An optimal control problem related to a 3D chemo-repulsion model with nonlinear production

Élder J. Villamizar-Roa
(joint with F. Guillén-González, M.A. Rodríguez-Bellido, E. Mallea-Zepeda)

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Chemotaxis

Is the biological process of the movement of living organisms in response to a chemical stimulus

Initiation of slime mold aggregation viewed as an instability

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Evelyn F. Keller, Lee A. Segel †

Keller-Segel system

$$
\begin{cases}
u_t - \Delta u = \pm\chi \mathrm{div}(u\nabla v) \quad \text{in } \Omega \times (0,T),\\
v_t - \Delta v = u - v \quad \text{in } \Omega \times (0,T),\\
u(0) = u_0 \quad v(0) = v_0 \quad \text{in } \Omega,\\
\partial_n u = \partial_n v = 0, \quad \text{on } \partial\Omega \times (0,T),\\
u \geq 0, \quad v \geq 0.
\end{cases}
$$

- u : Density of cells.
- v : Chemical concentration.
- Chemotaxis term: $\pm\chi\mathrm{div}(u\nabla v)$
  - **chemo-attraction** $(-)$
  - **chemo-repulsion** $(+)$.

Chemo-attraction vs chemo-repulsion

Chemo-attraction

- If $N = 1$, all solutions are global and uniformly bounded.
- If $N = 2$, for $\int_\Omega n_0 < \frac{4\pi}{\chi}$, the solution will be global and uniformly bounded, whereas for $\int_\Omega n_0 > \frac{4\pi}{\chi}$, the blows up can occur.
- If $N \geq 3$, existence of global solutions for small initial data, and blow-up for arbitrary $\int_\Omega n_0$.
- Energy identity:

$$\frac{d}{dt}\mathcal{E}(n,c) + \mathcal{D}(n,c) = 0$$

$$\mathcal{E}(n,c) = \frac{\chi}{2}\int_\Omega |\nabla c|^2 + \frac{\chi}{2}\int_\Omega c^2 - \int_\Omega nc + \int_\Omega n \ln n,$$

$$\mathcal{D}(n,c) = \int_\Omega |\nabla c - c + n|^2 + \int_\Omega \left|\frac{\nabla u}{\sqrt{n}} - \sqrt{n}\nabla c\right|^2$$

Chemo-repulsion

- If $N = 1, 2$ it holds the existence and uniqueness of classical global-in-time solutions. (Morales-Rodrigo *et al.* 2008).
- If $N = 3$, it holds the existence of global weak solutions.
- If $N = 3$, it is unclear whether regular bounded solutions exist globally in time.

Chemorepulsion-nonlinear production and control

$$\text{Min } J[u,v,f] = \frac{\gamma_u}{5p/2}\int_0^T \|u-u_d\|^{5p/2}_{L^{5p/2}(\Omega)} + \frac{\gamma_v}{2}\int_0^T \|v-v_d\|^2_{L^2(\Omega)} + \frac{\gamma_f}{5/2}\int_0^T \|f\|^{5/2}_{L^{5/2+}(\Omega_c)},$$

$$(P)\begin{cases} u_t - \Delta u = \chi \operatorname{div}(u\nabla v) + \overbrace{ru - \mu u^p}^{Reaction}, \\ v_t - \Delta v = \underbrace{u^p}_{Production} - v + \underbrace{f\, v 1_{\Omega_v}}_{Control}, \\ u(0) = u_0 \quad \text{in } \Omega, \\ v(0) = v_0 \quad \text{in } \Omega, \\ \partial_n u = \partial_n v = 0, \quad \text{on } \partial\Omega \times (0,T), \\ u \geq 0, \quad v \geq 0. \end{cases}$$

- $f \in \mathcal{F}$ being $\mathcal{F}$ a closet and convex subset of $L^{5/2}(L^{5/2+})$ and $[u,v]$ strong solution of (P).
- $\gamma_u > 0$, $\gamma_v \geq 0$, either $\gamma_f > 0$ or $\gamma_f = 0$ and $\mathcal{F}$ is bounded in $L^{5/2}(L^{5/2+}(\Omega_c))$.
- 2D-case (Guillén-González, Mallea-Zepeda, V-R (2020), $p \in (1,2]$

1. Existence of weak solutions (with or without logistic term) with $f \in L^{5/2}((0,T);L^{5/2}(\Omega_c))$.
2. Regularity of weak solutions.
3. Existence of optimal control and characterization.

