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 by certain chemicals in the environment.
In this paper we use the results of a paper of Zhou and Saito to validate our Finite-Volume solution method with respect to blow-up analysis and equilibrium solutions. Based on these results we study model variations and there blow-up behaviour numerically.
We will discuss the question if conservative numerical methods are able to model a blow up behaviour in the case of non global existence of solutions.

Key words: Chemotaxis model; Blow up phenomenom; 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, commonly known as slime mold. The Keller-Segel system, named after the American physicist Evelyn Fox Keller and the American mathematician Lee Aarom Segel, consists of an elliptic and a parabolic partial differential equation coupled with initial and homogenous Neumann boundary conditions [4]. 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. 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.

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. This behaviour is often referred to as the most interesting feature of the Keller-Segel equations.

2 Chemotaxis and Keller-Segel system

For a wide description of the Chemotaxis/Keller-Segel model we refer to the thesis [7] and the review paper [3]. There one can find extensive explanations and derivations of the models.

In its original form the Keller-Segel system consists of four coupled reaction-advection-diffusion equations. 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-dimensionalization and some very natural assumptions starting from the original Keller-Segel system one can 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 of equation for u

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

is the so called chemotactic flux (see Müller et al. [5]) where χ depends on the density of the attractant, called chemotactic sensitivity.

The equations (1), (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 done by Gajewski and Zacharias [1] introducing a Lyapunov function for the system (2). All other mathematical investigations of Keller-Segel systems followed the ideas of [1]. As the result of the analysis global existence of solutions in the sub-critical case were shown.

For the parabolic-elliptic Keller-Segel system one can find a mathematical and numerical analysis of the system (1) in the paper of Zhou and Saito [6].

The Keller-Segel system admits several a priori estimates which reflects the basic modeling assumptions which 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's interesting to consider modifications of the standard Keller-Segel system. The mathematical meaning of the modifications is more or less a regularisation. This leads to different behaviour of the solutions and in some cases blow up effects can be surpressed.

In this paper we will discuss and numerical 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

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

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 Zhou et al. [6] and Eymard et al. [2]. Let Ω be a convex polygonal domain in $\mathbb{R}$. First, we will define a very important notion following Eymard et al. [2]:

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 neigbourhood 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

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

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 neighbour L of control volume K or neighbour K of control volume L.

We will now introduce a linear finite volume scheme in order to discretize 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. The error of the upwind scheme is of order $\mathcal{O}(h)$ only, 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 schems Scharfetter-Gummel approximations

which control the order of approximation between one and 2 depending on the convection velocity are used.

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 $u_h \in X_h$:

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

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

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

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

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

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

which is the discrete to the parabolic equation

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

using implicit Euler for the time discretization. For the parabolic v-equation of (2) we use also 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

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

For (16) we have to modify the discretisation (15) by insert a factor $\varphi(u_L^{n-1}, v_L^{n-1})$. In other words we do a linearisazion.

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 and global existence of solutions, as we will see later.

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 [6] and the thesis [7]

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

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

Analogue 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 holds 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

In the one-dimensional case of (1) a blow-up can never occur, which was shown in [6]. We will shortly discuss some important properties of the system before turning to the finite volume scheme and the system of linear equations. After this, we will turn to the two-dimensional system in section 4.1. We will prove for which cases there can never occur blow-up and then discuss some important properties of the system. Throughout this chapter, we will distinguish between the conservative and non-conservative system and derive the finite volume scheme and the system of linear equations for the conservative and the non-conservative schemes, respectively, using both cartesian and polar coordinates.

4.1 Two-dimensional system

Blow-up behaviour

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

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

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

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

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

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.

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

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

This implies that if $\theta > 8\pi$ and $M_2(0)$ is sufficiently small, then we 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). We have for $n = 1, \ldots, J$,

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

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 intruduced above.

4.2 Non-conservative finite volume scheme

We will now consider the numerical scheme without conservation of positivity but satisfying (27). With the obvious notations for the forward and backward difference quotients $\nabla_x u = \frac{u_{i+1,j} - u_{i,j}}{h}$, $\nabla_{\bar{x}} u = \frac{u_{i,j} - u_{i-1,j}}{h}$ we obtain this so-called non-conservative scheme by replacing the conservative discretized parabolic equation by

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

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 intruduced 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

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 $u = 1$ and $v = 1 + 0.1\exp(-10((x-1)^2 + (y-1)^2))$ on Ω. In the figure captions one can find the model and the used parameters. For the simulations we used the conservative scheme. In alle examples we reached the steady state (global existence of the solution). The solution were going to be grid-independent.

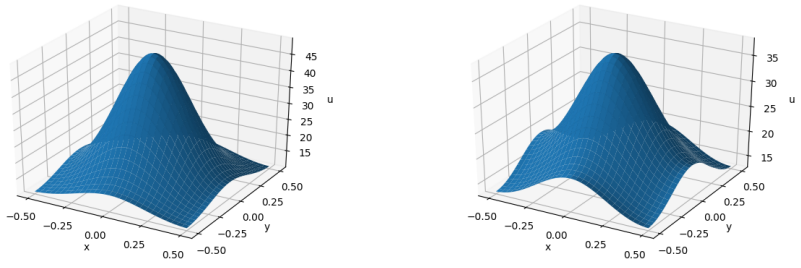

Fig. 1: cell density, cell density peak evolution, Problem (7),$D = 0.1, \chi = 5.0, \gamma = 3.0$, steady state

For the minimal Keller-Segel system (2) and the problem (6) we could only approximate the blow up behaviour with the conservative scheme. The possible maximum of the cell density depends on the used discretization, but with a very fine discretisation near the corner $(x, y) = (1, 1)$ a good approximation of the blow up behaviour is possible.

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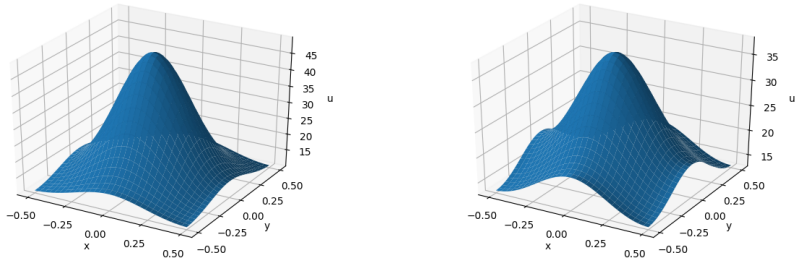

Fig. 2: cell density, cell density peak evolution, Problem (8),$D = 0.1, \chi = 5.0, \epsilon = 1.0$, steady state

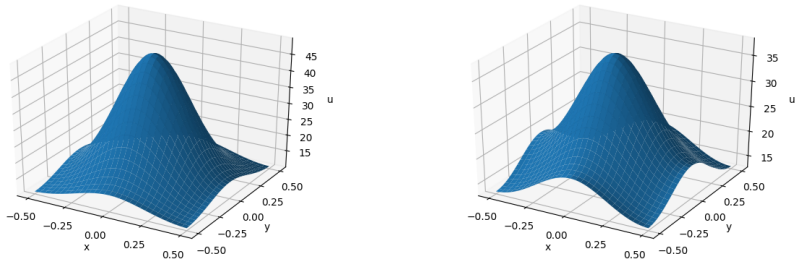

Fig. 3: cell density, cell density peak evolution, Problem (10),$D = 0.1, \chi = 5.0, r = 0.25$, steady state

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