Numerical and Analytical Investigation of Chemotaxis Models

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Abstract. The Keller-Segel system is a linear parabolic-elliptic system, which describes the aggregation of slime molds resulting from their chemotactic features. By chemotaxis we understand the movement of an organism (like bacteria) in response to chemical stimulus, for example attraction by certain chemicals in the environment.

In this paper, we use the results of a paper by Zhou and Saito to validate our finite volume method with respect to blow-up analysis and equilibrium solutions. Based on these results, we study model variations and their blow-up behavior numerically.

We will discuss the question whether or not conservative numerical methods are able to model a blow-up behavior in the case of non-global existence of solutions.

Keywords: Chemotaxis model · Blow-up phenomenon
Finite volume method

1 Introduction

In this paper, we will study models for chemotaxis, commonly known as the Keller-Segel system.

It describes the movement of cells, specifically the Dictyostelium discoïdeum, which is a species of soil-living amoeba, often referred to as slime mold. The Keller-Segel system, named after the American physicist Evelyn Fox Keller and the American mathematician Lee Aaron Segel, consists of an elliptic and a parabolic partial differential equation coupled with initial and homogeneous Neumann boundary conditions [10,11]. The Neumann boundary conditions imply that there is no flow through the boundary of the domain, meaning that there are no cells leaving or entering the system. Both boundary and initial conditions are needed in order to find a solution to the Keller-Segel system. The mere question of the solvability of such a system in general is very challenging and stands in focus of current research [3]. Additionally, it is difficult to state an universal method to solve partial differential equations. The finite volume method is used because of its conservation properties [1,5].

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If a solution of a system of partial differential equations becomes pointwise larger and larger until it eventually becomes infinite in finite time, we speak of numerical blow-up. The cell aggregation of the system is counterbalanced by diffusion, but if the cell density is sufficiently large, the chemical interaction dominates diffusion and may lead to finite-time blow-up of the cell density [13]. This behavior is often referred to as the most interesting feature of the Keller-Segel equations [8,9].

2 Chemotaxis and Keller-Segel System

For a wide description of the Chemotaxis/Keller-Segel model and extensive explanations and derivations of the models, we refer to the thesis [16] and the review paper [7].

In its original form, the Keller-Segel system consists of four coupled reaction-advection-diffusion equations [11]. These can be reduced under quasi-steady-state assumptions to a model for two unknown functions u and v which will form the basis for our study. With an appropriate non-dimensionalisation and some very natural assumptions starting from the original Keller-Segel system, we get the following systems of partial differential equations:

$$\begin{aligned} u_t &= \nabla \cdot (D\nabla u - \chi u \nabla v) \\ 0 &= \nabla^2 v + u - v \end{aligned} \tag{1}$$

and

$$\begin{aligned} u_t &= \nabla \cdot (D\nabla u - \chi u \nabla v) \\ v_t &= \nabla^2 v + u - v. \end{aligned} \tag{2}$$

(1) and (2) are the so-called minimal models with the density of the cellular slime molds u, the concentration of the chemical substance/attractant v and the diffusion coefficient of cell D.

The important term in the equation for u,

$$\Phi_{\text{chemo}} = \chi u \nabla v,$$

is the chemotactic flux (see Müller et al. [12]) where χ, the chemotactic sensitivity, depends on the density of the attractant.

Both (1) and (2) are considered in a bounded domain $\Omega \in \mathbb{R}^d$, $d = 1, 2, 3$. The mathematical models are closed by zero flux boundary conditions (homogeneous Neumann) on $\Gamma = \partial\Omega$ and initial conditions $u(x, 0) = u_0(x)$ and $v_0(x, 0) = v_0(x)$ (only necessary for (2)).

The first substantial mathematical analysis of the Keller-Segel model was performed by Gajewski and Zacharias [6] introducing a Lyapunov function for the system (2). All other mathematical investigations of Keller-Segel systems followed the ideas of [6]. As a result of the analysis, global existence of solutions in the sub-critical case were shown.

Extensive mathematical and numerical analysis of the minimal Keller-Segel system (1) can be found in the paper of Zhou and Saito [17].

The Keller-Segel system admits several a priori estimates which reflects the basic modeling assumptions that have been mentioned above: the solution remains positive

$$u(t,x) > 0 \tag{3}$$

and the total mass is conserved

$$\int_\Omega u(t,x)\mathrm{d}x = \int_\Omega u_0(x)\mathrm{d}x =: m^0, \tag{4}$$

which imply the conservation of the L^1 norm:

$$\|u(t)\|_{L^1(\Omega)} = \|u_0\|_{L^1(\Omega)}, \quad t \in [0,T].$$

2.1 Variations of the Minimal Keller-Segel System

From the view of mathematical biology, it is interesting to consider modifications of the standard Keller-Segel system. Roughly, the mathematical meaning of the modifications is a regularisation. This leads to different behavior of the solutions and in some cases blow-up effects can be suppressed.

In this paper, we will discuss and numerically analyse the following models.

Signal-dependent sensitivity models

Consideration of signal-dependent sensitivity leads to the receptor model

$$\begin{aligned} u_t &= \nabla \cdot (D\nabla u - \frac{\chi u}{(1+\alpha v)^2}\nabla v) \\ v_t &= \nabla^2 v + u - v, \end{aligned} \tag{5}$$

and the logistic model

$$\begin{aligned} u_t &= \nabla \cdot (D\nabla u - \chi u \frac{1+\beta}{v+\beta}\nabla v) \\ v_t &= \nabla^2 v + u - v. \end{aligned} \tag{6}$$

For $\alpha \to 0$, model (5) tends to the minimal model (2), and for $\beta \to \infty$, the model (6) approaches the minimal model.

