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Traveling waves in a Chemotaxis model

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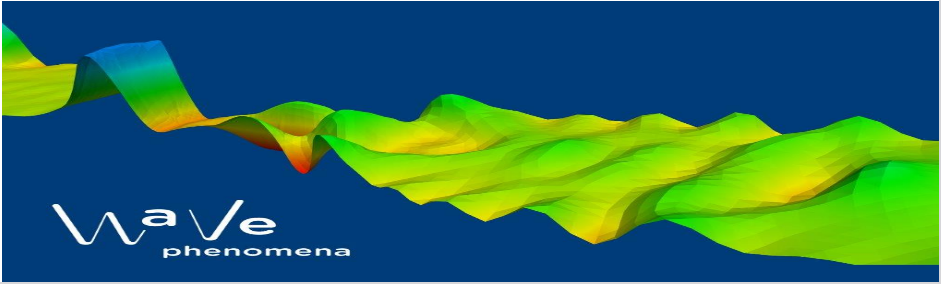

Outline

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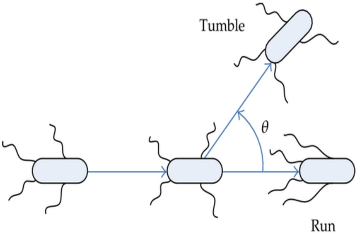

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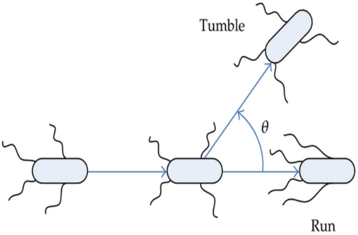
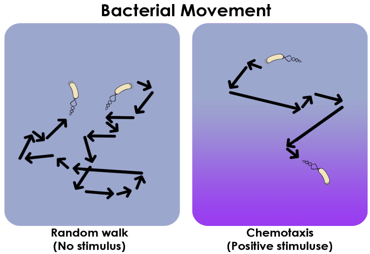


- Chemical stimulus: food (sugar), chemical substance, poison.



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- Meta level:
  - **Alzheimer's disease**
    - loss of neurons due to chemotactic processes
  - **Cancer research – Metastasis**
    - migration of cells

Outline

1. Motivation
2. System - Objectives
3. Methodology

System

- Classical mathematical model: Patlak-Keller-Segel [CITE] – Reaction-Diffusion system assuming diffusion of the species at hand.

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- Alternative model by Dolak-Hillen [CITE] that applies Cattaneo's law of heat propagation with finite speed based on the individual movement patterns of the species:

$$
\begin{aligned}
u_t + q_x &= \rho u(1 - \tfrac{1}{\lambda})(u - \tfrac{\lambda}{4}) \\
q_t + D\tau u_x &= \frac{\alpha}{\tau}\frac{S_x u}{(1+bS)^2} - \frac{1}{\tau} q \\
S_t - \frac{d}{\epsilon} S_{xx} &= \frac{1}{\epsilon}\frac{\lambda u}{(1+\gamma u)} - \frac{1}{\epsilon} S
\end{aligned} \tag{1}
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System

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$$S_t - \frac{d}{\epsilon} S_{xx} = \frac{1}{\epsilon}\frac{\lambda u}{(1 + \gamma u)} - \frac{1}{\epsilon} S$$

- u : cell density, q : population flux, S : signal concentration
- $\rho, \lambda, D, \tau, \alpha, \beta, \gamma, d, \epsilon$ are given constant parameters
- 2nd order, nonlinear, coupled system of PDEs of mixed hyperbolic-parabolic type.

Objectives

- Prove rigorously the existence of traveling wave (TW) solutions of the form:

$$u(x,t) = v_1(x-\mu t), \quad q(x,t) = v_2(x-\mu t), \quad S(x,t) = v_3(x-\mu t). \tag{2}$$

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  - Unbounded domain $\Omega = \mathbb{R}$

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  - Unbounded domain $\Omega = \mathbb{R}$
- Later, also stability properties of the traveling wave solutions shall be investigated.
- Approach: **Computer assisted method**
  - following the ideas from Plum [CITE] on elliptic problems
  - mathematical proof, at least partially generated by computer
  - interval arithmetics

Outline

Preparation

- Plugging (2) into system (1) and introducing $v_4 = v_3'$ yields

$$\begin{aligned}
v_1' &= \frac{1}{D-\tau\mu^2}\Big[\tau\mu\rho v_1(1-\frac{v_1}{\lambda})(v_1-\frac{\lambda}{4}) + \alpha\frac{v_1 v_4}{(1+\beta v_3)^2} - v_2\Big] \\
v_2' &= \frac{1}{D-\tau\mu^2}\Big[D\rho v_1(1-\frac{v_1}{\lambda})(v_1-\frac{\lambda}{4}) + \mu\alpha\frac{v_1 v_4}{(1+\beta v_3)^2} - \mu v_2\Big] \\
v_3' &= v_4 \\
v_4' &= -\frac{\lambda}{d}\frac{v_1}{1+\gamma v_1} + \frac{1}{d}v_3 - \frac{\epsilon\mu}{d}v_4
\end{aligned} \tag{3}$$

ODE system for $v = (v_1, v_2, v_3, v_4)^\top$, posed on $\mathbb{R}$.

