-stable with respect to the energy

$$\mathcal{E}^{h}_{\varepsilon}(u,\boldsymbol{\sigma}) = p(F_{\varepsilon}(u),1)^{h} + \frac{1}{2} \|\boldsymbol{\sigma}\|_{0}^{2}$$
(5.76)

if this energy is time decreasing, that is $\mathcal{E}^h_{\varepsilon}(u^n_{\varepsilon}, \boldsymbol{\sigma}^n_{\varepsilon}) \leq \mathcal{E}^h_{\varepsilon}(u^{n-1}_{\varepsilon}, \boldsymbol{\sigma}^{n-1}_{\varepsilon})$ for all $n \geq 1$.

Theorem 5.4.17 (Unconditional stability) The scheme $US\varepsilon$ is unconditional energy stable with respect to $\mathcal{E}^h_{\varepsilon}(u, \sigma)$. In fact, if $(u^n_{\varepsilon}, \sigma^n_{\varepsilon})$ is a solution of $US\varepsilon$, then the following discrete energy law holds

$$\delta_t \mathcal{E}^h_{\varepsilon}(u^n_{\varepsilon}, \boldsymbol{\sigma}^n_{\varepsilon}) + \frac{k\varepsilon^{2-p}p}{2} \|\delta_t u^n_{\varepsilon}\|^2_0 + \frac{k}{2} \|\delta_t \boldsymbol{\sigma}^n_{\varepsilon}\|^2_0 + p\varepsilon^{2-p} \|\nabla u^n_{\varepsilon}\|^2_0 + \|\boldsymbol{\sigma}^n_{\varepsilon}\|^2_1 \le 0.$$
(5.77)

Proof. Testing $(5.74)_1$ by $\bar{u} = p\Pi^h(F'_{\varepsilon}(u^n_{\varepsilon}))$, $(5.74)_2$ by $\bar{\boldsymbol{\sigma}} = \boldsymbol{\sigma}^n_{\varepsilon}$ and adding, the terms $p(u^n_{\varepsilon}\nabla\Pi^h(F'_{\varepsilon}(u_{\varepsilon})), \boldsymbol{\sigma}^n_{\varepsilon})$ cancel, and using that $\nabla\Pi^h(F'_{\varepsilon}(u^n_{\varepsilon})) = \Lambda^1_{\varepsilon}(u^n_{\varepsilon})^{-1}\nabla u^n_{\varepsilon}$, we arrive at

$$p(\delta_t u_{\varepsilon}^n, F_{\varepsilon}'(u_{\varepsilon}^n))^h + p \int_{\Omega} (\nabla u_{\varepsilon}^n)^T \cdot \Lambda_{\varepsilon}^1(u_{\varepsilon}^n)^{-1} \cdot \nabla u_{\varepsilon}^n d\boldsymbol{x} + \delta_t \left(\frac{1}{2} \|\boldsymbol{\sigma}_{\varepsilon}^n\|_0^2\right) + \frac{k}{2} \|\delta_t \boldsymbol{\sigma}_{\varepsilon}^n\|_0^2 + \|\boldsymbol{\sigma}_{\varepsilon}^n\|_1^2 = 0,$$

which, proceeding as in (5.65)-(5.66) and using Remark 5.4.5 and estimate (5.48), implies (5.77).

Corollary 5.4.18 (Uniform estimates) Assume that $(u_0, v_0) \in L^2(\Omega) \times H^1(\Omega)$. Let $(u_{\varepsilon}^n, \boldsymbol{\sigma}_{\varepsilon}^n)$ be a solution of scheme US_{ε} . Then, it holds

$$p(F_{\varepsilon}(u_{\varepsilon}^{n}),1)^{h} + \frac{1}{2} \|\boldsymbol{\sigma}_{\varepsilon}^{n}\|_{0}^{2} + k \sum_{m=1}^{n} \left(p \varepsilon^{2-p} \|\nabla u_{\varepsilon}^{m}\|_{0}^{2} + \|\boldsymbol{\sigma}_{\varepsilon}^{m}\|_{1}^{2} \right) \le \frac{C_{0}}{(p-1)^{2}}, \quad \forall n \ge 1,$$
(5.78)

with the constant $C_0 > 0$ depending on the data (Ω, u_0, v_0) , but independent of k, h, n and ε ; and the estimates given in (5.69) also hold.

