NUMERICAL COMPUTATIONS AND PATTERN FORMATION FOR CHEMOTAXIS-GROWTH MODEL

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Abstract. In [12], Mimura and Tsujikawa presented a sophisticated model for describing the process of pattern formation performed by bacteria. This paper is concerned with numerical simulations for their model. We find out various types of stationary solutions which show good correlation with experimental results due to Budrene-Berg [5, 6].

1 Introduction In 1991-95, E. O. Budrene and H. C. Berg [5, 6] found out that Escherichia coli form remarkable aggregating patterns by chemotaxis and growth. After this epoch-making result, some mathematical biologists tried to describe the process of pattern formation by mathematical models, see Woodward, Tyson, Myerscough, Murray, Budrene, and Berg [16], Kawasaki and Shigesada [10, 11], and Mimura and Tsujikawa [12].

Among others, Mimura and Tsujikawa presented in [12] a very sophisticated model which is based only on diffusion, chemotaxis and growth of the bacteria,

$$
(1) \qquad \begin{cases} \dfrac{\partial u}{\partial t} = a\Delta u - \mu\nabla\cdot[u\nabla\chi(\rho)] + f(u) & \text{in} \quad \Omega\times(0,\infty), \\ \dfrac{\partial \rho}{\partial t} = b\Delta\rho - c\rho + \nu u & \text{in} \quad \Omega\times(0,\infty), \\ \dfrac{\partial u}{\partial n} = \dfrac{\partial \rho}{\partial n} = 0 & \text{on} \quad \partial\Omega\times(0,\infty), \\ u(x,0) = u_0(x), \quad \rho(x,0) = \rho_0(x) & \text{in} \quad \Omega. \end{cases}
$$

Here, Ω is a bounded domain of $\mathbb{R}^2$ in which the bacteria are incubated. The unknown functions $u(x,t)$ and $\rho(x,t)$ denote the population density of the bacteria and the concentration of chemical substance in Ω at time $t \in [0,\infty)$, respectively. The mobility of individuals consists of two effects: one is random walking and the other is the directed movement in a sense that they have a tendency to move toward higher concentration of the chemical substance which is called chemotaxis. The flux of biological individuals is described by $\mu[u\nabla\chi(\rho)]$, where $\chi(\rho)$ denotes a sensitivity function of chemotaxis which is actually given by (3). $\mu > 0$ denotes a mobility rate. $a > 0$ and $b > 0$ are the diffusion rates of bacteria and chemical substance, respectively. $c > 0$ and $\nu > 0$ are the degradation and production rates of ρ, respectively. $f(u)$ is a growth function for the bacteria.

It is already known, under suitable assumptions on the functions $\chi(\rho)$ and $f(u)$, a global solution can be constructed for any nonnegative initial functions $u_0 \geq 0$ and $\rho_0 \geq 0$. Therefore, we can construct a dynamical system determined from the Cauchy problem of (1) in a certain phase space $\mathcal{K}$ considered in an infinite-dimensional universal space X.

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Furthermore, the dynamical system possesses exponential attractors $\mathcal{M}$. The exponential attractor is one of notions of attractors (see [17, 21]) which was presented by Eden, Foias, Nicolaenko and Temam [18] and has robustness. In fact, $\mathcal{M}$ is a subset of $\mathcal{K}$ which is a compact set of X with finite fractal dimension, $\mathcal{M}$ is positively invariant in the sense that every trajectory starting from $\mathcal{M}$ remains in $\mathcal{M}$, and $\mathcal{M}$ attracts all trajectories at an exponential rate. On the other hand, we can prove that, if $\mu\nu$ is sufficiently large, namely, chemotaxis is sufficiently strong, then any homogeneous stationary solution to (1) becomes unstable. These facts then indicate that any trajectory of the dynamical system stays in some space of finite freedoms but does not converge to any spatially homogeneous state.