Density-dependent sensitivity models

For the volume-filling model

$$\begin{aligned} u_t &= \nabla \cdot (D\nabla u - \chi u(1 - \frac{u}{\gamma})\nabla v) \\ v_t &= \nabla^2 v + u - v, \end{aligned} \tag{7}$$

we get the minimal model by $\gamma \to \infty$. Another type of a density-dependent sensitivity model is given by

$$\begin{aligned} u_t &= \nabla \cdot (D\nabla u - \chi u \frac{1}{1+\epsilon u}\nabla v) \\ v_t &= \nabla^2 v + u - v, \end{aligned} \tag{8}$$

where $\epsilon \to 0$ leads to the minimal model.

Signal and cell kinetics models

The nonlinear signal kinetics model reads as

$$\begin{aligned} u_t &= \nabla \cdot (D\nabla u - \chi u \nabla v) \\ v_t &= \nabla^2 v + \frac{u}{1+\Psi u} - v \end{aligned} \tag{9}$$

and approximates the minimal model for $\Psi \to 0$. The cell kinetics model is of the form

$$\begin{aligned} u_t &= \nabla \cdot (D\nabla u - \chi u \nabla v) + ru(1-u) \\ v_t &= \nabla^2 v + u - v \end{aligned} \tag{10}$$

and in the limit of zero growth $r \to 0$, it leads to the minimal model.

3 Finite Volume Scheme

We will next determine the terms which are necessary for the construction of the finite volume method. We will then present a linear finite volume scheme and take a look at the conservation laws.

We will follow the notation described in [17] and [5]. Let Ω be a convex polygonal domain in $\mathbb{R}$. First, we will define a very important notion following Eymard et al. [5]:

Definition 1 (Admissible mesh). *Let Ω be an open bounded polygonal subset of $\mathbb{R}$, $d = 2$ or $d = 3$. An* admissible finite volume mesh *of Ω, denoted by $\mathcal{T}$, is given by a family of control volumes, which are open polygonal convex subsets of Ω, a family of subsets of $\overline{\Omega}$ contained in hyperplanes of $\mathbb{R}^d$, denoted by $\mathcal{E}$ (these are edges (two-dimensional) or sides (three-dimensional) of the control volumes), with strictly positive $(d-1)$-dimensional measure, and a family of points of Ω denoted by $\mathcal{P}$ satisfying the following properties (in fact, we shall denote, somewhat incorrectly, by $\mathcal{T}$ the family of control volumes):*

(i) The closure of the union of all the control volumes is $\overline{\Omega}$, $\overline{\Omega} = \bigcup_{K\in\mathcal{T}} \overline{K}$.

(ii) For any $K \in \mathcal{T}$, there exists a subset $\mathcal{E}_K$ of $\mathcal{E}$ such that $\partial K = \overline{K} \backslash K = \bigcup_{\sigma\in\mathcal{E}_K} \overline{\sigma}$. Furthermore, $\mathcal{E} = \bigcup_{K\in\mathcal{T}} \mathcal{E}_K$.

(iii) For any $(K, L) \in \mathcal{T}^2$ with $K \neq L$, either the $(d-1)$-dimensional Lebesgue measure of $\overline{K} \cap \overline{L}$ is 0 or $\overline{K} \cap \overline{L} = \overline{\sigma}$ for some $\sigma \in \mathcal{E}$, which will then be denoted by $K|L$.

(iv) The family $\mathcal{P} = (x_K)_{K\in\mathcal{T}}$ is such that $x_K \in \overline{K}$ (for all $K \in \mathcal{T}$) and, if $\sigma = K|L$, it is assumed that $x_k \neq x_L$, and that the straight line $\mathcal{D}_{K,L}$ going through x_K and x_L is orthogonal to $K|L$.

(v) For any $\sigma \in \mathcal{E}$ such that $\sigma \subset \partial\Omega$, let K be the control volume such that $\sigma \in \mathcal{E}_K$. If $x_K \notin \sigma$, let $\mathcal{D}_{K,\sigma}$ be the straight line going through x_K and orthogonal to σ, then the condition $\mathcal{D}_{K,\sigma} \cap \sigma \neq \emptyset$ is assumed; let $y_\sigma = \mathcal{D}_{K,\sigma} \cap \sigma$.

Let $\mathcal{T}$ be an admissible mesh. As defined above, an element $K \in \mathcal{T}$ is called control volume. We introduce the neigborhood of $K \in \mathcal{T}$:

$$\mathcal{N}_K := \{L \in \mathcal{T} | \overline{L} \cap \overline{K} \neq \emptyset\}.$$

Let $K|L$ (or $\sigma_{K,L}$) denote the common edge $\overline{L} \cap \overline{K}$ of control volumes K and L. We introduce the set of interior (resp. boundary) edges inside Ω (resp. on Γ):

$$\begin{aligned}\mathcal{E}_{\text{int}} &= \{K|L \mid \forall K \in \mathcal{T}, \forall L \in \mathcal{N}_K\},\\ \mathcal{E}_{\text{ext}} &= \mathcal{E} \setminus \mathcal{E}_{\text{int}}.\end{aligned}$$

For every control volume K, let P_K (or denoted by x_K) be the control point. And the segment $\overline{P_K P_L}$ is perpendicular to $K|L$ for all $K \in \mathcal{T}$, $L \in \mathcal{N}_K$.

