Towards Global Existence and Optimal Equilibriation Rates for Reaction-Diffusion Models

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Overview

Towards bright sun and white snow for RD models

- Single Reversible Reaction: Quadratic RD system
  - Entropy-Dissipation structure
  - Global existence (classical vs. weak)
  - Convergence to equilibrium (optimal?)
- Networks of Reversible Reactions
  - Motivation
  - Entropy-Dissipation structure?
  - Quasi-Steady-State-Approximation
  - Volume-Surface RD models

Reaction-Diffusion Systems

Prototypical quadratic system: $\mathcal{A}_1 + \mathcal{A}_2 \leftrightarrow \mathcal{A}_3 + \mathcal{A}_4$

- One reversible reaction of four species $\mathcal{A}_i$

$$\mathcal{A}_1 + \mathcal{A}_2 \leftrightarrow \mathcal{A}_3 + \mathcal{A}_4$$

- mass action law kinetics: reaction rates $\sim a_1 a_2 - a_3 a_4$
- bounded, smooth domain $\Omega \subset \mathbb{R}^N$, $|\Omega| = 1$
  homogeneous Neumann boundary conditions

Reaction-Diffusion Systems

Prototypical quadratic system: $\mathcal{A}_1 + \mathcal{A}_2 \leftrightarrow \mathcal{A}_3 + \mathcal{A}_4$

Concentrations $a_i(t,x)$ of $\mathcal{A}_i$, different diffusivities $d_i > 0$

$$\partial_t a_1 - d_1 \triangle_x a_1 = -a_1\, a_2 + a_3\, a_4$$
$$\partial_t a_2 - d_2 \triangle_x a_2 = -a_1\, a_2 + a_3\, a_4$$
$$\partial_t a_3 - d_3 \triangle_x a_3 = +a_1\, a_2 - a_3\, a_4$$
$$\partial_t a_4 - d_4 \triangle_x a_4 = +a_1\, a_2 - a_3\, a_4$$

- quadratic non-linearities, Bootstrap?
- no comparison principle, no invariant regions, Turing instability?
- NO, there is an entropy functional!

Entropy and Entropy Dissipation

Prototypical quadratic model: $\mathcal{A}_1 + \mathcal{A}_2 \leftrightarrow \mathcal{A}_3 + \mathcal{A}_4$

Kinetic (free energy) entropy

$$H(a_i) = \int_\Omega \sum_{i=1}^{4} (a_i \ln(a_i) - a_i)\, dx$$

Entropy dissipation $\frac{d}{dt}H = -D \leq 0$

$$D(a_i) = 4\sum_{i=1}^{4} \int_\Omega d_i |\nabla \sqrt{a_i}|^2\, dx + \int_\Omega (a_1\, a_2 - a_3\, a_4) \ln \frac{a_1\, a_2}{a_3\, a_4}\, dx \geq 0$$

Programme

- Global (classical, weak, renormalised) solutions
- Large-time behaviour: explicit exponential convergence

Entropy and Entropy Dissipation

Prototypical quadratic model: $\mathcal{A}_1 + \mathcal{A}_2 \leftrightarrow \mathcal{A}_3 + \mathcal{A}_4$

Equilibrium state $\{a_{i\infty}\}_{i=1..4}$ is the unique vector of positive constants balancing the reaction rate

$$a_{1\infty}\, a_{3\infty} = a_{2\infty}\, a_{4\infty},$$

and satisfying the three (linear indep.) mass-conservation laws (homogeneous Neumann boundary conditions)

$$a_{1\infty} + a_{2\infty} = \frac{1}{|\Omega|}\int_\Omega (a_{10} + a_{20})\, dx,$$

$$a_{1\infty} + a_{4\infty} = \frac{1}{|\Omega|}\int_\Omega (a_{10} + a_{40})\, dx,$$

$$a_{2\infty} + a_{3\infty} = \frac{1}{|\Omega|}\int_\Omega (a_{20} + a_{30})\, dx.$$

The Entropy Method

Quantitative large-time behaviour

$E(f)$ non-increasing convex entropy functional

$D(f)$ entropy dissipation, f_∞ entropy minimising equilibrium

$$\frac{d}{dt}E(f) = \frac{d}{dt}(E(f) - E(f_\infty)) = -D(f) \leq 0$$

provided conservation laws: $D(f) = 0 \Longleftrightarrow f = f_\infty$

$$D \geq \Phi(E(f) - E(f_\infty)), \quad \Phi(0) = 0, \quad \Phi \geq 0$$

$\Rightarrow$ explicit convergence in entropy, exponential if $\Phi'(0) > 0$

$\Rightarrow$ convergence in L_1 : $\|f - f_\infty\|_1^2 \leq C(E(f) - E(f_\infty))$
Cziszár-Kullback-Pinsker inequalities of convex entropies

The Entropy Method

My Personal Entropy Method Dictionary

- Understanding Entropy-Dissipation Structure $\Longleftrightarrow$ Entropy Entropy-Dissipation (EDD) Estimate

$$D \geq \Phi(E(f) - E(f_\infty)), \quad \Phi(0) = 0, \quad \Phi \geq 0$$

- Really Understanding ED Structure $\Longleftrightarrow$ Optimal Rate/Constant in EED Estimate
- Gradient flow structure?

Entropy Entropy-Dissipation Estimate

$D \geq C\,(E - E_\infty)$

Theorem:[a] For any functions a_i, $i = 1, 2, 3, 4$ measurable, non-negative, satisfying the conservation laws holds

$$D(a_i) \geq C(M_{ij})(E(a_i|a_{i,\infty})).$$

Proof: Additivity $E(a_i|a_{i,\infty}) = E(a_i|\overline{a_i}) + E(\overline{a_i}|a_{i,\infty})$

$$E(a_i|\overline{a_i}) = \sum_{i=1}^{4} \int_\Omega a_i \ln\left(\frac{a_i}{\overline{a_i}}\right)\,dx \leq L(\Omega) \sum_{i=1}^{4} \int_\Omega |\nabla_x \sqrt{a_i}|^2\,dx\,,$$

+ Long long calculations + Conservation laws!

