XVIII SPANISH-FRENCH SCHOOL JACQUES-LOUIS LIONS ABOUT
NUMERICAL SIMULATION IN PHYSICS AND ENGINEERING
Las Palmas de Gran Canaria, 25-29 June 2018

Review of Numerical Schemes for the Classical Keller-Segel System - Nº 19

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Introduction and Previous Results

The movement of biological cells in response to chemical signals, also called as chemotaxis, was modelled by Keller-Segel in 1970. Although there are several models, we will focus on the classical one, which is given by the following equations in $\Omega \subset \mathbb{R}^n$:

$$\begin{cases} u_t = \Delta u - \alpha_1 \nabla \cdot (u \nabla v), & x \in \Omega,\ t > 0, \\ v_t = \alpha_2 \Delta v - \alpha_3 v + \alpha_4 u, & x \in \Omega,\ t > 0, \\ \dfrac{\partial u}{\partial \nu} = \dfrac{\partial v}{\partial \nu} = 0, & x \in \partial\Omega,\ t > 0, \\ u(x,0) = u_0(x),\ \ v(x,0) = v_0(x), & x \in \Omega, \end{cases} \tag{1}$$

where u and v represent the *density of cells* and *chemical-signal*, respectively.

Recently, a lot of research in this subject has been done from an analytical point of view (see e.g. [1] and references therein). Although the number of results related to numerical analysis of (1) is much lower. Here we focus on this topic.

1. Global in time existence and **boundedness** of the solution has been shown if the initial data is small enough. For instance, for $n = 2$ one has:

Theorem 1. Suppose that $n = 2$ and $\Omega \in \mathbb{R}^n$ is a bounded domain with smooth boundary, that $u_0 \in \mathcal{C}^0(\overline{\Omega})$ and $v \in \cup_{q>n} W^{1,q}(\Omega)$ are non-negative, and that (u,v) denotes the corresponding maximally extended classical solution of (1) in $\Omega \times (0, T_{\max})$. If $\int_\Omega u_0 < 4\pi$, then (u,v) exist globally and satisfies

$$\|u(\cdot,t)\|_{L^\infty(\Omega)} + \|v(\cdot,t)\|_{L^\infty(\Omega)} \le C \text{ for all } t > 0 \tag{2}$$

2. Energy law is important for a proof of Theorem 1 [1]:

Lemma 1. If (u,v) is a non-negative classical solution of (1) in $\Omega \times (0,T)$, then

$$\frac{d}{dt} E(u(\cdot,t), v(\cdot,t)) = -\mathcal{D}(u(\cdot,t), v(\cdot,t)), \tag{3}$$

for all $t \in (0,T)$, with energy

$$E(u,v) := \frac{1}{2}\int_\Omega |\nabla v|^2 + \frac{1}{2}\int_\Omega v^2 - \int_\Omega uv + \int_\Omega u \ln u$$

and the dissipation rate

$$\mathcal{D}(u,v) := \int_\Omega v_t^2 + \int_\Omega \left| \frac{\nabla u}{\sqrt{u}} - \sqrt{u} \nabla u \right|^2.$$

3. Blow-up phenomena have been detected for large initial data (e.g. $\int_\Omega u_0 > 4\pi$, $n = 2$) but only partial results exits and general case is an open problem [1]. Also (3) is a fundamental ingredient in this type of results. But (as far as we know) discrete versions of (3) like those ones we are dealing here have not yet been sistematically studied.

4. Positivity of solution is well known (but not trivially inherited by discrete schemes)

Proposition 1. Let be (u,v) a solution of (1) in $\Omega \times (0,T)$ for some $t > 0$. If $u_0 \ge 0$ and $v_0 \ge 0$, then u and v are non-negative functions in their domain.

Semi-Discretization in Time

Family of semi-discretizations in time: for a partition of $(0,T)$ into subintervals of size $k > 0$, We approximate u and v at each time step t^{m+1} by implicit Euler as follows:

$$\begin{cases} u^{m+1} - k\Delta u^{m+1} + k\nabla \cdot (u^{m+r_1} \nabla v^{m+r_2}) = u^m, \\ v^{m+1} - k\Delta v^{m+1} + k\nabla v^{m+r_3} + k u^{m+r_4} = v^m, \end{cases} \tag{4}$$

where $r_1, r_2, r_3, r_4 \in \{0,1\}$ and we fix $\alpha_i = 1$ $(i = 1, \dots, 4)$. We are interested energy-stability and positivity of FE approximations for those 12 tuplas (r_1, r_2, r_3, r_4) which result in linear uncoupled schemes (i.e. with $r_2 \cdot r_4 = 0$).

Acknowledgements and Contact Information

Second and third authors are partially supported by the research group FQM-315 of Junta de Andalucía.

