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Keller-Segel models for chemotaxis: stable and second order approximations

Master's dissertation in Mathematics - Applied Analysis and Computation, supervised by José Augusto Ferreira and submitted to the Department of Mathematics of the Faculty of Sciences and Technology of the University of Coimbra.

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Abstract

The main objective of this work is to study, from analytical and numerical perspectives, a Keller-Segel initial boundary value problem. In what concerns the mathematical analysis, we present a stability study for bounded domain in $\mathbb{R}$ with homogeneous Neumann boundary conditions. Although in numerical perspective our main goal is to obtain the discrete version of the continuous stability results, we start by studying the stability and convergence of a discrete version of the initial boundary value problem analyzed before but considering homogeneous Dirichlet boundary conditions and a one-dimensional spatial domain. Several numerical experiments are included to illustrate the qualitative behavior of the Keller-Segel problem. In the near future we intend to extend the discrete results presented here for a two-dimensional domain and Neumann boundary conditions. It is clear that, even for one-spatial domains, this new problem poses several challenges that we need to solve.

Keywords: Keller-Segel Model, Chemotaxis, Stability, Finite Difference Method

Resumo

O principal objetivo deste trabalho é o estudo, no ponto de vista analítico e numérico, de um problema Keller-Segel com condições inicial e de fronteira. No que diz respeito ao ponto de vista analítico, apresentamos um estudo de estabilidade considerando um domínio limitado unidimensional com condições de Neumann homogéneas para a fronteira. Embora no ponto vista numérico, o nosso objetivo central seja obter a versão discreta dos resultados de estabilidade estabelecidos para o caso contínuo, iniciamos o nosso estudo com a análise de estabilidade e a convergência de uma versão discreta do problema analisado anteriormente, mas considerando condições de fronteira de Dirichlet homogéneas. O comportamento qualitativo do sistema estudado é ilustrado numericamente. Num futuro próximo pretendemos estender os resultados discretos aqui apresentados para um domínio bidimensional e condições de fronteira de Neumann. É claro que, mesmo para domínios unidimensionais, este novo problema apresenta vários desafios que precisamos resolver.

Palavras-Chave: Modelo Keller-Segel, Quimiotaxia, Estabilidade, Método de Diferenças Finitas

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Chapter 1

Introduction

In this work we consider the following initial boundary value problem (IBVP)

$$\begin{cases} \dfrac{\partial u}{\partial t} = \nabla \cdot \big(D_u(u,v)\nabla u\big) - \nabla \cdot (\phi(u,v)\nabla v) + f(u,v), & x \in \Omega, t > 0, \\ \dfrac{\partial v}{\partial t} = \nabla \cdot \big(D_v(u,v)\nabla v\big) + g(u,v), & x \in \Omega, t > 0, \\ \dfrac{\partial u}{\partial \eta} = \dfrac{\partial v}{\partial \eta} = 0, & x \in \partial\Omega, t > 0, \\ u(x,0) = u_0(x) \geq 0, \, v(x,0) = v_0(x) \geq 0, & x \in \Omega, \end{cases} \tag{1.1}$$

where $\Omega \subset \mathbb{R}^n$, $\partial\Omega$ represents the boundary of Ω, η depends on $x \in \partial\Omega$ denotes the unitary exterior normal to Ω at $x \in \partial\Omega$, $f, g, \phi : \mathbb{R}^2 \to \mathbb{R}$, and both u and v represent the density of cells and the concentration of the chemical. The IBVP (1.1) is used to describe the bacteria transport that occurs by diffusion and convection enhanced by the presence of a chemical substance that induces a convective velocity given by $\phi(u,v)\nabla v$, $f(u,v)$ defines the population growth factor. The chemical species behaviour is defined by a diffusive transport and a chemical source/sink given by $g(u,v)$.For an overview on Keller- Segel models we recommend the [1].

In what concerns the behaviour on the boundary, as $\dfrac{\partial v}{\partial \eta} = 0$ and $\dfrac{\partial u}{\partial \eta} = 0$, then the bacteria convective fluxes are null. Consequently, the spatial domain is isolated for both species: bacteria and chemical. Then we can consider the following IBVP for bacteria and chemical concentrations

$$\begin{cases} \dfrac{\partial u}{\partial t} = \nabla \cdot \big(D_u(u,v)\nabla u\big) - \nabla \cdot (u\nabla v) + f(u), & x \in \Omega, t > 0, \\ \dfrac{\partial v}{\partial t} = \nabla \cdot \big(D_v(u,v)\nabla v\big) + g(u,v), & x \in \Omega, t > 0, \\ \dfrac{\partial u}{\partial \eta} = \dfrac{\partial v}{\partial \eta} = 0, & x \in \partial\Omega, t > 0, \\ u(x,0) = u_0(x) \geq 0, \, v(x,0) = v_0(x) \geq 0, & x \in \Omega, \end{cases} \tag{1.2}$$

the existence and uniqueness of solution of the IBVP (1.2) for $\Omega \subset \mathbb{R}^2$ with $D_u = D_v = 1$, and the reaction terms $f(u)$ and $g(u,v)$ are, respectively, the logistic term $-\mu u^2 + ru$, and $u - v$, that means that the time variation of the chemical is proportional to the difference between the bacteria and chemical concentrations, were the main objective of [5]. Here, upper bounds for the solution u and

v are established with respect to the $L^\infty(\Omega)$ norm for u and with respect to the $W^{1,\infty}(\Omega)$ for v. We remark that $u(\cdot,t) \in L^\infty(\Omega)$ if $u(\cdot,t)$ is bounded almost everywhere that means that $u(\cdot,t)$ is bounded except on a subset of null measure. The norm in $L^\infty(\Omega)$ is defined by

$$\|u(t)\|_{L^\infty(\Omega)} = \sup\{C > 0 : |u(x,t)| \le C \text{ almost everywhere in } \Omega\}.$$

The previous supremum is called the essential supremum of $u(\cdot,t)$ and it is denoted by $\operatorname{ess\,sup}_{\Omega} u$. Moreover, $u(\cdot,t) \in W^{1,\infty}(\Omega)$ if $u(\cdot,t) \in L^\infty(\Omega)$ and the partial derivatives with respect to the spatial components are also in $L^\infty(\Omega)$. In $W^{1,\infty}(\Omega)$ The usual norm is defined by

$$\|u(t)\|_{W^{1,\infty}(\Omega)} = \max\{\|u(t)\|_{L^\infty(\Omega)}, \|\frac{\partial u}{\partial x_i}(t)\|_{L^\infty(\Omega)}, i = 1,2\}.$$

Chapter 2, *Continuous Keller-Segel model: existence and uniqueness*, aims to present the results of [5] for $f(u) = -\mu u^2 + ru$, $g(u,v) = u - v$.

In general, the IBVP defined by a Keller-Segel model does not have solutions with a close form. Even for simple situations, the construction of the solution is a hard task. Numerical methods are powerful tools that allow us to obtain, at least approximately, the solution of such problems. The most popular approach to solve numerically IBVP defined by a Keller-Sequel equations is based on finite element methods. without being exhaustive we mention [4], [8]. Finite difference approach is also followed and we mention for instance [6]. Our initial main objective was to study a finite difference method for the IBVP (1.3)

$$\begin{cases} \dfrac{\partial u}{\partial t} = D_u \dfrac{\partial^2 u}{\partial x^2} - \dfrac{\partial}{\partial x}(\chi u \dfrac{\partial v}{\partial x}) + f(u,v), & x \in \Omega, t > 0, \\ \dfrac{\partial v}{\partial t} = D_v \dfrac{\partial^2 v}{\partial x^2} + g(v), & x \in \Omega, t > 0, \\ \dfrac{\partial u}{\partial x} = \dfrac{\partial v}{\partial x} = 0, & x \in \partial\Omega, t > 0, \\ u(x,0) = u_0(x) \ge 0,\ v(x,0) = v_0(x) \ge 0, & x \in \Omega. \end{cases} \tag{1.3}$$

where $\Omega \subset \mathbb{R}$, χ, D_u, D_v are positive constants and g does not depend on u, that is $g(u,v) = g(v)$. We follow the so called method of lines approach (MOL approach): we discretize the spatial derivatives using finite difference operators, and then the differential problem (1.3) is replaced by an ordinary differential problem. As the differential problem is characterized by Neumann boundary conditions and we would like to obtain second order approximations in space, several approaches can be used. Let $\{x_i, i = 0,\ldots,N\}$ be the spatial grid in $[0,1]$ defined by $x_i = x_{i-1} + h$, $i = 1,\ldots,N$, $x_0 = 0, x_N = 1, h > 0$. Then a second order approximations for the spatial derivatives at $x = x_0, x_N$ can be obtained considering the grid points $x_1,\ldots,x_p$ and $x_q,\ldots,x_{N-1}$, respectively, with $p,q \in \mathbb{N}$. In this case the finite difference approximations are specified for $i = 1,\ldots,N-1$. Another approach that we would like to follow is the use of fictitious points $x_{-1} = -x_1$, $x_{N+1} = 1 + h$, that lead to second order approximations. In this case, several difficulties arise in the establishment of error estimates with respect to a L^2 discrete norm. This fact motivates the replacement of the IBVP (1.3) by the following one

$$\begin{cases} \dfrac{\partial u}{\partial t} = D_u \dfrac{\partial^2 u}{\partial x^2} - \dfrac{\partial}{\partial x}(\chi u \dfrac{\partial v}{\partial x}) + f(u,v), & x \in (0,1), t > 0, \\ \dfrac{\partial v}{\partial t} = D_v \dfrac{\partial^2 v}{\partial x^2} + g(v), & x \in (0,1), t > 0, \\ u(x,t) = v(x,t) = 0, & x = 0,1, t > 0, \\ u(x,0) = u_0(x) \geq 0,\, v(x,0) = v_0(x) \geq 0, & x \in [0,1], \end{cases} \tag{1.4}$$

We observe that, under the previous assumptions, the two differential equations in (1.4) are decoupled. In Chapter 3, *Numerical approximation using the MOL approach*, we introduce a semi-discrete initial value problem that leads to a second order approximation for the solution of the IBVP (1.4) and we study its stability and convergence. We observe that, as the initial value problem is nonlinear, its stability requires the uniform boundness of the numerical approximation for the both unknowns. Such uniform boundness is obtained here using error estimates.

In Chapter 4, *Numerical Simulation*, we illustrate the theoretical results obtained in the last chapter and we also include several experiments that aim to illustrate the qualitative behaviour of the Keller-Segel model with different boundary conditions (4.4).

Finally, in the last chapter, Chapter 5, *Conclusions*, we present some conclusions and some topics that we would like to study in the near future.

Chapter 2

A continuous Keller-Segel model: existence and uniqueness

2.1 Introduction

This chapter aims to present the existence, uniqueness and stability of the solution of the IBVP (1.2) with $f(u) = -\mu u^2 + ru$, $g(u,v) = u - v$. The results that we present were taken from [5]. In what concerns the existence, we follow [10]. The stability of the solution of (1.2) for the previous choice of f and g is established constructing upper bounds for the solution.

For $p \in \mathbb{N}$, by $W^{1,p}(\Omega)$ we represent the Sobolev space of functions $u : \Omega \to \mathbb{R}$ with first order derivatives in $L^p(\Omega)$ where we consider the usual L^p-norm.

Let $0 < T_m \leq \infty$. By $C(\overline{\Omega} \times [0,T_m))$ we represent the space of functions defined in $\overline{\Omega} \times [0,T_m)$ that are continuous in this set, and by $C^{2,1}(\overline{\Omega} \times (0,T_m))$ we denote the space of functions defined in $\overline{\Omega} \times (0,T_m)$ that have continuous derivatives with respect to the spatial components until order 2 and have also continuous first order time derivatives in $\overline{\Omega} \times (0,T_m)$. By $L^\infty_{loc}([0,T_m), W^{1,p}(\Omega))$ we represent the space of function $u : \Omega \times [0,T_m) \to \mathbb{R}$ such that for each time t, $u(\cdot,t) \in W^{1,p}(\Omega)$ and for each compact K in $[0,T_m)$, $u \in L^\infty(K, W^{1,p}(\Omega))$ that is

$$\operatorname*{ess\,sup}_K \|u\|_{W^{1,p}(\Omega)} < +\infty.$$

In Section 2 we present an existence and uniqueness result following [10]. The stability is established in Section 3 following [5].

2.2 An existence and uniqueness result

We start by the existence and uniqueness result that can be seen in [10]. The formulation that we present here was presented in [5].

Theorem 1 *Let $\chi, \mu > 0$, $r \geq 0$, $\Omega \subset \mathbb{R}^n$, $n \geq 1$, be a bounded smooth domain and let the initial data $u_0 \in C(\overline{\Omega})$ and $v_0 \in W^{1,\infty}(\Omega)$ be nonnegative. Then there is a unique, nonnegative, and classical maximal solution (u,v) to the IBVP (1.2) with $f(u) = -\mu u^2 + ru$, $g(u,v) = u - v$, on some maximal* *interval* $[0,T_m)$ *with* $0<T_m\leq\infty$ *such that*

$$u\in C(\overline{\Omega}\times[0,T_m))\cap C^{2,1}(\overline{\Omega}\times(0,T_m)),$$

$$v\in C(\overline{\Omega}\times[0,T_m))\cap C^{2,1}(\overline{\Omega}\times(0,T_m))\cap L^{\infty}_{loc}([0,T_m),W^{1,p}(\Omega)),$$

with $p>n$.

2.3 Uniform boundness

To simplify the presentation we take $n=2$ and we use the notation u_t for the time derivative of u, Δu for the Laplacian of u and ∇u for the gradient of u. Moreover, we use $|\nabla u|^2$ to represent $\nabla u^T\nabla u$.

2.3.1 Auxiliary lemmas

Lemma 1 *For any* $t\in[0,T_m)$*, the non-negative solution* (u,v) *of (1.2) with* $f(u)=-\mu u^2+ru, g(u,v)=u-v$*, satisfies*

$$\|u(t)\|_{L^1(\Omega)}\leq\|u_0\|_{L^1(\Omega)}+\frac{(r+1)^2}{4\mu}|\Omega|=:k_1 \tag{2.1}$$

and

$$\|\nabla v(t)\|^2_{[L^2]^2(\Omega)}\leq\frac{2}{\mu}\left(\|u_0\|_{L^1(\Omega)}+\frac{\mu}{2}\|\nabla v_0\|^2_{[L^2]^2(\Omega)}+\frac{(r+2)^2}{4\mu}|\Omega|\right)=:k_2. \tag{2.2}$$

Proof: Let us start by establishing the following inequality

$$r\int_\Omega u\,dx-\mu\int_\Omega u^2\,dx\leq-\int_\Omega u\,dx+\frac{(r+1)^2}{4\mu}|\Omega|, \tag{2.3}$$

where $|\Omega|$ denotes the measure of Ω. The last inequality is consequence of

$$ru-\mu u^2\leq-u+\frac{(r+1)^2}{4\mu},$$

which is obtained taking into account that $\delta(u)\leq 0$, where $\delta(u):=ru-\mu u^2+u-\frac{(r+1)^2}{4\mu}$.

Applying the Divergence Theorem to the bacteria equation and then Using (2.3) we get

$$\frac{d}{dt}\int_\Omega u\,dx=r\int_\Omega u\,dx-\mu\int_\Omega u^2\,dx\leq-\int_\Omega u\,dx+\frac{(r+1)^2}{4\mu}|\Omega|, \tag{2.4}$$

that leads to

$$\frac{d}{dt}\int_\Omega u\,dx+\int_\Omega u\,dx-\frac{(r+1)^2}{4\mu}|\Omega|\leq 0,$$

and consequently

$$\frac{d}{dt}\left(\left(\int_\Omega u\,dx-\frac{(r+1)^2}{4\mu}|\Omega|\right)e^t\right)\leq 0,$$

that allow us to obtain (2.1).