$\Rightarrow$ obtain Functional Inequality Not sharp!

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[a] [L. Desvillettes, K.F.]

Entropy Entropy-Dissipation Estimate

$D \geq C\,(E - E_\infty)$

Entopry Entropy-Dissipation Estimate

$$D(a_i) \geq C(M_{ij})(E(a_i|a_{i,\infty}))$$

+ Gronwall argument + Cziszár-Kullback inequality

$\Rightarrow$ explicit exponential convergence to equilibrium in L^1.

As long a solutions exists?

Entropy A-priori Estimates

Entropy decay

The entropy decays

$$H(T) = H(0) - \int_0^T D(s)\,ds$$

with the entropy dissipation

$$D(a_i) = 4\sum_{i=1}^{4}\int_\Omega d_i|\nabla\sqrt{a_i}|^2\,dx + \int_\Omega (a_1\,a_2 - a_3\,a_4)\ln\frac{a_1\,a_2}{a_3\,a_4}\,dx$$

Entropy A-priori Estimates

Entropy decay

$$H(T):\Big\{\ a_i \in L^\infty([0,+\infty); L\log L(\Omega)) \qquad \forall i = 1,..,4$$

$$\int_0^T D(s):\Big\{\ \sqrt{a_i} \in L^2([0,+\infty); H^1(\Omega)) \qquad \forall i = 1,..,4 : d_i > 0$$

in 1D: $\|a_i\|^{3-\varepsilon}_{L^{3-\varepsilon}([0,T]\times[0,1])} \le C(1+T)$ + parabolic bootstrap

$\Rightarrow \ \|a_i\|_{L^\infty([0,T]\times[0,1])} \le C\left(1+T^{\frac{21}{2}}\right) \Rightarrow$ global classical solutions

in 2D: $a_i^2 \le a_i\, e^{\frac{s a_i}{\|\sqrt{a_i}(t)\|^2_{H^1(\Omega)}}} + \frac{a_i \|\sqrt{a_i}(t)\|^2_{H^1(\Omega)}}{s} \ln(a_i^2)$ for $\ln(a_i) > 1$

Trudinger ineq. $\Rightarrow$ global L^2 bound: $\|a_i\|^2_{L^2([0,T]\times\Omega)} \le C(1+T)$

$\Rightarrow$ global weak (super-)solutions [M. Pierre 2003][a]

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[a] [Desvillettes F. Pierre Vovelle]

Entropy A-priori Estimates

Entropy decay

$$H(T) : \left\{ \; a_i \in L^\infty([0,+\infty); L \log L(\Omega)) \qquad \forall i = 1,..,4 \right.$$

$$\int_0^T D(s) : \begin{cases} \sqrt{a_i} \in L^2([0,+\infty); H^1(\Omega)) & \forall i = 1,..,4 : d_i > 0 \\ \int_0^T \int_\Omega (a_1\, a_2 - a_3\, a_4) \, \ln\left(\frac{a_1\, a_2}{a_3\, a_4}\right) \, dxdt \le C & \end{cases}$$

in 3+D: $\|a_i\|^{1+2/N}_{L^{1+2/N}([0,T]\times\Omega)} \le C(1+T)$

$\Rightarrow$ renormalised solutions (in the sense of [DiPerna, Lions]) [a]

[a] [Desvillettes F. Pierre Vovelle]

Duality Argument for Entropy Density

Entropy density equation: $\mathcal{A}_1 + \mathcal{A}_2 \leftrightarrow \mathcal{A}_3 + \mathcal{A}_4$

Denote $z_i = a_i \ln(a_i) - a_i \quad \Rightarrow \quad H(a_i) = \int_\Omega \sum_{i=1}^4 z_i \, dx$

$$\begin{cases} \partial_t \left(\sum_{i=1}^4 z_i \right) - \Delta_x \left(\sum_{i=1}^4 d_i \, z_i \right) \leq 0, & t \in [0,T], \; x \in \Omega, \\ n \cdot \nabla_x z_i = 0, & t \in [0,T], \; x \in \partial\Omega, \end{cases}$$

Duality Argument for Entropy Density

Entropy density equation: $\mathcal{A}_1 + \mathcal{A}_2 \leftrightarrow \mathcal{A}_3 + \mathcal{A}_4$

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$$\begin{cases} \partial_t \left(\sum_{i=1}^4 z_i\right) - \Delta_x \left(\sum_{i=1}^4 d_i \, z_i\right) \leq 0, & t \in [0,T], \ x \in \Omega, \\ n \cdot \nabla_x z_i = 0, & t \in [0,T], \ x \in \partial\Omega, \end{cases}$$

rewrite with $z := \sum_{i=1}^4 z_i$ and $M(t,x) := \frac{\sum_{i=1}^4 d_i \, z_i}{z}$ as

$$\begin{cases} \partial_t z - \Delta_x [M \, z] \leq 0, & t \in [0,T], \ x \in \Omega, \\ n \cdot \nabla_x [M \, z] = 0, & t \in [0,T], \ x \in \partial\Omega, \end{cases}$$

coefficient M bounded by $\min\{d_i\} \leq M(t,x) \leq \max\{d_i\}$!