This paper is then concerned with some numerical computations for Problem (1). We will take a linear sensitivity function $\chi(\rho) = \rho$ and a cubic growth function $f(u) = u^2(1-u)$, and will fix all the parameters in a suitable way except the chemotaxis parameter μ. We consider the μ as a control parameter. It is clear that $(1, \frac{\nu}{c})$ is a stationary solution. If μ is small enough, then $(1, \frac{\nu}{c})$ is stable. But, if μ becomes large, then the stationary solution loses its stability and has a nontrivial unstable manifold. We are concerned with trajectories in this unstable manifold. Taking initial functions near $(1, \frac{\nu}{c})$, we perform numerical computations. Some time the numerical solutions are found to converge to some stationary solutions as $t \to \infty$. Other time, they show chaotic behaviors. These pattern solutions are in interesting agreement with the experimental results [5, 6]. Numerical computations for transit pattern solutions were performed by Aida-Yagi [4].

According to Aida-Yagi [3], the exponential attractors are known to attract not only all trajectories in the phase space but also approximate solutions into its neighborhood and to continue confining the approximate solutions in the neighborhood forever. This fact seems to ensure that numerical computations have global reliability at least in the sense that numerical solutions approximate always some trajectories in the neighborhood of the exponential attractor.

2 Dynamical System In this section, we shall review briefly known results on the dynamical system determined from (1). We assume the following conditions. The set Ω is a two-dimensional convex bounded domain. The sensitivity function $\chi(\rho)$ is a real smooth function of $\rho \in (0, \infty)$ with

$$\sup_{0<\rho<\infty} \left| \frac{d^i\chi}{d\rho^i}(\rho) \right| < \infty \qquad \text{for } i = 1, 2. \tag{2}$$

The possible forms of $\chi(\rho)$ are

$$\chi(\rho) = \rho, \; \log(\rho+1), \; \frac{\rho}{\rho+1}. \tag{3}$$

The growth function $f(u)$ is a real smooth function of $u \in [0, \infty)$ such that $f(0) = 0$ and

$$f(u) = (-\alpha u + \beta)u \qquad \text{for sufficiently large } u \tag{4}$$

with some constants $\alpha > 0$ and $\beta \geq 0$.

We set a space of initial functions by

$$\mathcal{K} = \left\{ \begin{pmatrix} u_0 \\ \rho_0 \end{pmatrix} ; \; 0 \leq u_0 \in L^2(\Omega) \qquad \text{and} \qquad 0 \leq \rho_0 \in H^2_N(\Omega) \right\}, \tag{5}$$

where $H^2_N(\Omega)$ is a subspace of $H^2(\Omega)$ consisting of functions $\rho \in H^2(\Omega)$ which satisfy the homogeneous Neumann boundary conditions on $\partial\Omega$. We set also an underlying space in which we work by

$$X = \left\{ \begin{pmatrix} u \\ \rho \end{pmatrix};\ u \in L^2(\Omega) \quad \text{and} \quad \rho \in H^2_N(\Omega) \right\}. \tag{6}$$

Then, global existence of solutions is obtained. For each $U_0 \in \mathcal{K}$, (1) possesses a unique global solution in the function space:

$$\begin{cases} 0 \le u \in \mathcal{C}^1((0,\infty);\ L^2(\Omega)) \cap \mathcal{C}([0,\infty);\ L^2(\Omega))) \cap \mathcal{C}((0,\infty);\ H^2_N(\Omega)), \\ 0 \le \rho \in \mathcal{C}^1((0,\infty);\ H^2_N(\Omega)) \cap \mathcal{C}([0,\infty);\ H^2_N(\Omega)) \cap \mathcal{C}([0,\infty);\ \mathcal{H}^4_{N^2}(\Omega)), \end{cases} \tag{7}$$

