Conservative finite-difference scheme to a chemotaxis system*

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Abstract

We consider a nonlinear parabolic system in mathematical biology that describes the aggregation of slime molds. An important property of solutions to the system is the conservation of the L^1 norm. Applying upwind technique and time increment control, we propose a finite-difference scheme satisfying the conservation of the discrete L^1 norm.

1 Introduction

In 1970, F. F. Keller and L. A. Segel ([5]) proposed the system of partial differential equations that described the aggregation of slime molds resulting from their chemotactic features. The system is now called the *Keller-Segel system modelling chemotaxis*, and a large number of works are devoted to mathematical analysis to the system (cf: [2], [3], [10] and [12]). In this paper, we consider a variant of the system in one dimensional spatial domain (cf: [6]):

$$\begin{cases} u_t = [D_u u_x - (\phi(v))_x u]_x \,, & (x,t) \in Q \equiv (0,1) \times (0,\infty) \\ \gamma v_t = D_v v_{xx} + g(u,v), & (x,t) \in Q \end{cases} \tag{1}$$

with the boundary and initial conditions:

$$\begin{cases} [D_u u_x - (\phi(v))_x u]|_{x=0,1} = 0, & u|_{t=0} = u_0(x), \\ v_x|_{x=0,1} = 0, & v|_{t=0} = v_0(x). \end{cases} \tag{2}$$

Here, we have used the following symbols.

- $u = u(x,t)$ is the density of the cellular slime molds and $v = v(x,t)$ the concentration of the chemical substance.
- $\phi(v)$ is a nondecreasing smooth function defined on $v > 0$ and is called chemotactical sensitivity function. Typical examples are $\phi(v) = \lambda v$ and $\phi(v) = \lambda \log v$ with $\lambda > 0$.
- $g(u,v) = \alpha_1 u - \alpha_2 v$ denotes the generation rates, where α_1 and α_2 are positive constants.
- D_u and D_v are diffusion coefficients, and γ is the relaxation time. They are assumed to be positive constants.

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- Smooth functions $u_0(x)$ and $v_0(x)$ are initial values. We assume that $u_0(x) \geq 0, \not\equiv 0$ and $v_0(x) > 0$.

The boundary condition for u in (2) is equivalently written as

$$u_x|_{x=0,1} = 0$$

because of $v_x|_{x=0,1} = 0$. However, we prefer the expression (2), since it is convenient when we consider an approximation of the boundary condition. By KS, we mean the initial-boundary value problem composed of (1) and (2).

It is known (cf: [1], [10], [12] and [13]) that KS admits a unique classical solution (u, v) globally in time. On the other hand, we obtain readily that

$$u(x,t) > 0, \ (x,t) \in \overline{Q} \equiv [0,1] \times [0,\infty) \quad \text{(conservation of positivity);} \tag{3}$$

$$\int_0^1 u(x,t)\ \mathrm{d}x = \int_0^1 u_0(x)\ \mathrm{d}x, \ t \in [0,\infty) \quad \text{(conservation of total mass).} \tag{4}$$

As a result, the L^1 norm of u is preserved:

$$\|u(t)\|_{L^1(0,1)} = \|u_0\|_{L^1(0,1)}, \qquad t \in [0,\infty). \tag{5}$$

This is actually a salient property; the steady-state problem corresponding to KS is reduced to a nonlocal eigenvalue problem by (5).

The purpose of this paper is to propose a finite-difference scheme that preserves the discrete analogues of (3), (4) and, consequently, (5). In a previous paper [9], we considered a reduced system of KS ($\gamma = 0$ and $\phi(v) = v$) and realize such conservative finite-difference schemes. There, we applied upwind technique to the spatial discretization and semi θ schemes with the time increment control to the time discretization. We extend our strategy to KS in this paper. Convergence analysis, which is not addressed in this paper, is another important subject. We are concerned with convergence analysis in the literature of the finite-element method in other papers ([7], [8]).