Proof. Proceeding as in (5.70) (using the fact that $(u^0, \boldsymbol{\sigma}^0) = (Q^h u_0, \widetilde{Q}^h(\nabla v_0)))$, we can deduce that

$$p \int_{\Omega} \Pi^{h}(F_{\varepsilon}(u^{0})) + \frac{1}{2} \|\boldsymbol{\sigma}^{0}\|_{0}^{2} \le \frac{C_{0}}{(p-1)^{2}},$$
(5.79)

where the constant $C_0 > 0$ depends on the data (Ω, u_0, v_0) , but is independent of k, h, n and ε . Therefore, from the discrete energy law (5.77) and estimate (5.79), we have

$$\mathcal{E}_{\varepsilon}^{h}(u_{\varepsilon}^{n},\boldsymbol{\sigma}_{\varepsilon}^{n}) + k \sum_{m=1}^{n} \left(p \varepsilon^{2-p} \| \nabla u_{\varepsilon}^{m} \|_{0}^{2} + \| \boldsymbol{\sigma}_{\varepsilon}^{m} \|_{1}^{2} \right) \leq \mathcal{E}_{\varepsilon}^{h}(u^{0},\boldsymbol{\sigma}^{0}) \leq \frac{C_{0}}{(p-1)^{2}}$$

which implies (5.78). Finally, the estimates given in (5.69) are proved as in Corollary 5.4.10.

Remark 5.4.19 (Approximated positivity of u_{ε}^{n}) The approximated positivity result for u_{ε}^{n} established in Remark 5.4.11 remains true for the scheme US_{ε} .

Well-posedness

The following two results are concerning to the well-posedness of the scheme $\mathbf{US}\varepsilon$.

Theorem 5.4.20 (Unconditional existence) There exists at least one solution $(u_{\varepsilon}^n, \sigma_{\varepsilon}^n)$ of scheme US_{ε} .

Proof. The proof follows as in Theorem 4.4.5, by using the Leray-Schauder fixed point theorem. \blacksquare

Lemma 5.4.21 (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 $US\varepsilon$ is unique.

Proof. The proof follows as in Lemma 4.4.6.

5.4.3 Scheme US0

In this section, we are going to study another unconditional energy-stable fully discrete scheme associated to model (5.1). With this aim, we consider the following reformulation of problem (5.1): Find $u: \Omega \times [0,T] \to \mathbb{R}$ and $\boldsymbol{\sigma}: \Omega \times [0,T] \to \mathbb{R}^d$, with $u \ge 0$, such that

$$\begin{cases} \partial_t u - \Delta u - \nabla \cdot (u\boldsymbol{\sigma}) = 0 \quad \text{in } \Omega, \ t > 0, \\ \partial_t \boldsymbol{\sigma} + \operatorname{rot}(\operatorname{rot} \boldsymbol{\sigma}) - \nabla (\nabla \cdot \boldsymbol{\sigma}) + \boldsymbol{\sigma} = \nabla (u^p) \quad \text{in } \Omega, \ t > 0, \\ \frac{\partial u}{\partial \mathbf{n}} = 0, \ \boldsymbol{\sigma} \cdot \mathbf{n} = 0, \ [\operatorname{rot} \boldsymbol{\sigma} \times \mathbf{n}]_{tang} = 0 \quad \text{on } \partial\Omega, \ t > 0, \\ u(\boldsymbol{x}, 0) = u_0(\boldsymbol{x}) \ge 0, \ \boldsymbol{\sigma}(\boldsymbol{x}, 0) = \nabla v_0(\boldsymbol{x}), \quad \text{in } \Omega. \end{cases}$$
(5.80)

Once system (5.80) is solved, we can recover v from u by solving

$$\begin{cases} \frac{\partial_t v - \Delta v + v = u^p \text{ in } \Omega, \ t > 0, \\ \frac{\partial v}{\partial \mathbf{n}} = 0 \quad \text{on } \partial\Omega, \ t > 0, \\ v(\boldsymbol{x}, 0) = v_0(\boldsymbol{x}) > 0 \quad \text{in } \Omega. \end{cases}$$
(5.81)

Observe that (formally) multiplying $(5.80)_1$ by $\frac{p}{p-1}u^{p-1}$, $(5.80)_2$ by $\boldsymbol{\sigma}$, integrating over Ω and adding both equations, the terms $\frac{p}{p-1}(u\boldsymbol{\sigma}, \nabla(u^{p-1}))$ and $(\nabla(u^p), \boldsymbol{\sigma})$ vanish, we obtain the following energy law

$$\frac{d}{dt} \int_{\Omega} \left(\frac{1}{p-1} |u|^p + \frac{1}{2} |\boldsymbol{\sigma}|^2 \right) d\boldsymbol{x} + \int_{\Omega} \frac{4}{p} |\nabla(u^{p/2})|^2 d\boldsymbol{x} + \|\boldsymbol{\sigma}\|_1^2 = 0$$

In particular, the modified energy

$$\mathcal{E}(u, \boldsymbol{\sigma}) = \int_{\Omega} \left(\frac{1}{p-1} |u|^p + \frac{1}{2} |\boldsymbol{\sigma}|^2 \right) d\boldsymbol{x}$$

is decreasing in time. Then, taking into account the reformulation (5.80)-(5.81), we consider a fully discrete approximation using a FE discretization in space and the backward Euler discretization in time (considered for simplicity on a uniform partition of [0, T] with time step $k = T/N : (t_n = nk)_{n=0}^{n=N})$. Concerning the space discretization, we consider the triangulation as in the scheme $\mathbf{UV}\varepsilon$, but in this case without imposing the constraint (**H**) related with the right-angles simplices. We choose the following continuous FE spaces for $u, \boldsymbol{\sigma}$ and v:

 $(U_h, \Sigma_h, V_h) \subset H^1(\Omega)^3$, generated by $\mathbb{P}_1, \mathbb{P}_m, \mathbb{P}_r$ with $m, r \ge 1$.

