

# ***Entropy- and Duality Methods for Dissipative PDE Models***

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# Entropy Methods in non-linear PDEs

## Introduction

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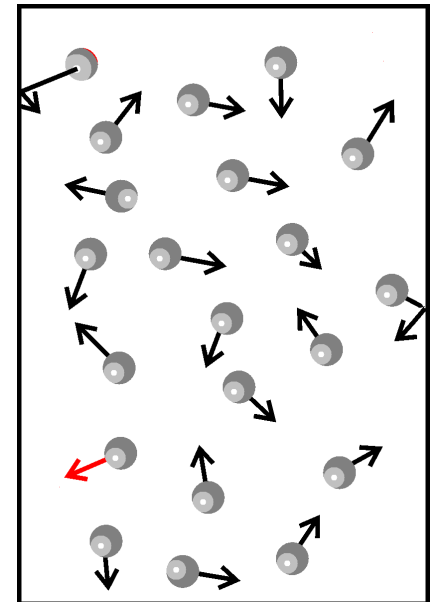
The Boltzmann's equation of gas dynamics describes the evolution of a phase-space density  $f(t, x, v)$  (time  $t \geq 0$ , position  $x \in \mathbb{R}^3$ , velocity  $v \in \mathbb{R}^3$ )

$$\partial_t f + v \cdot \nabla_x f = Q(f, f)$$

Boltzmann's H-theorem:  $H = \int_{\mathbb{R}^3} f \log(f) dv$

$$\frac{d}{dt} \int_{\mathbb{R}^3} H(f(t)) dx = \int_{\mathbb{R}^3} Q(f, f) \log(f) dv \leq 0$$

Lyapunov functional  $\Rightarrow$  irreversibility



# Entropy Methods in non-linear PDEs

## Overview

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More precisely: Entropy and Entropy Dissipation functional<sup>a</sup>

$$\frac{d}{dt} \int_{\mathbb{R}^3} H(f(t)) dx = - \int_{\mathbb{R}^3} D(f(t)) dx \leq 0$$

How to use such an entropy structure in the best possible way in the quantitative analysis of

- Reaction-Diffusion Systems
- Coagulation-Fragmentation Models

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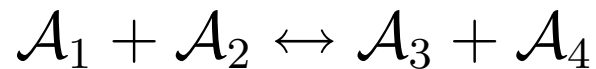
<sup>a</sup>e.g. [DiPerna, Lions, 1988], [Desvillettes, Villani, 2005]

# Reaction-Diffusion Systems

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

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



- 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  $d_i > 0$

$$\partial_t a_1 - d_1 \Delta_x a_1 = -a_1 a_2 + a_3 a_4$$

$$\partial_t a_2 - d_2 \Delta_x a_2 = -a_1 a_2 + a_3 a_4$$

$$\partial_t a_3 - d_3 \Delta_x a_3 = +a_1 a_2 - a_3 a_4$$

$$\partial_t a_4 - d_4 \Delta_x a_4 = +a_1 a_2 - a_3 a_4$$

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

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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

# Equilibrium and Entropy Dissipation

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

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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 of dissipative PDEs

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

$D(f)$  entropy dissipation,  $f_\infty$  entropy minimising equilibrium

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



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

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

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

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

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$\Rightarrow$  convergence in  $L_1$  :  $\|f - f_\infty\|_1^2 \leq C(E(f) - E(f_\infty))$

**Csiszár-Kullback-Pinsker** inequalities of convex entropies

# *The Entropy Method*

## My Personal Entropy Method Dictionary

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- **Understanding** Entropy-Dissipation Structure  $\iff$   
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  $\iff$  **Optimal**  
Rate/Constant in EED Estimate

# Entropy Entropy-Dissipation Estimate

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

---

Theorem:<sup>a</sup> 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  $E(a_i|a_{i,\infty}) = E(a_i|\bar{a}_i) + E(\bar{a}_i|a_{i,\infty})$

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

+ Long long calculations + Conservation laws!

⇒ obtain Functional Inequality      Not sharp!

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<sup>a</sup> [L. Desvillettes, K.F.]