Duality Argument for Entropy Density

Entropy density equation: $\mathcal{A}_1 + \mathcal{A}_2 \leftrightarrow \mathcal{A}_3 + \mathcal{A}_4$

Simplest case: $0 < d_0 \le \min\{d_i\} \le M(t,x) \le \max\{d_i\} < \infty$

$$\begin{cases} \partial_t \left(\sum_{i=1}^k z_i\right) - \Delta_x \left(\sum_{i=1}^k d_i\, z_i\right) \le 0, & t \in [0,T],\ x \in \Omega, \\ n \cdot \nabla_x z_i = 0, & t \in [0,T],\ x \in \partial\Omega, \end{cases}$$

uniform $L^2(\log L)^2$ bound + quadratic non-linearities

$\Rightarrow$ uniform integrability of non-linearities

$\Rightarrow$ convergence in $L^1(Q_T)$ of approximating sequence

$\Rightarrow$ global L^2-weak solutions in all space dimensions!

Duality Argument for Entropy Density

General systems $\partial_t a_i - \nabla_x \cdot (d_i \nabla_x a_i) = f_i(a)$

Quadratic Lotka-Volterra systems in $\mathbb{R}^N$: For $z \in (0,\infty)^q$

$$\begin{cases} \partial_t a_i = d_i \Delta_x a_i + a_i \sum_{j=1}^q p_{ij}(a_j - z_j), \quad i = 1 \ldots q \\ \nabla_x a_i \cdot n = 0 \quad \text{on} \quad \partial\Omega, \qquad a_i(0,\cdot) = a_{i,0}(\cdot) \in L^2(\Omega), \end{cases}$$

Then, there exists a global weak solution in $L^2(\Omega)$ in $\mathbb{R}^N$.

Improved Duality Argument

An improved duality argument

Let $\Omega \subset \mathbb{R}^N$ be a bounded domain with $\partial\Omega \in C^{2+\alpha}$. Let $T > 0$,

$$\begin{cases} \partial_t u - \Delta_x(M(t,x)u) = 0 & \text{on} \quad \Omega_T, \\ u(0,x) = u_0(x) \in L^p(\Omega) & \text{for} \quad x \in \Omega, \\ \nabla_x u \cdot \nu(x) = 0 & \text{on} \quad [0,T] \times \partial\Omega, \end{cases}$$

with $\quad 0 < a \leq M(t,x) \leq b < +\infty \quad$ for $\quad (t,x) \in \Omega_T$.

Then, any weak solution u satisfies $(1/p + 1/p' = 1)$

$$\|u\|_{L^p(\Omega_T)} \leq (1 + b\, D_{a,b,p'})\, T^{1/p}\, \|u_0\|_{L^p(\Omega)}, \qquad p \in (2, +\infty),$$

where $\quad D_{a,b,p'} := \dfrac{C_{\frac{a+b}{2},p'}}{1 - C_{\frac{a+b}{2},p'} \frac{b-a}{2}} \quad$ as long as $\quad C_{\frac{a+b}{2},p'} \frac{b-a}{2} < 1$. [a]

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[a] [Cañizo Desvillettes F., CPDE]

Summary

Results $\mathcal{A}_1 + \mathcal{A}_2 \leftrightarrow \mathcal{A}_3 + \mathcal{A}_4$

- 1D: global classical solutions based on entropy structure
  $\approx$ alternative to theory of [Amann],... (more general)
  explicit exponential decay (rates) in all Sobolev norms.
- 2D: global classical solutions [Goudon, Vasseur] [Cañizo Desvillettes F.]
  explicit exponential decay (rates) in L^2.
- allD: global weak L^2-solutions
  explicit exponential decay (rates) in L^p, $1 \le p < 2$.
  Blow-up example [M. Pierre D. Schmidt]

Towards optimal constants/rates?

Nonlinear mass action law system $\alpha\mathcal{A} \leftrightarrow \beta\mathcal{B}$

$$\begin{aligned} \partial_t a - d_a \triangle a &= \\ \partial_t b - d_b \triangle b &= \end{aligned} \begin{pmatrix} -\alpha & \alpha \\ \beta & -\beta \end{pmatrix} \cdot \begin{pmatrix} l\, a^\alpha \\ k\, b^\beta \end{pmatrix}$$

Linearisation around equilibrium $u = a - a_\infty$ and $v = b - b_\infty$

$\Rightarrow$ Rescaled linearised system

$$\begin{aligned} \partial_t u - d_a \triangle u &= \\ \partial_t v - d_b \triangle v &= \end{aligned} \begin{pmatrix} -\alpha^2 & \alpha\beta \\ \alpha\beta & -\beta^2 \end{pmatrix} \cdot \begin{pmatrix} u \\ v \end{pmatrix}$$

Fourier expansion $u = \sum_{k=0}^{\infty} u^k(t)\varphi_k$, $v = \sum_{k=0}^{\infty} v^k(t)\varphi_k$

$$\begin{cases} \Delta\varphi_k = \lambda_k \varphi_k & \text{in} \quad \Omega \\ n \cdot \nabla\varphi_k = 0 & \text{on} \quad \partial\Omega \end{cases} \qquad k = 0, 1, \ldots$$

Towards optimal constants/rates?

Nonlinear mass action law system $\alpha\mathcal{A} \leftrightarrow \beta\mathcal{B}$

For any eigenmode $k \in \mathbb{N}$, we have

$$\partial_t \begin{pmatrix} u^k \\ v^k \end{pmatrix} = \begin{pmatrix} d_a\lambda_k - \alpha^2 & \alpha\beta \\ \alpha\beta & d_b\lambda_k - \beta^2 \end{pmatrix} \cdot \begin{pmatrix} u^k \\ v^k \end{pmatrix}, \qquad k = 0, 1, \ldots$$

a pair of eigenvalues μ_i, $i = 1, 2$ and eigenvectors e_i, $i = 1, 2$:

$$\mu_1(0) = 0, \qquad \mu_2(0) = -(\alpha^2 + \beta^2) < 0,$$

$$\mu_1(k) = \tfrac{d_a+d_b}{2}\lambda_k - \tfrac{\alpha^2+\beta^2}{2} + \sqrt{\tfrac{(\lambda_k(d_b-d_a)+\alpha^2-\beta^2)^2}{4} + \alpha^2\beta^2} < 0,$$

$$\mu_2(k) = \tfrac{d_a+d_b}{2}\lambda_k - \tfrac{\alpha^2+\beta^2}{2} - \sqrt{\tfrac{(\lambda_k(d_b-d_a)+\alpha^2-\beta^2)^2}{4} + \alpha^2\beta^2} < 0,$$

We have $\mu_2(k) < \mu_1(k)$ and $\mu_1(k+1) < \mu_1(k)$ for all $k \in \mathbb{N}$.