where $\mathcal{H}^4_{N^2}(\Omega)$ is the space of functions $\rho \in H^2_N(\Omega)$ such that $\Delta\rho \in H^2_N(\Omega)$. Since the boundary $\partial\Omega$ of Ω is not of $\mathcal{C}^4$ class, $\Delta\rho \in H^2_N(\Omega)$ does not necessarily imply $\rho \in H^4(\Omega)$, namely, $\mathcal{H}^4_{N^2}(\Omega) \not\subset H^4(\Omega)$ (see [19]). Furthermore, we can build up a dissipative estimate such that

$$\|u(t)\|_{L^2} + \|\rho(t)\|_{H^2_N} \le P(e^{-\delta t} P(\|u_0\|_{L^2} + \|\rho_0\|_{H^2_N}) + 1), \qquad 0 < t < \infty \tag{8}$$

with some fixed exponent $\delta > 0$ and some continuous increasing functions $P(\cdot)$. For $U_0 \in \mathcal{K}$, let $U(t; U_0) = {}^t(u(t), \rho(t))$ be the global solution of (1) with initial value U_0. Then, $S(t)U_0 = U(t; U_0)$ defines a nonlinear semigroup $S(t)$, $0 \le t < \infty$, acting on $\mathcal{K}$ which is Lipschitz continuous with respect to the initial values U_0 in the topology of X. Hence, $(S(t), \mathcal{K}, X)$ is a dynamical system with the phase space $\mathcal{K}$ in the universal space X.

This result was first obtained by Osaki-Tsujikawa-Yagi-Mimura [13] when $\partial\Omega$ is of $\mathcal{C}^3$ class. Afterward, this was generalized to the case when Ω is convex by Aida-Efendiev-Yagi [1]. See also Osaki-Yagi [14].

i) Exponential Attractors. Let $(S(t), \mathcal{K}, X)$ be the dynamical system constructed above from (1). We can prove that the system enjoys exponential attractors. The notion of exponential attractors has been presented by Eden-Foias-Nicolaenko-Temam [18] as one of limiting sets of dynamical systems in infinite-dimensional spaces which are more robust than the global attractors. A subset $\mathcal{M} \subset \mathcal{K}$ is called an exponential attractor of $(S(t), \mathcal{K}, X)$ if $\mathcal{M}$ has the following properties:

1. $\mathcal{M}$ contains the global attractor $\mathcal{A}$;
2. $\mathcal{M}$ is a compact subset of X with finite fractal dimension;
3. $\mathcal{M}$ is a positively invariant set of $S(t)$, i.e., $S(t)\mathcal{M} \subset \mathcal{M}$ for every $t > 0$;
4. For any bounded subset B of $\mathcal{K}$, there exists a constant $C_B > 0$ such that

   $$h(S(t)B, \mathcal{M}) \le C_B e^{-\delta t}, \qquad 0 \le t < \infty$$

   with some fixed exponent $\delta > 0$, here $h(B_1, B_2) = \sup_{U \in B_1} \inf_{V \in B_2} \|U - V\|_X$ denotes the Hausdorff pseudo-distance for two bounded sets B_1 and B_2 of X.

It is known that the exponential attractors can depend on a parameter continuously. Indeed, consider a family of dynamical systems $(S_\mu(t), \mathcal{K}, X)$ which possess exponential attractors. If $S_\mu(t)$ depends on μ continuously for each t in a fixed finite interval $[0, T]$, then one can construct exponential attractors $\mathcal{M}_\mu$ in such a way that $\mathcal{M}_\mu$ is continuous with respect to the symmetric distance $d(B_1, B_2) = \max\{h(B_1, B_2),\, h(B_2, B_1)\}$. These results were shown in Eden-Foias-Nicolaenko-Temam [18] and Efendiev-Yagi [8].