Taking in the chemical equation of (1.2) the product with $-\Delta v$, with respect to the L^2 inner product, we obtain

$$\int_\Omega v_t(-\Delta v)\,dx = \int_\Omega (\Delta v - v + u)(-\Delta v)dx. \tag{2.5}$$

Taking into account the Divergence Theorem and the boundary conditions we get successively

$$\int_\Omega v_t(-\Delta v)\,dx = \int_\Omega \nabla v_t \nabla v\,dx = \int_\Omega \left(\frac{\partial}{\partial t}\nabla v\right)\nabla v\,dx = \frac{1}{2}\frac{d}{dt}\int_\Omega |\nabla v|^2\,dx.$$

As we have

$$\int_\Omega v\Delta v\,dx = -\int_\Omega |\nabla v|^2\,dx,$$

and

$$\int_\Omega u(-\Delta v)\,dx \le \int_\Omega u|\Delta v|\,dx \le \frac{1}{2}\int_\Omega |\Delta v|^2\,dx + \frac{1}{2}\int_\Omega u^2\,dx,$$

from (2.5) we deduce

$$\frac{1}{2}\frac{d}{dt}\int_\Omega |\nabla v|^2\,dx \le -\int_\Omega |\Delta v|^2\,dx - \int_\Omega |\nabla v|^2\,dx + \frac{1}{2}\int_\Omega |\Delta v|^2\,dx + \frac{1}{2}\int_\Omega u^2\,dx, \tag{2.6}$$

which is equivalent to

$$\frac{1}{2}\frac{d}{dt}\int_\Omega \mu|\nabla v|^2\,dx + \int_\Omega \mu|\nabla v|^2\,dx \le \frac{\mu}{2}\int_\Omega u^2\,dx. \tag{2.7}$$

From (2.4) we know that

$$\frac{d}{dt}\int_\Omega u\,dx \le r\int_\Omega u\,dx - \mu\int_\Omega u^2\,dx$$

that, with (2.3), leads to

$$\frac{d}{dt}\int_\Omega u + \frac{\mu}{2}|\nabla v|^2\,dx + 2\int_\Omega \frac{\mu}{2}|\nabla v|^2\,dx \le r\int_\Omega u\,dx - \frac{\mu}{2}\int_\Omega u^2\,dx,$$

and consequently

$$\frac{d}{dt}\int_\Omega u + \frac{\mu}{2}|\nabla v|^2\,dx + 2\int_\Omega u + \frac{\mu}{2}|\nabla v|^2\,dx \le (r+2)\int_\Omega u\,dx - \frac{\mu}{2}\int_\Omega u^2\,dx. \tag{2.8}$$

We observe that

$$(r+2)u - \frac{\mu}{2}u - \frac{(r+2)^2}{2\mu} \le 0. \tag{2.9}$$

This inequality can be easily shown considering $\zeta(u) := (r+2)u - \frac{\mu}{2}u - \frac{(r+2)^2}{2\mu}$ and evaluating its extremes.

Inserting in (2.8) the upper bound (2.9), we conclude

$$\frac{d}{dt}\int_\Omega u + \frac{\mu}{2}|\nabla v|^2\,dx + \int_\Omega 2u + \mu|\nabla v|^2 dx \le \frac{(r+2)^2}{2\mu}|\Omega|,$$

that can be rewritten in the equivalent form

$$\frac{d}{dt}\left(\int_\Omega j(u,v)\,dx\,e^{2t}-\frac{(r+2)^2}{4\mu}|\Omega|e^{2t}\right)\leq 0,$$

with $j(u,v):=u+\frac{\mu}{2}|\nabla v|^2$.

The last inequality leads to

$$\int_\Omega u+\frac{\mu}{2}|\nabla v|^2\,dx\leq\int_\Omega u_0+\frac{\mu}{2}|\nabla v_0|^2\,dx+\frac{(r+2)^2}{4\mu}|\Omega|$$

and rearranging terms we obtain (2.2).

■

Lemma 2 *Given $\tau\in(0,T_m)$, then, for any $t\in[0,T_m-\tau)$, the solution (u,v) of the IVBP (1.2) with $f(u)=-\mu u^2+ru, g(u,v)=u-v$, fulfills*

$$\int_t^{t+\tau}\int_\Omega u^2(s)\,dx\,ds\leq\frac{(r+1)k_1}{\mu}\max\{\tau,1\}=:k_3\max\{\tau,1\},\tag{2.10}$$

$$\int_t^{t+\tau}\int_\Omega|\nabla v(s)|^2\,dx\,ds\leq k_2\max\{\tau,1\},\tag{2.11}$$

and

$$\int_t^{t+\tau}\int_\Omega|\Delta v(s)|^2\,dx\,ds\leq(k_3+k_2)\max\{\tau,1\}=:k_4\max\{\tau,1\}.\tag{2.12}$$

Proof: Integrating the bacteria equation in (1.2) over $\Omega\times(t,t+\tau)$, considering the Divergence Theorem and the homogeneous boundary conditions for u and v, we obtain

$$\int_t^{t+\tau}\int_\Omega\frac{\partial u(s)}{\partial s}\,dx\,ds+\mu\int_t^{t+\tau}\int_\Omega u^2(s)\,dx\,ds=r\int_t^{t+\tau}\int_\Omega u(s)\,dx\,ds.$$

As we have

$$\int_\Omega u(t+\tau)\,dx+\mu\int_t^{t+\tau}\int_\Omega u^2(s)\,dx\,ds=r\int_t^{t+\tau}\int_\Omega u(s)\,dx\,ds+\int_\Omega u\,dx,$$

since u is non-negative, we get

$$\mu\int_t^{t+\tau}\int_\Omega u^2(s)\,dx\,ds\leq r\int_t^{t+\tau}\int_\Omega u(s)\,dx\,ds+\int_\Omega u\,dx.$$

Using (2.1) in the last inequality we deduce

$$\begin{aligned}r\int_t^{t+\tau}\int_\Omega u(s)\,dx\,ds+\int_\Omega u\,dx&\leq r\tau k_1+k_1\\&\leq k_1\max\{\tau,1\}(r+1).\end{aligned}$$

To prove (2.11) we integrate the chemical equation of (2.2) over $(t,t+\tau)$ obtaining

$$\int_t^{t+\tau}\|\nabla v(s)\|^2_{[L^2]^2(\Omega)}\,ds\leq\int_t^{t+\tau}k_2\,ds\leq k_2\max\{\tau,1\}.$$

To prove (2.12), we consider the equivalent expression to (2.6)

$$\frac{1}{2}\frac{d}{dt}\int_\Omega |\nabla v|^2\,dx + \frac{1}{2}\int_\Omega |\Delta v|^2\,dx \le \frac{1}{2}\int_\Omega u^2\,dx.$$

Integrating over $(t, t+\tau)$ we get

$$\int_t^{t+\tau} \frac{d}{dt}\int_\Omega |\nabla v(s)|^2\,dx\,ds + \int_t^{t+\tau}\int_\Omega |\Delta v(s)|^2\,dx\,ds \le \int_t^{t+\tau}\int_\Omega u^2(s)\,dx\,ds,$$

that, in combination with (2.10) and (2.2), leads to

$$\begin{aligned}\int_t^{t+\tau}\int_\Omega |\Delta v(s)|^2\,dx\,ds &\le \int_t^{t+\tau}\int_\Omega u^2(s)\,dx\,ds + \int_\Omega |\nabla v|^2\,dx\\ &\le (k_3+k_2)\max\{\tau,1\}.\end{aligned}$$

■

By the Gagliardo-Nirenberg Theorem there exists a positive constant C_{GN} such that

$$\|u(t)\|^2_{L^4(\Omega)} \le \left(C_{GN}\left(\|\nabla u(t)\|^{\frac{1}{2}}_{[L^2]^2(\Omega)}\|u(t)\|^{\frac{1}{2}}_{L^2(\Omega)} + \|u(t)\|_{L^1(\Omega)}\right)\right)^2, \tag{2.13}$$

(see for instance [5]).

Lemma 3 *Given $\tau \in (0, T_m)$, then the u-component of the solution (u, v) of (1.2), with $f(u) = -\mu u^2 + ru, g(u, v) = u - v$, satisfies the explicit uniform-in-time bound*

$$\begin{aligned}\|u(t)\|^2_{L^2(\Omega)} \le &\left(\|u_0\|^2_{L^2(\Omega)} + \frac{8\,\min\{1,\frac{2}{\chi}\}}{4C^4_{GN}} + 3\chi C^4_{GN}\left(\|u_0\|_{L^1(\Omega)} + \frac{(r+1)^2}{4\mu}|\Omega|\right)^4 + \right.\\ &\left. + \frac{r+1}{\mu}\|u_0\|_{L^1(\Omega)} + \frac{(r+1)^3}{4\mu^2}|\Omega| + \frac{8r^3}{9\mu^2}|\Omega|\right)\max\left\{1,\tau,\frac{1}{\tau}\right\}\times\\ &\times\exp\left\{\frac{\chi 4C^4_{GN}}{2\,\min\{1,\frac{2}{\chi}\}}\left(\frac{r+3}{\mu}\|u_0\|_{L^1(\Omega)} + \frac{(r+1)^3}{4\mu^2}|\Omega| + \right.\right.\\ &\left.\left. + \|\nabla v_0\|^2_{[L^2]^2(\Omega)} + \frac{(r+2)^2}{2\mu^2}|\Omega|\right)\max\{1,\tau\}\right\}\end{aligned} \tag{2.14}$$

and

$$\|u(t)\|_{L^2(\Omega)} \le C_1\left(1 + \frac{1}{\mu}\sqrt{\chi}\left(1+\frac{1}{\mu^2}\right)\right)\max\left\{\sqrt{\tau},\frac{1}{\sqrt{\tau}}\right\}C_2^{\max\{1,\tau\}}(\chi,\mu) \tag{2.15}$$

for all $t \in (0, T_m)$ and for some positive constants C_1, C_2.

Proof: From the bacteria equation of (1.2) we get

$$\int_\Omega u_t u\,dx = \int_\Omega (\Delta u)u\,dx - \chi\int_\Omega u^2\Delta v + (\nabla u\nabla v)u\,dx + \int_\Omega u^2(r-\mu u)\,dx,$$

and, considering the Divergence Theorem and the homogeneous boundary conditions for u and v, we get

$$\frac{1}{2}\frac{d}{dt}\int_\Omega u^2\,dx+\int_\Omega |\nabla u|^2\,dx=\chi\int_\Omega u^2\Delta v\,dx-\frac{\chi}{2}\int_\Omega u^2\Delta v\,dx+\int_\Omega u^2(r-\mu u)\,dx.$$

Using Cauchy-Schwarz we then deduce

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\int_\Omega u^2\,dx+\int_\Omega |\nabla u|^2\,dx\le \frac{\chi}{2}\left(\int_\Omega u^4\,dx\right)^{\frac{1}{2}}\left(\int_\Omega |\Delta v|^2\,dx\right)^{\frac{1}{2}}\\ +\int_\Omega u^2(r-\mu u)\,dx.\end{aligned}$$

As there exists a positive constant C_{GN} satisfying (2.13), using (2.1), we obtain

$$\left(\int_\Omega u^4\,dx\right)^{\frac{1}{2}}\le\left(2C_{GN}^2\left(\|\nabla u(t)\|_{[L^2]^2(\Omega)}\|u(t)\|_{L^2(\Omega)}+k_1^2\right)\right).$$

and consequently

$$\begin{aligned}\left(\int_\Omega u^4\,dx\right)^{\frac{1}{2}}\left(\int_\Omega |\Delta v|^2\,dx\right)^{\frac{1}{2}}&\le\|\nabla u(t)\|_{[L^2]^2(\Omega)}\|u(t)\|_{L^2(\Omega)}\|\Delta v(t)\|_{L^2(\Omega)}2C_{GN}^2+2k_1^2\|\Delta v(t)\|_{L^2(\Omega)}C_{GN}^2\\ &\le\varepsilon\|\nabla u(t)\|^2_{[L^2]^2(\Omega)}+\frac{C_{GN}^4}{\varepsilon}\|u(t)\|^2_{L^2(\Omega)}\|\Delta v(t)\|^2_{L^2(\Omega)}+\|\Delta v(t)\|^2_{L^2(\Omega)}+k_1^4C_{GN}^4.\end{aligned}$$

Finally, we have

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\int_\Omega u^2\,dx\quad&+\int_\Omega|\nabla u|^2\,dx\\ &\le\frac{\chi}{2}\left(\varepsilon\|\nabla u(t)\|^2_{[L^2]^2(\Omega)}+\frac{C_{GN}^4}{\varepsilon}\|u(t)\|^2_{L^2(\Omega)}\|\Delta v(t)\|^2_{L^2(\Omega)}+\|\Delta v(t)\|^2_{L^2(\Omega)}+k_1^4C_{GN}^4\right)\\ &+\int_\Omega u^2(r-\mu u)\,dx.\end{aligned}$$

Let $\varepsilon:=\min\left\{1,\frac{2}{\chi}\right\}$. If $\varepsilon=1$ then $\frac{\chi}{2}\varepsilon\|\nabla u(t)\|^2_{[L^2]^2(\Omega)}=\frac{\chi}{2}\|\nabla u(t)\|^2_{[L^2]^2(\Omega)}<\|\nabla u(t)\|^2_{[L^2]^2(\Omega)}$. Otherwise, if $\varepsilon=\frac{2}{\chi}$, then $\frac{\chi}{2}\varepsilon\|\nabla u(t)\|^2_{[L^2]^2(\Omega)}=\|\nabla u(t)\|^2_{[L^2]^2(\Omega)}$.

In both cases, we have

$$\begin{aligned}\frac{d}{dt}\int_\Omega u^2\,dx\quad&\le\chi\left(\frac{C_{GN}^4}{\varepsilon}\|u(t)\|^2_{L^2(\Omega)}\|\Delta v(t)\|^2_{L^2(\Omega)}+\|\Delta v(t)\|^2_{L^2(\Omega)}+k_1^4C_{GN}^4\right)\\ &+2\int_\Omega u^2(r-\mu u)\,dx.\end{aligned}\tag{2.16}$$

In what follows we establish an upper bound for $2\int_\Omega u^2(r-\mu u)dx$. Let $\delta(u):=2u^2(r-\mu u)-\frac{8r^3}{27\mu^2}$. It can be shown that $\delta(u)\le 0, u\in\mathbb{R}$.

Then

$$\int_\Omega u^2(r-\mu u)\,dx\le\frac{8r^3}{27\mu^2}|\Omega|.$$

Inserting the last upper bound in (2.16) we obtain

$$\begin{aligned}\frac{d}{dt}\int_\Omega u^2\,dx &\le \frac{\chi C_{GN}^4}{\varepsilon}\left(\|u(t)\|^2_{L^2(\Omega)}+\frac{2\varepsilon}{C_{GN}^4}\right)\|\Delta v(t)\|^2_{L^2(\Omega)}+\chi k_1^4 C_{GN}^4+\frac{8r^3}{27u^2}|\Omega| \\ &=: k_5 y(t)z(t)+k_6,\end{aligned}$$

where

$$\begin{aligned}&k_5=\frac{\chi C_{GN}^4}{\varepsilon},\, k_6=\chi k_1^4 C_{GN}^4+\frac{8r^3}{27u^2}|\Omega|,\\ &y(t)=\|u\|^2_{L^2(\Omega)}+\frac{\varepsilon}{2C_{GN}^4},\, z(t)=\|\Delta v\|^2_{L^2(\Omega)}.\end{aligned}$$

The last inequality leads to

$$\frac{d}{dt}\left(\exp\big(-k_5\int_0^t z(\mu)d\mu\big)y(t)-k_6\int_0^t \exp\big(-k_5\int_0^\eta z(\sigma)d\sigma\big)\right)\le 0,$$

and then

$$\begin{aligned}&y(t)\,\exp\left(-k_5\int_0^t z(\sigma)d\sigma\right)-k_6\int_0^t \exp\left(-k_5\int_0^\eta z(\sigma)d\sigma\right)d\eta\\ &\le y(s)\,\exp\left(-k_5\int_0^s z(\sigma)d\sigma\right)-k_6\int_0^s \exp\left(-k_5\int_0^\eta z(\sigma)d\sigma\right)d\eta,\end{aligned}$$

that implies the following

$$y(t)\le y(s)\,\exp\left(k_5\int_s^t z(\sigma)d\sigma\right)+k_6\int_s^t \exp\left(k_5\int_\eta^t z(\sigma)d\sigma,\right)d\eta, t\ge 0. \tag{2.17}$$

Considering some $s_i\in(i\tau,(i+1)\tau)$ and any natural number $i<\frac{T_m}{\tau}-1$. Using the upper bound (2.10) we establish

$$\begin{aligned}y(s_i)&=\frac{1}{\tau}\int_{i\tau}^{(i+1)\tau}y(s)ds\\ &\le\frac{1}{\tau}k_3\max\{\tau,1\}+\frac{2\varepsilon}{C_{GN}^2}\\ &\le\max\left\{1,\frac{1}{\tau}\right\}\left(k_3+\frac{2\varepsilon}{C_{GN}^2}\right)=:k_7\max\left\{1,\frac{1}{\tau}\right\},\end{aligned} \tag{2.18}$$

and considering (2.12) directly we have

$$\int_{i\tau}^{(i+1)\tau}z(s)ds=\int_{i\tau}^{(i+1)\tau}\|\Delta v(s)\|^2_{L^2(\Omega)}ds\le k_4\max\{\tau,1\}. \tag{2.19}$$

For $t\in[0,\tau]$, we set $s=0$ in (2.17) and $i=0$ to get

$$y(t)\le y(0)\exp\left(k_5\int_0^\tau z(\sigma)d\sigma\right)+k_6\int_0^\tau \exp\left(k_5\int_0^\tau z(\sigma)d\sigma\right)d\xi.$$

Using (2.19) we obtain

$$\begin{aligned} y(t) &\leq y(0)\exp\left(k_5 k_4\right) + k_6 \int_0^\tau \exp\left(k_5 k_4\right) d\xi \\ &\leq \left(y(0)+k_6\right)\max\{\tau,1\}\exp(\max\{\tau,1\}k_5 k_4). \end{aligned} \tag{2.20}$$

For $t \in [\tau, 2\tau]$, assuming $t < T_m$, we put $s = s_0 \in [0,\tau]$ in (2.17) from which we establish

$$\begin{aligned} y(t) &\leq y(s_0)\exp\left(k_5\int_{s_0}^t z(\sigma)d\sigma\right) + k_6\int_{s_0}^t \exp\left(k_5\int_{s_0}^t z(\sigma)d\sigma\right)d\xi \\ &\leq y(s_0)\exp\left(k_5\int_0^{2\tau} z(\sigma)d\sigma\right) + k_6\int_0^{2\tau}\exp\left(k_5\int_0^{2\tau} z(\sigma)d\sigma\right)d\xi. \end{aligned}$$

Introducing now (2.18) and (2.19)

$$\begin{aligned} y(t) &\leq k_7 \max\left\{1,\frac{1}{\tau}\right\}\exp\left(\max\{\tau,1\}\,2k_5k_4\right) + 2\tau k_6\exp\left(\max\{\tau,1\}\,2k_5k_4\right) \\ &\leq \left(k_7+2k_6\right)\max\left\{1,\tau,\frac{1}{\tau}\right\}\exp\left(\max\{\tau,1\}\,2k_5k_4\right). \end{aligned} \tag{2.21}$$

Adding (2.20) and (2.21) yields the desired result

$$\|u(t)\|^2_{L^2(\Omega)} + \frac{\varepsilon}{2C^4_{GN}} \leq \left(y(0)+k_7+3k_6\right)\max\left\{1,\tau\frac{1}{\tau}\right\}\exp\left(2k_5k_4\max\{\tau,1\}\right).$$

■

Lemma 4 *For $p \geq 1$, let*

$$\begin{cases} q \in [1,\frac{np}{n-p]}), & if\, p \leq n, \\ q \in [1,\infty], & if\, p > n. \end{cases} \tag{2.22}$$

Then there exists $C > 0$ such that the unique global-in-time classical solution (u,v) of the IBVP (1.2), with $f(u,v) = -\mu u^2 + ru, g(u,v) = u - v,$) satisfies

$$\|v(t)\|_{W^{1,q}(\Omega)} \leq C\left(1 + \sup_{s\in(0,t)}\|u(s)\|_{L^p(\Omega)}\right). \tag{2.23}$$

The proof of this result can be seen in [5].