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- Access to the whole data of experiments: `https://github.com/rrgalvan/keller-segel-schemes`

Discrete Energy Law and Positivity

Let us consider the following discrete counterpart of (3):

$$E_m = \int_\Omega \frac{1}{2}|\nabla v^m|^2 + \int_\Omega \frac{1}{2}|v^m|^2 - \int_\Omega u^m v^m + \int_\Omega u^m \log(u^m),$$

$$D_m = \int_\Omega |\delta_t v^m|^2 + \int_\Omega \left| \frac{\nabla u^m}{\sqrt{u^m}} - \sqrt{u^m} v^m \right|^2,$$

where we denote $\delta_t \Lambda^m = (\Lambda^m - \Lambda^{m-1})/k$ for any squence $\{\Lambda^m\}$, and let

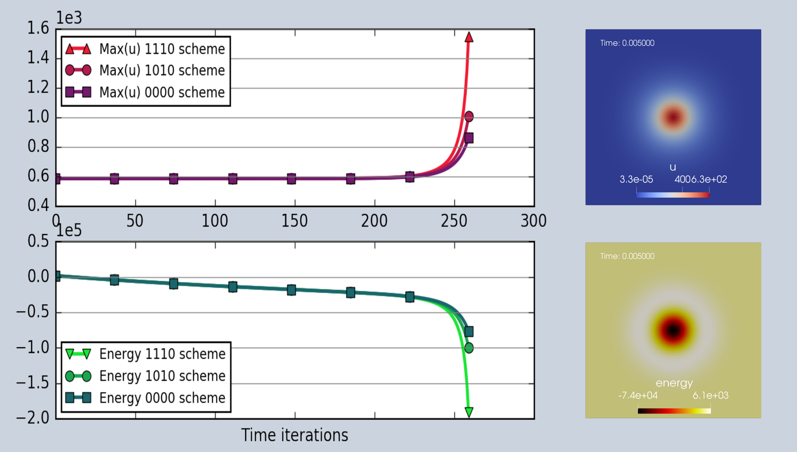
$$N_m = \frac{\gamma}{2}\int_\Omega |\delta_t v^m|^2 + \frac{1}{2}\int_\Omega |\delta_t(\nabla v^m)|^2, \quad \gamma \in \{0,1\}.$$

Theorem 2. Let us consider the schemes given by (4).

1. For any (r_1, r_2, r_3, r_4), the following energy law holds with $\gamma = 1$:
$$\frac{d}{dt} E_m \le -D_m - k\,N_m + k\,M_m, \tag{5}$$
where $M_m \ge 0$ (numerical source) does not depend on k.
2. The case $(r_1, r_2, r_3, r_4) = (1,1,1,0)$ is the only one with $M_m = 0$ (minimizes M_m)
3. The case $(r_1, r_2, r_3, r_4) = (1,0,1,0)$ also satisfies (5) with $\gamma = 0$ (minimizes N_m)
4. If $r_1 = 1$ then u^{m+1} and v^{m+1} are non-negative solutions of (4) for all m.

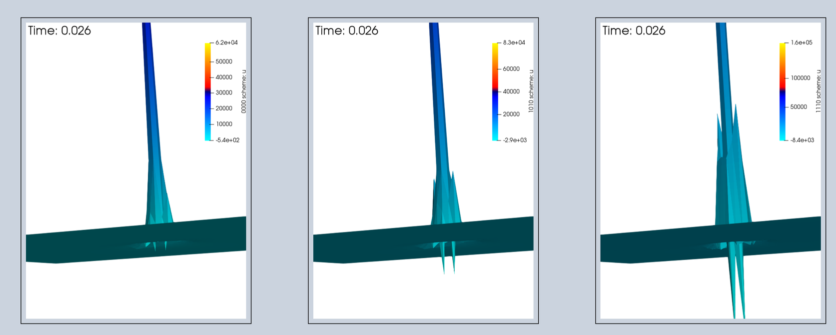
Numerical Tests. 1: Blow-up and Energy

$\Omega = [-2,2]^2 \subset \mathbb{R}^2$, $(\alpha_1, \alpha_2, \alpha_3, \alpha_4) = (0.2, 1, 0.1, 1)$, $u_0 = 1.15 e^{-(x^2+y^2)}(4-x^2)^2(4-y^2)^2$, $v_0 = 0.55 e^{-(x^2+y^2)}(4-x^2)^2(4-y^2)^2$. Blow-up expected [5]. Discretization: 30×30 mesh ($h \sim 10^{-1}$), $k = 10^{-4}$.



Experiment 1.
- *Left*: $\max_\Omega(u^m)$ and E_m for schemes **1110**, **1010** and **0000**.
- *Right*: plot of u^m (top) and E_m (bottom) a time step $m = 50$.

As expected from Theorem 2, energy is lower (and blow-up is earlier) for **1110**.