# Entropy Entropy-Dissipation Estimate

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

---

Entropy Entropy-Dissipation Estimate

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

+ Gronwall argument + Csiszár-Kullback inequality

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

As long as suitable solutions exist?

# Entropy A-priori Estimates

## Entropy decay

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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

---

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

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

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

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

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

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

$\Rightarrow$  **global weak (super-)solutions** [M. Pierre 2003]<sup>a</sup>

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<sup>a</sup>[Desvillettes F. Pierre Vovelle]



# Entropy A-priori Estimates

## Entropy decay

---

$$H(T) : \left\{ \begin{array}{l} a_i \in L^\infty([0, +\infty); L \log L(\Omega)) \quad \forall i = 1, \dots, 4 \\ \int_0^T D(s) : \left\{ \begin{array}{l} \sqrt{a_i} \in L^2([0, +\infty); H^1(\Omega)) \quad \forall i = 1, \dots, 4 : d_i > 0 \\ \int_0^T \int_\Omega (a_1 a_2 - a_3 a_4) \ln \left( \frac{a_1 a_2}{a_3 a_4} \right) dx dt \leq C \end{array} \right. \end{array} \right.$$

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

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

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<sup>a</sup>[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  $z_i = a_i \ln(a_i) - a_i \Rightarrow H(a_i) = \int_{\Omega} \sum_{i=1}^4 z_i dx$

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

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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

## A duality argument

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

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

Dual problem (inhomogeneous),  $Q_T = (0, T) \times \Omega$

$$-(w_t + M \Delta w) = \psi \in C_0^\infty(Q_T), \quad w(T) = 0, \quad n \cdot \nabla_x w \text{ on } \partial\Omega$$

one can show  $\int_{Q_T} z \psi \leq \int_{\Omega} z(0) w(0) \leq C_T \|z(0)\|_{L^2} \|\psi\|_{L^2(Q_T)}$

$$\forall \psi \geq 0 \quad \Rightarrow \quad \|z\|_{L^2(Q_T)} \leq C_T \|z(0)\|_{L^2(\Omega)}$$

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<sup>a</sup>[Pierre, Schmidt, 2000]

# Duality Argument for Entropy Density

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

---

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

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

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!!<sup>a</sup>

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<sup>a</sup>[Desvillettes, F., Pierre, Vovelle, Adv. Nonlinear Stud. 2007]

# 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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Degenerate Diffusion: Enhanced entropy duality argument for

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

proves  $\left( \sum_{i=1}^k z_i \right) \left( \sum_{i=1}^k d_i z_i \right) \in L^1([0, T] \times \Omega)$ <sup>a</sup>

if  $d_i(x) = 0$ , but  $\sum_{i=1}^4 d_i \geq d_0 > 0$  and  $\nabla_x \sqrt{d_i} \in L^\infty(Q_T)$

$\Rightarrow$  still global weak solutions in all space dimensions!

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<sup>a</sup>[Desvillettes, F., Pierre, Vovelle, Adv. Nonlinear Stud. 2007]

# Duality Argument for Entropy Density

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

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

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

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

# Improved Duality Argument

## An improved duality argument

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

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

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

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

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

where  $D_{a,b,p'} := \frac{C_{\frac{a+b}{2}, p'}}{1 - C_{\frac{a+b}{2}, p'} \frac{b-a}{2}}$  as long as  $C_{\frac{a+b}{2}, p'} \frac{b-a}{2} < 1$ .<sup>a</sup>

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<sup>a</sup>[Cañizo Desvillettes F., CPDE]



# Improved Duality Argument

## Maximal regularity for dual problem

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For  $m > 0$  and  $p' \in (1, 2)$ , the constant  $C_{m,p'} > 0$  is the best parabolic regularity constant in

$$\|\Delta_x v\|_{L^{p'}(\Omega_T)} \leq C_{m,p'} \|f\|_{L^{p'}(\Omega_T)},$$

where  $v : [0, T] \times \Omega \rightarrow \mathbb{R}$  solves the backward heat equation

$$\begin{cases} \partial_t v + m \Delta_x v = f & \text{on } \Omega_T, \\ v(T, x) = 0 & \text{for } x \in \Omega, \\ \nabla_x v \cdot \nu(x) = 0 & \text{on } [0, T] \times \partial\Omega. \end{cases}$$

Note that  $C_{m,p'} = C_{m,p'}(\Omega, N) < \infty$  does not depend on  $T$ .