Set

$$\begin{aligned} d_{K,L} &:= \text{dist}(P_K, P_L), \qquad \tau_{K,L} := \tfrac{m(K|L)}{d_{K,L}}, \quad K, L \in \mathcal{T},\\ d_{K,\sigma} &:= \text{dist}(P_K, \sigma_{K,\Gamma}), \quad \tau_{K,\sigma} := \tfrac{m(\sigma_{K,\Gamma})}{d_{K,\sigma}}, \quad \tau_{K,\sigma} \in \mathcal{E}_{\text{ext}}.\end{aligned}$$

Here, $m(\mathcal{O}) = m_{d-1}(\mathcal{O})$ denotes the $(d-1)$-dimensional Lebesgue measure of $\mathcal{O} \subset \mathbb{R}^{d-1}$.

Note that

$$\tau_{K,L} = \tau_{L,K},$$

which means that it does not make any difference whether we consider the neighbor L of control volume K or the neighbor K of control volume L.

We will now introduce a linear finite volume scheme in order to discretise the Keller-Segel system.

3.1 Linear Finite Volume Scheme

An important issue of the discretisation of the Keller-Segel system is the handling of the convective terms. Upon computing a convection-diffusion problem, there often occur problems when the convective term gets by far bigger than the diffusion term. In our example, when the cell density is very large, the cell aggregation outbalances diffusion. To handle this, an upwind scheme is used [15]. The error of the upwind scheme is of order $\mathcal{O}(h)$, however, the physics of the system is better reproduced than by use of the central difference quotient. Especially in convection dominated cases like drift diffusion, instead of simple upwind schemes, Scharfetter-Gummel approximations are used. They control the order of approximation between one and two, depending on the convection velocity.

We set the function space X_h for the discrete solution (u_h, v_h):

$$X_h = \text{span}\{\phi_K \mid K \in \mathcal{T}\},$$

where ϕ_K is the characteristic (or indicator) function of K ($\phi_K = 1$ in K, $\phi = 0$ otherwise). With the assumptions on the mesh from above, we define the discrete

$W^{1,p}$ semi-norm for $u_h \in X_h$:

$$|u_h|^p_{1,p,\mathcal{T}} = \sum_{K|L\in\mathcal{E}_{\rm int}} \tau_{K,L} d^{2-p}_{K,L} \left|u_K - u_L\right|^p, \quad \text{for } p \in [1,\infty), \tag{11}$$

$$|u_h|_{1,\infty,\mathcal{T}} = \max_{K|L\in\mathcal{E}_{\rm int}} \frac{|u_K - u_L|}{d_{K,L}}. \tag{12}$$

We further set the discrete $W^{1,p}$ norm for X_h: For any $u_h \in X_h$,

$$\|u_h\|_{1,p,\mathcal{T}} := |u_h|_{1,p,\mathcal{T}} + \|u_h\|_p.$$

For $u_h \in X_h$ and $K \in \mathcal{T}$, we set $u_K = u_h(P_K)$. Given the initial condition

$$u^0_h \in X_h, \quad u^0_h \geq 0,$$
$$\int_\Omega u^0_h {\rm d}x = \sum_{K\in\mathcal{T}} m(K) u^0_K \equiv \theta > 0, \tag{13}$$

we state the finite volume scheme for the Keller-Segel system (1):

Find $(u^n_h, v^n_h) \in X_h \times X_h$ for $n \in \mathbb{N}_+$, such that:

$$\begin{aligned}
&\sum_{L\in\mathcal{N}_K} \tau_{K,L}(v^{n-1}_K - v^{n-1}_L) + m(K) v^{n-1}_K = m(K) u^{n-1}_K \\
&\Leftrightarrow \sum_{L\in\mathcal{N}_K} \frac{m(K|L)}{d_{K,L}}(v^{n-1}_K - v^{n-1}_L) + m(K) v^{n-1}_K = m(K) u^{n-1}_K,
\end{aligned} \tag{14}$$

which is the discrete to the elliptic equation

$$-\Delta v + v = u,$$

and

$$\begin{aligned}
&m(K)\partial_{\tau_n} u^n_K + \sum_{L\in\mathcal{N}_k} \tau_{K,L}(u^n_K - u^n_L) \\
&\qquad + \sum_{L\in\mathcal{N}_k} \tau_{K,L}\left[(Dv^{n-1}_{K,L})_+ u^n_K - (Dv^{n-1}_{K,L})_- u^n_L\right] = 0 \\
&\Leftrightarrow m(K)\frac{u^n_K - u^{n-1}_K}{\tau_n} + \sum_{L\in\mathcal{N}_k} \frac{m(K|L)}{d_{K,L}}(u^n_K - u^n_L) \\
&\quad + \sum_{L\in\mathcal{N}_k} \frac{m(K|L)}{d_{K,L}}\left[\max\left(v^{n-1}_L - v^{n-1}_K, 0\right) u^n_K - \max\left(-(v^{n-1}_L - v^{n-1}_K), 0\right) u^n_L\right] = 0,
\end{aligned} \tag{15}$$

which is the discrete to the parabolic equation

$$u_t = \Delta u - \nabla\cdot(u\nabla v),$$

using implicit Euler for the time discretisation. For the parabolic v-equation of (2), we also use the implicit Euler method, as in the case of the parabolic u-equation.