We describe our finite-difference scheme in Section 2 and then study the conservation of the L^1 norm in Section 3. Finally, we give a remark on the conservation of positivity in the finite-difference method for a parabolic equation in Section 4.

2 Finite-difference scheme

Take a positive integer N and put $h = 1/N$. We introduce two kinds of grid points over $[0, 1]$ as:

$$x_i = \left(i - \frac{1}{2}\right) h \quad (i = 1, \ldots, N), \quad \hat{x}_i = ih \quad (i = 0, \ldots, N).$$

Grid points over $[0, \infty)$ is defined by

$$t_n = \tau_1 + \cdots + \tau_n \quad (n = 1, 2, \ldots),$$

where the time increment $\tau_n > 0$ will be determined later. We consider approximations of $u(x,t)$ and $v(x,t)$ on (x_i, t_n) and $(\hat{x}_i, t_n)$, respectively. Thus, we would like to find

$$u_i^n \approx u(x_i, t_n) \quad \text{and} \quad v_i^n \approx v(\hat{x}_i, t_n).$$

Posit that

$$\mathbf{u}^n = (u_1^n, \ldots, u_N^n)^T \quad \text{and} \quad \mathbf{v}^n = (v_0^n, \ldots, v_N^n)^T.$$

For the time being, we suppose that $\mathbf{u}^{n-1}$ and $\mathbf{v}^{n-1}$ have been obtained and describe schemes for solving $\mathbf{u}^n$ and $\mathbf{v}^n$ separately.

Scheme for solving $\mathbf{v}^n$

We introduce

$$\hat{u}_i^n = \begin{cases} u_1^n & (i=0) \\ \frac{1}{2}(u_{i+1}^n + u_i^n) & (i=1,\ldots,N-1) \\ u_N^n & (i=N) \end{cases}, \quad \hat{\mathbf{u}}^n = (\hat{u}_0^n, \ldots, \hat{u}_N^n)^T.$$

Let $\theta \in [0,1]$. Then, $\mathbf{v}^n$ is computed by the standard θ scheme. That is,

$$\gamma \frac{v_i^n - v_i^{n-1}}{\tau_n} = \theta D_v \frac{v_{i-1}^n - 2v_i^n + v_{i+1}^n}{h^2} + (1-\theta) D_v \frac{v_{i-1}^{n-1} - 2v_i^{n-1} + v_{i+1}^{n-1}}{h^2} + g(\hat{u}_i^{n-1}, v_i^{n-1}) \quad (0 \le i \le N), \tag{6}$$

where v_{-1}^n and v_{N+1}^n are eliminated by the boundary condition

$$v_{-1}^n = v_1^n, \quad v_{N+1}^n = v_{N-1}^n \qquad (n = 1, \cdots, m). \tag{7}$$

The scheme (6) with (7) is equivalently written as:

$$(\gamma \mathbf{I} + \theta \lambda_n D_v \mathbf{L})\mathbf{v}^n = [\gamma \mathbf{I} - (1-\theta)\lambda_n D_v \mathbf{L}]\mathbf{v}^{n-1} + \tau_n \mathbf{g}^{n-1}, \tag{8}$$

where $\mathbf{I}$ is the identity matrix, and

$$\mathbf{L} = \begin{bmatrix} 2 & -2 & 0 & & 0 \\ -1 & 2 & -1 & & \\ & \cdots & \cdots & & \\ & -1 & 2 & -1 & \\ & & & \cdots & \cdots \\ 0 & & & -2 & 2 \end{bmatrix}, \quad \mathbf{g}^n = \begin{bmatrix} g(\hat{u}_0^n, v_0^n) \\ g(\hat{u}_1^n, v_1^n) \\ \vdots \\ \vdots \\ g(\hat{u}_N^n, v_N^n) \end{bmatrix}, \quad \lambda_n = \frac{\tau_n}{h^2}. \tag{9}$$