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

• <u>Scheme</u> USO: Initialization: Let $(u^0, \boldsymbol{\sigma}^0) = (Q^h u_0, \widetilde{Q}^h(\nabla v_0)) \in U_h \times \boldsymbol{\Sigma}_h$. Time step n: Given $(u^{n-1}, \boldsymbol{\sigma}^{n-1}) \in U_h \times \boldsymbol{\Sigma}_h$, compute $(u^n, \boldsymbol{\sigma}^n) \in U_h \times \boldsymbol{\Sigma}_h$ solving $\begin{cases} (\delta_t u^n, \bar{u})^h + \frac{1}{p-1}((u^n_+)^{2-p} \nabla (\Pi^h((u^n_+)^{p-1})), \nabla \bar{u}) = -(u^n \boldsymbol{\sigma}^n, \nabla \bar{u}), & \forall \bar{u} \in U_h, \\ (\delta_t \boldsymbol{\sigma}^n, \bar{\boldsymbol{\sigma}}) + (B_h \boldsymbol{\sigma}^n, \bar{\boldsymbol{\sigma}}) = \frac{p}{p-1}(u^n \nabla (\Pi^h((u^n_+)^{p-1})), \bar{\boldsymbol{\sigma}}), & \forall \bar{\boldsymbol{\sigma}} \in \Sigma_h, \end{cases}$ (5.82)

where $u_{+}^{n} := \max\{u^{n}, 0\} \geq 0$. Recall that Q^{h} is the L^{2} -projection on U_{h} defined in (5.43), \widetilde{Q}^{h} is the standard L^{2} -projection on Σ_{h} , $\Pi^{h} : C(\overline{\Omega}) \to U_{h}$ is the Lagrange interpolation operator, $(B_{h}\boldsymbol{\sigma}^{n}, \bar{\boldsymbol{\sigma}}) = (\operatorname{rot} \boldsymbol{\sigma}^{n}, \operatorname{rot} \bar{\boldsymbol{\sigma}}) + (\nabla \cdot \boldsymbol{\sigma}^{n}, \nabla \cdot \bar{\boldsymbol{\sigma}}) + (\boldsymbol{\sigma}^{n}, \bar{\boldsymbol{\sigma}})$ and the discrete semi-inner product $(\cdot, \cdot)^{h}$ was defined in (5.42).

Once the scheme **US0** is solved, given $v^{n-1} \in V_h$, we can recover $v^n = v^n(u^n) \in V_h$ solving:

$$(\delta_t v^n, \bar{v}) + (\nabla v^n, \nabla \bar{v}) + (v^n, \bar{v}) = ((u^n_+)^p, \bar{v}), \quad \forall \bar{v} \in V_h.$$

$$(5.83)$$

Given $u^n \in U_h$ and $v^{n-1} \in V_h$, Lax-Milgram theorem implies that there exists a unique $v^n \in V_h$ solution of (5.83).

Remark 5.4.22 (Positivity of v^n) Imposing the geometrical property of the triangulation where the interior angles of the triangles or tetrahedra must be at most $\pi/2$, the result concerning to the positivity of v^n stablished in Remark 5.4.7 remains true for the scheme **USO**.

Mass-conservation, Energy-stability and Solvability

Since $\bar{u} = 1 \in U_h$ and $\bar{v} = 1 \in V_h$, we deduce that the scheme **US0** is conservative in u^n , that is,

$$(u^n, 1) = (u^n, 1)^h = (u^{n-1}, 1)^h = \dots = (u^0, 1)^h = (u_0, 1) = m_0,$$
 (5.84)

and we have the following behavior for $\int_{\Omega} v^n$:

$$\delta_t \left(\int_{\Omega} v^n \right) = \int_{\Omega} (u^n_+)^p - \int_{\Omega} v^n.$$

Definition 5.4.23 A numerical scheme with solution (u^n, σ^n) is called energy-stable with respect to the energy

$$\mathcal{E}^{h}(u,\boldsymbol{\sigma}) = \frac{1}{p-1} ((u_{+})^{p}, 1)^{h} + \frac{1}{2} \|\boldsymbol{\sigma}\|_{0}^{2},$$
(5.85)

if this energy is time decreasing, that is $\mathcal{E}^{h}(u^{n}, \boldsymbol{\sigma}^{n}) \leq \mathcal{E}^{h}(u^{n-1}, \boldsymbol{\sigma}^{n-1})$, for all $n \geq 1$.