Here, $w_+ = \max(w, 0)$, $w_- = \max(-w, 0)$, hence following the technique of an upwind approximation, and

$$Dv_{K,L} = v_L - v_K \text{ for } v_h \in X_h, \quad Dv_{K,\sigma} = 0 \text{ for } \sigma \in \mathcal{E}_{\text{ext}}.$$

In the scheme, $\tau > 0$ is the time-step increment, $t_n = \tau_1 + \cdots \tau_n$, and $\partial_{\tau_n} u_K^n$ is the backward Euler difference quotient approximating to $\partial_t u(t_n)$, which is defined by

$$\partial_{\tau_n} u_K^n = \frac{u_K^n - u_K^{n-1}}{\tau_n}.$$

For the modified models (5)−(10), we have the more general equations

$$u_t = \nabla \cdot (D\nabla u - \varphi(u, v)u\nabla v) \quad \text{and} \quad v_t = \Delta v + \psi(u)u - v. \tag{16}$$

Finally, for (16), we have to modify the discretisation (15) by inserting a factor $\varphi(u_L^{n-1}, v_L^{n-1})$. In other words, we perform a linearisation.

3.2 Conservation Laws

We consider the Keller-Segel system (1). The solution (u, v) satisfies the conservation of positivity

$$u(x, t) > 0, \quad (x, t) \in \bar{\Omega} \times [0, T], \tag{17}$$

and the conservation of total mass

$$\int_\Omega u(x, t)\mathrm{d}x = \int_\Omega u_0(x)\mathrm{d}x, \quad t \in [0, T], \tag{18}$$

which imply the conservation of the L^1 norm.

Remark 1. The value of $\|u_0\|_{L^1(\Omega)}$ plays a crucial role in the blow-up behavior and global existence of solutions, as we will see in Theorem 3.

The conservation properties (17) and (18) are essential requirements and it is desirable that numerical solutions preserve them when we solve the Keller-Segel system by numerical methods.

In the following, we will state some important theorems when working with conservation laws. For the proofs, we refer to the paper [17] and the thesis [16].

Theorem 1 (Conservation of total mass). *Let $\{(u_h^n, v_h^n)\}_{n\geq 0} \subset X_h$ be the solution of the finite volume scheme (14−15). Then we have*

$$(v_h^n, 1) = (u_h^n, 1) = (u_h^0, 1), \quad \forall n \geq 0. \tag{19}$$

Theorem 2 (Well-posedness and conservation of positivity). *Let $u_h^0 \geq 0$, $u_h \not\equiv 0$. Then (14)−(15) admits a unique solution $\{(u_h^n, v_h^n)\}_{n\geq 0} \subset X_h \times X_h$, such that $u_h^n > 0$ for $n \geq 1$ and $v_h^n > 0$ for $n \geq 0$.*

3.3 Discrete Free Energy

As mentioned before, the L^1 conservation (which follows from the conservation of positivity and the conservation of total mass) is an important feature of the Keller-Segel system. Another important feature of the Keller-Segel system is the existence of free energy. By free energy we understand the energy in a physical system that can be converted to do work. It is desirable that the numerical solution preserves both these properties.

For the free energy

$$W(u(t), v(t)) = \int_\Omega (u \log u - u) \mathrm{d}x - \frac{1}{2} \int_\Omega uv \mathrm{d}x, \tag{20}$$

one can show the important energy inequality. The free energy is expressed as

$$\frac{d}{dt} W(u(t), v(t)) \leq 0, \quad t \in [0, T].$$

In the following, we will discuss a discrete version of the energy equality (20). For the solution $\{(u_h^n, v_h^n)\}_{n \geq 0}$ of the finite volume scheme (14)−(15), we set

$$H_h^n := \sum_{K \in \mathcal{T}} m(K)(u_K^n \log u_K^n - u_K^n). \tag{21}$$

For any internal edge $K|L \in \mathcal{E}_{\mathrm{int}}$, we set

$$\tilde{u}_{K,L}^n = \frac{u_K^n - u_L^n}{\log u_K^n - \log u_L^n}, \quad \text{for } u_K^n \neq u_L^n. \tag{22}$$

Let $\tilde{u}_{K,L}^n = u_K^n$, if $u_K^n = u_L^n$. Then there exists $s_{K,L}^n \in [0, 1]$ such that

$$\tilde{u}_{K,L}^n = s_{K,L}^n u_K^n + (1 - s_{K,L}^n) u_L^n. \tag{23}$$

Analogous to the energy function $W(u, v)$, we define the discrete energy function

$$W_h^n = H_h^n - \frac{1}{2} \sum_{K \in \mathcal{T}} m(K) u_K^n v_K^n.$$

However, we can not obtain the inequality $\partial_{\tau_n} W_h^n \leq 0$. Instead of that, we have the following estimate on $\partial_{\tau_n} W_h^n$. For the discrete energy W_h^n, we have the inequality

$$\begin{aligned} \partial_{\tau_n} W_h^n \leq & - \sum_{K|L \in \mathcal{E}_{\mathrm{int}}} \tau_{K,L} \left| \frac{D u_{K,L}^n}{\sqrt{\tilde{u}_{K,L}^n}} - D v_{K,L}^{n-1} \sqrt{\tilde{u}_{K,L}^n} \right|^2 \\ & - \frac{\tau_n}{2} \left[\sum_{K \in \mathcal{T}} |\partial_{\tau_n} v_K^n|^2 + \sum_{K|L \in \mathcal{E}_{\mathrm{int}}} \tau_{K,L} \left| \partial_{\tau_n} (D v_{K,L}^n) \right|^2 \right] + C_h(u_h^n, v_h^n), \end{aligned}$$