Towards optimal constants/rates?

Nonlinear mass action law system $\alpha\mathcal{A} \leftrightarrow \beta\mathcal{B}$

Two dominant negative eigenvalues

$$\mu_2(0) = \; -(\alpha^2 + \beta^2) < 0,$$

$$\mu_1(1) = \frac{d_a + d_b}{2}\lambda_k - \frac{\alpha^2 + \beta^2}{2} + \sqrt{\frac{(\lambda_k(d_b - d_a) + \alpha^2 - \beta^2)^2}{4} + \alpha^2\beta^2},$$

Special case: $d_1 = d_2 = d \quad \Rightarrow \quad \mu_1(1) = d\lambda_k$.

Optimal rate of convergence depends on

$$|\mu_1(1)| > |\mu_2(0)| \; \Leftrightarrow \; \pi^2 > \frac{\alpha^2}{d_2} + \frac{\beta^2}{d_1}$$

Geometry + stoichiometric coefficients + diffusion rates

Towards optimal constants/rates?

Nonlinear mass action law system $\alpha\mathcal{A} \leftrightarrow \beta\mathcal{B}$

Optimal constant in Entropy Entropy-Dissipation Estimate[a]

$$I = \min_{\substack{\beta\overline{u}+\alpha\overline{v}=0,\\ u,v\in C^\infty}} \left\{ \frac{d_a \int_\Omega |\nabla u|^2 + d_b \int_\Omega |\nabla v|^2 dx + \int_\Omega (\alpha u - \beta v)^2 dx}{\int_\Omega u^2 + v^2} \right\}$$

$$= \min_{c^0=0} \left\{ \frac{\sum_{k=0}^\infty |\mu_1(k)|(c^k)^2 + |\mu_2(k)|(d^k)^2}{\sum_{k=0}^\infty (c^k)^2 + (d^k)^2} \right\} \geq \min\{|\mu_1(1)|, |\mu_2(0)|\}$$

Minimising functions are $\sim \varphi_0$ (“large diffusion”) and $\sim \varphi_1$ (“small diffusion”)!?

Conjecture: nonlinear constants/minimisers are the same!

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[a] [G. Pissante, E. Latos, K. F.]

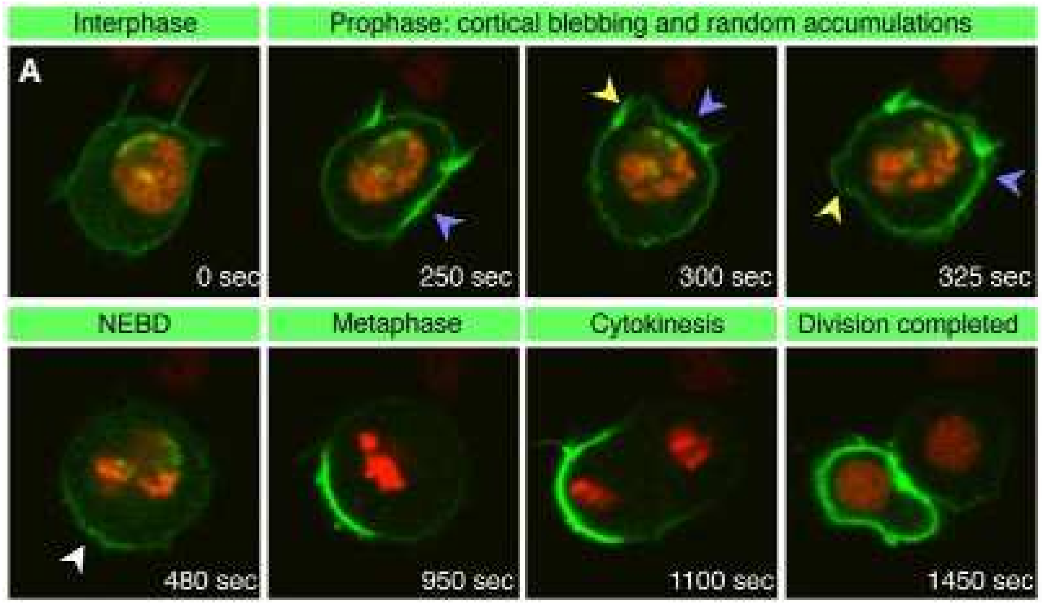
Overview

Towards bright sun and white snow for RD models

- Single Reversible Reaction: Quadratic RD system
  - Entropy-Dissipation Structure
  - Global existence (classical vs. weak)
  - Convergence to equilibrium (optimal?)
- Networks of Reversible Reactions
  - Motivation
  - Entropy-Dissipation Structure? (beyond detailed balance)
  - Quasi-Steady-State-Approximation
  - Volume-Surface RD models