Notation: ⋆ $L^p(L^q) := L^p((0,T);L^q(\Omega))$,
⋆ $L^p(Q)$ means $L^p(L^p)$,
⋆ L^{p+} means $L^{p+\delta}$.

1. Existence of solutions (formal computations)

$$\begin{cases} u_t - \Delta u = \chi \mathrm{div}(u\nabla v), \\ v_t - \Delta v = u^p - v + f\, v 1_{\Omega_v}, \end{cases}$$

- Multiplying u-eq by $\frac{1}{p-1}u^{p-1}$ and v-eq by by $-\frac{1}{p}\Delta v$, adding the corresponding results in order to cancel the chemotaxis and production effects, we get

$$\frac{d}{dt}\left(\frac{1}{p(p-1)}\|u^{p/2}\|^2 + \frac{1}{2p}\|\nabla v\|^2\right) + \frac{4}{p^2}\|\nabla(u^{p/2})\|^2 + \frac{1}{4p}\|\Delta v\|^2 + \frac{1}{p}\|\nabla v\|^2 \le C\|f\|_{L^{5/2}}^{5/2}\|v\|_{H^1}^2.$$

- Integrating v-eq in Ω, then multiplying the resulting equation by $\frac{1}{p}\int_\Omega v$ we obtain

$$\begin{aligned} \frac{1}{2p}\frac{d}{dt}\left(\int_\Omega v\right)^2 + \frac{1}{2p}\left(\int_\Omega v\right)^2 &\le \frac{1}{p}\left(\int_\Omega u^p\right)^2 + C\|f\|_{L^2}^2\|v\|_{L^2}^2 \\ &\le \frac{1}{p}\|u\|_{L^p}^{2p} + C\|f\|_{L^2}^2\|v\|_{L^2}^2. \end{aligned}$$

Remark:

$$\|u\|_{H^1}^2 \equiv \|\nabla u\|^2 + \left(\int_\Omega u\right)^2, \ \forall\, u \in H^1(\Omega), \quad \|u\|_{H^2}^2 \equiv \|\Delta u\|^2 + \left(\int_\Omega u\right)^2 \ \forall\, u \in H^2_{\mathrm{n}}(\Omega).$$

Energy inequality

To bound the term $\|u\|_{L^p}^{2p}$, from the 3D-Gagliardo-Nirenberg inequality, we have

$$\|u\|_{L^p}^{2p} = \|u^{p/2}\|^4 \leq C\left(\|\nabla(u^{p/2})\|^{12(p-1)/(3p-1)}\|u^{p/2}\|_{L^{2/p}}^{8/(3p-1)} + \|u^{p/2}\|_{L^{2/p}}^4\right).$$

At this point, we distinguish three cases:

- If $p \in (1, 5/3)$, then $12(p-1)/(3p-1) < 2$; thus, from the Young inequality, and noting that $\|u(t,\cdot)\|_{L^1} = \|u_0\|_{L^1}$, we get

$$\begin{aligned}\frac{1}{p}\|u\|_{L^p}^{2p} &\leq \frac{2}{p^2}\|\nabla u^{p/2}\|^2 + C\|u^{p/2}\|_{L^{2/p}}^{8/(5-3p)} + C\|u^{p/2}\|_{L^{2/p}}^4 \\ &= \frac{2}{p^2}\|\nabla u^{p/2}\|^2 + C\left(\int_\Omega u_0\right)^{8/(5-3p)} + C\left(\int_\Omega u_0\right)^4.\end{aligned}$$