Lemma 5 *The u component of the unique global-in-time classical solution of the IBVP (1.2), with $f(u) = -\mu u^2 + ru, g(u,v) = u - v$, satisfies the uniform estimate*

$$\|u(t)\|_{L^3(\Omega)} \leq C\left(1 + \frac{1}{\mu} + \frac{\chi^{\frac{8}{3}}}{\mu}M^{\frac{8}{3}}E^{\frac{8}{3}}\right), \tag{2.24}$$

for all $t \in (0,\infty)$ and for some C depending on u_0, v_0, r and Ω, where M is given by

$$M(\chi,\mu) = \left(1 + \frac{1}{\mu} + \sqrt{\chi}(1+\frac{1}{\mu^2})\right)$$

and

$$E(\chi,\mu) = \exp\left[\frac{\chi 2C_{GN}^2}{2\min\{2,\frac{2}{\chi}\}}\left(\frac{(r+3)}{\mu}\|u_0\|_{L^1(\Omega)} + \frac{(r+1)^3}{4\mu^2}|\Omega| + \|\nabla v_0\|^2_{[L^2]^2(\Omega)} + \frac{(r+2)^2}{2\mu^2}|\Omega|\right)\right]. \tag{2.25}$$

Proof: Considering the uniform L^2-bound of u in (2.15) with $\tau = 1$ we have

$$\|u(t)\|^2_{L^2(\Omega)} \leq C\left(1+\frac{1}{\mu}p\sqrt{\chi}(1+\frac{1}{\mu^2})\right)E(\chi,\mu),$$

using Lemma 4 with $p = 2$, for any $1 < q < \infty$, we get

$$\begin{aligned}\|\nabla v(t)\|_{[L^q]^2(\Omega)} \leq \|v(t)\|_{W^{1,q}(\Omega)} &\leq C(1+\sup_{s\in(0,t)}\|u(s)\|_{L^2(\Omega)})\\ &= C\left(1+\frac{1}{\mu}+\sqrt{\chi}(1+\frac{1}{\mu^2})\right)E(\chi,\mu)\\ &= CM(\chi,\mu)E(\chi,\mu).\end{aligned} \tag{2.26}$$

From the bacteria equation of (1.2) we deduce

$$\int_\Omega u_t u^2\,dx = \int_\Omega \Delta u u^2\,dx - \chi\left(\int_\Omega \nabla u\nabla v u^2\,dx + \int_\Omega u^3\Delta v\,dx\right) + \int_\Omega ru^3 - \mu u^4\,dx.$$

As we have

$$\int_\Omega u_t u^2 dx = \frac{1}{3}\frac{d}{dt}\int_\Omega u^3 dx,$$

$$\int_\Omega \Delta u u^2\,dx = -2\int_\Omega u|\nabla u|^2\,dx = -2\int_\Omega u|\nabla u|^2\,dx,$$

$$\int_\Omega u^3\Delta v\,dx = -3\int_\Omega u^2\nabla u\nabla v\,dx,$$

we have

$$\frac{1}{3}\frac{d}{dt}\int_\Omega u^3\,dx + 2\int_\Omega u|\nabla u|^2\,dx = 2\chi\int_\Omega u^2\nabla u\nabla v\,dx + \int_\Omega ru^3 - \mu u^4\,dx.$$

Cauchy's inequality with $\varepsilon = 1$ leads to

$$\begin{aligned}&\frac{1}{3}\frac{d}{dt}\int_\Omega u^3\,dx + 2\int_\Omega u|\nabla u|^2\,dx\\ &\leq 2\int_\Omega u|\nabla u|^2\,dx + \frac{\chi^2}{2}\int_\Omega u^3|\nabla v|^2\,dx + \int_\Omega ru^3 - \mu u^4\,dx.\end{aligned} \tag{2.27}$$

Using now Young's inequality, $ab \le \dfrac{a^c}{c} + \dfrac{b^d}{d}$ with $a = (\frac{4}{3})^{\frac{3}{4}} \frac{\mu}{\mu^{\frac{1}{4}}} u^3$, $b = (\frac{3}{4})^{\frac{3}{4}} \frac{\chi^2 |\nabla v|^2}{\mu^{\frac{3}{4}}}$, $c = 4$ and $d = \frac{4}{3}$ in the second term of the right hand side of (2.27) we establish

$$\begin{aligned} &\frac{1}{3}\frac{d}{dt}\int_\Omega u^3\,dx + 2\int_\Omega u|\nabla u|^2\,dx \\ &\le 2\int_\Omega u|\nabla u|^2\,dx + \frac{\mu}{2}\frac{3}{4}\frac{4}{3}\int_\Omega u^4\,dx + \frac{3^3\chi^8}{2\cdot 4\cdot 4^3\mu^3}\int_\Omega |\nabla v|^8\,dx + \int_\Omega ru^3 - \mu u^4\,dx. \end{aligned} \tag{2.28}$$

To get an upper bound for $\int_\Omega ru^3 - \mu u^4\,dx$, we consider $\zeta(u) := ru^3 - \frac{\mu}{2}u^4 + \frac{1}{3}u^3 - \frac{27(r+\frac{1}{3})^4}{32\mu^3}$.

It can be shown that $\zeta(u) < 0$ for all $u \in \mathbb{R}$, and consequently $ru^3 - \dfrac{\mu}{2}u^4 \le -\dfrac{1}{3}u^3 + \dfrac{3^3(r+\frac{1}{3})^4}{2^5\mu^3}$. Then we deduce

$$\int_\Omega ru^3\,dx - \frac{\mu}{2}\int_\Omega u^4\,dx \le -\frac{1}{3}\int_\Omega u^3\,dx + \frac{3^3(r+\frac{1}{3})^4}{2^5\mu^3}|\Omega|,$$

and hence

$$\begin{aligned} &\frac{1}{3}\frac{d}{dt}\int_\Omega u^3\,dx + \frac{1}{3}\int_\Omega u^3\,dx + 2\int_\Omega u|\nabla u|^2\,dx \\ &\le 2\int_\Omega u|\nabla u|^2\,dx + \frac{3^3\chi^8}{2\cdot 4^4\mu^3}\|\nabla v(t)\|^8_{[L^8]^2(\Omega)} + \frac{3^3(r+\frac{1}{3})^4}{2^5\mu^3}|\Omega|, \end{aligned}$$

Considering now (2.26) for $q = 8$, we obtain

$$\frac{d}{dt}\int_\Omega u^3\,dx + \int_\Omega u^3\,dx \le \frac{3^4\chi^8}{2\cdot 4^4\mu^3}CM(\chi,\mu)E(\chi,\mu) + \frac{3^4(r+\frac{1}{3})^4}{2^5\mu^3}|\Omega|,$$

that is

$$\frac{d}{dt}\left(e^t\left(\int_\Omega u^3\,dx - \frac{3^4\chi^8}{2\cdot 4^4\mu^3}CM(\chi,\mu)E(\chi,\mu) + \frac{3^4(r+\frac{1}{3})^4}{2^5\mu^3}|\Omega|\right)\right) \le 0, t > 0.$$

The last inequality leads to (2.24).

■

2.3.2 Main result

We are now able to establish the following result:

Theorem 2 *Let $\chi,\mu > 0, r \le 0, \Omega \subset \mathbb{R}^2$ be a bounded domain with a smooth boundary and let the initial data $u_0 \in C(\bar{\Omega})$ and $v_0 \in W^{1,\infty}(\Omega)$ be non-negative. Then the Keller-Segel IBVP (1.2), with $f(u) = -\mu u^2 + ru, g(u,v) = u - v$, has a unique a global classical non-negative solution (u,v) defined in $\Omega \times [0,\infty)$ such that*

$$\|u(t)\|_{L^\infty(\Omega)} \le C\big(1 + \frac{1}{\mu}\chi KN\big) =: CL \tag{2.29}$$

and

$$\|v(t)\|_{W^{1,\infty}(\Omega)} \le C\big(1 + \frac{1}{\mu} + \frac{\chi^{\frac{8}{3}}}{\mu}K^{\frac{8}{3}}\big) =: CN \tag{2.30}$$

uniformly on $[0,\infty)$ *and for some* C *depending on* u_0, v_0, r *and* $|\Omega|$, *where*

$$K = M(\chi,\mu)E(\chi,\mu)$$

and M *and* E *defined by (2.25).*

Proof: We obtain the following $W^{1,\infty}$ bound of v directly from Lemmas 5 and 4 with $n=2$, $p=3$ and $q=\infty$

$$\begin{aligned}\|v(t)\|_{W^{1,\infty}(\Omega)} &\leq C\left(1+\sup_{s\in(0,\infty)}\|u(s)\|_{L^3(\Omega)}\right)\\ &\leq C\left(1+\frac{1}{\mu}+\frac{\chi^{\frac{8}{3}}}{\mu}M^{\frac{8}{3}}(\chi,\mu)E^{\frac{8}{3}}(\chi,\mu)\right).\end{aligned}$$

For the L^∞ estimate of u we start by considering that solution u of the bacteria equation (1.2) with χ constant, admits the formal representation

$$\begin{aligned}u(t) &= e^{t(\Delta-I)}u_0 - \chi\int_0^t e^{(t-s)(\Delta-I)}\nabla\cdot((u\nabla v)(s))\,ds\\ &+\int_0^t e^{(t-s)(\Delta-I)}\left((r+1)u(s)-\mu^2(s)\right)ds. \end{aligned}\tag{2.31}$$

Then $u(t) = u_1(t)+u_2(t)+u_3(t)$ where

$$\begin{aligned}u_1 &:= e^{t(\Delta-I)}u_0,\\ u_2 &:= -\chi\int_0^t e^{(t-s)(\Delta-I)}\nabla\cdot((u\nabla v)(s))\,ds,\\ u_3 &:= \int_0^t e^{(t-s)(\Delta-I)}\left((r+1)u(s)-\mu^2(s)\right)ds.\end{aligned}$$

Given that u is non-negative and smooth we have

$$\|u(t)\|_{L^\infty(\Omega)} = \sup_{x\in\Omega}u(x,t) \leq \sup_{x\in\Omega}u_1(x,t)+\sup_{x\in\Omega}u_2(x,t)+\sup_{x\in\Omega}u_3(x,t).$$

As $\|e^{t\Delta}u_0\|_{L^\infty} \leq \|u_0\|_{L^\infty(\Omega)}$, we get

$$\|u_1(t)\|_{L^\infty(\Omega)} = \|e^{t(\Delta-I)}u_0\|_{L^\infty(\Omega)} \leq e^{-t}\|u_0\|_{L^\infty(\Omega)} \leq \|u_0\|_{L^\infty(\Omega)}.$$

We remark that if $w\geq 0$ then $e^{(t-s)(\Delta-I)}w\geq 0$. Consequently we deduce

$$\begin{aligned}u_3(t) &= \int_0^t e^{(t-s)(\Delta-I)}((r+1)u(s)-\mu^2(s))\,ds\\ &\leq \int_0^t e^{(t-s)(\Delta-I)}\frac{(r+1)^2}{4\mu}\,ds\\ &\leq \frac{(r+1)^2}{4\mu}.\end{aligned}$$

To obtain an upper bound for u_2 we observe that holds the following: for any $< q \leq p \leq \infty$ there exist $k_{11} > 0$ and λ_1 such that

$$\|e^{t\Delta}\nabla \cdot w(t)\|_{L^p(\Omega)} \leq k_{11}\left(1 + t^{-\frac{1}{2}-\frac{n}{2}\left(\frac{1}{q}-\frac{1}{p}\right)}\right) e^{-\lambda_1 t}\|w\|_{L^q(\Omega)}, \forall t > 0, w(t) \in (W^{1,p})^n,$$

applying this result to u_2 with $n = 2, q = \frac{5}{2}, p = 4$

$$\begin{aligned}\|u_2(t)\|_{L^\infty(\Omega)} &\leq \chi \int_0^t \|e^{(t-s)(\Delta-I)}\nabla \cdot (u(s)\nabla v(s))\|_{L^\infty(\Omega)}\, ds \\ &\leq k_{11}\chi \int_0^t \left(1 + (t-s)^{\frac{1}{2}-\frac{2}{5}}\right) e^{-(\lambda_1+1)(t-s)}\|u(s)\nabla v(s))\|_{L^{\frac{5}{2}}(\Omega)}\, ds.\end{aligned}$$

Using Hölder's inequality $\int fg\,dx \leq (\int f^p\,dx)^{\frac{1}{p}}\,(\int g^q\,dx)^{\frac{1}{q}}$ with $f = u$, $g = \nabla v$, $p = \frac{6}{5}$, $q = 6$, to the last inequality allow us to deduce

$$\|u_2(t)\|_{L^\infty(\Omega)} \leq k_{11}\chi \int_0^t \left(1 + (t-s)^{\frac{1}{2}-\frac{2}{5}}\right) e^{-(\lambda_1+1)(t-s)}\|u(s)\|_{L^3(\Omega)}\|\nabla v(s)\|_{[L^{15}]^2(\Omega)}\, ds.$$

Considering now the change of variable $s = t - \sigma$, that is $\sigma = s - t$, we obtain successively

$$\|u_2(t)\|_{L^\infty(\Omega)} \leq k_{11}\chi \int_0^\infty \left(1 + \sigma^{\frac{1}{2}-\frac{2}{5}}\right) e^{-(\lambda_1+1)\sigma}\|u(s)\|_{L^3(\Omega)}\|\nabla v(s)\|_{[L^{15}]^2(\Omega)}\, d\sigma$$

$$\begin{aligned}\|u_2(t)\|_{L^\infty(\Omega)} &\leq k_{11} \sup_{s\in(0,\infty)} \left(\|u(s)\|_{L^3(\Omega)}\|\nabla v(s)\|_{[L^{15}]^2(\Omega)}\right)\chi \int_0^\infty \left(1 + \sigma^{-\frac{9}{10}}\right) e^{-(\lambda_1+1)(\sigma)}\, d\sigma \\ &\leq k_{11} \sup_{s\in(0,\infty)} \|u(s)\|_{L^3(\Omega)} \sup_{s\in(0,\infty)} \|\nabla v(s)\|_{[L^{15}]^2(\Omega)}\chi \int_0^\infty \left(1 + \sigma^{-\frac{9}{10}}\right) e^{-(\lambda_1+1)\sigma}\, d\sigma.\end{aligned}$$

Introducing $k_{12} := k_{11}\int_0^\infty \left(1 + \sigma^{-\frac{9}{10}}\right) e^{-(\lambda_1+1)\sigma}\, d\sigma$ we can rewrite the last upper bound as follows

$$\|u_2(t)\|_{L^\infty(\Omega)} \leq k_{12} \sup_{s\in(0,\infty)} \|u(s)\|_{L^3(\Omega)} \sup_{s\in(0,\infty)} \|\nabla v(s)\|_{[L^{15}]^2(\Omega)}\chi.$$

Using Lemma 5 and (2.26) with $q = 15$ we obtain the following upper bound

$$\|u_2(t)\|_{L^\infty(\Omega)} \leq C\chi M(\chi,\mu)E(\chi,\mu)\left(1 + 1\frac{1}{u} + \frac{\chi^{\frac{8}{3}}}{\mu}M^{\frac{8}{3}}(\chi,\mu)E^{\frac{8}{3}}(\chi,\mu)\right).$$

Finally, the desired result is established taking in (2.31) the estimates for u_1, u_2, u_3 previously constructed.