Motivation

Protein-localisation before asymmetric stem-cell division



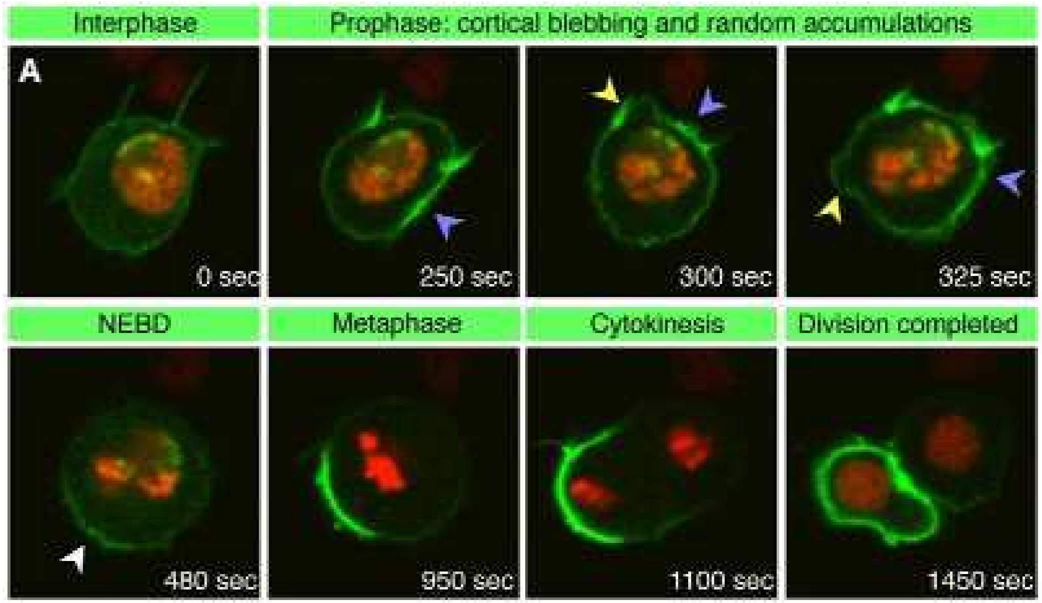
Asymmetric stem-cell division:

Cell-diversity by localisation of cell-fate determinants into one side of the cell cortex and into one of two daughter cells.[a]

[a] GFP-Pon in SOP precursor cells in living Drosophila larvae [Meyer, Emery, Berdnik, Wirtz-Peitz, Knoblich, Current Biology, 2005]

Motivation

Protein-localisation before asymmetric stem-cell division



Mathematical model:

- "high" concentrations, insignificant stochastic effects
- system of (reversible) reaction-diffusion equations
- volume(cytoplasm)-surface(membran) dynamics

Mixed Volume-Surface Reaction-Diffusion Systems

Model Assumptions and Quantities

Key protein Lgl in cell cortex and cytoplasm.

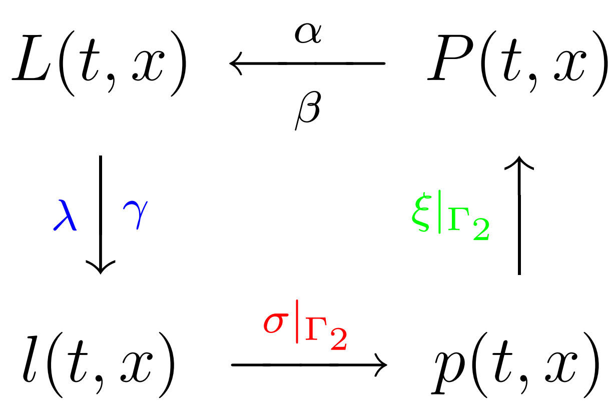
Kinase aPKC phosphorylates Lgl on a part Γ_2 of cell cortex.

$L(t,x)$: cytoplasmic concentration of Lgl

$l(t,x)$: cortical concentration of Lgl

$p(t,x)$: cortical phosphorylated Lgl

$P(t,x)$: cytoplasmic phosphorylated Lgl



Mixed Volume-Surface Reaction-Diffusion Systems

A prototypical model I

Volume equations with diffusion coefficients $d_L, d_P > 0$

$$
\text{(V)} \quad \begin{cases} L_t - d_L \Delta L = \alpha P - \beta L, & x \in \Omega, t > 0, \\ P_t - d_P \Delta P = -\alpha P + \beta L, & x \in \Omega, t > 0, \\ L(0,x) = L_0(x), \ P(0,x) = P_0(x), & x \in \Omega \end{cases}
$$

Boundary conditions on $\partial\Omega = \Gamma = \Gamma_1 \cup \Gamma_2$ and $\Gamma_1 \cap \Gamma_2 = \emptyset$

$$
\text{(BC)} \quad \begin{cases} d_L \frac{\partial L}{\partial \nu} = \gamma l - \lambda L, & x \in \Gamma, t > 0, \\ d_P \frac{\partial P}{\partial \nu} = 0, & x \in \Gamma_1, t > 0, \\ d_P \frac{\partial P}{\partial \nu} = \xi p, & x \in \Gamma_2, t > 0, \end{cases}
$$

Reaction rates $\alpha, \beta, \gamma, \lambda, \sigma, \xi$ are positive constants

Mixed Volume-Surface Reaction-Diffusion Systems

A prototypical model II

Boundary dynamics

(BD)
$$\begin{cases} l_t - d_l \Delta_\Gamma l = \lambda L - \gamma l - \sigma \chi_{\Gamma_2} l, & x \in \Gamma, t > 0 \\ p_t - d_p \Delta_{\Gamma_2} p = \sigma l - \xi p, & x \in \Gamma_2, t > 0, \\ d_p \frac{\partial p}{\partial \nu_{\Gamma_2}} = 0, & x \in \partial\Gamma_2, \\ l(0,x) = l_0(x), & x \in \Gamma, \\ p(0,x) = p_0(x), & x \in \Gamma_2, \end{cases}$$

Δ is the usual Laplacian in the domain Ω

Δ_Γ and Δ_{Γ_2} are Laplace-Beltrami operator on Γ and Γ_2

χ_{Γ_2} is the characteristic function of Γ_2

Mixed Volume-Surface Reaction-Diffusion Systems

Local well-posedness

Conservation law:

$$\frac{d}{dt}\Big[\int_\Omega (L(t,x)+P(t,x)) + \int_\Gamma l(t,x) + \int_{\Gamma_2} p(t,x)\Big] = 0$$

For a $T>0$ there exists a unique weak solution L, P, l, p on $(0,T)$, which remains nonnegative if the intital data are so.