In particular  $C_{m,2} \leq \frac{1}{m}$ .

# Improved Duality Argument

## Meyer's type argument

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We take  $m := (a + b)/2$  and rewrite

$$\partial_t v + m \Delta_x v = (m - M) \Delta_x v + f.$$

Then, from the above estimate, we get with  $\|m - M\|_\infty \leq \frac{b-a}{2}$

$$\|\Delta_x v\|_{L^{p'}(\Omega_T)} \leq C_{m,p'} \left( \frac{b-a}{2} \|\Delta_x v\|_{L^{p'}(\Omega_T)} + \|f\|_{L^{p'}(\Omega_T)} \right).$$

Thus,  $\|\Delta_x v\|_{L^{p'}(\Omega_T)} \leq C \|f\|_{L^{p'}(\Omega_T)}$  provided  $C_{m,p'} \frac{b-a}{2} < 1$ .

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

where  $D_{a,b,p'} := \frac{C_{\frac{a+b}{2},p'}}{1 - C_{\frac{a+b}{2},p'} \frac{b-a}{2}}$  provided  $C_{\frac{a+b}{2},p'} \frac{b-a}{2} < 1$ <sup>a</sup>

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<sup>a</sup>[Cañizo Desvillettes F., CPDE]

# Summary

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

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- 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  $L^p$ ,  $1 \leq p < 2$ .  
Blow-up example [M. Pierre D. Schmidt]

# Towards optimal constants/rates?

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

---

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

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

$\Rightarrow$  Rescaled linearised system

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

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

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

## 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

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

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

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

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

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

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

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  $\alpha\mathcal{A} \leftrightarrow \beta\mathcal{B}$

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Optimal constant in Entropy Entropy-Dissipation Estimate<sup>a</sup>

$$I = \min_{\substack{\beta\bar{u} + \alpha\bar{v} = 0, \\ u, v \in C^\infty}} \left\{ \frac{d_a \int_{\Omega} |\nabla u|^2 + d_b \int_{\Omega} |\nabla v|^2 dx + \int_{\Omega} (\alpha u - \beta v)^2 dx}{\int_{\Omega} u^2 + v^2} \right\}$$
$$= \min_{c^0=0} \left\{ \frac{\sum_{k=0}^{\infty} |\mu_1(k)| (c^k)^2 + |\mu_2(k)| (d^k)^2}{\sum_{k=0}^{\infty} (c^k)^2 + (d^k)^2} \right\} \geq \min\{|\mu_1(1)|, |\mu_2(0)|\}$$

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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<sup>a</sup>[G. Pissante, E. Latos, K. F.]

# Coagulation-fragmentation models with diffusion

## Background

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The **Formation** and the **Break-up** of **Clusters/Polymers**



assume particles fully described by **mass/size**  $y \in Y$ .

full/realistic models can quickly get very difficult



# Introduction

## Coagulation-fragmentation models with diffusion

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evolution of a polymer/cluster density  $f(t, x, y) \geq 0$

$$\partial_t f - d(y) \Delta_x f = Q_{coag}(f, f) + Q_{frag}(f)$$

time  $t \geq 0$ , space  $x \in \Omega$  normalised with  $|\Omega| = 1$

size-dependent diffusion coefficients  $d(y)$ ,  $y$  measures size

homogeneous Neumann B.C.  $\nabla_x f(t, x, y) \cdot \nu(x) = 0$  on  $\partial\Omega$

non-negative initial data  $f_0(x, y) \geq 0$

# Continuous coagulation-fragmentation models

## inhomogeneous CF with constant kernel

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Continuous in size density  $f(t, x, y)$  with  $y \in [0, \infty)$

$$\begin{aligned} \partial_t f - d(y) \Delta_x f &= \int_0^y f(y - y') f(y') dy' - 2f(y) \int_0^\infty f(y') dy' \\ &\quad + 2 \int_y^\infty f(y') dy' - y f(y) \end{aligned}$$

homogeneous Neumann, non-negative initial density  $f_0(x, y)$

diffusion may **degenerate at most linearly for large sizes**

$$d(y) \leq d^*(\delta), \quad \forall y \in [\delta, \delta^{-1}], \quad 0 < \frac{d_*}{1 + y} \leq d(y), \quad \forall y \in [0, \infty).$$