Scheme for solving $\mathbf{u}^n$

The key point is to introduce a *reasonable* approximation of the flux $F = -D_u u_x + (\phi(v))_x u$ of u by applying upwind technique. We set

$$b_i^n = \frac{\phi(v_i^n) - \phi(v_{i-1}^n)}{h} \quad (1 \le i \le N), \quad \mathbf{b}^n = (b_1^n, \ldots, b_N^n)^T. \tag{10}$$

Further, we set

$$b_i^{n,+} = \max\{0, b_i^n\} \quad \text{and} \quad b_i^{n,-} = \max\{0, -b_i^n\}.$$

Obviously, b_i^n is an approximation of $(\phi(v))_x$ at $x = x_i$. We note that

$$F = -D_u u_x + [b]_+ u - [b]_- u,$$

where $b = (\phi(v))_x$ and $[b]_\pm = \max\{0, \pm b\}$. Hence, following a technique of upwind approximation, we may suppose that u_i^n and u_{i+1}^n are carried into a point $\hat{x}_i$ on flows $b_i^{n-1,+}$ and $-b_{i+1}^{n-1,-}$, respectively. That is, a discrete flux F_i^n of $\mathbf{u}^n$ at $x = \hat{x}_i$ is given by

$$F_i^n = -D_u \frac{u_{i+1}^n - u_i^n}{h} + b_i^{n-1,+} u_i^n - b_{i+1}^{n-1,-} u_{i+1}^n \quad (i = 1, \ldots, N-1).$$

Similarly, an discrete flux $\tilde{F}_i^n$ of $\mathbf{u}^{n-1}$ at $x = \hat{x}_i$ is given by

$$\tilde{F}_i^{n-1} = -D_u \frac{u_{i+1}^{n-1} - u_i^{n-1}}{h} + b_i^{n-1,+} u_i^{n-1} - b_{i+1}^{n-1,-} u_{i+1}^{n-1} \quad (i = 1, \ldots, N-1).$$

By the boundary condition ($F|_{x=0,1} = 0$), we set

$$F_0^n = 0, \quad F_N^n = 0, \quad \tilde{F}_0^n = 0, \quad \tilde{F}_N^n = 0. \tag{11}$$

Then our proposed scheme is as follows:

$$\frac{u_i^n - u_i^{n-1}}{\tau_n} = -\theta \frac{F_i^n - F_{i-1}^n}{h} - (1-\theta) \frac{\tilde{F}_i^{n-1} - \tilde{F}_{i-1}^{n-1}}{h} \quad (i = 1, \ldots, N) \tag{12}$$

with the boundary condition (11).

In order to state the matrix representation, we introduce an $N \times N$ matrix $\mathbf{H}^n = [H_{i,j}]$ by

$$H_{i,j} = \begin{cases} D_u + h b_1^{n,+} & (i = j = 1) \\ -D_u - h b_2^{n,-} & (i = 1,\ j = 2) \\ -D_u - h b_{i-1}^{n,+} & (2 \leq i \leq N-1,\ j = i-1) \\ 2D_u + h[b_k^{n,+} + b_k^{n,-}] & (2 \leq i \leq N-1,\ j = i) \\ -D_u - h b_{k+1}^{n,-} & (2 \leq i \leq N-1,\ j = i+1) \\ -D_u - h b_{N-1}^{n,-} & (i = N,\ j = N-1) \\ D_u + h b_N^{n,+} & (i = j = N) \\ 0 & (\text{otherwise}). \end{cases}$$

Then, the scheme (12) with (11) is equivalently written as

$$\mathbf{M}^{n-1} \mathbf{u}^n = \mathbf{K}^{n-1} \mathbf{u}^{n-1}, \tag{13}$$

where

$$\mathbf{M}^{n-1} = [M_{i,j}] = \mathbf{I} + \theta \lambda_n \mathbf{H}^{n-1}, \quad \mathbf{K}^{n-1} = [K_{i,j}] = \mathbf{I} - (1-\theta) \lambda_n \mathbf{H}^{n-1}.$$

3 Conservation of the L^1 norm

In this section, we describe how to choose the time increment τ_n such that $\mathbf{u}^n$ generated by (13) and (8) satisfies

$$\|\mathbf{u}^n\|_{1,h} = \|\mathbf{u}^0\|_{1,h},$$

where $\|\cdot\|_{1,h}$ is the discrete L^1 norm defined as

$$\|\mathbf{u}\|_{1,h} = \sum_{i=1}^{N} |u_i| h \qquad (\mathbf{u} = (u_1, \ldots, u_N)^T \in \mathbf{R}^N).$$

We still suppose that $\mathbf{u}^{n-1}$ and $\mathbf{v}^{n-1}$ have been obtained, unless otherwise stated explicitly.