where $C_h(u_h^n, v_h^n)$ is defined by

$$C_h(u_h^n, v_h^n) := \\ -\sum_{K|L\in\mathcal{E}_{\text{int}}} \tau_{K,L}\left[(Dv_{K,L}^{n-1})_+^2(1-s_{K,L}^n)(u_K^n-u_L^n)+(Dv_{K,L}^{n-1})_-^2 s_{K,L}(u_L^n-u_K^n)\right],$$

and it admits the estimate:

$$|C_h(u_h^n, v_h^n)| \le Ch\,|u_h^n|_{1,\infty,\mathcal{T}}\,|v_h^n|_{1,2,\mathcal{T}}\,.$$

Here, $s_{K,L}^n$ satisfies (23) and $|\cdot|_{1,p,\mathcal{T}}$ is defined by (11) and (12).

Thus, the finite volume scheme conserves the energy inequality in the above noted sense.

4 Numerical Blow-Up

When organisms, such as the amoeba Dictyostelium discoïdeum, secrete an attracting chemical and move towards areas of higher chemical concentration, this leads to aggregation of organisms. The cell aggregation is counterbalanced by diffusion, in particular by the use of the upwind type approximation. However, if the cell density is sufficiently large, the chemical interaction dominates the diffusion and this may lead to finite-time blow-up of the cell density.

This blow-up phenomenon, or chemotactic collapse, can never occur in one dimension, which was shown in [17]. In two dimensions, it can occur if a total cell number on Ω is larger than a critical number but it can never occur for the total cell number on Ω less than the critical number [2,4]. We will focus on the two-dimensional case, shortly discuss some important properties of the system before turning to the finite volume scheme. Throughout this section, we will distinguish between the conservative and non-conservative system and derive the finite volume scheme for both, using Cartesian coordinates.

4.1 Two-Dimensional System

We consider the finite volume scheme with mesh $\mathcal{T}$:

$$-L = x_{\frac{1}{2}} < x_{1+\frac{1}{2}} < \cdots < x_{N+\frac{1}{2}} = L,$$

where $0 < N \in \mathbb{N}$ is the number of control volumes, $h = \frac{2L}{N}$ is the uniform mesh size in both directions. We set

$$u_{i,j}^0 = u_0(x_i, y_j), \quad i = 1,\dots,N,\ j = 1,\dots,M.$$

Let $(u_{i,j}^n, v_{i,j}^n)$ be the approximation of $(u(t_n, x_i, y_j), v(t_n, x_i, y_j))$. With the obvious notations for the forward and backward difference quotients

$$\nabla_x u^n = \frac{u_{i+1,j}^n - u_{i,j}^n}{h}, \quad \nabla_{\bar{x}} u^n = \frac{u_{i,j}^n - u_{i-1,j}^n}{h},$$

we formulate the finite volume scheme for the minimal Keller-Segel system. It is to find

$$u^n = (u^n_{i,j})^{N,M}_{i,j=1}, \quad v^n = (v^n_{i,j})^{N,M}_{i,j=1}$$

for $n = 1, 2, ..., J$, such that

$$\begin{aligned} -\nabla_x \nabla_{\bar{x}} v^n_{i,j} - \nabla_y \nabla_{\bar{y}} v^n_{i,j} + v^n_{i,j} &= u^{n-1}_{i,j}, \\ \partial_\tau u^n_{i,j} - \nabla_x \nabla_{\bar{x}} u^n_{i,j} - \nabla_y \nabla_{\bar{y}} u^n_{i,j} + \frac{\chi}{h} convup(\nabla v, u) &= 0\ , \\ v^n_{0,j} = v^n_{1,j},\ v^n_{i,0} = v^n_{i,1},\ v^n_{0,N} = v^n_{0,N+1},\ v^n_{N,0} &= v^n_{N+1,0}, \\ u^n_{0,j} = u^n_{1,j},\ u^n_{i,0} = u^n_{i,1},\ u^n_{0,N} = u^n_{0,N+1},\ u^n_{N,0} &= u^n_{N+1,0}. \end{aligned}$$

with the upwind-discretisation

$$\begin{aligned} convup(\nabla v, u) = &[\max(\nabla_x v^n, 0) + \max(-\nabla_{\bar{x}} v^n, 0)] u^n_{i,j} \\ &+ [\max(\nabla_y v^n, 0) + \max(-\nabla_{\bar{y}} v^n, 0)] u^n_{i,j} \\ &- \max(-\nabla_x v^n, 0) u^n_{i+1,j} - \max(\nabla_{\bar{x}} v^n, 0) u^n_{i-1,j} \\ &- \max(-\nabla_y v^n, 0) u^n_{i,j+1} - \max(\nabla_{\bar{y}} v^n, 0) u^n_{i,j-1} \end{aligned}$$

where $\tau > 0$ is the time-step increment and $\{u^0_{ij}\}^{N,M}_{i,j=1} \geq 0$ and not identically zero.