Proof: [Bao Quoc Tang, S. Rosenberger, K. F.]

- fix-point argument between (V),(BC) and (BD).
- local weak solutions of (V),(BC) and (BD)
- non-negativity of solutions of (V),(BC) and (BD)
- uniqueness

Mixed Volume-Surface Reaction-Diffusion Systems

Global existence

The unique solution (L, P, l, p) exists globally.

Proof: $H(t) = \frac{1}{2}\left(\|L(t)\|_{\Omega}^2 + \|P(t)\|_{\Omega}^2 + \|l(t)\|_{\Gamma}^2 + \|p(t)\|_{\Gamma_2}^2\right)$

$$\frac{dH}{dt} \leq \eta H$$

where $\eta = \max\left\{d_L + \frac{\alpha+\beta}{2}, d_P + \frac{\alpha+\beta}{2}, \frac{C_P(\lambda+\gamma)^2}{4d_L} + \frac{\sigma}{2}, \frac{C_P\xi^2}{4d_P} + \frac{\sigma}{2}\right\}$

- Convergence to equilibrium for all initial data and parameter?
- Problem: Decaying entropy functional?

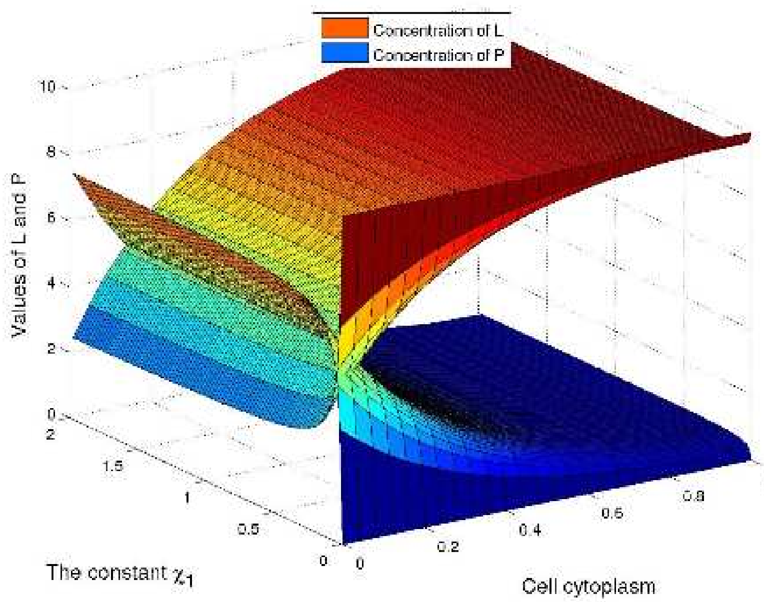
Simple 1D model

Equilibrium: Asymmetric Protein Localisation

1D Cell $x \in [0,1]$, aPKC is located at $x = 0$.

$\Rightarrow$ Explicit solution ($\beta = 0$): $\frac{l(\infty,1)}{l(\infty,0)} = 1 + a(1 + bh(g))$

with $a = \frac{\sigma}{\gamma}$, $b = \frac{\lambda}{d_L}$, $g^2 = \frac{\alpha}{d_P}$, $h(x) = \frac{(e^x-1)^2}{x(e^{2x}-1)}$,



Remark: ξ does not enter stationary state!

Convergence of Network of Reversible Linear Reactions

Deviation around the stationary state

$$X := L - L_\infty, \quad Y := P - P_\infty, \quad x := l - l_\infty, \quad y := p - p_\infty$$

Network of four linear reversible reactions: general structure

$$\begin{array}{ccc} X & \xleftarrow[\beta]{\alpha} & Y \\ \lambda \Big\downarrow \gamma & & \xi \Big\uparrow \mu \\ x & \xrightarrow[\nu]{\sigma} & y \end{array}$$

Conservation law

$$\int [X + Y + x + y] = 0, \qquad \forall t \geq 0.$$

Systems of Reaction-Diffusion Equations

Detailed balance vs. complex kinetics

Then, the detailed balance condition $\frac{\alpha\lambda\sigma\xi}{\beta\mu\nu\gamma} = 1$ is sufficient (and necessary?) for a convex entropy of the form:

$$\frac{d}{dt}\int \left[\Phi_1(X) + \Phi_2(Y) + \Phi_3(x) + \Phi_4(y)\right] \leq 0.$$

- Incompatibility of diffusion and reaction eigen-structure.
- RD-systems allow potentially for oscillations ([BZ]).
- From numerics: Decaying entropy after transient phase?

Systems of Reaction-Diffusion Equations

Network of Reversible Linear Reactions

Closed system of reactions between n substances:

$$\mathcal{U}_i \underset{a_{ij}}{\overset{a_{ji}}{\Longleftrightarrow}} \mathcal{U}_j \qquad\qquad i, j = 1, 2, \ldots, n$$

Concentrations $U = [u_1, u_2, \ldots, u_n]^T$, $D = diag(d_1, d_2, \ldots, d_n)$

$$\begin{cases} U_t = D \triangle U + RU, \\ \frac{\partial U}{\partial \nu} = 0, \quad U(0) = [u_{1,0}, u_{2,0}, \ldots, u_{n,0}]^T \geq 0. \end{cases}$$

$a_{ii} = -\sum_{j=1, j\neq i}^{n} a_{ij}$, $\qquad R = \begin{pmatrix} a_{11} & a_{12} & \ldots & a_{1n} \\ a_{21} & a_{22} & \ldots & a_{2n} \\ \ldots & \ldots & \ldots & \ldots \\ a_{n1} & a_{n2} & \ldots & a_{nn} \end{pmatrix}$