Consequently, we conclude the energy inequality

$$\begin{aligned}\frac{d}{dt}\left(\frac{1}{p(p-1)}\|u^{p/2}\|^2 + \frac{1}{2p}\|v\|_{H^1}^2\right) &+ \frac{C}{p}\|v\|_{H^2}^2 + \frac{2}{p^2}\|\nabla u^{p/2}\|^2 \\ &\leq C\left(\|f\|_{L^{5/2}}^{5/2} + \|f\|_{L^{5/2}}^2\right)\|v\|_{H^1}^2 + C. \qquad (1)\end{aligned}$$

Energy inequality

- For $p = 5/3$,

$$\begin{aligned}\frac{1}{p}\|u\|_{L^p}^{2p} &= \frac{3}{5}\|u^{5/6}\|^4 \leq \frac{3}{5}\left(C\|\nabla u^{5/6}\|^2\|u^{5/6}\|_{L^{6/5}}^2 + C\|u^{5/6}\|_{L^{6/5}}^4\right)\\ &\leq C\left(\|\nabla u^{5/6}\|^2\left(\int_\Omega u_0\right)^{5/3} + \left(\int_\Omega u_0\right)^{10/3}\right) \leq C\left(\|\nabla u^{5/6}\|^2 + 1\right).\end{aligned}$$

Then, we also can obtain the energy inequality (1).

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- The condition $p \leq 5/3$ to get (1) means that we can control the energy only with the random diffusion.

The case $p > \frac{5}{3}$

- Energy is controlled by the logistic growth

$$(P) \begin{cases} u_t - \Delta u - \chi \mathrm{div}(u \nabla v) = ru - \mu u^p \quad \text{in } \Omega \times (0,T), \\ v_t - \Delta v = u^p - v + f v 1_{\Omega_v} \quad \text{in } \Omega \times (0,T), \\ u(0) = u_0 \ \ v(0) = v_0 \ \text{ in } \Omega, \\ \partial_n u = \partial_n v = 0, \ \text{ on } \partial\Omega \times (0,T), \\ u \geq 0, \ v \geq 0. \end{cases}$$

$$\|u\|_{L^p}^{2p} = \|u^{p/2}\|^4 \leq C \|u^{p/2}\|_{L^{2(2p-1)/p}}^{2(2p-1)/p} \|u^{p/2}\|_{L^{2/p}}^{2/p} = C(\|u_0\|_{L^1}, r, \mu) \, \|u\|_{L^{2p-1}}^{2p-1} .$$

Consequently,

$$\frac{d}{dt}\left(\frac{1}{p(p-1)}\|u^{p/2}\|^2 + \frac{1}{2p}\|v\|_{H^1}^2\right) + \frac{4}{p^2}\|\nabla(u^{p/2})\|^2 + C\|v\|_{H^2}^2 + C\|u\|_{L^{2p-1}}^{2p-1}$$
$$\leq r\|u\|_{L^p}^p + C\left(\|f\|_{L^{5/2}}^{5/2} + \|f\|_{L^{5/2}}^2\right)\|v\|_{H^1}^2 + C.$$

Weak solutions

$$
(P)\begin{cases}
u_t - \Delta u - \chi \operatorname{div}(u\nabla v) = ru - \mu u^p & \text{in } \Omega\times(0,T),\\
v_t - \Delta v = u^p - v + f v 1_{\Omega_v} & \text{in } \Omega\times(0,T),\\
u(0) = u_0 \quad v(0) = v_0 \quad \text{in } \Omega, & \\
\partial_n u = \partial_n v = 0, \quad \text{on } \partial\Omega\times(0,T), & \\
u\ge 0,\ v\ge 0. &
\end{cases}
$$

.

Definition. Let $f \in L^{5/2}(Q_c) := L^{5/2}(L^{5/2}(\Omega_c))$, $(u_0, v_0) \in L^p(\Omega)\times H^1(\Omega)$, with $u_0 \ge 0$ and $v_0 \ge 0$ a.e. in Ω. A pair (u, v) is called **weak solution,** if $u \ge 0$ and $v \ge 0$ a.e. in Q,

$$
(2) \qquad u \in L^\infty(L^p) \cap L^{5p/3}(Q), \quad v \in L^\infty(H^1) \cap L^2(H^2_n),
$$