[LM 2002] global existence of weak, solutions

# *inhomogeneous CF with constant kernel*

## Macroscopic densities

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amount of monomers  $N$ , number density  $M$

$$N = \int_0^{\infty} y' f(y') dy' , \quad M = \int_0^{\infty} f(y') dy'$$

conservation of the total mass

$$\partial_t N - \Delta_x \left( \int_0^{\infty} y' d(y') f(y') dy' \right) = 0$$

$$\partial_t M - \Delta_x \left( \int_0^{\infty} d(y') f(y') dy' \right) = N - M^2$$

# *inhomogeneous CF with constant kernel*

## Entropy (free energy functional)

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Entropy

$$H(f)(t, x) = \int_0^\infty (f \ln f - f) dy,$$

Entropy dissipation

$$\frac{d}{dt} \int_{\Omega} H(f) dx = -D_H(f)$$

$$D_H(f) = \int_{\Omega} \int_0^\infty d(y) \frac{|\nabla_x f|^2}{f} dy dx \\ + \int_{\Omega} \int_0^\infty \int_0^\infty (f'' - f f') \ln \left( \frac{f''}{f f'} \right) dy dy' dx$$

# *inhomogeneous CF with constant kernel*

## Inequality by [Aizenman, Bak]'79

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$$\int_0^\infty \int_0^\infty (f(y+y') - f(y)f(y')) \ln \left( \frac{f(y+y')}{f(y)f(y')} \right) dy dy' \geq$$
$$M H(f|f_N) + 2(M - \sqrt{N})^2$$

Entropy dissipation

$$D_H(f) \geq \int_\Omega \int_0^\infty d(y) \frac{|\nabla_x f|^2}{f} dy dx$$
$$+ M H(f|f_N) + 2(M - \sqrt{N})^2$$

# *inhomogeneous CF with constant kernel*

## Local and global equilibria

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Intermediate equilibria with the moments  $N$  and  $M = \sqrt{N}$

$$f_N = e^{-\frac{1}{\sqrt{N}}y}$$

the global equilibrium

$$f_\infty = e^{-\frac{y}{\sqrt{N_\infty}}}$$

- is constant in  $x$  satisfying  $M_\infty^2 = N_\infty$
- preserves the initial mass  $N_\infty = \int_0^\infty N(x) dx$

# *inhomogeneous CF with constant kernel*

## relative entropy, additivity

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relative entropy

$$H(f|g) = H(f) - H(g)$$

additivity

$$H(f|f_\infty) = H(f|f_N) + H(f_N|f_\infty)$$

$f_N$  and  $f_\infty$  do not need to have the same  $L_y^1$ -norm, but nevertheless

$$\int_{\Omega} H(f_N|f_\infty) dx = 2 \left( \sqrt{\int_{\Omega} N dx} - \int_{\Omega} \sqrt{N} dx \right) \geq 0$$

# *inhomogeneous CF with constant kernel*

## Theorem

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Nonnegative initial data  $(1 + y + \ln f_0)f_0 \in L^1((0, 1) \times (0, \infty))$   
with positive initial mass  $\int_0^1 N_0(x) dx = N_\infty > 0$  on  $\Omega = (0, 1)$ .  
**At most linearly degenerating** diffusion coefficients.

Then, for  $\beta < 2$  and  $t > 0$

$$\|f(t, \cdot, \cdot) - f_\infty\|_{L^1_{x,y}} \leq C_\beta e^{-(\ln t)^\beta},$$

and

$$\int_0^\infty (1 + y)^q \|f(t, \cdot, y) - f_\infty(y)\|_{L^\infty_x} dy \leq C_{\beta,q} e^{-(\ln t)^\beta},$$

for all  $t \geq t_* > 0$ .