■

Chapter 3

A numerical approximation using the MOL approach

3.1 Introduction

The aim of this chapter is to introduce a semi-discrete problem obtained using the MOL approach: the spatial derivatives are discretized using finite difference operators that allows the replacing the IBVP (1.4) by an ordinary differential problem. As mentioned before, we would like to extend the results presented here to (1.4) with Neumann boundary conditions.

The stability and convergence are analysed considering L^2 discrete norm. In what concerns stability, we will observe that the upper bounds depend on discrete solutions. This fact motivates the need to impose a uniform boundness assumption. However, as such assumption is not natural, we investigate how we can construct such upper bounds using errors estimates. The convergence analysis is then presented. We remark that the error estimate obtained for the bacteria concentration depends on the error for the approximation for the chemical concentration and on the numerical derivative of such approximation. The decoupled reaction terms is crucial to get the desired results.

In section 2 we present the notations and the basic results. The energy estimates for the numerical approximations are constructed in Section 3 - Theorems 3 and 4. The error analysis is presented in Section 4- Theorems 5, 6 and 7. In this section, is also concluded uniform boundness of the upper bounds that arise in Theorems 3 and 4.

3.2 Auxiliary Results

In $\Omega = (0,1)$ and for $h > 0$, we introduce in Ω the grid

$$\overline{\Omega}_h = \{x_i, i = 0, \ldots, N : x_{i+1} = x_i + h, i = 0, \ldots, N-1, x_0 = 0, x_N = 1\}.$$

Let $\Omega_h = \overline{\Omega}_h - \{x_0, x_N\}$.

By V_h we denote the space of grid functions defined in $\overline{\Omega}_h$. Let $V_{h,0}$ represents the space of functions in V_h that are null on the boundary points x_0, x_N. In this space we introduce the inner product

$$(u_h, w_h)_h = \sum_{i=1}^{N-1} h u_h(x_i) w_h(x_i), u_h, w_h \in V_{h,0}.$$

By $\|.\|_h$ we denote the norm induced by $(.,.)_h$. We also introduce the following notation

$$(u_h, w_h)_+ = \sum_{i=1}^{N} h u_h(x_i) w_h(x_i),\ u_h, w_h \in V_h,$$

$$\|u_h\|_+ = \sqrt{(u_h, u_h)_+},\ u_h \in V_h.$$

By $\|.\|_\infty$ we represent the usual infinite norm.

Let D_{-x} be the finite difference backward operator. By D_2 and D_c we represent the centered operators

$$D_2 w_h(x_i) = \frac{1}{h^2}(u_h(x_{i-1}) - 2u_h(x_i) + u_h(x_{i+1})),$$

and

$$D_c u_h(x_i) = \frac{1}{2h}(u_h(x_{i+1}) - u_h(x_{i-1})).$$

We now recall the following discrete Poincaré-Friedrich inequality.

Proposition 1 *If $w_h \in V_{h,0}$ then*

$$\|w_h\|_h \le \|D_{-x} w_h\|_+$$

Proof: To conclude the proof, we observe that we have

$$\begin{aligned} w_h(x_i)^2 &= \Big(\sum_{j=1}^{i} h D_{-x} w_h(x_j)\Big)^2 \\ &\le \sum_{j=1}^{N} h \sum_{j=1}^{N} h D_{-x} w_h(x_j)^2 \\ &\le \|D_{-x} w_h\|_+. \end{aligned}$$

■

Proposition 2 *If $w_h \in V_{h,0}$ then*

$$\|u_h\|_\infty \le \|D_{-x} u_h\|_+, u_h \in V_{h,0}.$$

Proof: It follows directly from the proof of the last result.

■

Proposition 3 *If $u_h, w_h \in V_{h,0}$, then*

$$(D_2 u_h, w_h)_h = -(D_{-x} u_h, D_{-x} w_h)_+.$$

Proof: Taking into account that the grid functions are null on the boundary points, we have successively the following

$$\begin{aligned}
(D_2u_h(t), w_h(t))_h &= h\sum_{i=1}^{N+1}\frac{D_{-x}u_{i+1} - D_{-x}u_i}{h}w_i \\
&= \sum_{i=1}^{N-1} D_{-x}u_{i+1}w_i - \sum_{i=1}^{N-1} D_{-x}u_iw_i \\
&= \sum_{i=2}^{N} D_{-x}u_iw_{i-1} - \sum_{i=1}^{N} D_{-x}u_iw_i \\
&= \sum_{i=1}^{N} D_{-x}u_iw_{i-1} - \sum_{i=1}^{N} D_{-x}u_iw_i \\
&= -\sum_{i=1}^{N} hD_{-x}u_i\frac{(w_i - w_{i-1})}{h} \\
&= -(D_{-x}u_h, D_{-x}w_h]_+.
\end{aligned} \tag{3.1}$$

■

Proposition 4 *If* $w_0 = w_N = u_0 = u_N = 0$*, then*

$$(D_c(w_h), u_h)_h = -(M_h(w_h), D_{-x}u_h)_+.$$

Proof:

$$
\begin{aligned}
D_c(w_h),u_h(t))_h &= h\sum_{i=1}^{N-1}\frac{w_{i+1}-w_{i-1}}{2h}u_i\\
&= \frac{1}{2}(\sum_{i=1}^{N-1} w_{i+1}u_i - \sum_{i=1}^{N-1} w_{i-1}u_i)\\
&= \frac{1}{2}(\sum_{i=2}^{N} w_i u_{i-1} - \sum_{i=0}^{N-2} w_i u_{i+1})\\
&= \frac{1}{2}(\sum_{i=1}^{N-1} w_i u_{i-1} - \sum_{i=1}^{N-1} w_i u_{i+1})\\
&= -\frac{1}{2}\sum_{i=1}^{N-1} hw_i\frac{u_{i+1}-u_{i-1}}{h}\\
&= -\frac{1}{2}\sum_{i=1}^{N-1} hw_i\frac{u_{i+1}-u_i+u_i-u_{i-1}}{h}\\
&= -\frac{1}{2}\sum_{i=1}^{N-1} hw_iD_{-x}u_{i+1} - \frac{1}{2}\sum_{i=1}^{N-1} hw_iD_{-x}u_i\\
&= -\frac{1}{2}\sum_{i=2}^{N} hw_{i-1}D_{-x}u_i - \frac{1}{2}\sum_{i=1}^{N} hw_iD_{-x}u_i\\
&= -\frac{1}{2}\sum_{i=1}^{N} hw_{i-1}D_{-x}u_i - \frac{1}{2}\sum_{i=1}^{N} hw_iD_{-x}u_i\\
&= -\sum_{i=1}^{N} h\frac{w_{i-1}+w_i}{2}D_{-x}u_h\\
&= -\sum_{i=1}^{N} hM_h(w_i)D_{-x}u_i\\
&= -(M_h(w_h),D_{-x}u_h)_+.
\end{aligned}
\tag{3.2}
$$

■

In what follows we denote by $R_h : C(\overline{\Omega}) \to V_h$ the restriction operator $R_u(x_i)u(x_i), i = 0,\dots,N, u \in C(\overline{\Omega})$.

Discretizing the first spatial derivative using C_c and the second order spatial derivatives in (1.4) using D_2 we introduce the following ordinary differential system

$$
\begin{cases}
u_h'(t) = D_uD_2u_h(t) - D_c(D_cv_h(t)u_h(t)) + f(u_h(t),v_h(t)),\\
v_h'(t) = D_vD_2v_h(t) + g(v_h(t)) \text{ in } \Omega_h \times (0,T],\\
u_h(0,t) = u_h(1,t) = 0, t \in (0,T],\\
v_h(0,t) = v_h(1,t)) = 0, t \in (0,T],\\
u_h(x_i,t) = R_hu_0(x_i), i = 1,\dots,N-1,\\
v_h(x_i,t) = R_hv_0(x_i), i = 1,\dots,N-1,
\end{cases}
\tag{3.3}
$$

where $u(x_i,t) \simeq u_h(x_i,t), v(x_i,t) \simeq v_h(x_i,t), i = 0,\dots,N, t \in [0,T]$.

System (3.3) is then solved solving the ordinary differential problems

$$\begin{cases} v_h'(t) = D_v D_2 v_h(t) + g(v_h(t)) \text{ in } \Omega_h \times (0,T], \\ v_h(0,t) = v_h(1,t) = 0, t \in (0,T], \\ v_h(x_i,0) = R_h v_0(x_i), i = 1,\dots,N-1, \end{cases} \tag{3.4}$$

and then, using v_h as input, we solve the following problem

$$\begin{cases} u_h'(t) = D_u D_2 u_h(t) - D_c(D_c v_h(t) u_h(t)) + f(u_h(t), v_h(t)) \text{ in } \Omega_h \times (0,T], \\ u_h(0,t) = u_h(1,t) = 0, t \in (0,T], \\ u_h(x_i,0) = R_h u_0(x_i), i = 1,\dots,N-1. \end{cases} \tag{3.5}$$

In what concerns the existence and uniqueness of the solutions v_h of (3.4), we observe that the last problem can be rewritten as

$$Z'(t) = D_v A_h Z(t) + G(Z(t)), t > 0, Z(0) \text{ given},$$

where $Z_i(t) = v_h(x_i,t), i = 1,\dots,N-1$, A_h denotes the matrix associated with the operator D_2 and $G_i(Z) = g(Z_i(t)), i = 1,\dots,N-1$. Then if g is a Lipschitz function with Lipschitz constant L_g and $P_1(Z(t)) = D_v A_h Z + G(Z)$, we obtain

$$\begin{aligned} \|P_1(Z) - P_1(\tilde{Z})\|_\infty &= ||D_v A_h Z + G(Z) - D_v A_h \tilde{Z} - G(\tilde{Z})||_\infty \\ &\leq D_v ||A_h(Z - \tilde{Z})||_\infty + L_g ||Z - \tilde{Z}||_\infty \\ &\leq \frac{4D_v}{h^2} ||Z - \tilde{Z}||_\infty + L_g ||Z - \tilde{Z}||_\infty \\ &= \left(\frac{4D_v}{h^2} + L_g \right) ||Z - \tilde{Z}||_\infty, \forall Z, \tilde{Z} \in \mathbb{R}^{N-1}. \end{aligned}$$

Then, applying Picard's Theorem [3], we conclude that there exists a unique solution.

Analogously, problem (3.5) admits the representation

$$W'(t) = D_u A_h W(t) + B_h(Z(t)) W(t) + F(W(t), Z(t)), t > 0, W(0) \text{ given}.$$

In this representation, $W_i(t) = u_h(x_i,t), i = 1,\dots,N-1$, $B_h(Z(t))W(t)$ is induced by $D_c(\chi D_c v_h(t) u_h(t))$ and $F_i(W(t), Z(t)) = f(W_i(t), Z_i(t)) = f(u_h(x_i,t), v_h(x_i,t))$. Assuming that f is a Lipschitz function with L_f as a Lipschitz constant and $P_2(W,Z) = D_u A_h W + B_h(Z) W + F(W,Z)$, for $Z \in \mathbb{R}^{N-1}$, we obtain,

$$\begin{aligned} \|P_2(W,Z) - P_2(\tilde{W},Z)\|_\infty &= ||D_u A_h(Z - \tilde{Z}) + B_h(Z)(W - \tilde{W}) + F(W,Z) - F(\tilde{W},Z)||_\infty \\ &\leq \left(\frac{4D_u}{h^2} + \frac{||Z||_\infty}{h^2} \right) ||W - \tilde{W}\|_\infty + ||F(W,Z) - F(\tilde{W},Z)||_\infty \\ &\leq \left(\frac{4D_u}{h^2} + \frac{||Z||_\infty}{h^2} + L_f \right) ||W - \tilde{W}\|_\infty, \end{aligned}$$

for all $W, \tilde{W} \in \mathbb{R}^{N-1}$. Again by Picard's Theorem we conclude that (3.5) has a unique solution.

3.3 Energy Estimates

We start by establishing an upper bound for $u_h(t)$. Taking in the first equation of (3.5) the inner product $(.,.)_h$ by u_h, we deduce

$$(u_h'(t), u_h(t))_h = D_u(D_2 u_h(t), u_h(t))_h - (D_c(D_c v_h u_h), u_h(t))_h + (f(u_h, v_h), u_h(t))_h.$$

Assuming that that $f(0,0) = 0$ and the first order partial derivatives of f are bounded by C_f, for the reaction term, we easily get

$$\begin{aligned}
(f(u_h, v_h), u_h(t))_h &= (f(0,0) + \frac{\partial f}{\partial x}(\theta_1 u_h, v_h)u_h + \frac{\partial f}{\partial y}(0, \theta_2 v_h)v_h, u_h(t)) \\
&\leq C_f||u_h||_h^2 + C_f(|u_h|, |u_h|)_h \\
&\leq C_f||u_h||_h^2 + \frac{C_f}{2}||u_h||_h^2 + \frac{C_f}{2}||v_h||_h^2,
\end{aligned}$$

where $\theta_1, \theta_2 \in [0,1]$.

Using Propositions 3 and 4 we obtain the inequality,

$$\frac{1}{2}\frac{d}{dt}||u_h(t)||_h^2 + D_u||D_c u_h(t)||_+^2 \leq -(M_h(D_c v_i u_i), D_{-x}u_h)_+ + \frac{3}{2}C_f||u_h||_h^2 + \frac{C_f}{2}||v_h||_h^2. \tag{3.6}$$

Furthermore we estimate now the term $(M_h(D_c v_i u_i), D_{-x}u_h)$. We deduce, successively,

$$\begin{aligned}
&(M_h(D_c v_i u_i), D_{-x}u_h) \leq ||D_c v_h||_\infty \sum_{i=1}^{N} h\frac{|u_i| + |u_{i-1}|}{2}|D_{-x}u_i| \\
&\leq ||D_c v_h||_\infty \left(\sum_{i=1}^{N} h\frac{1}{4}(|u_i|^2 + |u_{i-1}|^2)\right)^{\frac{1}{2}} \left(\sum_{i=1}^{N} h(D_{-x}u_i)^2\right)^{\frac{1}{2}} \\
&\leq \frac{1}{2}||D_c v_h||_\infty ||u_h||_h ||D_{-x}u_h||_+ \\
&\leq \frac{1}{4\varepsilon^2}||D_c v_h||_\infty^2 ||u_h||_h^2 + \varepsilon^2||D_{-x}u_h||_+^2.
\end{aligned}$$

From (3.6) we get

$$\frac{d}{dt}||u_h(t)||_h^2 + 2\left(D_u - \varepsilon^2\right)||D_{-x}u_h(t)||_+^2 \leq \left(3C_f + \frac{1}{2\varepsilon^2}||D_{-x}v_h(t)||_\infty^2\right)||u_h(t)||_h^2 + C_f e^{2C_g t}||v_h(t)||_h^2,$$

and, consequently,

$$\begin{aligned}
&\frac{d}{dt}\Bigg(||u_h(t)||_h^2 e^{-\int_0^t Q_h(s)\,ds} + 2\left(D_u - \varepsilon^2\right)\int_0^t e^{-\int_0^s Q_h(\mu)\,d\mu}||D_{-x}u_h(s)||_+^2\,ds \\
&-\int_0^t C_f e^{-\int_0^s Q_h(\mu)d\mu + 2C_g s}||v_h(s)||_h^2 ds\Bigg) \leq 0,
\end{aligned}$$

where $Q_h(t) := 3C_f\frac{1}{2\varepsilon^2}||D_{-x}v_h(t)||_\infty^2$.
The last inequality allows us to conclude the next result.

Theorem 3 *Let u_h and v_h be defined by (3.3). Then*

$$||u_h(t)||_h^2 + 2(D_u-\varepsilon^2)\int_0^t e^{\int_s^t Q_h(\mu)\,d\mu}||D_{-x}u_h(0)||_+^2\,ds$$
$$\leq e^{\int_0^t Q_h(s)\,ds}||u_h(0)||_h^2 + \int_0^t C_f e^{\int_s^t Q_h(\mu)\,d\mu+2C_g s}||v_h(s)||_h^2 ds, t\geq 0, \tag{3.7}$$

where ε is a non zero constant.