Blow-Up Behavior

Theorem 3 (2D Blow-Up). *In* $\mathbb{R}^2$, *assume* $\int_{\mathbb{R}^2} |x|^2 u_0(x) \mathrm{d}x < \infty$.

(i) (Blow-up) When the initial mass satisfies

$$m^0 := \int_{\mathbb{R}^2} u_0(x) \mathrm{d}x > m_{crit} := 8\pi$$

then any solution to the Keller-Segel system (1) becomes a singular measure in finite time.

(ii) When the initial data satisfies

$$\int_{\mathbb{R}^2} u_0 |log(u_0(x))| \mathrm{d}x < \infty \quad and \quad m^0 := \int_{\mathbb{R}^2} u_0(x) \mathrm{d}x < m_{crit} := 8\pi,$$

there are weak solutions to the Keller-Segel system (1) satisfying the a priori estimates

$$\int_{\mathbb{R}^2} u \left[|\ln(u(t))| + |x|^2 \right] \mathrm{d}x \leq C(t), \quad \|u(t)\|_{L^p(\mathbb{R}^2)} \leq C(p, t, u^0)$$

for $\|u_0\|_{L^p(\mathbb{R}^2)} < \infty,\ 1 < p < \infty$.

The mathematical interest here is to prove existence with an energy method rather than direct estimates based on Sobolev inequalities. For the proof, we refer to [14] or [16].

Remark 2. In general bounded domains, with no-flux boundary conditions, the critical mass is 8π because blow-up may occur on the boundary which intuitively acts as a reflection wall.

Properties of the System. In order to consider the blow-up solution, the moment is introduced:

$$M_2(t) = \int_\Omega u(x,t)|x|^2 \mathrm{d}x = 2\pi \int_0^L u(r,t) r^3 \mathrm{d}r, \tag{24}$$

which, with $\theta = \int_\Omega u_0 dx$, satisfies

$$\frac{d}{dt} M_2(t) \leq 4\theta - \frac{1}{2\pi}\theta^2 + \frac{1}{\pi L^2}\theta M_2(t) + \frac{1}{2e\pi}\theta^{\frac{3}{2}} M_2(t)^{\frac{1}{2}}. \tag{25}$$

This implies that if $\theta > 8\pi$ and $M_2(0)$ is sufficiently small, we then have

$$\frac{d}{dt} M_2(t) < 0, \quad t > 0, \tag{26}$$

which means that $M_2(t) \to 0$ at some time $t = t_b$. Since $u > 0$ and $\int_\Omega u(x,t) = \theta$, the function u actually blows up in finite time t_b. We call t_b the blow-up time.

We aim to show the discrete version of inequality (25). For $n = 1, \ldots, J$, we have

$$\frac{M_2^n - M_2^{n-1}}{\tau} \leq \frac{4\theta}{2\pi} - \left(\frac{\theta}{2\pi}\right)^2 + C_1 \theta M_2^{n-1} + C_2 \theta^{\frac{3}{2}} \sqrt{M_2^{n-1}} + C_3 h \theta^2, \tag{27}$$

where C_1, C_2, C_3 are independent of h, θ and M_2^{n-1}.

We should mention that (27) is not satisfied for the conservative scheme introduced above.

4.2 Non-conservative Finite Volume Scheme

We will now consider the numerical scheme without conservation of positivity but satisfying (27). With the above defined notations, we obtain this so-called non-conservative scheme by replacing the conservative discretised parabolic equation by

$$\begin{aligned} &\partial_\tau u_{i,j}^n - \nabla_x \nabla_{\bar{x}} u_{i,j}^{n-1} - \nabla_y \nabla_{\bar{y}} u_{i,j}^{n-1} \\ &+ \frac{\chi}{h}(\nabla_x v_{i,j}^{n-1} u_{i,j}^n + \nabla_y v_{i,j}^{n-1} u_{i,j}^n + \nabla_{\bar{x}} v_{i,j}^{n-1} u_{i-1,j}^n + \nabla_{\bar{y}} v_{i,j}^{n-1} u_{i,j-1}^n) = 0. \end{aligned} \tag{28}$$

We will now state that (27) is satisfied for the non-negative solution of the non-conservative scheme. In view of (27), for $\theta > 8\pi$ and sufficiently small M_2^0, M_2^n decreases by n. When M_2^n approaches 0, we have

$$\frac{M_2^n - M_2^{n-1}}{\tau} \approx \frac{4\theta}{2\pi} - (\frac{\theta}{2\pi})^2.$$

Theorem 4. *For the non-conservative scheme introduced above, let J be the largest time step such that $(u_h^n, v_h^n) \geq 0$, for any $1 \leq n \leq J$. Then we have the moment inequality*

$$\frac{M_2^n - M_2^{n-1}}{\tau} \leq \frac{4\theta}{2\pi} - \left(\frac{\theta}{2\pi}\right)^2 + C_1 \theta M_2^{n-1} + C_2 \theta^{\frac{3}{2}} \sqrt{M_2^{n-1}} + C_3 h \theta^2,$$

where C_1, C_2, C_3 are independent of h, θ and M_2^{n-1}.

5 Numerical Examples

In order to verify the theoretical results, we conducted various numerical simulations. We implemented the presented finite volume schemes using Python. The model and used parameters can be found in the figure captions. For the simulations, we used the conservative scheme.