# *inhomogeneous CF with constant kernel*

## Entropy Entropy-Dissipation Estimate

Let  $f := f(x, y) \geq 0$  be measurable with moments

$$0 < \mathcal{M}_* \leq M(x) = \int_0^\infty f(x, y) dy \leq \|M\|_{L_x^\infty},$$

$$0 < N_\infty = \int_\Omega \int_0^\infty y f(x, y) dy dx, \int_\Omega \int_0^\infty y^{2p} f(x, y) dx dy \leq \mathcal{M}_{2p}.$$

Then, for all  $A \geq 1$  and  $p > 1$

$$D_1(f) \geq \frac{C}{A \|M\|_{L_x^\infty}} \int_\Omega H(f|f_\infty) dx - C \frac{\mathcal{M}_{2p}}{A^{2p+1}},$$

with a constant  $C = C(\mathcal{M}_*, N_\infty, d_*, P(\Omega))$  depending only on  $\mathcal{M}_*$ ,  $N_\infty$ ,  $d_*$ , and the Poincaré constant  $P(\Omega)$ .

# *Proof of Theorem*

**Algebraic rate for all  $p > 1$**

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**Algebraic rate for all  $p > 1$**

We have for any  $A > 1$

$$\frac{d}{dt} \int_0^1 H(f|f_\infty) dx \leq -\frac{C}{\|M\|_{L_x^\infty}} \frac{1}{A} \int_0^1 H(f|f_\infty) dx + \frac{C_p 2^{8p^2}}{A^{2p+1}},$$

where  $\|M\|_{L_x^\infty}(t) \leq m_\infty + m_2(t)$ .

balance r.h.s. by choosing  $A = A(t) > 2$  as

$$\frac{1}{A} \leq C_3^{-1/2} \left( \frac{C_4 \int_0^1 H(f|f_\infty) dx}{\|M\|_{L_x^\infty} 2^{8p^2}} \right)^{\frac{1}{2p}},$$

Thus, Gronwall yields algebraic rate for all  $p > 1$ .

# *Proof of Theorem*

**Algebraic rate for all  $p > 1$**

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**Faster than polynomial rate**

Then, by summing w.r.t.  $p \in \mathbb{N}$

$$\int_0^1 H(f(t)|f_\infty) dx \leq L(t - C_7),$$

where (for all  $1 < \alpha < 2$ )

$$\begin{aligned} L^{-1}(t) &= \sum_{q \geq 1, \text{ even}} \frac{t^q}{(C_{10} q)^q 2^{2q^2}} = \sum_{q \geq 1, \text{ even}} t^q e^{-2q^2 \ln 2 - q \ln(q C_{10})} \\ &\geq C(\alpha) e^{[\ln^2(\alpha-1)(t)]} \end{aligned}$$

for all  $t$  large enough and  $1 < \alpha < 2$ .

# *Proof of Entropy Entropy-Dissipation Estimate*

**needs**  $\|M\|_{L_x^\infty}$ ,  $\|M\|_{L_t^\infty(L_x^1)}$ ,  $\mathcal{M}_* > 0$

---

## **Step 1) Additivity**

$$\int_0^1 H(f|f_\infty) dx = \int_0^1 H(f|f_N) dx + 2 \left( \sqrt{\overline{N}} - \overline{\sqrt{N}} \right)$$

# *Proof of Entropy Entropy-Dissipation Estimate*

**needs**  $\|M\|_{L_x^\infty}$ ,  $\|M\|_{L_t^\infty(L_x^1)}$ ,  $\mathcal{M}_* > 0$

---

**Step 2) "Reacting" Moments  $N$  and  $M$**

$$\int_0^1 H(f|f_\infty) dx = \int_0^1 H(f|f_N) dx + 2 \left( \sqrt{\overline{N}} - \overline{\sqrt{N}} \right)$$

$$\sqrt{\overline{M_1}} - \overline{\sqrt{M_1}} \leq \frac{2}{\sqrt{N_\infty}} \left[ \|M - \sqrt{M_1}\|_{L_x^2}^2 + \|M - \overline{M}\|_{L_x^2}^2 \right].$$