The energy estimate established in the last theorem has meaning if $||D_{-x}v_h(t)||_\infty^2$ is bounded. To conclude the desired result we establish in what follows an upper bound for v_h. Analogously, following the procedure used to estimate u_h, we deduce

$$\frac{d}{dt}||v_h(t)||_h^2 + 2D_v||D_{-x}v_h(t)||_+^2 \leq 2(g(v_h),v_h)_h \leq 2C_g||v_h(t)||_h^2.$$

Rearranging the terms we obtain the following inequality

$$\frac{d}{dt}\left(||v_h(t)||_h^2 e^{-2C_g t} + 2D_v\int_0^t e^{-2C_g s}||D_{-x}v_h(s)||_+^2\,ds\right) \leq 0, t\geq 0.$$

The last inequality allow us to conclude the next result:

Theorem 4 *Let $v_h(t)$ be defined by (3.3). Then*

$$||v_h(t)||_h^2 + 2D_v\int_0^t e^{2C_g(t-s)}||D_{-x}v_h(s)||_+^2\,ds \leq e^{2C_g t}||v_h(0)||_h^2, t\geq 0, \tag{3.8}$$

Inserting the last upper bound in the estimate (3.7) of Theorem 3, we get

$$||u_h(t)||_h^2 + 2(D_u-\varepsilon^2)\int_0^t e^{\int_s^t Q_h(\mu)\,d\mu}||D_{-x}u_h(0)||_+^2\,ds$$
$$\leq e^{\int_0^t Q_h(s)\,ds}||u_h(0)||_h^2 + C_f||v_h(0)||_h^2\int_0^t e^{\int_s^t Q_h(\mu)\,d\mu+4C_g s}ds, t\geq 0.$$

We finalize this section remarking that the last upper bound gives useful information if $\int_s^t Q_h(\mu)\,d\mu$ is uniformly bounded in $t\in[0,T]$ and h.

3.4 Convergence Analysis

To show that $||D_{-x}v_h(t)||_\infty$ is uniformly bounded in t and h, we observe that $||D_{-x}v(t)||_\infty$ is bounded. Let $E_v(x_i,t) = R_h v(x_i,t) - v_h(x_i,t), i=0,\ldots,N$. We have

$$||D_{-x}v_h(t)||_\infty^2 \leq 2||D_{-x}E_v(t)||_\infty^2 + 2||D_{-x}v(t)||_\infty^2,$$

and then we will obtain an upper bound for $||D_{-x}E_v(t)||_\infty^2$.

We start by point out that

$$E_v'(t) = \frac{\partial v}{\partial t}(t) - v_h'(t) = D_v \frac{\partial^2 v}{\partial x^2}(t) - D_v D_2 v_h(t) + g(v(t)) - g(v_h(t)),$$

Considering now Taylor's formula we can rewrite

$$D_v \frac{\partial^2 v}{\partial x^2}(x_i,t) = D_v D_2 v(x_i,t) + D_v \frac{h^2}{24}\left(\frac{\partial^4 v}{\partial x^4}(\xi_i,t) + \frac{\partial^4 v}{\partial x^4}(\eta_i,t)\right), \xi_i, \eta_i \in [x_{i-1}, x_{i+1}],$$

Let $T_v(x_i,t) := D_v \frac{h^2}{24}\left(\frac{\partial^4 v}{\partial x^4}(\xi_i,t) + \frac{\partial^4 v}{\partial x^4}(\eta_i,t)\right)$ denote the truncation error. Then

$$E_v'(t) = D_v D_2 E_v(t) + g(v(t)) - g(v_h(t)) + T_v(t),$$

and, consequently, we obtain

$$(E_v'(t), E_v(t))_h = (D_v D_2 E_v(t), E_v(t))_h + (g(v(t)) - g(v_h(t)), E_v(t))_h + (T_v(t), E_v(t))_h.$$

Using Proposition 3, Cauchy's inequality and imposing $|g'| \leq C_{g'}$ we establish

$$\frac{1}{2}\frac{d}{dt}||E_v(t)||_h^2 = -D_v||D_{-x}E_v(t)||_+^2 + C_{g'}||E_v(t)||_h^2 + \frac{1}{2}||T_v(t)||_h^2 + \frac{1}{2}||E_v(t)||_h^2,$$

that leads to

$$\frac{d}{dt}\left(||E_v(t)||_h^2 e^{-2(C_{g'}+\frac{1}{2})t} + \int_0^t \left(2D_v||D_{-x}E_v(s)||_h^2 + ||T_v(t)||_h^2\right) e^{-2(C_{g'}+\frac{1}{2})s} ds\right) \leq 0$$

From the last inequality we conclude

$$\begin{aligned} &||E_v(t)||_h^2 + 2D_v \int_0^t ||D_{-x}E_v(s)||_+^2 e^{-2(C_{g'}+\frac{1}{2})(t-s)} ds \\ &\quad \leq e^{-2(C_{g'}+\frac{1}{2})}||E_v(0)||_h^2 + \int_0^t e^{-2(C_{g'}+\frac{1}{2})(t-s)}||T_v(s)||_h^2 ds. \end{aligned}$$

Therefore, there exists a positive constant C, h and t independent, such that

$$||E_v(t)||_h^2 + 2D_v \int_0^t ||D_{-x}E_v(s)||_+^2 ds \leq Ch^4, t \in [0,T]. \tag{3.9}$$

Theorem 5 *Let $v(t) \in C^4([0,1]), t \in [0,T]$, be solution of the IBVP for v defined by (1.4) and let $v_h(t)$ be defined by (3.4). Then for $E_v(t) = v(t) - v_h(t)$ we have (3.9).*

Corollary 1 *Under the conditions of Theorem 5, we have*

$$\begin{aligned} \int_0^t ||D_{-x}v_h(s)||_\infty^2 ds &\leq \int_0^t \frac{2}{h}||D_{-x}E_v(s)||_+^2 ds + 2\int_0^t \left\|\frac{\partial v}{\partial x}(s)\right\|_\infty^2 ds \\ &\leq Ch^3 + 2\int_0^t \left\|\frac{\partial v}{\partial x}(s)\right\|_\infty^2 ds, \end{aligned} \tag{3.10}$$

for $t \in [0,T]$.

From the last Corollary we obtain

$$\int_s^t ||D_{-x}v_h(\mu)||_\infty^2 \, d\mu \leq C, 0 \leq s < t, t \in [0,T]. \tag{3.11}$$

This upper bound enable us to conclude that $\int_s^t Q_h(\mu)\, d\mu$ is uniformly bounded in Theorem 3.

We consider now an upper bound for the error the spatial error $E_u(t) = R_h u(t) - u_h(t)$, where $u_h(t)$ is defined by (3.3). We have

$$\begin{aligned} E_u'(x_i,t) = {} & D_u \frac{\partial^2 u}{\partial x^2}(x_i,t) - D_u D_2 u_h(x_i,t) + \frac{\partial}{\partial x}(\chi \frac{\partial}{\partial x} vu)(x_i,t) - D_c(\chi D_c v_h u_h)(x_i,t) \\ & + f(u(x_i,t), v(x_i,t)) - f(u_h(x_i,t), v_h(x_i,t)), \end{aligned}$$

where

$$D_c(D_c vu)(x-i,t) = \frac{D_c v(x_{i+1},t)u(x_{i+1},t) - D_c v(x_{i-1},t)u(x_{i-1},t)}{2h}.$$

Using Taylor's formula, we obtain the following expansion for $D_c v(x_i,t)$,

$$v(x_{i+1},t) = v(x_i,t) + h\frac{\partial v}{\partial x}(x_i,t) + \frac{h^2}{2}\frac{\partial^2 v}{\partial x^2}(x_i,t) + \frac{h^3}{6}\frac{\partial^3 v}{\partial x^3}(\xi_i,t),$$

$$v(x_{i-1},t) = v(x_i,t) - h\frac{\partial v}{\partial x}(x_i,t) + \frac{h^2}{2}\frac{\partial^2 v}{\partial x^2}(x_i,t) - \frac{h^3}{6}\frac{\partial^3 v}{\partial x^3}(\eta_i,t),$$

$$\frac{v(x_{i+1},t) - v(x_{i-1},t)}{2h} = \frac{\partial v}{\partial x}(x_i,t) + \frac{h^2}{12}\left(\frac{\partial^3 v}{\partial x^3}(\xi_i,t) + \frac{\partial^3 v}{\partial x^3}(\eta_i,t)\right),$$

where $\xi_i, \eta_i \in [x_{i-1}, x_{i+1}]$.

Let $T_{c,v}(x_i,t) := \frac{h^2}{12}\big(\frac{\partial^3 v}{\partial x^3}(\xi_i,t) + \frac{\partial^3 v}{\partial x^3}(\eta_i,t)\big)$. Then

$$\begin{aligned} D_c(D_c vu)(x_i,t) &= \left(\frac{\partial v}{\partial x}(x_{i+1},t) + T_{c,v}(x_{i+1},t)\right)u(x_{i+1},t) \\ &\quad - \left(\frac{\partial v}{\partial x}(x_{i-1},t) + T_{c,v}(x_{i-1},t)\right)u(x_{i-1},t) \\ &= \frac{\frac{\partial v}{\partial x}(x_{i+1},t)u(x_{i+1},t) - \frac{\partial v}{\partial x}(x_{i-1},t)u(x_{i-1},t)}{2h} \\ &\quad + \frac{1}{2h}\big(T_{c,v}(x_{i+1},t)u(x_{i+1},t) - T_{c,v}(x_{i-1},t)u(x_{i-1},t)\big). \end{aligned}$$

Therefore

$$\begin{aligned} D_c(D_c vu)(x_i,t) = {} & \frac{\partial}{\partial x}\left(\frac{\partial v}{\partial x}u\right)(x_i,t) + \frac{h^2}{12}\left(\frac{\partial^3}{\partial x^3}(\frac{\partial v}{\partial x}u)(\bar{\xi}_i,t) + \frac{\partial^3}{\partial x^3}(\frac{\partial v}{\partial x}u)(\bar{\eta}_i,t)\right) \\ & + \frac{1}{2h}\big(T_{c,v}(x_{i+1},t)u(x_{i+1},t) - T_{c,v}(x_{i-1},t)u(x_{i-1},t)\big), \end{aligned}$$

with $\bar{\xi}_i, \bar{\eta}_i \in [x_{i-1}, x_{i+1}]$.

The truncation error is given by,

$$\begin{aligned}
|T_u(x_i,t)| \ &= |\tfrac{h^2}{24}\left(\tfrac{\partial^4 u}{\partial x^4}(\tilde{\xi}_i,t)+\tfrac{\partial^4 u}{\partial x^4}(\tilde{\eta}_i,t))\right)+\tfrac{h^2}{12}\left(\tfrac{\partial^3}{\partial x^3}(\tfrac{\partial v}{\partial x}u)(\bar{\xi}_i,t)+\tfrac{\partial^3}{\partial x^3}(\tfrac{\partial v}{\partial x}u)(\bar{\eta}_i,t)\right)\\
&+\tfrac{h}{24}\Big(\big(\tfrac{\partial^3 v}{\partial x^3}(\xi_{i+1},t)+\tfrac{\partial^3 v}{\partial x^3}(\eta_{i+1},t)\big)u(x_{i+1},t)\\
&\quad-\big(\tfrac{\partial^3 v}{\partial x^3}(\xi_{i-1},t)+\tfrac{\partial^3 v}{\partial x^3}(\eta_{i-1},t)\big)u(x_{i-1},t)\Big)|\\
&\le Ch^2\Big(\|\tfrac{\partial^4 u}{\partial x^4}(t)\|_\infty+\|\tfrac{\partial^3}{\partial x^3}(\tfrac{\partial v}{\partial x}(t)u(t))\|_\infty+\|\tfrac{\partial^4 v}{\partial x^4}(t)\|_\infty\|u(t)\|_\infty+\|\tfrac{\partial^3 v}{\partial x^3}(t)\|_\infty\|\tfrac{\partial u}{\partial x}(t)\|_\infty\Big).
\end{aligned}$$

We can rewrite the error equation as

$$\begin{aligned}
E_u'(x_i,t) = D_u D_2 E_u(x_i,t) + D_c(\chi D_c v u)(x_i,t) - D_c(\chi D_c v_h u_h)(x_i,t)\\
+ f(u(x_i,t),v(x_i,t)) - f(u_h(x_i,t),v_h(x_i,t)) + T_u(x_i,t).
\end{aligned}$$

We observe that we have

$$\begin{aligned}
(f(u,v)-f(u_h,v_h),E_u(t))_h \ &= (f(u,v)-f(u_h,v)+f(u_h,v)-f(u_h,v_h),E_u(t))_h\\
&= \Big(\tfrac{\partial f}{\partial x}(\theta_1,v(t))E_u(t)+\tfrac{\partial f}{\partial y}(u_h(t),\theta_2(t))E_v(t),E_u(t)\Big)_h\\
&\le C_{f'}\left(||E_u(t)||_h+||E_v(t)||_h\right)||E_u(t)||_h = C_{f'}||E_u(t)||_h^2 + C_{f'}||E_v(t)||_h\\
&\le C_{f'}||E_u||_h^2+\tfrac{C_{f'}}{2}\left(||E_v(t)||_h^2+||E_u(t)||_h^2\right),
\end{aligned}$$

where θ_1,θ_2 belong to the intervals defined by $u(t)$ and $u_h(t)$ and by $v(t)$ and $v_h(t)$, respectively, and $C_{f'}$ is the upper bound for the first order partial derivatives of f. Then we easily get

$$\begin{aligned}
(E_u'(t),E_u(t))_h = -D_u||D_cE_u(t)||_h^2 + (D_c(\chi D_c v u, E_u(t)))_h - (D_c(\chi D_c v_h(t)u_h(t),E_u(t)))_h\\
+C_{f'}||E_u(t)||_h^2+\frac{C_{f'}}{2}\left(||E_v(t)||_h^2+||E_u(t)||_h^2\right)+\frac{1}{2}||T_u(t)||_h^2+\frac{1}{2}||E_u(t)||_h^2. \qquad (3.12)
\end{aligned}$$

Let, $V(x_i,t) := (\chi D_c v)(x_i,t)$, $V_h(x_i,t) := (\chi D_c v_h)(x_i,t)$,

$$(D_c(V(t)u(t)),E_u(t))_h - (D_c(V_h(t)u_h(t)),E_u(t))_h = (D_c(V(t)u(t)-V_h(t)u_h(t)),E_u(t))_h\,,$$

and

$$\begin{aligned}
D_c(V(x_i,t)u(x_i,t)) - D_c(V_h(x_i,t)u_h(x_i,t)) &= D_c(V(x_i,t)u(x_i,t)) - D_c(V_h(x_i,t)u(x_i,t))\\
&\quad + D_c(V_h(x_i,t)u(x_i,t)) - D_c(V_h(x_i,t)u_h(x_i,t))\\
&= D_c(V(x_i,t)u(x_i,t)) - D_c(V_h(x_i,t)u(x_i,t))\\
&\quad + D_c(V_h(x_i,t)(u(x_i,t)-u_h(x_i,t)))\\
&= D_c(E_V(x_i,t)u(x_i,t)) + D_c(V_h(x_i,t)E_u(x_i,t)).
\end{aligned}$$

Considering $w := Vu - V_h u_h$ in Proposition 4, it follows

$$\begin{aligned}\big(D_c w(t), E_u(t)\big)_h &= -\big(M_h w(t), D_{-x}E_u(t)\big)_+\\&= -\big(M_h E_V(t)u(t), D_{-x}E_u(t)\big)_+ - \big(M_h V_h(t)E_u(t), D_{-x}E_u(t)\big)_+\\&\leq ||u(t)||_\infty ||M_h D_c E_v(t)||_+ ||D_{-x}E_u(t)||_+\\&+ ||D_c v_h(t)||_\infty ||M_h E_u(t)||_+ ||D_{-x}E_u(t)||_+\end{aligned}$$

Note that $||M_h u_h(t)||_+ \leq ||u_h(t)||_h^2$. In fact,

$$||M_h u_h(t)||_+ = \sum_{i=1}^{N} h\left(\frac{u_{i-1}+u_i}{2}\right)^2 \leq \frac{1}{2}\sum_{i=1}^{N} hu_{i-1}^2 + \frac{1}{2}\sum_{i=1}^{N} hu_i^2 = ||u_h(t)||_h^2.$$

Therefore,

$$\begin{aligned}&\big(D_c(\chi D_c v(t)u(t) - \chi D_c v_h(t)u_h(t)), E_u(t)\big)_h \leq\\&\leq ||u(t)||_\infty ||D_c E_v(t)||_h ||D_{-x}E_u(t)||_+ + ||D_c v_h(t)||_\infty ||E_u(t)||_h ||D_{-x}E_u(t)||_+ \leq\\&\leq \frac{1}{4\varepsilon^2}||u(t)||_\infty^2 ||D_c E_v(t)||_h^2 + \varepsilon^2 ||D_{-x}E_u(t)||_+^2\\&+ \frac{1}{4\eta^2}||D_c v_h(t)||_\infty^2 ||E_u(t)||_h^2 + \eta^2 ||D_{-x}E_u(t)||_+^2.\end{aligned}$$