The following lemma is a direct consequence of the expression (12) and the boundary condition (11).

Lemma 3.1. *Let* $\mathbf{u}^n$ *be a solution of* (13). *Then,* $\displaystyle\sum_{i=1}^{N} u_i^n = \sum_{i=1}^{N} u_i^{n-1}$.

We introduce

$$\|\mathbf{b}\|_\infty = \max_{1\le i\le N} |b_i| \qquad (\mathbf{b}=(b_1,\ldots,b_N)^T\in\mathbf{R}^N).$$

Lemma 3.2. *If*

$$2(1-\theta)\left(D_u + \|\mathbf{b}^{n-1}\|_\infty\right)\tau_n \le h^2, \tag{14}$$

then we have

$$K_{i,i}\ge 0 \quad \textit{and} \quad K_{i,j}\begin{cases} >0 & (j=i\pm 1),\\ =0 & (i\ne j,\ j\ne i\pm 1).\end{cases} \tag{15}$$

Lemma 3.3. *We have*

$$M_{i,i}> 0 \quad \textit{and} \quad M_{i,j}\begin{cases} <0 & (j=i\pm 1),\\ =0 & (i\ne j,\ j\ne i\pm 1).\end{cases} \tag{16}$$

In particular, $\mathbf{M}^{n-1}$ *is irreducible.*

Proofs of Lemmas 3.2 and 3.3. Since $b_i^{n-1,\pm}\ge 0$, we have $H_{i,i}>0$ and $H_{i,i\pm1}<0$. Other entries of $\mathbf{H}^{n-1}$ vanish. Hence, (15) and (16) follows. Irreducibility is a consequence of (16).

Lemma 3.4. *If*

$$2\theta\|\mathbf{b}^{n-1}\|_\infty\tau_n \le h, \tag{17}$$

then $\mathbf{M}^{n-1}$ *is diagonally dominant with strict inequalities holding for* $i=1,N$.

Proof. By (17), we deduce

$$\sum_{k=1}^{N} M_{i,k} = M_{i,i-1}+M_{i,i}+M_{i,i+1} \ge 1-2h\lambda_n\theta\|\mathbf{b}^{n-1}\|_\infty \ge 0$$

for $i=2,\ldots,N-1$. Similarly, we have

$$\sum_{k=1}^{N} M_{1,k}>0, \qquad \sum_{k=1}^{N} M_{N,k}>0.$$

Thus, strict inequalities hold for $i=1,N$. □

For $\mathbf{u}=(u_1,\ldots,u_N)^T\in\mathbf{R}^N$, we write $\mathbf{u}\ge\mathbf{0}$, if and only if $u_i\ge 0$ for $1\le i\le N$. The meaning of $\mathbf{u}>\mathbf{0}$ is similar.

Lemma 3.5. *Let* $\mathbf{u}^{n-1}\ge\mathbf{0}$. *If*

$$\tau_n \le \min\left\{\frac{h^2}{2(1-\theta)(D_u+\|\mathbf{b}^{n-1}\|_\infty)},\ \frac{h}{2\theta\|\mathbf{b}^{n-1}\|_\infty)}\right\},$$

then there exists a solution $\mathbf{u}^n$ *of* (13) *satisfying* $\mathbf{u}^n>\mathbf{0}$.