Theorem 5.4.24 (Unconditional stability) The scheme **USO** is unconditional energy stable with respect to $\mathcal{E}^{h}(u, \sigma)$. In fact, if (u^{n}, σ^{n}) is a solution of **USO**, then the following discrete energy law holds

$$\delta_t \mathcal{E}^h(u^n, \boldsymbol{\sigma}^n) + \frac{k}{2} \|\delta_t \boldsymbol{\sigma}^n\|_0^2 + \frac{p}{(p-1)^2} \int_{\Omega} (u^n_+)^{2-p} |\nabla(\Pi^h((u^n_+)^{p-1}))|^2 d\boldsymbol{x} + \|\boldsymbol{\sigma}^n\|_1^2 \le 0.$$
(5.86)

Proof. Testing $(5.82)_1$ by $\bar{u} = \frac{p}{p-1} \Pi^h((u_+^n)^{p-1})$, $(5.82)_2$ by $\bar{\boldsymbol{\sigma}} = \boldsymbol{\sigma}^n$ and adding, the terms $\frac{p}{p-1}(u^n \nabla(\Pi^h((u_+^n)^{p-1})), \boldsymbol{\sigma}^n)$ cancel, and we obtain

$$\frac{p}{p-1} \int_{\Omega} \Pi^{h} (\delta_{t} u^{n} \cdot (u_{+}^{n})^{p-1}) d\boldsymbol{x} + \frac{1}{2} \delta_{t} \|\boldsymbol{\sigma}^{n}\|_{0}^{2} + \frac{k}{2} \|\delta_{t} \boldsymbol{\sigma}^{n}\|_{0}^{2} + \frac{p}{(p-1)^{2}} \int_{\Omega} (u_{+}^{n})^{2-p} |\nabla(\Pi^{h}((u_{+}^{n})^{p-1}))|^{2} d\boldsymbol{x} + \|\boldsymbol{\sigma}^{n}\|_{1}^{2} = 0.$$
(5.87)

Denoting by $F(u^n) = \frac{1}{p}(u^n_+)^p$, we have that F is differentiable and convex, and then, from (5.5) we have that

$$\delta_t u^n \cdot (u^n_+)^{p-1} = \frac{1}{k} F'(u^n)(u^n - u^{n-1}) \ge \frac{1}{k} (F(u^n) - F(u^{n-1})) = \delta_t F(u^n),$$

and therefore,

$$\int_{\Omega} \Pi^{h}(\delta_{t}u^{n} \cdot (u_{+}^{n})^{p-1}) \ge \delta_{t}\left(\int_{\Omega} \Pi^{h}F(u^{n})\right) = \frac{1}{p}\delta_{t}\left(\int_{\Omega} \Pi^{h}((u_{+}^{n})^{p})\right).$$
(5.88)

Therefore, from (5.87) and (5.88) we deduce (5.86).

Corollary 5.4.25 (Uniform estimates) Let (u^n, σ^n) be a solution of scheme **USO**. Then, it holds for all $n \ge 1$,

$$\frac{1}{p-1}((u_{+}^{n})^{p},1)^{h} + \frac{1}{2}\|\boldsymbol{\sigma}^{n}\|_{0}^{2} + k\sum_{m=1}^{n} \left(\frac{p}{(p-1)^{2}} \int_{\Omega} (u_{+}^{m})^{2-p} |\nabla(\Pi^{h}((u_{+}^{m})^{p-1}))|^{2} d\boldsymbol{x} + \|\boldsymbol{\sigma}^{m}\|_{1}^{2}\right) \leq \frac{C_{0}}{p-1}$$
(5.89)

$$\int_{\Omega} |u^n| \le C_1, \tag{5.90}$$

with the constants $C_0, C_1 > 0$ depending on the data (Ω, u_0, v_0) , but independent of (k, h)and n.

Proof. In order to obtain (5.89), by multiplying (5.86) by k and adding from m = 1 to m = n, it suffices to bound the initial energy $\mathcal{E}^h(u^0, \boldsymbol{\sigma}^0)$. Taking into account that $(u^0, \boldsymbol{\sigma}^0) = (Q^h u_0, \tilde{Q}^h(\nabla v_0))$ and $u_0 \ge 0$ (and therefore, $u^0 \ge 0$), we have

$$\mathcal{E}^{h}(u^{0},\boldsymbol{\sigma}^{0}) \leq \frac{C}{p-1} \int_{\Omega} \Pi^{h}((u^{0})^{2}+1) + \frac{1}{2} \|v_{0}\|_{1}^{2} \leq \frac{C}{p-1} (\|u_{0}\|_{0}^{2}+\|v_{0}\|_{1}^{2}+1).$$

On the other hand, by considering $u_{-}^{n} = \min\{u^{n}, 0\} \ge 0$, taking into account that $|u^{n}| = 2u_{+}^{n} - u^{n}$, using the Hölder and Young inequalities as well as (5.84), we have

$$\int_{\Omega} |u^{n}| \leq \int_{\Omega} \Pi^{h} |u^{n}| = 2 \int_{\Omega} \Pi^{h} (u^{n}_{+}) - \int_{\Omega} u^{n} \\ \leq C \Big(\int_{\Omega} (\Pi^{h} (u^{n}_{+}))^{p} + 1 \Big) \leq C \Big(\int_{\Omega} \Pi^{h} ((u^{n}_{+})^{p}) + 1 \Big).$$
(5.91)

Therefore, from (5.89) and (5.91), we deduce (5.90).