Preparation

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$$v' = f(v, \mu) \quad \text{on } \mathbb{R} \tag{4}$$

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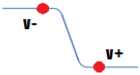
- The connecting orbit/TW v is called a homoclinic/pulse if $v^- = v^+$ and heteroclinic/front if $v^- \neq v^+$.



Preparation

- System (4) ($v' = f(v,\mu)$) is autonomous and posed on $\mathbb{R}$, hence every translate of v, is a solution too. To remove this degeneracy, we adjoint a suitable shift fixing condition, namely

$$\psi(v) = 0, \tag{6}$$

with

$$\psi(v) := \langle \hat{v}', v - \hat{v} \rangle_{L^2}. \tag{7}$$

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Function $\hat{v} \in C^1(\mathbb{R})^4$ denotes a very rough approximate solution where for some "large" $R > 0$,

$$\hat{v}(x) = \begin{cases} v_-, & \text{for } -\infty < x \leq -R \\ v_+, & \text{for } R \leq x < +\infty. \end{cases} \tag{8}$$

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- With ψ from (7), condition (6) represents minimization of $\|\hat{v} - v(\cdot + s)\|_{L^2(\mathbb{R})}$ over all shifts $s \in \mathbb{R}$ and thus fixes the shift position of v.

Preparation

- If v satisfies diff.eq. (4), b.c. (5) and s.f.c. (6), $w := v - \hat{v}$ satisfies

$$w' = \tilde{f}(x, w, \mu), \quad w \xrightarrow{x \to \pm\infty} 0 \quad \tilde{\psi}(w) = 0 \tag{9}$$

where

$$\tilde{f}(x, y, \mu) := f(\hat{v}(x) + y, \mu) - \hat{v}'(x) \quad \text{and} \quad \tilde{\psi}(w) = \langle \hat{v}', w \rangle_{L^2(\mathbb{R})}$$

- Note that

$$\tilde{f}(x, 0, \mu) = \begin{cases} f(v^-, \mu) = 0, & \text{for } x \leq -R \\ f(v^+, \mu) = 0, & \text{for } x \geq R \end{cases} \tag{10}$$

- Thus, we can look for solutions $w \in H^1(\mathbb{R})^4$.

Preparation

- Henceforth, the problem reads

$$F(w,\mu) = 0, \tag{11}$$

where $F : H^1(\mathbb{R})^4 \times \mathbb{R} \to L^2(\mathbb{R})^4 \times \mathbb{R}$ is given by

$$F(w,\mu) := (w' - \tilde{f}(\cdot, w, \mu), \quad \tilde{\psi}(w)) \tag{12}$$

which is well-shaped for a computer-assisted existence proof.

Existence proof - Sketch:

- **Step 1**: Compute, by numerical means, an approximate solution $(\tilde{w}, \tilde{\mu}) \in H_0^1(-x_0, x_0)^4 \times \mathbb{R}$ for some "large" x_0, via a Newton-Collocation method (using cubic splines). Then, define $\omega \in H^1(\mathbb{R}^4)$ by zero extension of $\tilde{w}$.
  - This will give an approximate solution $(\omega, \tilde{\mu}) \in H^1(\mathbb{R})^4$ of problem (11).
  - **No** rigorous computations needed for Step 1.

Existence proof - Sketch:

- **Step 2:** Compute a rigorous upper bound δ for the residual (defect) of $(\omega, \tilde{\mu})$:

$$\left\|\omega' - \tilde{f}(\cdot, \omega, \mu)\right\|^2_{L^2(\mathbb{R})} + \zeta |\tilde{\psi}(\omega)|^2 \leq \delta^2. \tag{13}$$

  - ζ is a scaling factor in $\|\cdot\|_{L^2(\mathbb{R})^4 \times \mathbb{R}}$.
  - Use quadrature with remainder term bound and interval arithmetic.

Existence proof - Sketch:

- **Step 3:** For $x \in \mathbb{R}$, let

$$C(x) := \frac{\partial \tilde{f}}{\partial y}(x, \omega(x), \tilde{\mu}) = \frac{\partial \tilde{f}}{\partial y}(\hat{v}(x) + \omega(x), \tilde{\mu}) \in \mathbb{R}^{4,4},$$

$$\varphi(x) := \frac{\partial \tilde{f}}{\partial \mu}(x, \omega(x), \tilde{\mu}) = \frac{\partial \tilde{f}}{\partial \mu}(\hat{v}(x) + \omega(x), \tilde{\mu}) \in \mathbb{R}^4$$

(φ has compact support) and let $L : H^1(\mathbb{R})^4 \times \mathbb{R} \to L^2(\mathbb{R})^4 \times \mathbb{R}$ be the Fréchet derivative of F at (ω, μ), i.e.