Proof. By Lemma 3.2, we have $\mathbf{w}=\mathbf{K}^{n-1}\mathbf{u}^{n-1}\ge\mathbf{0}$ and $\mathbf{w}\ne\mathbf{0}$. Hence, in view of Lemmas 3.3 and 3.4, we can apply [14, Corollary 3.20] to obtain $\mathbf{u}^n>\mathbf{0}$ satisfying (13). □

The following result is standard.

Lemma 3.6. *If* $\mathbf{v}^{n-1}\ge\mathbf{0}$ *and* $2D_v(1-\theta)\lambda_n\le\gamma$, *then there exists a solution* $\mathbf{v}^n>\mathbf{0}$ *of* (8).

Remark 3.1. If $\mathbf{v}^n > \mathbf{0}$, then $\phi(v_i^n)$ is well-defined.

Now we can state our numerical algorithm.

Step 0. Take $N \in N$, $\theta \in [0,1]$, $T > 0$, and $\varepsilon \in (0,1]$. Set $h = 1/N$, $n = 1$ and $t_0 = 0$. $\mathbf{u}^0$ and $\mathbf{v}^0$ are defined by $u_i^0 = u_0(x_i)$ and $v_i^0 = v(\hat{x}_i)$.

Step 1. Compute $\mathbf{b}^{n-1}$ by (10). Set

$$\tau_n = \min\left\{\tau,\ \frac{\varepsilon h^2}{2(1-\theta)(D_u + \|\mathbf{b}^{n-1}\|_\infty)},\ \frac{\varepsilon h}{2\theta\|\mathbf{b}^{n-1}\|_\infty}\right\} \tag{18}$$

and $t_n = t_{n-1} + \tau_n$. Here, τ is defined as

$$\tau = \begin{cases} \text{an arbitrary fixed positive constant} & (\theta = 1), \\ \dfrac{\gamma h^2}{2D_v(1-\theta)} & (\theta \neq 1). \end{cases}$$

Step 2. Find $\mathbf{u}^n$ and $\mathbf{v}^n$ by solving (13) and (8), respectively.

Step 3. If $t_n \geq T$, then finish the computation. Otherwise, renew n by $n+1$ and return to Step 1.

Summarizing lemmas mentioned above, we establish the following.

Theorem 3.1. *Let $\{\mathbf{u}^n, \mathbf{v}^n\}$ be the solution generated by the algorithm mentioned above. Suppose that $\mathbf{u}^0 \geq \mathbf{0}$ and $\mathbf{v}^0 > \mathbf{0}$. Then, we have $\mathbf{u}^n > \mathbf{0}$ and $\mathbf{v}^n > \mathbf{0}$ for $n \geq 1$. Moreover, $\mathbf{u}^n$ satisfies*

$$\|\mathbf{u}^n\|_{1,h} = \|\mathbf{u}^0\|_{1,h} \tag{19}$$

for $n \geq 1$.

Remark 3.2. We have a priori estimate

$$\|\mathbf{u}^n\|_\infty \leq \sum_{i=1}^{N} u_i^n = \frac{1}{h}\sum_{i=1}^{N} u_i^n h = \frac{1}{h}\sum_{i=1}^{N} u_0(x_i) h$$

by (19). Hence, we obtain $C = C(h, u_0) > 0$ such that $\tau_n \geq \min\{\tau, C\}$ which implies that τ_n never converge to zero as n increases. Thus, our algorithm always works.

4 A remark on the conservation of positivity

In this section, we briefly mention an issue on the conservation of positivity in the finite-difference method for a parabolic equation. Thus, we consider a linear convection-diffusion equation for the function $u = u(x,t)$ defined on $\overline{Q}$:

$$u_t = [u_x - b(x,t)u]_x \tag{20}$$

where $b(x,t) \geq 0$ denotes a given flow. We assume that $u(\cdot,t)$ and $b(\cdot,t)$ are periodic in $[0,1]$. The standard explicit finite-difference approximation to (20) is

$$\frac{u_i^{n+1} - u_i^n}{\tau} = \frac{u_{i-1}^n - 2u_i^n + u_{i+1}^n}{h^2} - \frac{b_{i+1}^n u_{i+1}^n - b_{i-1}^n u_{i-1}}{2h} \tag{21}$$