Applying these results in (3.12) we get

$$\begin{aligned}&\frac{1}{2}\frac{d}{dt}||E_u(t)||_h^2 + (D_u - \varepsilon^2 - \eta^2)||D_{-x}E_u(t)||_+^2 \leq\\&\leq C_{f'}(\frac{1}{2}||E_u(t)||_h^2 + \frac{1}{2}||E_v(t)||_h^2 + ||E_u(t)||_h^2) + \frac{1}{2}||T_h(t)||_h^2 + \frac{1}{\varepsilon}||E_u(t)||_h^2\\&+ \frac{1}{4\varepsilon^2}||u(t)||_\infty^2 ||D_{-x}E_v(t)||_h^2 + \frac{1}{4\eta^2}||D_c v_h(t)||_\infty^2 ||E_u(t)||_h^2.\end{aligned}$$

Rearranging the terms,

$$\begin{aligned}&\frac{1}{2}\frac{d}{dt}||E_u(t)||_h^2 + (D_u - \varepsilon^2 - \eta^2)||D_{-x}||E_u(t)||_+^2 \leq\\&\leq \left(3C_{f'} + 1 + \frac{1}{2\eta^2}||D_c v_h(t)||_\infty^2\right)||E_u(t)||_h^2\\&+ C_{f'}||E_v(t)||_h^2 + \frac{1}{2\varepsilon^2}||u(t)||_\infty^2 ||D_c E_v(t)||_h^2 + ||T_u(t)||_h^2.\end{aligned}$$

The last inequality allow us to conclude the following result:

Theorem 6 *Let $u(t) \in C^4([0,1]), t \in [0,T]$ be a solution of 1.4 and let $u_h(t)$ be defined by 3.3. Then for $E_u(t) = R_h u(t) - u_h(t)$ we have*

$$\begin{aligned}&||E_u(t)||_h^2 + 2(D_u - \varepsilon^2 - \eta^2)\int_0^t e^{\int_s^t S_h(\mu)d\mu}||D_{-x}E_u(s)||_+^2\, ds\\&\leq e^{\int_0^t S_h(s)ds}||E_u(0)||_h^2 + \int_0^t e^{\int_s^t S_h(\mu)d\mu}\gamma(s)ds, t \in [0,T],\end{aligned}$$

where ε and η arbitrary non zero constants,

$$\gamma(t) = C_{f'}||E_v(t)||_h^2 + \frac{1}{2\varepsilon^2}||u(t)||_\infty^2||D_cE_v(t)||_h^2 + ||T_u(t)||_h^2,$$

and

$$S_h(t) = \left(3C_{f'} + 1 + \frac{1}{2\eta^2}||D_cv_h(t)||_\infty^2\right).$$

■

We remark that from (3.9) we have

$$||E_v(t)||_h^2 \le Ch^4,$$

$$\int_0^t ||D_{-x}E_v(s)||_+^2 ds \le Ch^4.$$

Moreover, using the representation of T_u we also have

$$||T_u(t)||_h \le Ch^2.$$

Considering the last upper bounds in Theorem 6 we establish the next result:

Theorem 7 *From Theorem 6 and Corollary 1 we conclude*

$$||E_u(t)||_h^2 + \int_0^t ||D_{-x}E_u(s)||_h^2 ds \le Ch^4, t \in [0,T].$$

■

Taking into account Corollary 1 that holds for $v_h(0) = v(0)$, we are able to conclude that there exists a positive constant C such that

$$||u_h(t)||_h^2 + \int_0^t ||D_{-x}u_h(s)||_+^2 ds \le C\big(||u_h(0)||_h^2 + ||v_h(0)||_h^2\big), t \in [0,T], \tag{3.13}$$

and

$$||v_h(t)||_h^2 + \int_0^t ||D_{-x}v_h(s)||_+^2 ds \le C||v_h(0)||_h^2, t \in [0,T]. \tag{3.14}$$

From the previous error estimates we obtain the following energy inequalities:

1.

$$\begin{aligned} ||u_h(t)||_\infty^2 &\le ||E_u(t)||_\infty^2 + 2||R_hu(t)||_\infty^2 \\ &\le \tfrac{2}{h}\textstyle\sum_{i=1}^{N-1} hE_i^2 + 2||R_hu(t)||_\infty^2 \\ &= \frac{2}{h}||E_u(t)||_h^2 + 2||R_hu(t)||_\infty^2. \end{aligned}$$

Considering now Theorem 6, we obtain

$$||u_h(t)||_\infty^2 \le \frac{2C}{h}(||E_u(0)||^2 + h^4) + 2||R_hu(t)||_\infty^2.$$

Finally, from Theorem 7, we deduce

$$||u_h(t)||_\infty^2 \leq 2C(1+h^3) + 2||R_h u(t)||_\infty^2$$

2.

$$\begin{aligned} ||u_h(t)||_\infty^2 &\leq 2||E_u(t)||_\infty^2 + 2||R_h u(t)||_\infty^2 \\ &\leq 2||D_{-x}E_u(t)||_+^2 + 2||R_h u(t)||_\infty^2 \end{aligned}$$

that leads to

$$\int_0^t ||u_h(t)||_\infty^2 \leq 2\int_0^t ||D_{-x}E_u(s)||_+^2\, ds + 2\int_0^t ||R_h u(s)||_\infty^2\, ds$$

Once again by Theorem 7,

$$||u_h(t)||_\infty^2 \leq 2C(||E_u(0)||_h^2 + h^4) + 2\int_0^t ||R_h u(s)||_\infty^2\, ds.$$

If $||E_u(0)||_h \leq C$ then

$$\int_0^t ||u_h(s)||_\infty^2\, ds \leq C, t \in [0,T],$$

where C is h and t independent.

Chapter 4

Numerical Simulation

4.1 Introduction

The main goal of this chapter is to illustrate the results presented in the last chapter. As in the last chapter we considered MOL approach that reduces the IBVP for bacteria and chemical concentrations to an ordinary differential system, numerical methods for this kind of problems will be used to obtain the numerical approximations for dependent variables.

Several approaches can be followed: implicit, explicit or implicit-explicit methods. It is well known that in general explicit methods are less stable than implicit methods being implicit-explicit methods a compromise between the two previous classes of methods ([2], [9]).In this chapter we consider methods belonging to the last three classes of methods.

In the theoretical support developed in Chapter 3, the semi-discrete approximations for the IBVP (1.4), with Dirichlet boundary conditions, defined by (3.3) was studied. In the present chapter we illustrate the qualitative behavior of (1.4) considering fully discrete schemes obtained integration (3.3) with Euler's method (implicit, explicit, implicit-explicit). Neumann boundary conditions will be also considered.

The chapter is organized as follows: in Section 4.2 we present the different methods, the illustration of the error behaviour is presented in Section 4.3, the stability behaviour is illustrated in Section 4.4 and finally in Section 4.5 we illustrate the qualitative behaviour of bacteria and chemical concentrations in different scenarios.

4.2 Euler's methods

We discretize our spatial domain $[0,1]$ into N uniform intervals of the form $[x_n, x_{n+1}]$, where $n = 1,\ldots,N$ and $x_n = x_{n-1} + h$, where $x_0 = 0$ and $h = \frac{1}{N}$. Similarly we discretize the time domain $[0,T]$ into M uniform intervals with time step size denoted as $\Delta t = \frac{T}{M}$. We consider U_n^m and V_n^m as the approximations to the exact solutions of u and v, at (x_n,t_m), respectively. For the time discretization, of both u and v, we use forward Euler approximations

$$\frac{\partial u}{\partial t}(x_n,t_m) \approx \frac{u(x_n,t_{m+1}) - u(x_n,t_m)}{\Delta t}.$$

Explicit Method

Considering an explicit Euler's method in the time integration of (3.3) with $f=0, g=0$ and Dirichlet boundaries, we obtain

$$\begin{cases} \dfrac{U_n^{m+1}-U_n^m}{\Delta t} = D_u \dfrac{U_{n+1}^m - 2U_n^m - U_{n-1}^m}{h^2} \\ -\dfrac{\chi}{4h^2}\left((V_{n+2}^m - V_n^m)U_{n+1}^m - (V_n^m - V_{n-2}^m)U_{n-1}^m\right), \quad n = 2,\dots,N-2, \\ \dfrac{V_n^{m+1}-V_n^m}{\Delta t} = D_v \dfrac{V_{n+1}^m - 2V_n^m - V_{n-1}^m}{h^2}, \quad m = 1,\dots,M-1. \end{cases} \tag{4.1}$$

Then

$$\begin{aligned}
U_0^{m+1} &= 0,\\
U_1^{m+1} &= U_1^m + \frac{\Delta t D_u}{h^2}(U_2^m - 2U_1^m) - \frac{\Delta t \chi}{4h^2}\left((V_4^m - V_2^m)U_2^m\right),\\
U_N^{m+1} &= 0,\\
U_{N-1}^{m+1} &= U_{N-1}^m + \frac{\Delta t D_u}{h^2}(-2U_{N-1}^m + U_{N-2}^m) + \frac{\Delta t \chi}{4h^2}\left((V_{N-1}^m - V_{N-3}^m)U_{N-2}^m\right),\\
&\text{and}\\
V_0^{m+1} &= 0,\\
V_1^{m+1} &= V_2^m + \frac{\Delta t D_v}{h^2}(V_2^m - 2V_1^m),\\
V_N^{m+1} &= 0,\\
V_{N-1}^{m+1} &= V_{N-1}^m + \frac{\Delta t D_v}{h^2}(-2V_{N-1}^m + V_{N-2}^m).
\end{aligned}$$

Imex Method

If we consider the diffusion term implicitly and maintain the convective part explicitly, we obtain

$$\begin{cases} \dfrac{U_n^{m+1}-U_n^m}{\Delta t} = D_u \dfrac{U_{n+1}^{m+1} - 2U_n^{m+1} - U_{n-1}^{m+1}}{h^2} \\ -\dfrac{\chi}{4h^2}\left((V_{n+2}^m - V_n^m)U_{n+1}^m - (V_n^m - V_{n-2}^m)U_{n-1}^m\right), \quad n = 2,\dots,N-2, \\ \dfrac{V_n^{m+1}-V_n^m}{\Delta t} = D_v \dfrac{(V_{n+1}^{m+1} - 2V_n^{m+1} - V_{n-1}^{m+1})}{h^2}, \quad m = 1,\dots,M-1. \end{cases} \tag{4.2}$$

To obtain the numerical solution we need to solve two systems of linear equations, $A_v V^{m+1} = V^m$ and $A_u U^{m+1} = B_u U^m$, where A_v, A_u, B_u are tridiagonal matrices defined by:

Matrix A_v

$$a_{00} = a_{NN} = 1,$$

for $i = 1, \dots, N-1$

$$a_{ii} = \frac{2\Delta t D_v}{h^2} + 1, \quad a_{ii+1} = -\frac{\Delta t D_u}{h^2}, \quad a_{ii-1} = -\frac{\Delta t D_v}{h^2}.$$

Matrix A_u

$$a_{00} = a_{NN} = 1,$$

for $i = 1, \dots, N-1$

$$a_{ii} = \frac{2\Delta t D_u}{h^2} + 1, \quad a_{ii+1} = -\frac{\Delta t D_u}{h^2}, \quad a_{ii-1} = -\frac{\Delta t D_u}{h^2}.$$

Matrix B_u

$$b_{00} = b_{11} = b_{N-1N-1} = b_{NN} = 1,$$

$$b_{12} = -\frac{\Delta t \chi}{4h^2}(V_4^m - V_2^m), \quad b_{N-1N-2} = \frac{\Delta t \chi}{4h^2}(V_{N-1} - V_{N-3}),$$

for $i = 2, \dots, N-2$

$$b_{ii} = 1, \quad b_{ii+1} = -\frac{\Delta t \chi}{h^2}(V_{j+2}^m - V_j^m), \quad b_{ii-1} = \frac{\Delta t \chi}{h^2}(V_j^m - V_{j-2}^m).$$

Implicit Method

If we consider the the diffusion and the convective parts implicitly we obtain the implicit method

$$\begin{cases} \dfrac{U_n^{m+1} - U_n^m}{\Delta t} = D_u \dfrac{U_{n+1}^{m+1} - 2U_n^{m+1} - U_{n-1}^{m+1}}{h^2} \\ \\ -\dfrac{\chi}{4h^2}\left((V_{n+2}^{m+1} - V_n^{m+1})U_{n+1}^{m+1} - (V_n^{m+1} - V_{n-2}^{m+1})U_{n-1}^{m+1}\right), \quad n = 2, \dots, N-2, \\ \\ \dfrac{V_n^{m+1} - V_n^m}{\Delta t} = D_v \dfrac{(V_{n+1}^{m+1} - 2V_n^{m+1} - V_{n-1}^{m+1})}{h^2}, \qquad m = 1, \dots, M-1. \end{cases} \tag{4.3}$$

Then,

Matrix A_u:

$$a_{00} = a_{NN} = 1,$$

$$a_{11} = \frac{2\Delta t D_u}{h^2} + 1, \quad a_{12} = -\frac{\Delta t D_u}{h^2} + \frac{\Delta t \chi}{4h^2}(V_4^{m+1} - V_2^{m+1}),$$

$$a_{N-1N-1} = \frac{2\Delta t D_u}{h^2} + 1, \quad a_{N-1N-2} = -\frac{\Delta t D_u}{h^2} - \frac{\Delta t \chi}{4h^2}(V_{N-1}^{m+1} - V_{N-3}^{m+1}),$$

for $i = 2,\ldots,N-2$

$$a_{i\,i-1} = -\frac{\Delta t D_u}{h^2} + \frac{\Delta t \chi}{4h^2}(V_{i-2}^{m+1} - V_i^{m+1}), \quad a_{i\,i} = \frac{2\Delta t D_u}{h^2} + 1, \quad a_{i\,i+1} = -\frac{\Delta t D_u}{h^2} + \frac{\Delta t \chi}{4h^2}(V_{i+2}^{m+1} - V_i^{m+1}).$$

We remark that matrix A_v is defined the same way as in the Imex method.

4.3 Explicit differentiation of the convective term

Another class of methods can be constructed if we compute

$$\frac{\partial}{\partial x}(\chi \frac{\partial v}{\partial x} u) = \chi \frac{\partial^2 v}{\partial x^2} u + \chi \frac{\partial v}{\partial x}\frac{\partial u}{\partial x},$$

and then approximate each term of the second member of the last equality.

Explicit Method

The following explicit method is obtained if we consider an explicit approach

$$\begin{cases} \dfrac{U_n^{m+1} - U_n^m}{\Delta t} = D_u \dfrac{U_{n+1}^m - 2U_n^m - U_{n-1}^m}{h^2} \\ \\ -\chi \dfrac{4(U_{n+1}^m - U_{n-1}^m)(V_{n+1}^m - V_{n-1}^m)}{h^2} - \chi \dfrac{U_n^m (V_{n+1}^m - 2V_n^m - V_{n-1}^m)}{h^2}, & n = 1,\ldots,N-1, \\ \\ \dfrac{V_n^{m+1} - V_n^m}{\Delta t} = D_v \dfrac{(V_{n+1}^m - 2V_n^m - V_{n-1}^m)}{h^2}, & m = 1,\ldots,M-1. \end{cases} \tag{4.4}$$

For the Dirichlet boundary conditions we considered

$$U_0^m = U_N^m = V_0^m = V_N^m = 0,$$

while for the Neumann boundary conditions we took in (4.4) $n = 0,\ldots,N$ with $x_{-1} = -x_1$ and $x_{N+1} = 1 + h$ and $U_{-1}^m = U_1^M, U_{N+1}^m = U_{N-1}^m$, $V_{-1}^m = V_1^M, V_{N+1}^m = V_{N-1}^m$. Then we have

$$U_0^{m+1} = U_0^m + \Delta t \left(D_u \frac{U_2^m - 2U_1^m - U_1^m}{h^2} - \chi \frac{4(U_2^m - U_1^m)(V_2^m - V_1^m)}{h^2} - \chi \frac{U_n^m (V_2^m - 2V_1^m - V_1^m)}{h^2} \right),$$

$$U_N^{m+1} = U_N^m + \Delta t \left(D_u \frac{U_N^m - 2 * U_N^m - U_{N-1}^m}{h^2} - \chi \frac{4(U_N^m - U_{N-1}^m)(V_N^m - V_{N-1}^m)}{h^2} - \chi \frac{U_n^m (V_N^m - 2V_N^m - V_{N-1}^m)}{h^2} \right),$$

$$V_1^{m+1} = V_1^m + \frac{(V_2^m) + V_1^m}{h^2}, V_N^{m+1} = V_N^m + \frac{(V_N^m) + V_{N-1}^m}{h^2}.$$

Implicit Method

If an implicit approach is considered, with Dirichlet Boundaries, we obtain the following method

$$\begin{cases} \dfrac{U_n^{m+1}-U_n^m}{\Delta t} = D_u \dfrac{U_{n+1}^{m+1}-2U_n^{m+1}-U_{n-1}^{m+1}}{h^2} \\ \\ -\chi \dfrac{4(U_{n+1}^{m+1}-U_{n-1}^{m+1})(V_{n+1}^{m+1}-V_{n-1}^{m+1})}{h^2} - \chi \dfrac{U_n^{m+1}(V_{n+1}^{m+1}-2V_n^{m+1}-V_{n-1}^{m+1})}{h^2}, \quad n=1,\dots,N-1, \\ \\ \dfrac{V_n^{m+1}-V_n^m}{\Delta t} = D_v \dfrac{V_{n+1}^{m+1}-2V_n^{m+1}-V_{n-1}^{m+1}}{h^2}, \quad m=1,\dots,M-1. \end{cases} \tag{4.5}$$