$$L[(u, \sigma)] := (u' - Cu - \sigma\varphi, \tilde{\psi}(u)) \quad \text{where } (u, \sigma) \in H^1(\mathbb{R})^4 \times \mathbb{R}.$$

Existence proof - Sketch:

- Compute constant K such that

$$\left\|(u,\sigma)\right\|_{H^1(\mathbb{R})^4\times\mathbb{R}} \leq K\left\|L[(u,\sigma)]\right\|_{L^2(\mathbb{R})^4\times\mathbb{R}} \qquad (14)$$

  for all $(u,\sigma) \in H^1(\mathbb{R})^4 \times \mathbb{R}$ by means of a **positive lower bound** $\underline{\kappa}$ for the smallest spectral point of the eigenvalue problem

$$\langle L[(u,\sigma)], L[(v,\rho)]\rangle_{L^2(\mathbb{R})^4\times\mathbb{R}} = \kappa\langle (u,\sigma),(v,\rho)\rangle_{H^1(\mathbb{R})^4\times\mathbb{R}} \qquad (15)$$

  for all $(v,\rho) \in H^1(\mathbb{R})^4 \times \mathbb{R}$. (Significant work. Heavy use of computer assistance.)
- Then (13) holds for $K := \frac{1}{\sqrt{\underline{\kappa}}}$.

Existence proof - Sketch:

- **Step 4:** Prove that $L : H^1(\mathbb{R})^4 \times \mathbb{R} \to L^2(\mathbb{R})^4 \times \mathbb{R}$ is surjective by showing that $L^* : H^1(\mathbb{R})^4 \times \mathbb{R} \to L^2(\mathbb{R})^4 \times \mathbb{R}$ is injective. This can be achieved again by spectral bounds:
- Compute a **positive lower bound** $\underline{\kappa}^*$ for the smallest spectral point of the eigenvalue problem

$$\langle L^*[(u,\sigma)], L^*[(v,\rho)]\rangle_{L^2(\mathbb{R})^4\times\mathbb{R}} = \kappa^*\langle (u,\sigma),(v,\rho)\rangle_{H^1(\mathbb{R})^4\times\mathbb{R}}. \quad (16)$$

Existence proof - Sketch:

- **Step 5:** Calculate $g_1, g_2 : [0,\infty) \to [0.\infty)$, non-decreasing, such that for all $(u,\sigma) \in H^1(\mathbb{R})^4 \times \mathbb{R}$

$$\left\| \frac{\partial \tilde{f}}{\partial y}(\cdot, \omega + u, \tilde{\mu} + \sigma) - \frac{\partial \tilde{f}}{\partial y}(\cdot, \omega, \tilde{\mu}) \right\|_{L^\infty(\mathbb{R})^4} \leq g_1(\|(u,\sigma)\|_{H^1(\mathbb{R})^4 \times \mathbb{R}}),$$

$$\left\| \frac{\partial \tilde{f}}{\partial \mu}(\cdot, \omega + u, \tilde{\mu} + \sigma) - \frac{\partial \tilde{f}}{\partial \mu}(\cdot, \omega, \tilde{\mu}) \right\|_{L^2(\mathbb{R})^4} \leq g_2(\|(u,\sigma)\|_{H^1(\mathbb{R})^4 \times \mathbb{R}}).$$

- Let c_1 denote an embedding constant for the embedding $H^1(\mathbb{R}) \hookrightarrow L^2(\mathbb{R})$ and define (for η : scaling factor in $\|\cdot\|_{H^1(\mathbb{R})^4 \times \mathbb{R}}$)

$$g(t) := \sqrt{c_1^2 g_1(t)^2 + \frac{1}{\eta} g_2(t)^2} \quad \text{and} \quad G(t) := \int_0^t g(s) ds.$$

Existence proof - Sketch:

- **Step 6:** Suppose that, for some $\alpha > 0$,

$$\delta \leq \frac{\alpha}{K} - G(\alpha) \quad \text{and} \quad Kg(\alpha) < 1.$$

  - Side note: Constant δ is "small" if the approximate solution $(\omega, \tilde{\mu})$ is sufficiently accurate and $G(t) = \mathcal{O}(t)$ as $t \to 0$.

Theorem

There exists some solution $(w, \mu) \in H^1(\mathbb{R})^4 \times \mathbb{R}$ *of problem* (10) $(F(w, \mu) = 0)$ *satisfying*

$$\left\|(w, \mu) - (\omega, \tilde{\mu})\right\|_{H^1(\mathbb{R})^4 \times \mathbb{R}} \leq \alpha.$$

(Proof: Banach's Fixed Point Theorem)
Hence, there exists a connecting orbit (v, μ) *of our traveling wave problem* (3), (5) *such that*

$$\left\|(v, \mu) - (\hat{v} + \omega, \tilde{\mu})\right\|_{H^1(\mathbb{R})^4 \times \mathbb{R}} \leq \alpha.$$

References

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Thank you!