$$
(3) \qquad \nabla u \in L^{\gamma(p)}(Q); \quad \gamma(p) = \begin{cases} 5p/(3+p) & \text{when } 1 < p \le 2,\\ 25p/(18+5p) & \text{when } 2 < p < 12/5,\\ 2 & \text{when } p \ge 12/5, \end{cases}
$$

satisfying the variational formulation of the u-equation

$$
(4) \qquad \int_0^T \langle \partial_t u, \overline{u}\rangle + \int_0^T\int_\Omega \nabla u\cdot\nabla\overline{u} + \int_0^T\int_\Omega u\nabla v\cdot\nabla\overline{u} = \int_0^T\int_\Omega (r\,u - \mu\,u^p)\overline{u},
$$

for all $\overline{u} \in L^{5/2}(Q)$ with $\nabla\overline{u} \in L^{10}(Q)$, the **$v$-equation holds a.e** $(t,x)\in Q$ and the initial conditions. Moreover, $u \in L^{2p-1}(Q)$ for the logistic problem.

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Existence of weak solutions

Theorem.

- If $1 < p \leq 5/3$, then there exists a weak solution of system in the **no** logistic case.

- If $1 < p < \infty$, then there exists a weak solution of system in the logistic case.

Existence of weak solutions

Proof is obtained as a limit of a family of regularized problems: Given $\varepsilon > 0$, find $[u_\varepsilon, w_\varepsilon]$ such that:

$$(5) \quad \left\{ \begin{array}{rcl} \partial_t u_\epsilon - \Delta u_\varepsilon & = & \nabla \cdot (u_\varepsilon \nabla v_\varepsilon) + r u_\varepsilon - \mu u_\varepsilon^p, \quad \text{in } \Omega \times (0, T), \\ \partial_t w_\varepsilon - \Delta w_\varepsilon + w_\varepsilon & = & u_\varepsilon^p + f v_\varepsilon 1_{\Omega_c}, \quad \text{in } \Omega \times (0, T), \\ [u_\varepsilon(0), w_\varepsilon(0)] & = & [u_{0,\epsilon}, w_{0,\varepsilon}] \quad \text{in } \Omega, \\ \partial_{\mathrm{n}} u_\varepsilon(x,t) & = & \partial_{\mathrm{n}} w_\varepsilon(x,t) = 0, \quad \text{on } \partial\Omega \times (0, T), \end{array} \right.$$

where $v_\varepsilon(\cdot, t)$ for any $t \in [0, T]$ is the unique solution of the elliptic problem

$$\left\{ \begin{array}{l} v_\varepsilon - \varepsilon \Delta v_\varepsilon = w_\varepsilon \text{ in } \Omega, \\ \partial_{\mathrm{n}} v_\varepsilon(x,t) = 0 \text{ on } \partial\Omega. \end{array} \right.$$

In (5), $(u_{0,\varepsilon}, w_{0,\varepsilon})$ are initial data satisfying

$$\left\{ \begin{array}{l} u_{0,\varepsilon} \in L^{\infty-}(\Omega), \ u_{0,\varepsilon} \geq 0, \text{ with } \displaystyle\int_\Omega u_{0,\varepsilon} = \int_\Omega u_0, \\ u_{0,\varepsilon} \to u_0 \text{ in } L^p(\Omega), \text{ as } \varepsilon \to 0, \\ v_{0,\varepsilon} \in W_{\mathrm{n}}^{2+6/5,5/2}(\Omega), \ v_{0,\varepsilon} \to v_0 \text{ in } H^1(\Omega), \text{ as } \varepsilon \to 0, \\ w_{0,\varepsilon} = v_{0,\varepsilon} - \varepsilon \Delta v_{0,\varepsilon} \in W^{6/5,5/2}(\Omega). \end{array} \right.$$

Regularity criterion and existence of strong solutions

Theorem. Let (u, v) be a weak solution. Assume $[u_0, v_0] \in L^{r(p)}(\Omega) \times W^{6/5,5/2}(\Omega)$, $r(p) = \text{máx}\{3, 3(p-1)\}$.

$$\text{If } f \in L^{5/2}(L^{5/2+}(\Omega_c)) \quad \text{and} \quad u^p \in L^{5/2}(Q),$$

then

$$u, \nabla v \in L^5(Q) \text{ for } p \leq 2 \quad \text{and} \quad u, \nabla v \in L^{5(p-1)}(Q) \text{ for } p > 2.$$

The strong solution is unique.