Systems of Reaction-Diffusion Equations

Network of Reversible Linear Reactions

Convergence to the unique equilibrium?

$$\begin{cases} \sum_{j=1}^n a_{ji} u_{i,\infty} = 0, \qquad i = 1, 2, \ldots, n, \\ |\Omega| \sum_{i=1}^n u_{i,\infty} = M > 0 \end{cases}$$

Exists a quadratic entropy $E[U](t) = \frac{1}{2} \sum_{i=1}^n \alpha_i \int_\Omega |u_i(t,x)|^2 dx$,

for a multiplier $B = diag(\alpha_1, \alpha_2, \ldots, \alpha_n)$ with $\alpha_i > 0$ to get

$$D[U](t) = -\frac{dE}{dt} = \sum_{i=1}^n \alpha_i d_i \|\nabla u_i\|^2 - U^T BRU \geq 0 \, ?$$

Systems of Reaction-Diffusion Equations

Network of Reversible Linear Reactions

Algebra Theorem: Assume that $R = (a_{ij})_{i,j=1}^n$ such that

(i) $a_{ij} \geq 0$, $i, j = 1, 2, \ldots, n$,

(ii) $\sum_{i=1}^n a_{ji} = 0$ for all $i = 1, 2, \ldots, n$,

(iii) $\sum_{j=1}^n a_{ji}^2 \times \sum_{k=1}^n a_{ik}^2 \neq 0$ for all $i = 1, 2, \ldots, n$.

Then, the matrix BR, where $B = diag(1/\rho_{11}, 1/\rho_{22}, \ldots, 1/\rho_{nn})$, is negative semi-definite, ρ_{ij} are some co-factors.

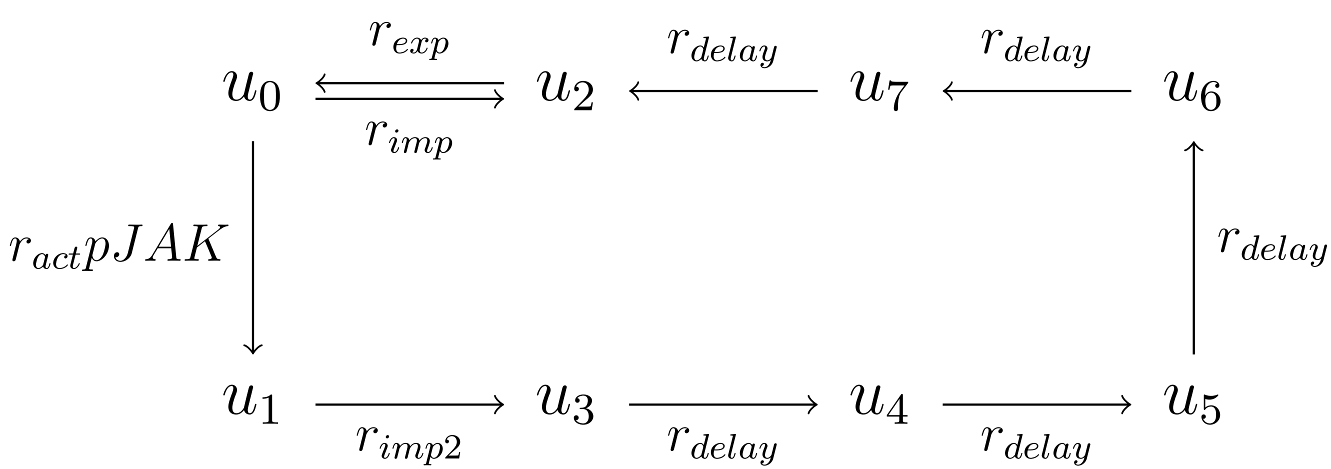
BR has n eigenvalues $0 = \lambda_1 > \lambda_2 \geq \lambda_3 \geq \ldots \lambda_n$.

Interpretation: B transforms to relative entropy!

Systems of Reaction-Diffusion Equations

Network of Reversible Linear Reactions

Friedmann-Neumann-Rannacher model[a]



Yes, if assume that reactions occur only within one domain

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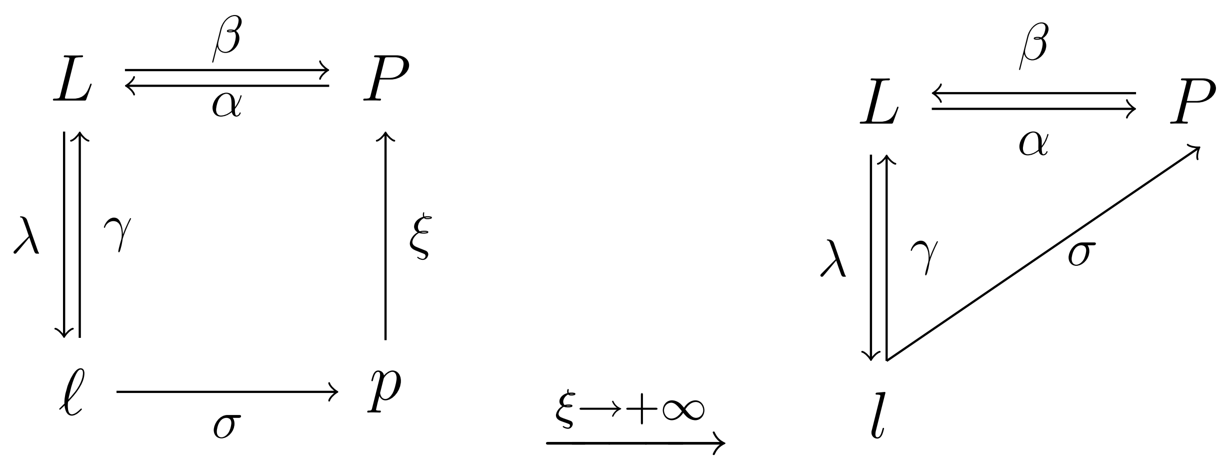
[a] E. Friedmann, R. Neumann, R. Rannacher, *Well-posedness of a linear spatio-temporal model of the JAK2/STAT5 signaling pathway*, Comm. Math. Anal. 15 (2013) 76-102.