Theorem 5.4.26 (Unconditional existence) There exists at least one solution (u^n, σ^n) of scheme **USO**.

Proof. The proof follows as in Theorem 4.4.5, by using the Leray-Schauder fixed point theorem. \blacksquare

5.5 Numerical simulations

In this section, we will compare the results of several numerical simulations using the schemes derived through the paper. We have chosen the 2D domain $[0, 2]^2$ using a structured mesh (then the right-angled constraint (**H**) holds and the scheme **UV** ε can be defined), the spaces for u and σ generated by \mathbb{P}_1 -continuous FE, and all the simulations are carried out using **FreeFem++** software. We will also compare with the usual Backward Euler scheme for problem (5.1), which is given for the following first order in time, nonlinear and coupled scheme:

• <u>Scheme</u> UV:

Initialization: Let $(u^0, v^0) \in U_h \times V_h$ an approximation of (u_0, v_0) as $h \to 0$. **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

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

Remark 5.5.1 The scheme UV 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 $UV\varepsilon$ (which is the "closest" approximation to the scheme UV considered in this paper) differs from the scheme UV in the use of the regularized functions F_{ε} and its derivatives (see Figure 5.1) and in the approximation of cross-diffusion and production terms, $(u\nabla v, \nabla \bar{u})$ and (u^p, \bar{v}) respectively, which are crucial for the proof of the energy-stability of the scheme $UV\varepsilon$.

The linear iterative methods used to approach the solutions of the nonlinear schemes $UV\varepsilon$, $US\varepsilon$, US0 and UV are the following Picard methods:

(i) Picard method to approach a solution $(u_{\varepsilon}^n, v_{\varepsilon}^n)$ of the scheme $\mathbf{UV}\varepsilon$:

Initialization (l = 0): Set $(u_{\varepsilon}^{0}, v_{\varepsilon}^{0}) = (u_{\varepsilon}^{n-1}, v_{\varepsilon}^{n-1}) \in U_{h} \times V_{h}$. **Algorithm:** Given $(u_{\varepsilon}^{l}, v_{\varepsilon}^{l}) \in U_{h} \times V_{h}$, compute $(u_{\varepsilon}^{l+1}, v_{\varepsilon}^{l+1}) \in U_{h} \times V_{h}$ such that

$$\begin{cases} \frac{1}{k}(u_{\varepsilon}^{l+1},\bar{u})^{h} + (\nabla u_{\varepsilon}^{l+1},\nabla\bar{u}) = \frac{1}{k}(u_{\varepsilon}^{n-1},\bar{u})^{h} - (\Lambda_{\varepsilon}^{2}(u_{\varepsilon}^{l})\nabla v_{\varepsilon}^{l},\nabla\bar{u}), \quad \forall \bar{u} \in U_{h}, \\ \frac{1}{k}(v_{\varepsilon}^{l+1},\bar{v}) + (A_{h}v_{\varepsilon}^{l+1},\bar{v}) = \frac{1}{k}(v_{\varepsilon}^{n-1},\bar{v}) + p(p-1)(\Pi^{h}F_{\varepsilon}(u_{\varepsilon}^{l+1}),\bar{v}), \quad \forall \bar{v} \in V_{h}. \end{cases}$$

until the stopping criteria $\max\left\{\frac{\|u_{\varepsilon}^{l+1} - u_{\varepsilon}^{l}\|_{0}}{\|u_{\varepsilon}^{l}\|_{0}}, \frac{\|v_{\varepsilon}^{l+1} - v_{\varepsilon}^{l}\|_{0}}{\|v_{\varepsilon}^{l}\|_{0}}\right\} \leq tol.$

(ii) Picard method to approach a solution $(u_{\varepsilon}^{n}, \boldsymbol{\sigma}_{\varepsilon}^{n})$ of the scheme $\mathbf{US}_{\varepsilon}$: **Initialization** (l = 0): Set $(u_{\varepsilon}^{0}, \boldsymbol{\sigma}_{\varepsilon}^{0}) = (u_{\varepsilon}^{n-1}, \boldsymbol{\sigma}_{\varepsilon}^{n-1}) \in U_{h} \times \Sigma_{h}$. **Algorithm:** Given $(u_{\varepsilon}^{l}, \boldsymbol{\sigma}_{\varepsilon}^{l}) \in U_{h} \times \Sigma_{h}$, compute $(u_{\varepsilon}^{l+1}, \boldsymbol{\sigma}_{\varepsilon}^{l+1}) \in U_{h} \times \Sigma_{h}$ such that