Existence of such exponential attractors for $(S(t), \mathcal{K}, X)$ was first proved by Osaki-Tsujikawa-Yagi-Mimura [13] when $\partial\Omega$ is of $\mathcal{C}^3$ class by verifying the squeezing property of the semigroup $S(t)$. The squeezing property which was presented by Eden, Foias, Nicolaenko and Temam [18] can ensure existence of exponential attractors for the dynamical systems in Hilbert spaces. Afterward, Aida-Efendiev-Yagi [1] constructed exponential attractors under the assumption of convexity of Ω by showing the fact that $S(t)$ is a compact perturbation of contraction operator. According to Efendiev-Miranville-Zelik [7] (cf. also Takei-Yagi [15]), if the semigroup $S(t)$ is a compact perturbation of contraction, then one can always construct exponential attractors. It is as well known that, if $S(t)$ satisfies the squeezing property, then one can obtain precise dimension estimates for exponential attractors.

ii) Instability of Homogeneous Stationary Solution. Let $\overline{u} > 0$ be a solution of the equation $f(u) = 0$. We assume that $f'(\overline{u}) < 0$ and $f(u)$ is real analytic in a neighborhood of $\overline{u}$. Let in addition $\overline{\rho} = \frac{\nu\overline{u}}{c}$. Then, $\overline{U} = {}^t(\overline{u}, \overline{\rho})$ is a homogeneous stationary solution to (1) and is an equilibrium of $(S(t), \mathcal{K}, X)$. We can then show that $\overline{U}$ is unstable provided that $\mu\nu$ is sufficiently large. These results were proved by Aida-Tsujikawa-Efendiev-Yagi-Mimura [2]. The degree of instability of $\overline{U}$ is also estimated from below. This naturally implies a lower estimate of dimension of exponential attractors. As $\mu\nu \to \infty$, $\dim \mathcal{M}$ also tends to ∞.

3 Numerical Simulations

In this section, we present some numerical results for the problem

$$
(9) \qquad \begin{cases} \dfrac{\partial u}{\partial t} = 0.0625\Delta u - \mu\nabla\cdot[u\nabla\rho] + u^2(1-u) & \text{in } \Omega\times(0,+\infty),\\ \dfrac{\partial \rho}{\partial t} = \Delta\rho - 32\rho + u & \text{in } \Omega\times(0,+\infty),\\ \dfrac{\partial u}{\partial n} = \dfrac{\partial \rho}{\partial n} = 0 & \text{on } \partial\Omega\times(0,\infty),\\ u(x,0) = u_0(x),\ \rho(x,0) = \rho_0(x) & \text{in } \Omega \end{cases}
$$

in a rectangular domain $\Omega = [-8, 8]\times[-8, 8]$. We fixed all coefficients but μ, the chemotaxis parameter, which is also a parameter of the numerical simulations. Obviously, (9) has a homogeneous stationary solution $\overline{U} = {}^t(1, \frac{1}{32})$. The initial values for u and ρ are set as $\overline{U}$ plus a small perturbation, namely,

$$
\begin{bmatrix} u_0(x) \\ \rho_0(x) \end{bmatrix} = \begin{bmatrix} 1+\varepsilon(x) \\ \frac{1}{32}, \end{bmatrix},
$$

where $\varepsilon(x)$ is a small perturbation which is zero except in a small disk centered at the origin. We use the finite difference method with uniform spatial step sizes,

$$
\Delta x = \Delta y = \frac{1}{16}.
$$

The diffusion terms are approximated by second-order central differences. The chemotaxis term is approximated by using the limited third-order $\frac{1}{3}$-scheme, see [9]. The result of the spatial discretization is the autonomous semi-discrete system $w'(t) = F(w(t))$ assembling at all grid cells the approximations to the population density and chemical concentration.