.

$$\text{weak: } \boxed{f \in L^{5/2}(Q),\ u^p \in L^{5/3}(Q),\ [u_0, v_0] \in L^p \times H^1}$$

vs

$$\text{Regularity criterion: } \boxed{f \in L^{5/2}(L^{5/2+}),\ u^p \in L^{5/2}(Q),\ [u_0, v_0] \in L^{r(p)} \times W^{6/5,5/2}}$$

Existence of ptimal solution

- Setting:
  - $X := \{u : u \in L^\infty(L^{r(p)}) \cap L^{s(p)}(Q),\ \nabla u \in L^2(Q),\ \partial_t u \in L^2((H^1)')\}$, $s(p) = \text{máx}\{5, 5(p-1)\}$.
  - $$X_u := \{u \in X \ :\ u \text{ is a variational solution of a heat problem } \partial_t u - \Delta u = g^0 - \nabla\cdot \mathrm{g}^1,\ u(0) = w_0,\ (-\nabla u + \mathrm{g}^1)\cdot \mathrm{n}|_{\partial\Omega} = 0 \text{ with } w_0 \in L^{r(p)}(\Omega),\ g^0 \in L^{5r(p)/(2r(p)+3)}(Q) \text{ and } \mathrm{g}^1 \in L^{5r(p)/(r(p)+3)}(Q)^3\Big\},$$
  - $X_v := \left\{u \in C([0,T]; W^{6/5,5/2}) \cap L^{5/2}(W^{2,5/2}) \ :\ \partial_t u \in L^{5/2}(Q)\right\}$.
- Admissible set:

$$\mathcal{S}_{ad} = \{[u,v,f] \in X_u \times X_v \times \mathcal{F} \ :\ [u,v] \text{ is the strong solution with control } f\}.$$

The optimal control problem is given by:

$$\begin{cases} \text{mín } J([u,v,f]), \\ \text{subject to } [u,v,f] \in \mathcal{S}_{ad}, \end{cases}$$

$$J[u,v,f] = \frac{\gamma_u}{5p/2}\int_0^T \|u-u_d\|^{5p/2}_{L^{5p/2}(\Omega)} + \frac{\gamma_v}{2}\int_0^T \|v-v_d\|^2_{L^2(\Omega)} + \frac{\gamma_f}{5/2}\int_0^T \|f\|^{5/2}_{L^{5/2+}(\Omega_c)}.$$

Theorem. Assume that $\mathcal{S}_{ad} \neq \emptyset$. Then, there exists at least one global optimal solution.

Control-state mapping

Let $(u^*, v^*, f^*) \in X_u \times X_v \times L^{5/2}(L^{5/2+}(\Omega_c))$ such that $\mathcal{S}(u^*, v^*, f^*) = 0$.

- The equality operator $\mathcal{S} \in C^1$, and

$$\frac{\partial \mathcal{S}(u^*, v^*, f^*)}{\partial(u, v)}(\overline{U}, \overline{V}) = \begin{pmatrix} \partial_t \overline{U} - \Delta \overline{U} - \nabla \cdot (\overline{U} \nabla v^*) - \nabla \cdot (u^* \nabla \overline{V}) - r\overline{U} + \mu p(u^*)^{p-1}\overline{U} \\ \partial_t \overline{V} - \Delta \overline{V} + \overline{V} - p(u^*)^{p-1}\overline{U} - f^* \overline{V} 1_{\Omega_c} \end{pmatrix}.$$

  - $\frac{\partial \mathcal{S}(u^*, v^*, f^*)}{\partial(u, v)}$ is an isomorphism from $X_u \times X_v$ onto $Y_u \times Y_v$.
  - T.F.I. gives the existence of a C^1 control-to-state map $\mathcal{E} : \mathcal{B}_{f^*} \to \mathcal{B}_{(u^*, v^*)}$ such that $\mathcal{S}(\mathcal{E}(f), f) = (0, 0)$, for each $f \in \mathcal{B}_{f^*}$. Then, $\mathcal{E}(f) = (u_f, v_f)$ is the strong solution.
  - If $(U, V) = D\mathcal{E}(f)[F]$, for some $f \in \mathcal{B}_{f^*}$, then (U, V) is the unique solution of the "linearized" problem.