$$\begin{cases} \frac{1}{k}(u_{\varepsilon}^{l+1},\bar{u})^{h} + (\nabla u_{\varepsilon}^{l+1},\nabla\bar{u}) + (u_{\varepsilon}^{l+1}\boldsymbol{\sigma}_{\varepsilon}^{l},\nabla\bar{u}) = \frac{1}{k}(u_{\varepsilon}^{n-1},\bar{u})^{h}, \quad \forall \bar{u} \in U_{h}, \\ \frac{1}{k}(\boldsymbol{\sigma}_{\varepsilon}^{l+1},\bar{\boldsymbol{\sigma}}) + (B_{h}\boldsymbol{\sigma}_{\varepsilon}^{l+1},\bar{\boldsymbol{\sigma}}) = \frac{1}{k}(\boldsymbol{\sigma}_{\varepsilon}^{n-1},\bar{\boldsymbol{\sigma}}) + p(u_{\varepsilon}^{l+1}\nabla\Pi^{h}(F_{\varepsilon}'(u_{\varepsilon}^{l+1})),\bar{\boldsymbol{\sigma}}), \quad \forall \bar{\boldsymbol{\sigma}} \in \Sigma_{h}, \\ \int \|u_{\varepsilon}^{l+1} - u_{\varepsilon}^{l}\|_{0} \, \|\boldsymbol{\sigma}_{\varepsilon}^{l+1} - \boldsymbol{\sigma}_{\varepsilon}^{l}\|_{0} \, d\boldsymbol{\sigma}_{\varepsilon}^{l+1} - \boldsymbol{\sigma}_{\varepsilon}^{l+1}\|_{0} \, d\boldsymbol{\sigma}_{\varepsilon}^{l+1} - \boldsymbol{\sigma}_{\varepsilon}^{l+1}\|_{$$

until the stopping criteria max $\left\{ \frac{\|u_{\varepsilon}^{l+1} - u_{\varepsilon}^{l}\|_{0}}{\|u_{\varepsilon}^{l}\|_{0}}, \frac{\|\boldsymbol{\sigma}_{\varepsilon}^{l+1} - \boldsymbol{\sigma}_{\varepsilon}^{l}\|_{0}}{\|\boldsymbol{\sigma}_{\varepsilon}^{l}\|_{0}} \right\} \leq tol.$

(iii) Picard method to approach a solution (uⁿ, σⁿ) the scheme US0:
Initialization (l = 0): Set (u⁰, σ⁰) = (uⁿ⁻¹, σⁿ⁻¹) ∈ U_h × Σ_h.
Algorithm: Given (u^l, σ^l) ∈ U_h × Σ_h, compute (u^{l+1}, σ^{l+1}) ∈ U_h × Σ_h such that

$$\begin{cases} \frac{1}{k}(u^{l+1},\bar{u})^{h} + (\nabla u^{l+1},\nabla\bar{u}) - (\nabla u^{l},\nabla\bar{u}) + (u^{l+1}\boldsymbol{\sigma}^{l},\nabla\bar{u}) \\ &= \frac{1}{k}(u^{n-1},\bar{u})^{h} - \frac{1}{p-1}((u^{l}_{+})^{2-p}\nabla(\Pi^{h}(u^{l}_{+})^{p-1}),\nabla\bar{u}), \quad \forall \bar{u} \in U_{h}, \\ \frac{1}{k}(\boldsymbol{\sigma}^{l+1},\bar{\boldsymbol{\sigma}}) + (B_{h}\boldsymbol{\sigma}^{l+1},\bar{\boldsymbol{\sigma}}) = \frac{1}{k}(\boldsymbol{\sigma}^{n-1},\bar{\boldsymbol{\sigma}}) + \frac{p}{p-1}(u^{l+1}\nabla(\Pi^{h}(u^{l+1}_{+})^{p-1}),\bar{\boldsymbol{\sigma}}), \quad \forall \bar{\boldsymbol{\sigma}} \in \Sigma_{h}, \end{cases}$$

until the stopping criteria max $\left\{ \frac{\|u^{l+1} - u^l\|_0}{\|u^l\|_0}, \frac{\|\boldsymbol{\sigma}^{l+1} - \boldsymbol{\sigma}^l\|_0}{\|\boldsymbol{\sigma}^l\|_0} \right\} \leq tol.$ Observe that the residual term $(\nabla(u^{l+1} - u^l), \nabla \bar{u})$ is considered.