We consider $\Omega = (0,1)^2$ and use a direction equidistant discretisation with $1 < N \in \mathbb{N}$, $h = \frac{1}{N-1}$ and $\tau = \tau_n = 0.2h$, $N = 41$ and $N = 61$. As initial conditions, we use

$$u = 1, \quad v = 1 + 0.1\exp(-10((x-1)^2 + (y-1)^2))$$

on Ω. In all examples, we reached the steady state (global existence of the solution), as can be seen in Figs. 1, 2 and 3. The solutions were grid-independent.

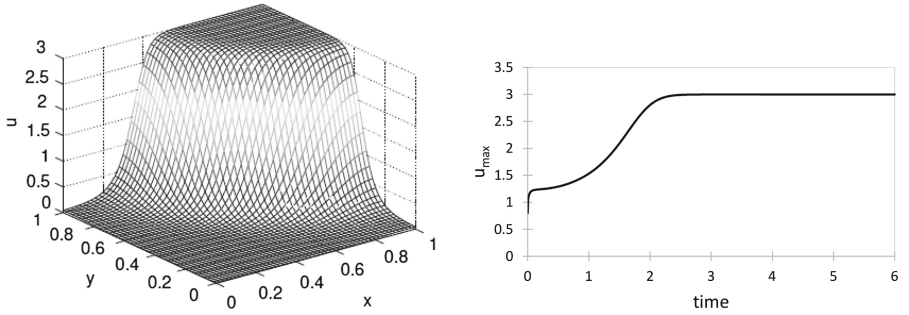

Fig. 1. Cell density (left) and cell density peak evolution (right) for problem (7), using $D = 0.1, \chi = 5.0, \gamma = 3.0$ (steady state)

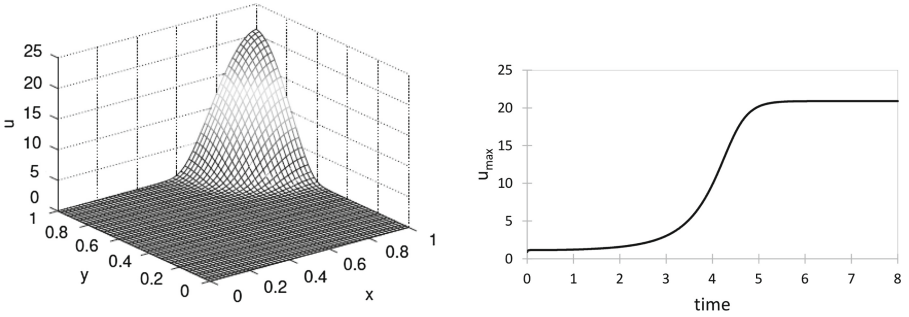

Fig. 2. Cell density (left) and cell density peak evolution (right) for problem (8), using $D = 0.1, \chi = 5.0, \epsilon = 1.0$ (steady state)

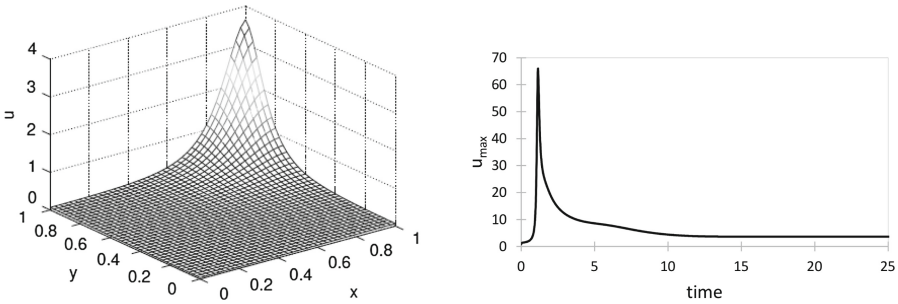

Fig. 3. Cell density (left) and cell density peak evolution (right) for problem (10), using $D = 0.1, \chi = 5.0, r = 0.25$ (steady state)

With the same setting, we define the function

$$W_{(x_0,y_0)} = \frac{M}{2\pi\theta} \exp\left(-\frac{(x-x_0)^2 + (y-y_0)^2}{2\theta}\right),$$

where $(x_0, y_0) \in (0,1)^2$, $M = 6\pi$, $\theta = \frac{1}{500}$ and choose the initial function

$$u_0 = W_{(\frac{1}{3},\frac{1}{3})} + W_{(\frac{1}{3},\frac{2}{3})} + W_{(\frac{2}{3},\frac{1}{3})} + W_{(\frac{2}{3},\frac{2}{3})}. \tag{29}$$

We also consider a non-symmetric situation given by the initial function

$$u_0 = \frac{1}{3}W_{(\frac{1}{3},\frac{2}{3})} + \frac{1}{2}W_{(\frac{1}{3},\frac{1}{3})} + W_{(\frac{2}{3},\frac{2}{3})}. \tag{30}$$

The initial mass is $24\pi > 8\pi$ and $11\pi > 8\pi$, respectively and thus, we expect the solutions to blow up in finite time.