With matrix A_v defined as previously and A_u a tridiagonal defined as follows:

Matrix A_u

$$a_{00} = a_{NN} = 1,$$

for $i=1,\dots,N-1$,

$$a_{ii} = \frac{2\Delta t D_u}{h^2} + \frac{\Delta t \chi}{h^2}\left(V_{i+1}^{m+1} - 2V_i^{m+1} + V_{i-1}^{m+1}\right) + 1,$$

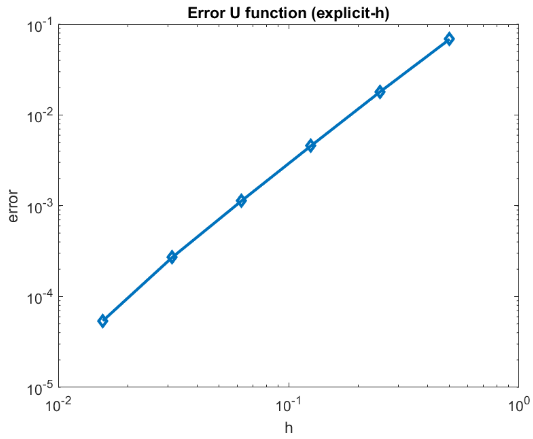
$$a_{ii+1} = -\frac{\Delta t D_u}{h^2} + \frac{\Delta t \chi}{4h^2}(V_{i+1}^{m+1} - V_{i-1}^{m+1}), \quad a_{ii-1} = -\frac{\Delta t D_u}{h^2} - \frac{\Delta t \chi}{4h^2}(V_{i+1}^{m+1} - V_{i-1}^{m+1}).$$

4.4 Error Behaviour

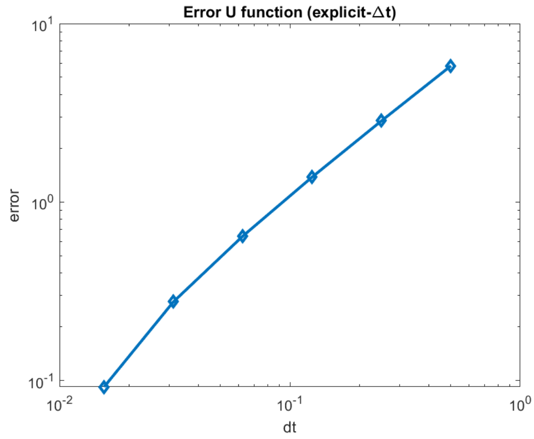
In what follows we illustrate the convergence order p in space considering the $\|.\|_\infty$ for the error with the following approximation

$$p = \frac{\ln\left(\frac{Error_1}{Error_2}\right)}{\ln\left(\frac{h_1}{h_2}\right)},$$

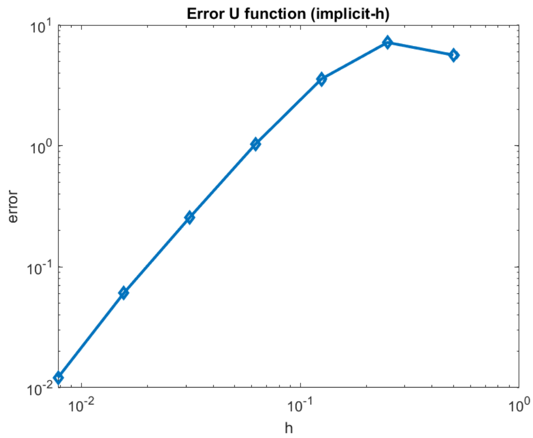
where $Error_i$, $i=1,2$ are computed with the grids defined by h_1 and h_2, respectively. For the space convergence the errors are computed considering the numerical solution obtained with $h = 7.8\cdot 10^{-3}$ and $\Delta t = 10^{-4}$ as the exact solution while for the time convergence the errors are computed considering the numerical solution obtained with $h = 10^{-1}$ and $\Delta t = 7.8\cdot 10^{-3}$. For both convergences, we took the constants $D_u = 10^{-2} = D_v$, $\chi = 3\cdot 10^{-1}$, and $T = 1$. The error is taken the maximum of the error at each time level. Considered only for the bacteria concentration. In Table 4.4 we present the results obtained for the explicit method (4.4) that are plotted in Figures 4.2(a) and 4.1(b). From these results the we conclude that the method is second convergence order in space and first convergence order in time. We point out that similar results were obtained for the implicit method (4.5). These results illustrate the error estimate obtained in last chapter for the spatial discretization (Theorems 5 and 7).



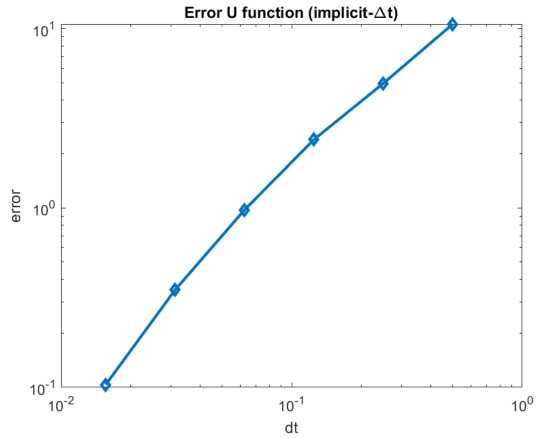
(a) Explicit method: Convergence order in h.



(b) Explicit method:Convergence order in Δt



(c) Implicit method: Convergence order in h



(d) Implicit method: Convergence order in Δt

Fig. 4.1 Error Behaviour Graphs

Explicit Method Error Table

h-step	Error-u	Order-u	Δt-step	Error-u	Order-u
0.5	6.84629e-02	1.92	0.5	5.79235	1.02
0.25	1.80974e-02	1.98	0.25	2.85171	1.05
0.125	4.57514e-03	2.01	0.125	1.38023	1.10
0.0625	1.13427e-03	2.07	0.0625	6.44194e-01	1.22
0.03125	2.70297e-04	2.32	0.03125	2.76102e-01	1.58
0.01562	5.40710e-05		0.01562	9.20372e-02	

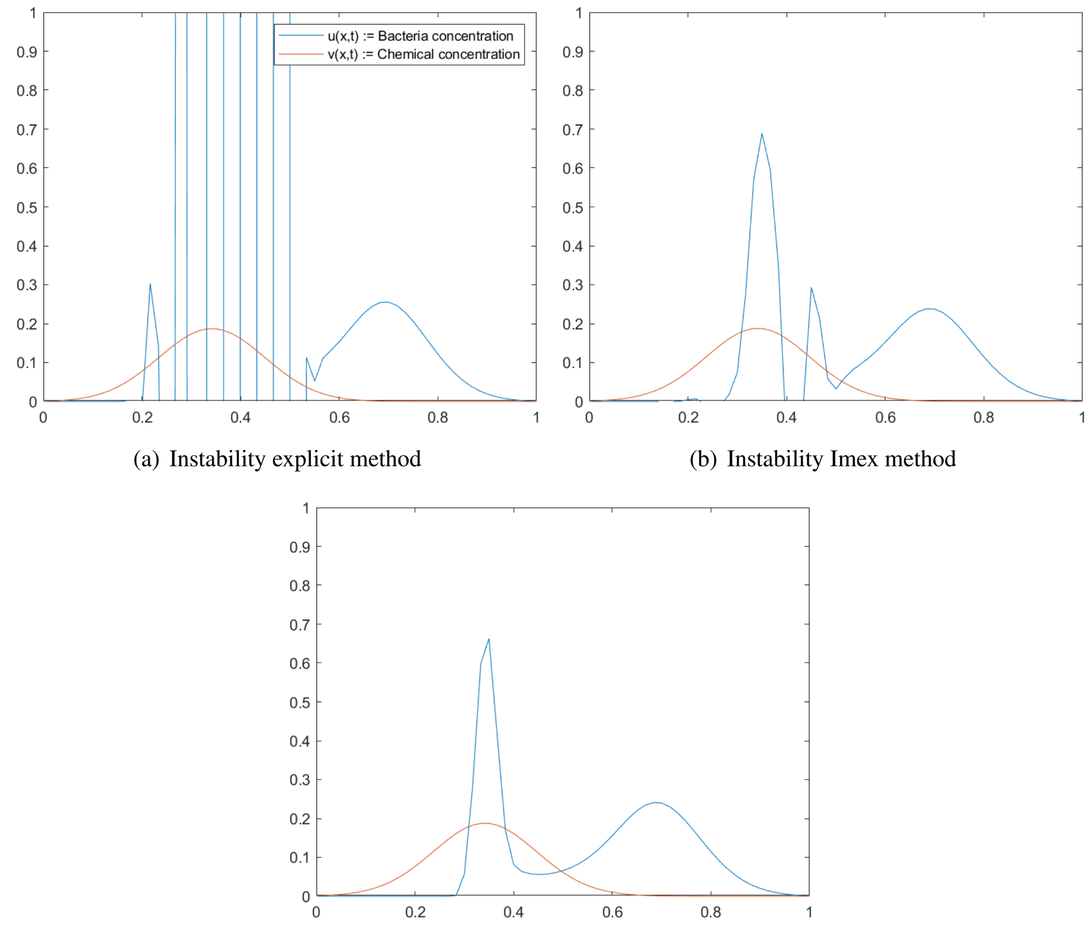
4.5 Stability

This section aims to illustrate the stability behaviour of the methods presented before. We consider

$$D_u = 5.2 * 10^{-3} = D_v,\ \chi = 8.6 \cdot 10^{-1}, T = 1, N = 61; M = 41, h = 0.01666,\ \Delta t = 0.0250.$$

The results obtained for $t_M = T$ are plotted in Figures (4.2(a)- 4.2(c)). As observe in this figures, the explicit method (4.1) is less stable than the implicit-explicit method (4.2) which is less stable than the implicit method (4.3).

We obtain the following graphs at the final time $t_M = T$.



(a) Instability explicit method

(b) Instability Imex method

(c) Instability implicit method

Fig. 4.2 Instability Graphs

4.6 Qualitative Behaviour

In what follows we illustrate the qualitative behaviour of the Keller-Segel model (1.4) considering the explicit method (4.4). The results were computed using the initial concentrations defined by

$$u(x,0) = 1, x \in [0.6, 0.69], u(x,0) = 0, x \notin [0.6, 0.69], \; v(x,0) = 0.5, x \in [0.3, 0.39], \; v(x,0) = 0, x \notin [0.3, 0.39],$$

plotted in Figure 4.3 and the following parameters

$$D_u = 10^{-2} = D_v, \; \chi = 3 \cdot 10^{-1}, \; T = 1, \; N = 101, \; M = 501, \; h = 0.01, \; \Delta t = 0.002.$$

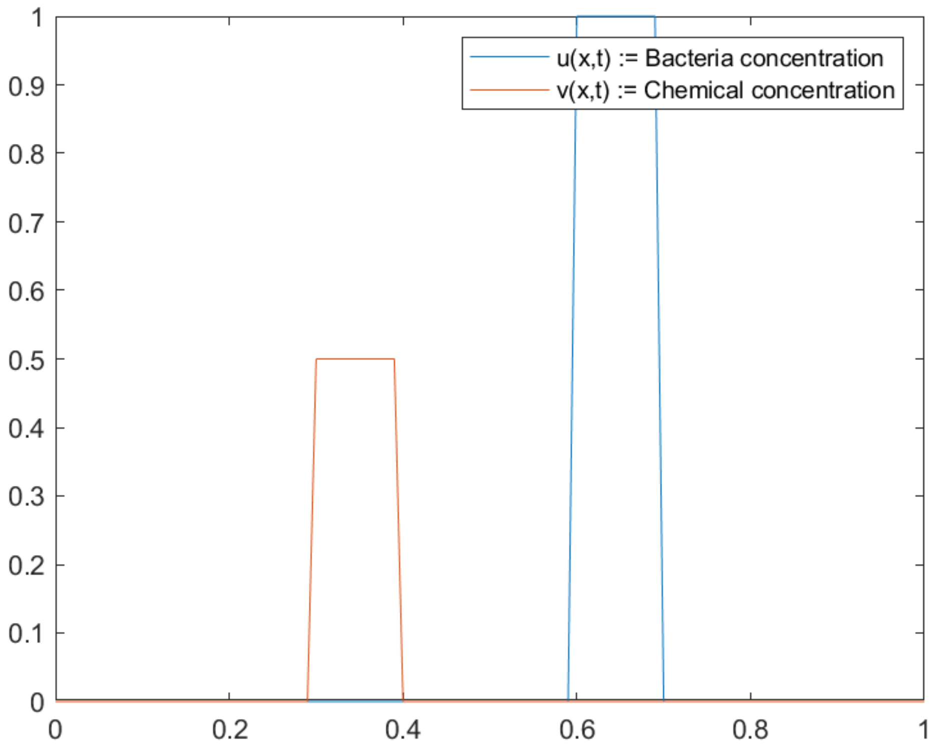


Fig. 4.3 Initial concentration of bacteria and chemical

In Figure 4.4(a) we plot the bacteria and chemical concentrations and chemical gradient, for Dirichlet boundary conditions, that will be our reference plot.

In the Figures 4.4(b) - 4.5(f) we plot the bacteria and chemical concentration as well as the chemical gradient in different scenarios defined by different parameters and initial conditions.

In Figure 4.4(b) and Figure 4.4(c) we consider $D_u = 2 \cdot 10^{-2}, 0.5 \cdot 10^{-2}$. We observe that higher bacteria diffusion coefficient leads to a smaller concentration of bacteria aggregating around the peak of the concentration of chemical. Due to Dirichlet boundary conditions the higher coefficient allows more bacteria to spread out towards the boundary on the right hand side along with the fact that the chemotaxis attraction effect is weaker the further they are from the chemical peak allowing them to escape the bounds of the simulation.

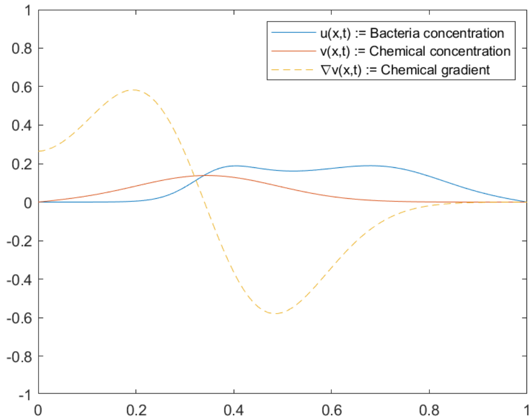
In Figure 4.4(d) and Figure 4.4(e) we take $D_v = 2 \cdot 10^{-2}, 0.5 \cdot 10^{-2}$. We observe that higher chemical diffusion coefficient causes the chemical to disperse faster which affects the chemotaxis movement of the bacteria to start earlier which doesn't allow as many bacteria to go out of bounds from dispersing due to diffusion.

Figure 4.5(a) and Figure 4.5(b) intend to illustrate the behaviour of the variables of interest for different values of χ. We take $\chi = 2 \cdot 3 \cdot 10^{-1}, 0.5 \cdot 3 \cdot 10^{-1}$. Higher χ increases bacteria sensitivity to variations in the chemical concentration.

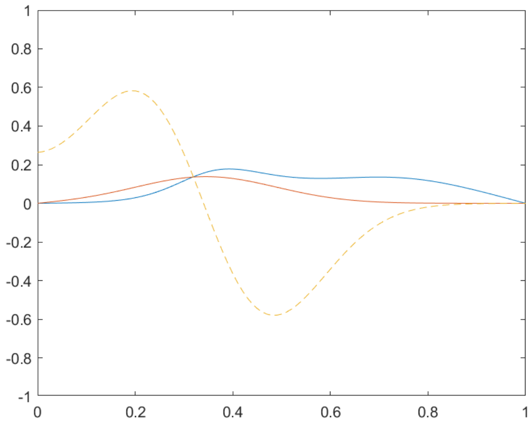
The effect of an increase and decrease of the initial concentration of bacteria on u is illustrated by Figure 4.5(c) and Figure 4.5(d). This leads to a vertical scaling of the u function.

For the Figures 4.5(e) and 4.5(f) we change the initial concentration of chemical to the double and to a half. An of the chemical increases leads to a bacteria higher peak and an aggregation around this peak. This behaviour is a consequence of an increase of the gradient.