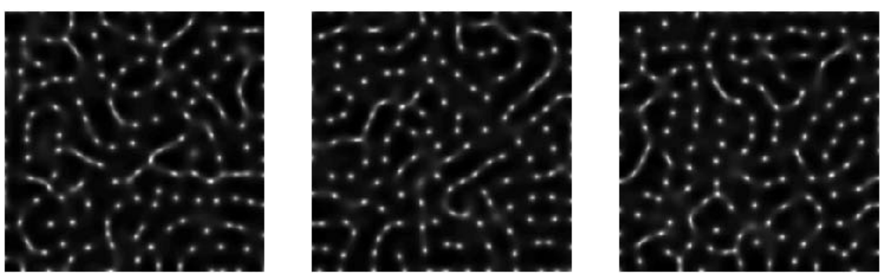
For temporal discretization, we use a three-stage AMF-Rosenbrock method of order two, see [20]. A cheap first-order embedded solution is also in use for variable time step size control.

When μ is sufficient small, the homogeneous stationary solution $\overline{U}$ is observed. With larger values of chemotaxis parameter, $\overline{U}$ is no longer stable and the stationary solutions turn to be inhomogeneous. For $\mu = 7.2$ the swarm rings pattern appears, as in Figure 1(a). In figures, white shows high concentration of bacteria and black the opposite. As μ increases from 7.2 to 8.4, the stationary solution changes its structure to stripes patterns. When $\nu = 8.2$, continuous stripes pattern is observed, and when $\mu = 8.4$, perforated stripes pattern.

(a) Swarm rings (b) Continuous stripes (c) Perforated stripes

Fig. 1: μ for these patterns are 7.2, 8.2 and 8.4, respectively.

If we increase ν, ordered stationary solutions are replaced by some chaotic moving patterns. With $\mu = 10$, a moving meandering pattern is observed as in Figure 2.



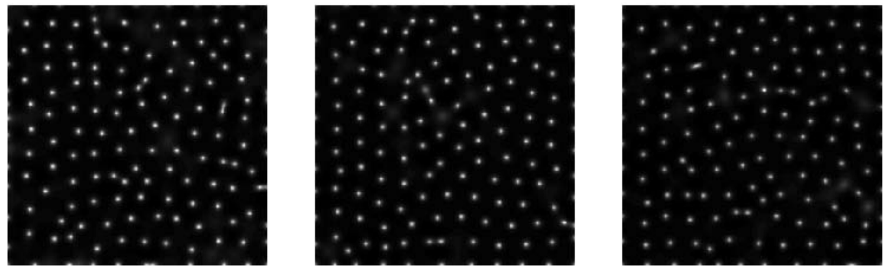
(a) $t = 896$ (b) $t = 1195$ (c) $t = 1493$

Fig. 2: Short-perforated-lines move chaotically with $\mu = 10$.

And a chaotic spots pattern is observed with $\nu = 12$ as in Figure 3.

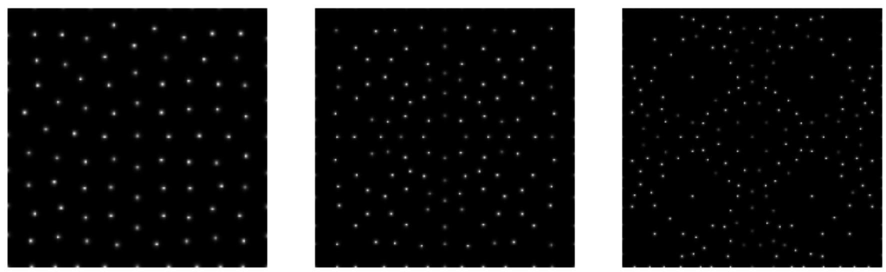
For bigger chemotaxis μ's, e.g.$\nu = 20, 40$ and 70, stationary solutions reappear with isolated-spots patterns as in Figure 4.

Some of these patterns observed here seem to be in good agreement with the experimental results by Budrene-Berg [5, 6].



(a) $t = 365$ (b) $t = 547$ (c) $t = 729$

Fig. 3: Dots move chaotically with $\mu = 12$.



(a) $\mu = 20$ (b) $\mu = 40$ (c) $\mu = 70$

Fig. 4: Stabilized-isolated-dots patterns.

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