for $1 \le i \le N$ and $n \ge 0$, where $u_i^n \approx u(ih, n\tau)$, $b_i^n = b(ih, n\tau)$, $h = 1/N$ and $\tau > 0$. As readily see, if

$$\tau \le \frac{1}{2}h^2, \quad h \le \frac{1}{2\beta^n} \quad \left(\beta^n = \max_{x\in[0,1]} b(x, n\tau)\right), \tag{22}$$

then we have

$$u_i^n \ge 0 \ (1 \le i \le N) \quad \Rightarrow \quad u_i^{n+1} \ge 0 \ (1 \le i \le N). \tag{23}$$

If we apply this method of approximation to KS, $b(x,t)$ corresponds to $(\phi(v))_x$. However, since we do not know a priori bound for $(\phi(v))_x$, we cannot guarantee that (22) holds. On the other hand, a simple upwind finite-difference approximation to (20) is

$$\frac{u_i^{n+1} - u_i^n}{\tau} = \frac{u_{i-1}^n - 2u_i^n + u_{i+1}^n}{h^2} - \frac{b_i^n u_i^n - b_{i-1}^n u_{i-1}}{h}$$

for $1 \le i \le N$ and $n \ge 0$. In this scheme, (23) is satisfied, if

$$\tau \le \frac{h^2}{2 + h\beta^n}. \tag{24}$$

Therefore, in order to guarantee (23), we take a variable time increment τ_n subject to (24) instead of the fixed time increment τ. This is a reason why we have employed upwind method and time increment control to our finite-difference scheme.

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References

[1] P. Biler: *Local and global solvability of some parabolic systems modelling chemotaxis*, Adv. Math. Sci. Appl. **8** (1998) 715-743.

[2] D. Horstmann: *From 1970 until present: the Keller-Segel model in chemotaxis and its consequences I*, Jahresber. Deutsch. Math.-Verein. **105** (2003) 103-165.

[3] D. Horstmann: *From 1970 until present: the Keller-Segel model in chemotaxis and its consequences II*, Jahresber. Deutsch. Math.-Verein. **106** (2004) 51-69.

[4] R. Gorenflo: *Conservative difference schemes for diffusion problems* In; *Numerische Behandlung von Differentialgleichungen mit besonderer Berücksichtigung freier Randwertaufgaben*, (Tagung Math. Forschungsinst., Oberwolfach, 1977), pp. 101-124, Internat. Ser. Numer. Math. **39**, Birkhäuser, Basel-Boston, Mass., 1978.

[5] F. F. Keller and L. A. Segel: *Initiation on slime mold aggregation viewed as instability*, J. Theor. Biol. **26** (1970) 399-415.

[6] V. Nanjundiah: *Chemotaxis, signal relaying and aggregation morphology*, J. Theor. Biol. **42** (1973) 63-105.

[7] N. Saito: *Conservative upwind finite-element method for a simplified Keller-Segel system modelling chemotaxis*, to appear in IMA J. of Numer. Anal.

[8] N. Saito: *Finite-element approximation for a nonlinear parabolic system modelling chemotaxis*, in preparation.

[9] N. Saito and T. Suzuki: *Notes on finite difference schemes to a parabolic-elliptic system modelling chemotaxis*, Appl. Math. Comput. **171** (2005) 72-90.

[10] T. Suzuki: Free Energy and Self-Interacting Particles, Birkhauser, Boston, 2005.

[11] T. Suzuki: Mean Field Theories and Dual Variation, Elsevier, to appear.

[12] T. Suzuki and T. Senba: Applied Analysis: Mathematical Methods in Natural Science. Imperial College Press, 2004.

[13] A. Yagi: *Norm behavior of solutions to a parabolic system of chemotaxis*, Math. Japon. **45** (1997) 241-265.

[14] R. S. Varga: Matrix Iterative Analysis, (Second revised and expanded edition), Springer Series in Computational Mathematics **27**, Springer-Verlag, Berlin, 2000.