Quasi-steady-state approximation

QSSA as $\xi \to +\infty$

Fast expulsion limit $\xi \to +\infty$:



Convergence towards reduced QSSA[a]

Proof: ideas from duality method and entropy dissipation.

[a] [T.Q.Bao, K.F., S. Rosenberger]

Nonlinear Boundary Model

Toy model system

Volume-concentrations $u(x,t)$, Surface-concentration $v(x,t)$

Nonlinear Robin-type boundary condition and matching reversible reaction source term on $\Gamma = \partial\Omega$

$$(\text{NBV}) \qquad \begin{cases} u_t - \delta_u \Delta u = 0, & x \in \Omega, t \geq 0, \\ \delta_u \frac{\partial u}{\partial \nu} = -\alpha(k_u u^\alpha - k_v v^\beta), & x \in \Gamma, t \geq 0, \\ v_t - \delta_v \Delta_\Gamma v = \beta(k_u u^\alpha - k_v v^\beta), & x \in \Gamma, t \geq 0, \\ u(0,x) = u_0(x) \geq 0, & x \in \Omega, \\ v(0,x) = v_0(x) \geq 0, & x \in \Gamma \end{cases}$$

Stoichiometric coefficients $\alpha, \beta \in [1, +\infty)$

Reaction rates $k_u(t,x), k_v(t,x)$

Nonlinear Boundary Model

Model properties

Mass conservation law

$$M = \beta \int_\Omega u(t,x)\,dx + \alpha \int_\Gamma v(t,x)\,dS, \qquad \forall t \geq 0.$$

The unique equilibrium (u_∞, v_∞) balances the reaction,

$$u_\infty^\alpha = v_\infty^\beta,$$

and satisfies the mass conservation

$$\beta|\Omega|u_\infty + \alpha|\Gamma|v_\infty = M.$$

Uniqueness from monotonicity of $u_\infty^\alpha = \left(\frac{M}{\alpha|\Gamma|} - \frac{\beta|\Omega}{\alpha|\Gamma|}|u_\infty)\right)^\beta$

Exponential Convergence to Equilibrium

Entropy and entropy dissipation

Entropy functional:

$$E(u,v) = \int_\Omega u(\log u - 1)dx + \int_\Gamma v(\log v - 1)dS$$

Entropy dissipation:

$$\begin{aligned} D(u,v) &= -\frac{d}{dt}E(u,v) \\ &= \delta_u \int_\Omega \frac{|\nabla u|^2}{u}dx + \delta_v \int_\Gamma \frac{|\nabla_\Gamma v|^2}{v}dS \\ &\quad + \int_\Gamma (v^\beta - u^\alpha)\log\frac{v^\beta}{u^\alpha}\,dS \geq 0 \end{aligned}$$

Two cases: non-degenerate $\delta_v > 0$ and degenerate $\delta_v = 0$.

Exponential Convergence to Equilibrium

Explicit exponential convergence to equilibrium

Theorem:

Assume $\Omega \subset \mathbb{R}^n$ with smooth boundary $\Gamma = \partial\Omega$.
Assume initial data $(u_0, v_0) \in L^\infty(\Omega) \times L^\infty(\Gamma)$.

Then, the global bounded solution (u, v) satisfies the following exponential convergence to equilibrium

$$\|u(t) - u_\infty\|_{L^1(\Omega)}^2 + \|v(t) - v_\infty\|_{L^1(\Gamma)}^2 \leq C_1 e^{-C_0 t} \left(E(u_0, v_0) - E(u_\infty, v_\infty)\right),$$

where the constants $C_0 > 0, C_1 > 0$ depending on α, β, Ω and the initial mass $M = \beta \int_\Omega u_0 dx + \alpha \int_\Gamma v_0 dS$.

Exponential Convergence to Equilibrium

Entropy entropy dissipation estimate

For all functions $u : \Omega \to \mathbb{R}_+$ and $v : \Omega \to \mathbb{R}_+$ satisfying mass conservation

$$\beta \int_\Omega u\,dx + \alpha \int_\Gamma v\,dS = M,$$

there exists $C_0 > 0$ such that

$$D(u,v) \geq C_0\,(E(u,v) - E(u_\infty, v_\infty))$$

Proof for two cases:

non-degenerate boundary diffusion $\delta_v > 0$

degenerate boundary diffusion $\delta_v = 0$: need L^∞-bounds

Conclusions and Open Problems

Towards bright sun and white snow for RD models

- Good existence theory in 2D for quadratic nonlinearities
- Higher dimensions?
- Algebraic Structure of Networks
- How to combine entropy and duality method?

THANK YOU VERY MUCH!!

References

J. A. Cañizo, L. Desvillettes, K. F., *Improved duality estimates and applications to reaction-diffusion equations*, to appear in CPDE

L. Desvillettes, K. F., M. Pierre, J. Vovelle, *About Global Existence for Quadratic Systems of Reaction-Diffusion*, J. Advanced Nonlinear Studies, **7** no. 3 (2007) pp. 491–511.

L. Desvillettes, K. F., *Entropy Methods for Reaction-Diffusion Equations: Slowly Growing A-priori Bounds*, Revista Matemática Iberoamericana, **24** no. 2 (2008) pp. 407–431.

T. Goudon, A. Vasseur. *Regularity analysis for systems of reaction- diffusion equations*, Ann. Sci. Ec. Norm. Super., (4) **43** no. 1 (2010) pp. 117–141.

M. Pierre, *Weak solutions and supersolutions in L^1 for reaction-diffusion systems*, J. Evol. Equ., **3**, no. 1 (2003) 153–168.