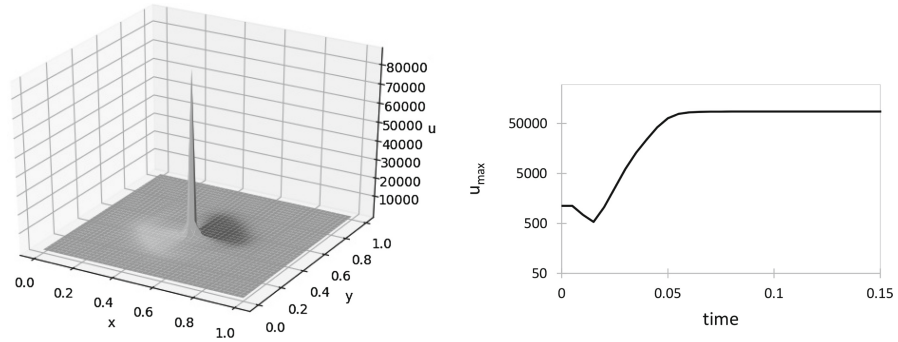

Fig. 4. Cell density (left) and cell density peak evolution (right) for problem (1) with initial data (29), using parameters $D = 0.1, \chi = 1$ (approximation of blow-up)

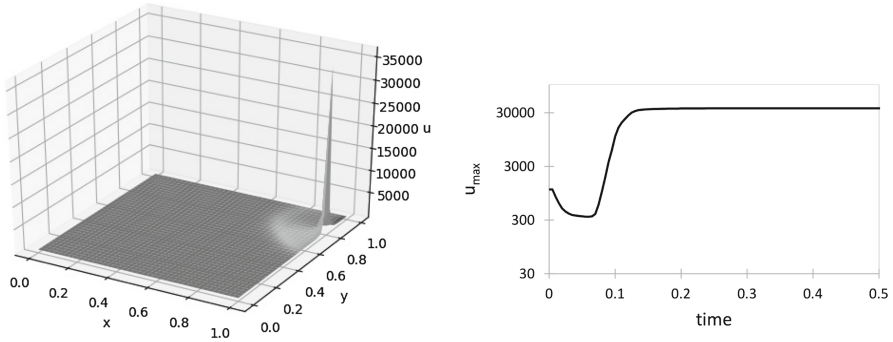

Fig. 5. Cell density (left) and cell density peak evolution (right) for problem (1) with initial data (30), using parameters $D = 1, \chi = 1$, (approximation of blow-up)

Let then $\Omega = (-0.5, 0.5)^2$. We consider the initial value

$$u_0 = 40 \exp\left(-10(x^2 + y^2)\right) + 10, \tag{31}$$

where $\|u_0\|_1 \approx 21.93 < 8\pi$. Therefore the solution will not blow up. With the same setting but the initial data

$$\begin{aligned} u_0 =& 100 \exp\left(-\frac{x^2 + y^2}{0.04}\right) + 60 \exp\left(-\frac{(x - 0.2)^2 + y^2}{0.05}\right) \\ &+ 30 \exp\left(-\frac{x^2 + (y - 0.02)^2}{0.05}\right), \end{aligned} \tag{32}$$

where $\|u_0\|_1 \approx 26.26 > 8\pi$.

Remark 3. Note that it is only possible to approximate the blow-up behavior with the finite volume scheme. Due to the conservation of mass, the solution will

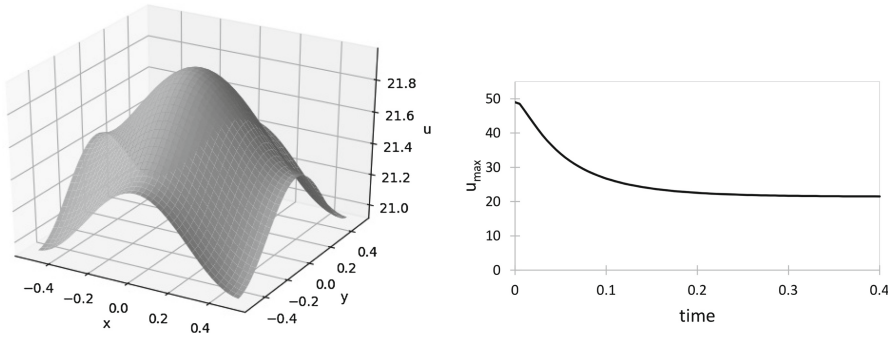

Fig. 6. Cell density (left) and cell density peak evolution (right) for problem (1) with initial data (31), using parameters $D = 0.1, \chi = 1$ (steady state)

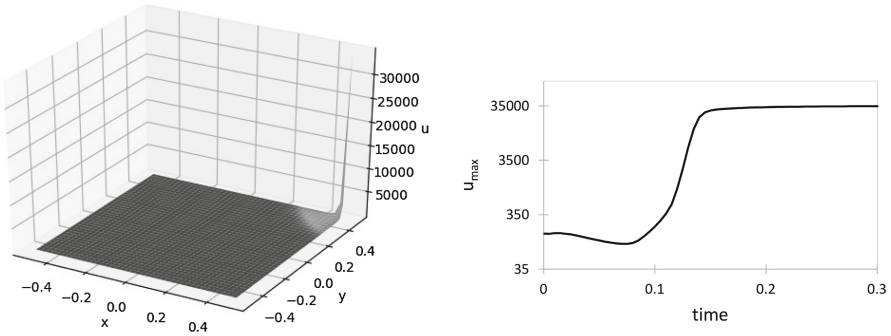

Fig. 7. Cell density (left) and cell density peak evolution (right) for problem (1) with initial data (32), using parameters $D = 0.1, \chi = 1$ (approximation of blow-up)

never become infinite in time. The possible maximum of the cell density depends on the used discretisation. Thus, with a very fine discretisation near the corner $(x, y) = (1, 1)$ a good approximation of the blow-up behavior is possible, as can bee seen in Figs. 4, 5 and 7.

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