# *Proof of Entropy Entropy-Dissipation Estimate*

**needs**  $\|M\|_{L_x^\infty}$ ,  $\|M\|_{L_t^\infty(L_x^1)}$ ,  $\mathcal{M}_* > 0$

---

**Step 2) "Reacting" Moments  $N$  and  $M > \mathcal{M}_* > 0$**

$$\begin{aligned} \int_0^1 H(f|f_\infty) dx &\leq C \left[ \int_0^1 M H(f|f_N) dx + 2\|M - \sqrt{M_1}\|_{L_x^2}^2 \right] \\ &\quad + \frac{4}{\sqrt{N_\infty}} \|M - \overline{M}\|_{L_x^2}^2 \\ &\leq C \int_0^1 \int_0^\infty \int_0^\infty (f'' - f f') \ln \left( \frac{f''}{f f'} \right) dy dy' dx \\ &\quad + \frac{4}{\sqrt{N_\infty}} \|M - \overline{M}\|_{L_x^2}^2, \end{aligned}$$

# Proof of Entropy Entropy-Dissipation Estimate

needs  $\|M\|_{L_x^\infty}$ ,  $\|M\|_{L_t^\infty(L_x^1)}$ ,  $\mathcal{M}_* > 0$

---

**Step 3) Diffusion** For a cut-off size  $A > 0$ , denote

$$M_A(t, x) := \int_0^A f(t, x, y) dy \text{ and } M_A^c(t, x) := \int_A^\infty f(t, x, y) dy$$

$$\begin{aligned} \|M - \overline{M}\|_{L_x^2}^2 &= \int_{\Omega} (M_A - \overline{M}_A + M_A^c - \overline{M}_A^c)^2 dx \\ &\leq 2\|M_A - \overline{M}_A\|_{L_x^2}^2 + \frac{4}{A^{2p}} \int_{\Omega} \left( \int_0^\infty y^p f(y) dy \right)^2 dx \\ &\leq C(P, d_*) A \|M\|_{L_x^\infty} \int_{\Omega} \int_0^\infty d(y) \frac{|\nabla_x f|^2}{f} dy dx \\ &\quad + \frac{4}{A^{2p}} \|M\|_{L_x^\infty} \mathcal{M}_{2p} \end{aligned}$$

for any  $p > 1$ .

# *Proof of Entropy Entropy-Dissipation Estimate*

**needs**  $\|M\|_{L_x^\infty}$ ,  $\|M\|_{L_t^\infty(L_x^1)}$ ,  $\mathcal{M}_* > 0$

---

## **Entropy Entropy Dissipation Estimate**

Let  $f := f(x, y) \geq 0$  be measurable with moments

$$0 < \mathcal{M}_* \leq M(x) = \int_0^\infty f(x, y) dy \leq \|M\|_{L_x^\infty},$$

$$0 < N_\infty = \int_\Omega \int_0^\infty y f(x, y) dy dx, \int_\Omega \int_0^\infty y^{2p} f(x, y) dx dy \leq \mathcal{M}_{2p}.$$

Then, for all  $A \geq 1$  and  $p > 1$

$$D_1(f) \geq \frac{C}{A \|M\|_{L_x^\infty}} \int_\Omega H(f|f_\infty) dx - C \frac{\mathcal{M}_{2p}}{A^{2p+1}}, \quad (1)$$

with a constant  $C = C(\mathcal{M}_*, N_\infty, d_*, P(\Omega))$  depending only on  $\mathcal{M}_*$ ,  $N_\infty$ ,  $d_*$ , and the Poincaré constant  $P(\Omega)$ .



# *Conclusions and Open Problems*

## **Entropy- and Duality Methods for PDE models**

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- Good existence theory higher nonlinearities?
- Higher dimensions?
- Algebraic Structure of Reaction Networks?
- How to combine entropy and duality method?

THANK YOU VERY MUCH!!

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