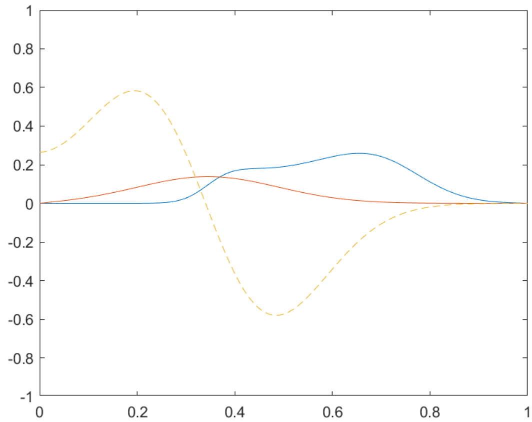
In the Figures 4.6(a) up to 4.7(f) we plot the bacteria and chemical concentration as well the chemical gradient similarly to before but with Neumann boundary conditions. There is no significant difference between the two cases except the expected behaviour at the boundaries.



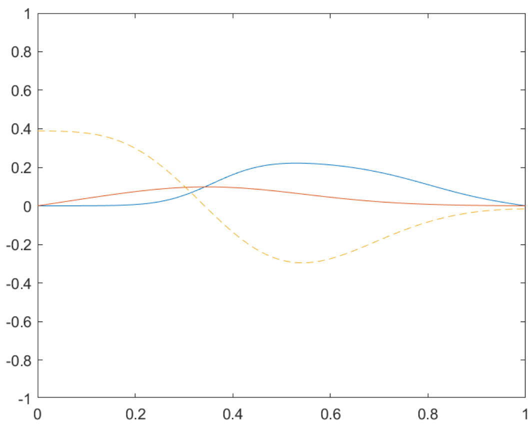
(a) Dirichlet Reference Graph



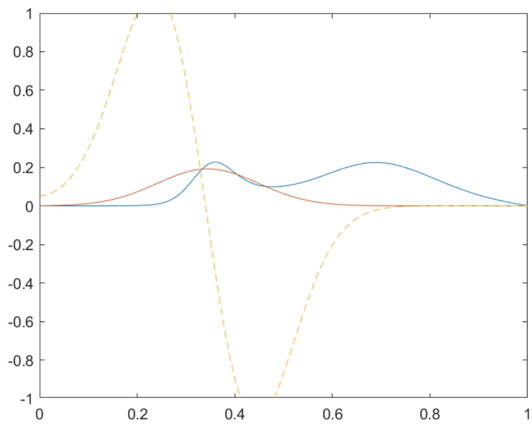
(b) $D_u = 2 \cdot 10^{-2}$



(c) $D_u = 0.5 \cdot 10^{-2}$

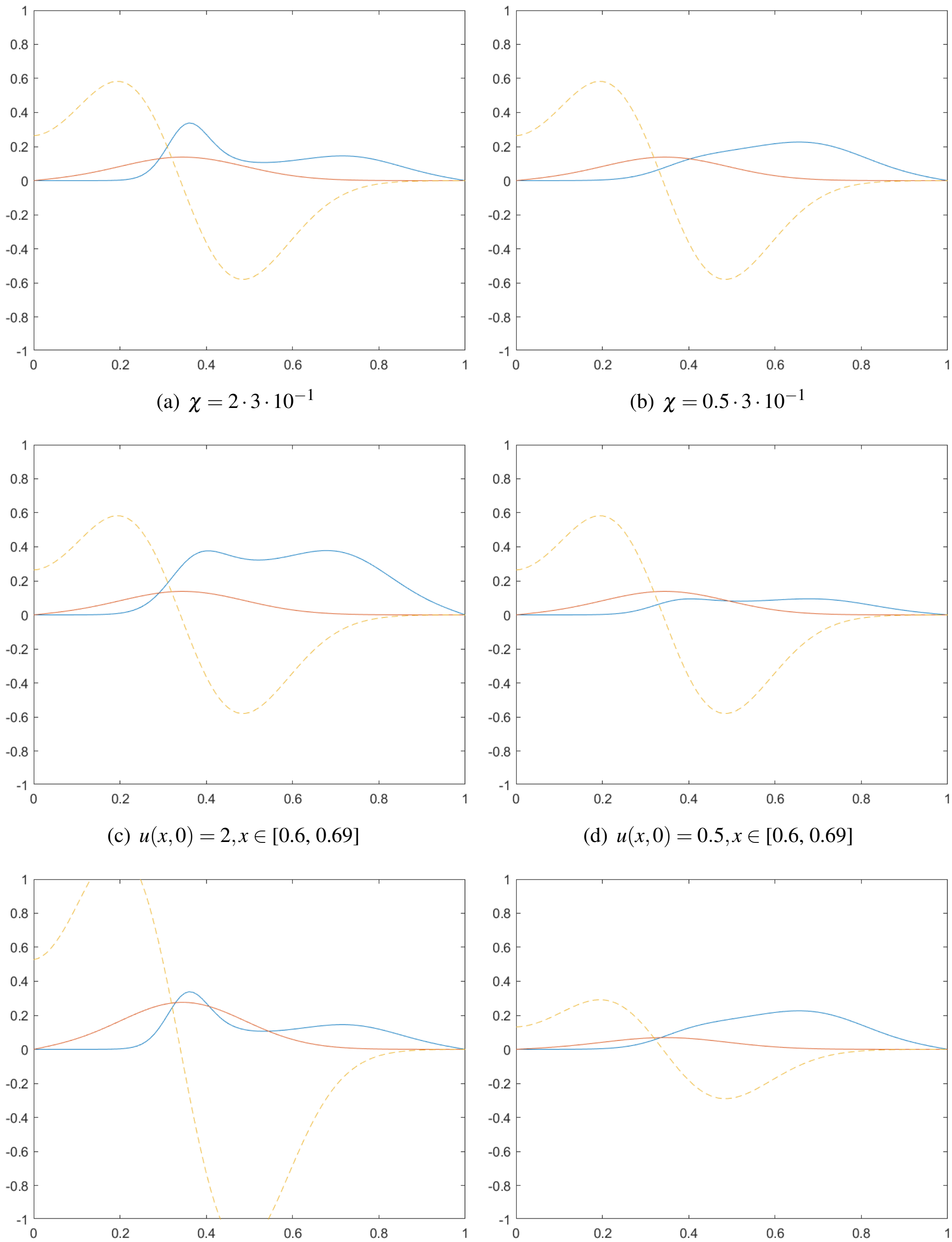


(d) $D_v = 2 \cdot 10^{-2}$



(e) $D_v = 0.5 \cdot 10^{-2}$

Fig. 4.4 Dirichlet Boundary Graphs



(a) $\chi = 2 \cdot 3 \cdot 10^{-1}$

(b) $\chi = 0.5 \cdot 3 \cdot 10^{-1}$

(c) $u(x,0) = 2, x \in [0.6, 0.69]$

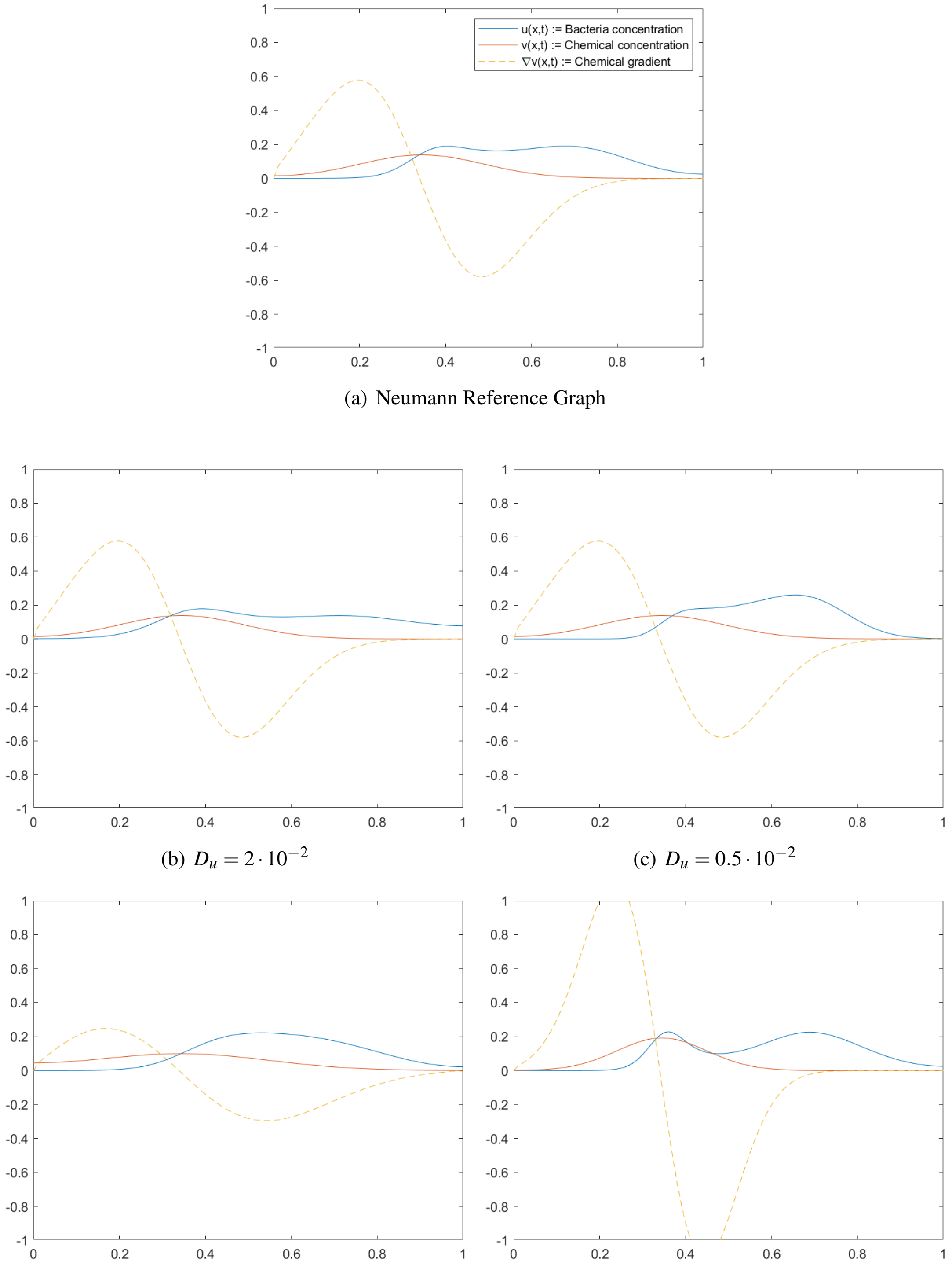
(d) $u(x,0) = 0.5, x \in [0.6, 0.69]$

(e) $v(x,0) = 1, x \in [0.3, 0.39]$

(f) $v(x,0) = 0.25, x \in [0.3, 0.39]$

Fig. 4.5 Dirichlet Boundary Graphs

Neumann Boundary Condition



(a) Neumann Reference Graph

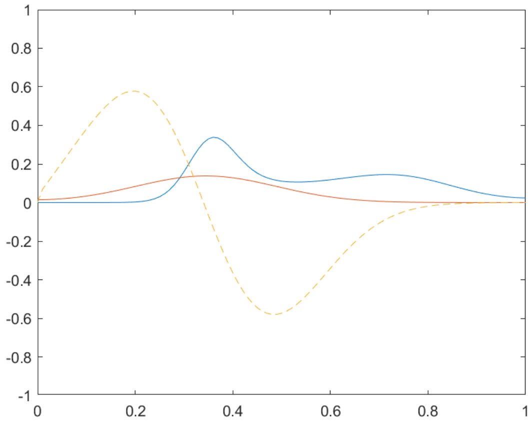
(b) $D_u = 2 \cdot 10^{-2}$

(c) $D_u = 0.5 \cdot 10^{-2}$

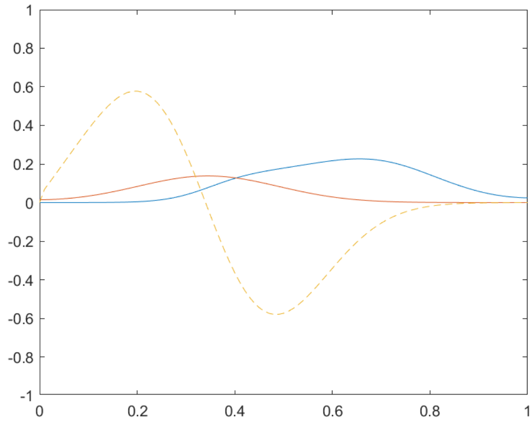
(d) $D_v = 2 \cdot 10^{-2}$

(e) $D_v = 0.5 \cdot 10^{-2}$

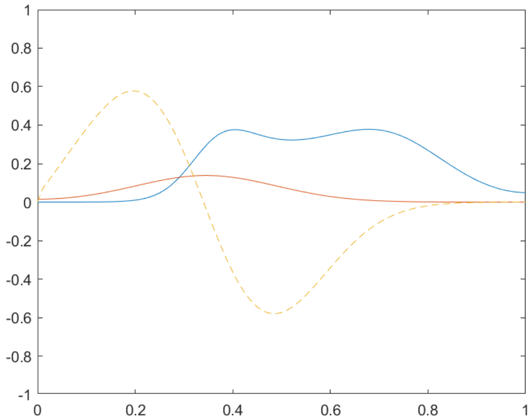
Fig. 4.6 Neumann Boundary Graphs



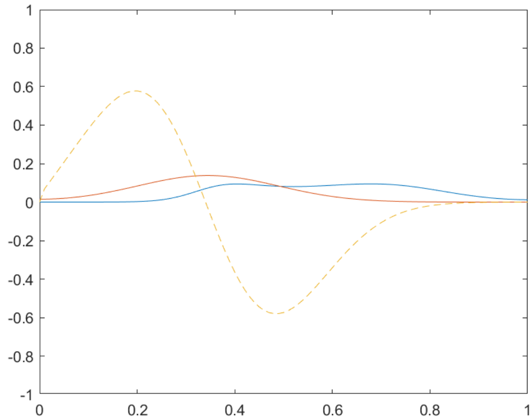
(a) $\chi = 2 \cdot 3 \cdot 10^{-1}$



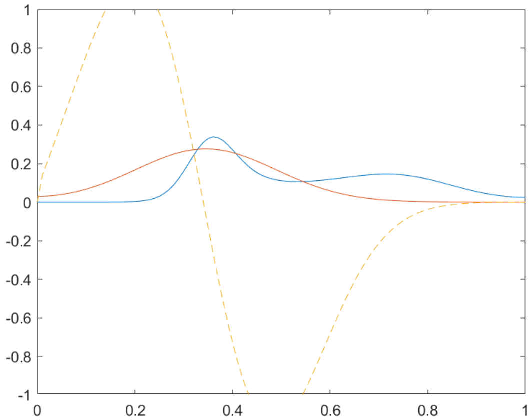
(b) $\chi = 0.5 \cdot 3 \cdot 10^{-1}$



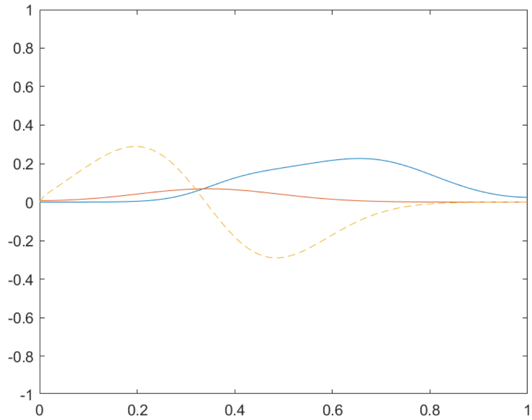
(c) $u(x,0) = 2, x \in [0.6,\ 0.69]$



(d) $u(x,0) = 0.5, x \in [0.6,\ 0.69]$



(e) $v(x,0) = 1, x \in [0.3,\ 0.39]$



(f) $v(x,0) = 0.25, x \in [0.3,\ 0.39]$

Fig. 4.7 Neumann Boundary Graphs

Chapter 5

Conclusion

In this work we studied from an analytical and numerical point of view, a Keller-Segel model that is used to describe the spread of bacteria induced by a chemical substance. In what concerns the analytical perspective, we establish an existence result Theorem 1 and a stability result Theorem 2. We recall that these results are established for Neumann boundary conditions. Although our initial objective was to study numerical methods for the IBVP (1.2), several difficulties arose associated with the Neumann boundary conditions. To gain sensibility in the treatment of these difficulties, we decided to proceed our work considering Dirichlet boundary conditions. We believe that in the end of this work, we are in conditions to return to our initial objective that will be considered in the near future.

In Chapter 3, we introduce a semi-discrete approach to compute an approximation for the IBVP (1.4) and we studied its stability and convergence. We realize that to conclude the stability of the bacteria semi-discrete approximation a uniform boundness assumption is needed for the chemical concentration. This assumption was avoided using the convergence analysis. The qualitative behaviour of the solution of the IBVP (1.4) with Dirichlet and Neumann boundary conditions is illustrated in Chapter 4.

To conclude, we remark, as stated before, that we would like to extend our results for Neumann boundary value problems with uniform and nonuniform spatial grids considering smooth and non-smooth solutions following the approach considered for instance in [7].

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