(iv) Picard method to approach a solution (uⁿ, vⁿ) of the scheme UV:
Initialization (l = 0): Set (u⁰, v⁰) = (uⁿ⁻¹, vⁿ⁻¹) ∈ U_h × V_h.
Algorithm: Given (u^l, v^l) ∈ U_h × V_h, compute (u^{l+1}, v^{l+1}) ∈ U_h × V_h such that

$$\begin{cases} \frac{1}{k}(u^{l+1},\bar{u}) + (\nabla u^{l+1},\nabla \bar{u}) + (u^{l+1}\nabla v^l,\nabla \bar{u}) = \frac{1}{k}(u^{n-1},\bar{u}), & \forall \bar{u} \in U_h, \\ \frac{1}{k}(v^{l+1},\bar{v}) + (\nabla v^{l+1},\nabla \bar{v}) + (v^{l+1},\bar{v}) = \frac{1}{k}(v^{n-1},\bar{v}) + ((u^{l+1}_+)^p,\bar{v}), & \forall \bar{v} \in V_h, \end{cases}$$
until the stopping criteria max
$$\begin{cases} \frac{\|u^{l+1} - u^l\|_0}{\|u^l\|_0}, \frac{\|v^{l+1} - v^l\|_0}{\|v^l\|_0} \end{cases} \le tol. \end{cases}$$

Remark 5.5.2 In all cases, first we compute u^{l+1} solving the u-equation, and then, inserting u^{l+1} in the v-equation (resp. σ -system), we compute v^{l+1} (resp. σ^{l+1}).

5.5.1 Positivity of u^n

In this subsection, we compare the positivity of the variable u^n in the four schemes. Here, we choose the space for v generated by \mathbb{P}_2 -continuous FE. We recall that for the three schemes studied in this paper, namely schemes $\mathbf{UV}\varepsilon$, $\mathbf{US}\varepsilon$ and $\mathbf{US0}$, it is not clear the positivity of the variable u^n . Moreover, for the schemes $\mathbf{UV}\varepsilon$ and $\mathbf{US}\varepsilon$, it was proved that $\Pi^h(u_{\varepsilon^-}^n) \to 0$ as $\varepsilon \to 0$ (see Remarks 5.4.11 and 5.4.19). For this reason, in Figures 5.3-5.9 we compare the positivity of the variable u_{ε}^n in the schemes, for different values of $1 and taking <math>\varepsilon = 10^{-3}$, $\varepsilon = 10^{-5}$ and $\varepsilon = 10^{-8}$ in the schemes $\mathbf{UV}\varepsilon$ and $\mathbf{US}\varepsilon$. We consider $k = 10^{-5}$, $h = \frac{1}{40}$, the tolerance parameter $tol = 10^{-3}$ and the initial conditions (see Figure 5.2)

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

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



(a) Initial cell density u_0



(b) Initial chemical concentration v_0

Figure 5.2: Initial conditions.

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

- (i) All the schemes take negative values for the minimum of u^n in different times $t_n \ge 0$, for the different values taken for p and ε . However, in the case of the schemes $\mathbf{UV}\varepsilon$ and $\mathbf{US}\varepsilon$, it is observed that these values are closer to 0 as $\varepsilon \to 0$ (see Figures 5.3-5.9).
- (ii) In all cases, the scheme $UV\varepsilon$ "preserves" better the positivity than the schemes UV, $US\varepsilon$ and US0 (see Figures 5.3-5.9).



Figure 5.3: Minimum values of u_{ε}^{n} for p = 1.1, computed using the scheme $\mathbf{UV}\varepsilon$.

Remark 5.5.3 In Figures 5.3 and 5.6 there are also negative values of minimum of u_{ε}^{n} for $\varepsilon = 10^{-8}$, but those are of order 10^{-8} and 10^{-5} , respectively.

5.5.2 Energy stability

In this subsection, we compare numerically the stability of the schemes $UV\varepsilon$, $US\varepsilon$, USo and UV with respect to the "exact" energy

$$\mathcal{E}_e(u,v) = \int_{\Omega} \frac{1}{p-1} (u_+)^p d\mathbf{x} + \frac{1}{2} \|\nabla v\|_0^2.$$
(5.92)

It was proved that the schemes $\mathbf{UV}\varepsilon$, $\mathbf{US}\varepsilon$ and $\mathbf{US0}$ are unconditionally energy-stables with respect to modified energies defined in terms of the variables of each scheme, and some energy inequalities are satisfied (see Theorems 5.4.9, 5.4.17 and 5.4.24). 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 (5.92), which comes from the continuous problem (5.1) (see (5.8)-(5.9)). Therefore, it is interesting to compare numerically the schemes with respect to this energy $\mathcal{E}_e(u, v)$, and to study the behaviour of the corresponding discrete energy law residual

$$RE_e(u^n, v^n) := \delta_t \mathcal{E}_e(u^n, v^n) + \frac{4}{p} \int_{\Omega} |\nabla((u^n_+)^{p/2})|^2 d\boldsymbol{x} + \|\Delta_h v^n\|_0^2 + \|\nabla v^n\|_0^2.$$
(5.93)



Figure 5.4: Minimum values of u_{ε}^{n} for p = 1.1, computed using the scheme $\mathbf{US}\varepsilon$.