Here $Y_v := L^{5/2}(Q)$, and $Y_u \equiv Z'$ with

$$Z := \{\varphi \in L^{5r(p)/(3r(p)-3)}(Q) : \ \nabla\varphi \in (L^{5r(p)/(4r(p)-3)}(Q))^3\}.$$

Adjoint system

Proposition. There exists a unique solution $[\sigma, \eta] \in Y_u' \times L^{5/3}(Q)$ of the adjoint problem:

$$\begin{cases} -\partial_t \sigma - \Delta\sigma + \nabla\sigma \cdot \nabla v^* - p(u^*)^{p-1}\eta - r\sigma + p\mu(u^*)^{p-1}\sigma = \gamma_u h(u^* - u_d), \\ -\partial_t \eta - \Delta\eta - \nabla \cdot (u^* \nabla\sigma) + \eta - f^* \eta \, 1_{\Omega_c} = \gamma_v (v^* - v_d), \\ \sigma(T) = 0, \ \eta(T) = 0 \ \text{ in } \ \Omega, \\ \partial_{\mathrm{n}} \sigma = 0, \ \ \partial_{\mathrm{n}} \eta = 0 \ \text{ on } \ \partial\Omega \times (0, T). \qquad \textbf{Here: } h(w) = |w|^{(5p-4)/2}(w) \end{cases}$$

- Reduced cost functional $J_0 : \mathcal{B}_{f^*} \to \mathbb{R}$ by $J_0(f) := J([u_f, v_f, f])$, for any f near of f^* and $[u_f, v_f]$ near of $[u^*, v^*]$
- From the chain rule

$$
\begin{aligned}
J_0'(f^*)[f] &= \frac{\partial J([u^*, v^*, f^*])}{\partial [u, v]}(D\mathcal{E}(f^*)[f]) + \frac{\partial J([u^*, v^*, f^*])}{\partial f}[f] \\
&= \frac{\partial J([u^*, v^*, f^*])}{\partial [u, v]}([U, V]) + \frac{\partial J([u^*, v^*, f^*])}{\partial f}[f] \\
&= \gamma_u \int_0^T \int_\Omega h(u^* - u_d)U + \gamma_v \int_0^T \int_\Omega (v^* - v_d)V \\
&\quad + \gamma_f \int_0^T \int_{\Omega_c} \frac{\operatorname{sgn}(f^*)|f^*|^{(3/2)+} f}{\|f^*\|^{0+}_{L^{(5/2)+}(\Omega_c)}}\, f.
\end{aligned}
$$

- Testing the adjoint by U and V, integrating by parts we get

$$
\gamma_u \int_0^T \int_\Omega h(u^* - u_d)U + \gamma_v \int_0^T \int_\Omega (v^* - v_d)V = \gamma_u \int_0^T \int_{\Omega_c} v^* \eta f.
$$

- Therefore, replacing

$$
J_0'(f^*)[f] = \int_0^T \int_{\Omega_c} \left(\gamma_f \frac{\operatorname{sgn}(f^*)|f^*|^{(3/2)+} f^*}{\|f^*\|^{0+}_{L^{(5/2)+}(\Omega_c)}} + v^* \eta \right) f \geq 0, \quad \forall f \in \mathcal{F}.
$$

In particular, identifying $(L^{5/2}(L^{(5/2)+}))' \equiv L^{5/3}(L^{(5/3)-})$, we have the identification

$$J_0'(f^*) \equiv \gamma_f \frac{\mathrm{sgn}(f^*)|f^*|^{(3/2)+}}{\|f^*\|^{0+}_{L^{(5/2)+}(\Omega_c)}} + v^*\eta.$$

- Steep-descent gradient: $\boxed{f^{k+1} = f^k - \alpha J_0'(f^k).}$

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