Experiment 2.
Detail of finite-time blow-up for u (time step $m = 260$). Left to right: **0000**, **1010** and **1110** schemes. Spurious oscillations appear. They are bigger in those schemes with lower energy and earlier blow-up.

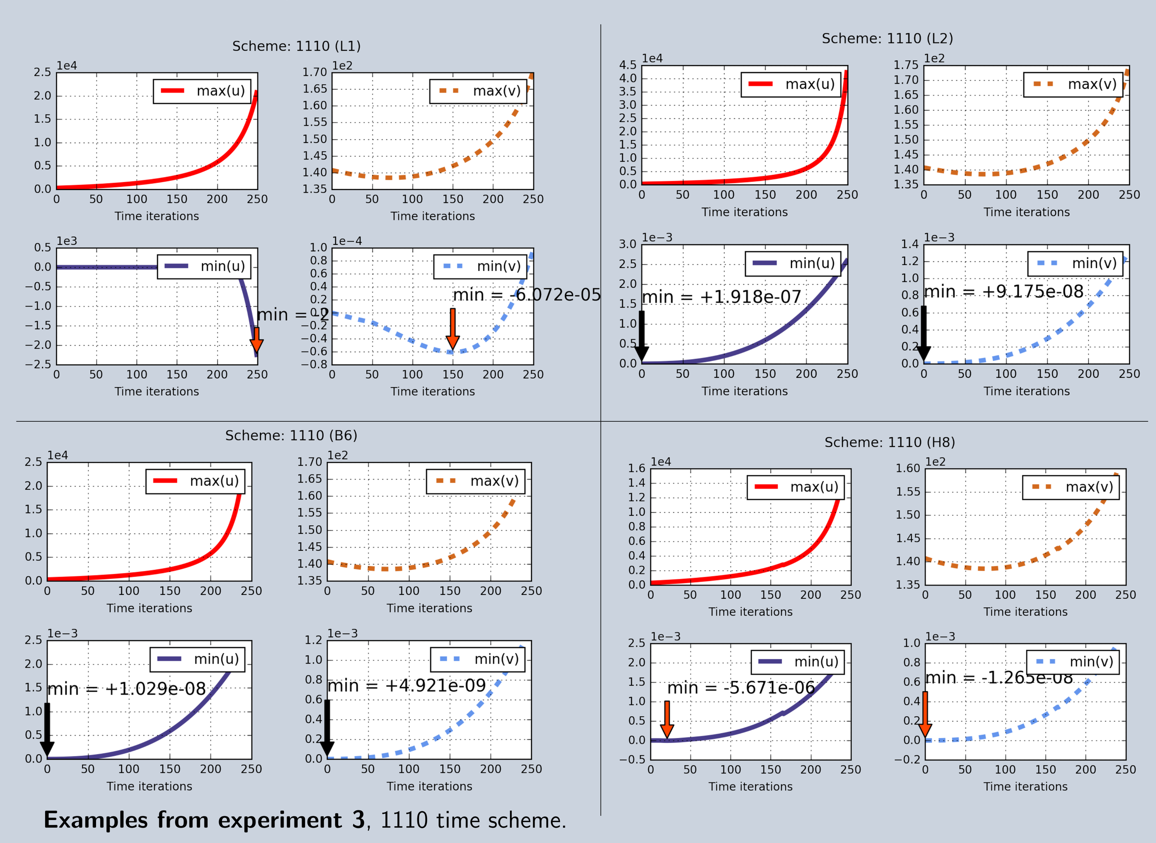
Numerical Tests. 2: Positivity Test Suite

Same data than in Numerical Test 1. We used FreeFem++ [2, 3] (for usual P_k Lagrange elements) and Libmesh [4] (for Lobatto hierarchic and Bernstein FE families of basis functions). Results for 3 schemes are summarized in the table below.

L=Lagrange FE family,
H=Hierarchic FE family,
B=Bernstein FE family.
✓=positive, ✗=non-positive.

Order	1110			1010			0000		
	L	H	B	L	H	B	L	H	B
1	✗	✗	✗	✗	✗	✗	✗	✗	✗
2	✓	✓	✓	✓	✗	✓	✓	✓	✓
3		✗	✗		✗	✗		✗	✗
4		✓	✓		✗	✓		✓	✓
5		✓	✓		✗	?		✗	✓
6		✗	✓		✗	✗		✗	✓
7		✗			✗			✗	
8		✗			✗			✗	

Experiment 3.
Positivity of three time schemes. For each scheme, three FE families (FE basis functions) are compared.



Examples from experiment 3, 1110 time scheme.
- Top row, left to right: Lagrange order 1 (non-positive ✗) and Lagrange order 2 (positive ✓).
- Bottom row, left to right: Bernstein order 6 (positive ✓) and Hierarchic order 8 (non-positive ✗).

References

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