We consider $k = 10^{-5}$, $h = \frac{1}{25}$, p = 1.4, $tol = 10^{-3}$ and the initial conditions (see Figure 5.10)

$$u_0 = 14\cos(2\pi x)\cos(2\pi y) + 14.0001$$
 and $v_0 = -14\cos(2\pi x)\cos(2\pi y) + 14.0001$

We choose the space for v generated by \mathbb{P}_1 -continuous FE. Then, we obtain that:

(i) All the schemes $\mathbf{UV}\varepsilon$, $\mathbf{US}\varepsilon$, \mathbf{UV} and $\mathbf{US0}$ satisfy the energy decreasing in time property for the exact energy $\mathcal{E}_e(u, v)$ (see Figure 5.11), that is,

$$\mathcal{E}_e(u^n, v^n) \le \mathcal{E}_e(u^{n-1}, v^{n-1}) \quad \forall n.$$

(ii) The schemes **US0** and **US** ε satisfy the discrete energy inequality $RE_e(u^n, v^n) \leq 0$, for $RE_e(u^n, v^n)$ defined in (5.93), independently of the choice of ε ; while the schemes **UV** and **UV** ε have $RE(u^n, v^n) > 0$ for some $t_n \geq 0$. However, it is observed that the scheme **UV** ε introduces lower numerical source than the scheme **UV**, and lower numerical dissipation than the schemes **US0** and **US** ε (see Figure 5.12).

5.6 Conclusions

In this paper we have developed three new mass-conservative and unconditionally energystable fully discrete FE schemes for the chemorepulsion production model (5.1), namely



Figure 5.5: Minimum values of u_{ε}^{n} for p = 1.1, computed using the schemes **UV** and **US0**.

 $\mathbf{UV}\varepsilon$, $\mathbf{US}\varepsilon$ and $\mathbf{US0}$. From the theoretical point of view we have obtained:

- (i) The solvability of the numerical schemes.
- (ii) The schemes $\mathbf{UV}\varepsilon$ and $\mathbf{US}\varepsilon$ are unconditionally energy-stables with respect to the modified energies $\mathcal{E}^h_{\varepsilon}(u, v)$ (given in (5.62)) and $\mathcal{E}^h_{\varepsilon}(u, \sigma)$ (given in (5.76)) respectively, under the right-angles constraint (**H**); while the scheme **US0** is unconditionally energy-stable with respect to the modified energy $\mathcal{E}^h(u, \sigma)$ given in (5.85), without this restriction (**H**) on the mesh.
- (iii) It is not clear how to prove the energy-stability of the nonlinear scheme UV (see Remark 5.5.1).
- (iv) In the schemes $\mathbf{U}\mathbf{V}\varepsilon$ and $\mathbf{U}\mathbf{S}\varepsilon$ there is a control for $\Pi^h(u_{\varepsilon^-}^n)$ in L^2 -norm, which tends to 0 as $\varepsilon \to 0$. This allows to conclude the nonnegativity of the solution u_{ε}^n in the limit as $\varepsilon \to 0$.

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

(i) The four schemes have decreasing in time energy $\mathcal{E}_e(u, v)$, independently of the choice of ε .



Figure 5.6: Minimum values of u_{ε}^{n} for p = 1.5, computed using the scheme $\mathbf{UV}\varepsilon$.

- (ii) The schemes **US0** and **US** ε satisfy the discrete energy inequality $RE_e(u^n, v^n) \leq 0$, for $RE_e(u^n, v^n)$ defined in (5.93), independently of the choice of ε ; while the schemes **UV** and **UV** ε have $RE(u^n, v^n) > 0$ for some $t_n \geq 0$. However, it was observed that the scheme **UV** ε introduces lower numerical source than the scheme **UV**, and lower numerical dissipation than the schemes **US0** and **US** ε .
- (iii) Finally, it was observed numerically that for the schemes $\mathbf{U}\mathbf{V}\varepsilon$ and $\mathbf{U}\mathbf{S}\varepsilon$, $\min_{\overline{\Omega}\times[0,T]} u_{\varepsilon}^n \to 0$ as $\varepsilon \to 0$.



Figure 5.7: Minimum values of u^n for p = 1.5, computed using the schemes **UV**, **US** ε and **US0**.



Figure 5.8: Minimum values of u_{ε}^{n} for p = 1.9, computed using the scheme $\mathbf{UV}\varepsilon$.



Figure 5.9: Minimum values of u^n for p = 1.9, computed using the schemes **UV**, **US** ε and **US0**.



(a) Initial cell density u_0



(b) Initial chemical concentration v_0

Figure 5.10: Initial conditions.



Figure 5.11: $\mathcal{E}_e(u^n, v^n)$ of the schemes **UV**, **US0**, **UV** ε and **US** ε (for $\varepsilon = 10^{-4}, 10^{-7}$).



Figure 5.12: $RE_e(u^n, v^n)$ of the schemes **UV**, **US0**, **UV** ε and **US** ε (for $\varepsilon = 10^{-4}, 10^{-7}$).

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