Global solutions to quadratic systems of stochastic reaction-diffusion equations in space-dimension two

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Plan of the talk

1. Modelling of chemical reactions
2. Stochastic system of reaction-diffusion equations
3. Some elementary facts
4. Main result and main steps of the proof

Modelling of chemical reactions

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Related Questions:

1. Justify the limit $N \to +\infty$: [Ethier-Kurtz 1986], [Oelschläger 1989], [Lim, Lu, Nolen 2020].

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jump process on a family of N particles.

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(in most cases, limit N large of the probabilistic modelling) systems of ODEs/ system of reaction-diffusion equations (PDEs) if displacement is taken into account.

Related Questions:

1. Justify the limit $N \to +\infty$: [Ethier-Kurtz 1986], [Oelschläger 1989], [Lim, Lu, Nolen 2020].
2. Study the system of reaction-diffusion equations, in particular: impact of the structure of the system on the existence of global weak/classical solutions (and subsequently, large-time behaviour). [...], [Survey M. Pierre 2010].

Modelling of chemical reactions: second-order approximation

Consider the binary reversible chemical reaction

$$A_1 + A_3 \rightleftharpoons A_2 + A_4.$$

Each reaction happens at a random exponential time, with rates

$$r_{\rightarrow} = \lambda_{\rightarrow} \frac{1}{N} N_1 N_3, \quad r_{\leftarrow} = \lambda_{\leftarrow} \frac{1}{N} N_2 N_4,$$

where N is the total number of reactants and N_i the number of molecules of type i.

Modelling of chemical reactions: second-order approximation

Generator $\mathscr{L}_N$ of the rescaled process $A_N(t) = (N_i(t)/N)_{1 \le i \le 4}$:

$$\mathscr{L}_N \varphi(a) = \sum_{\ell} N \eta_\ell(a) \left[\varphi(a + \ell/N) - \varphi(a) \right],$$

where $a \in \mathbb{R}^4$,

$$\ell_{\rightarrow} = (-1, 1, -1, 1), \quad \ell_{\leftarrow} = -\ell_{\rightarrow},$$

and (with $\lambda_{\rightarrow} = \lambda_{\leftarrow} = 1$)

$$\eta_{\ell_{\rightarrow}}(a) = a_1 a_3, \quad \eta_{\ell_{\leftarrow}}(a) = a_2 a_4.$$

Modelling of chemical reactions: second-order approximation

Expand $\mathscr{L}_N$:

$$\mathscr{L}_N \varphi(a) = f(a) \cdot D_a \varphi(a) + \frac{1}{N} \sum_{\ell} \eta_\ell(a) \ell \ell^* : D_a^2 \varphi(a) + \mathcal{O}\left(\frac{1}{N^2}\right),$$

where

$$f(a) = \sum_{\ell} \ell \eta_\ell(a), \quad A : B = \sum_{i,j} A_{ij} B_{ij}.$$

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At first order:

$$\mathscr{L} \varphi(a) = f(a) \cdot D_a \varphi(a)$$

is the generator associated to the ODE

$$\frac{da}{dt} = f(a).$$

Modelling of chemical reactions: second-order approximation

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where

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At second order (diffusion-approximation):

$$\mathscr{L} \varphi(a) = f(a) \cdot D_a \varphi(a) + \frac{1}{N} \sum_\ell \eta_\ell(a) \ell \ell^* : D_a^2 \varphi(a)$$

is the generator associated to the SDE

$$da = f(a) dt + \sqrt{\frac{2}{N}} \sum_\ell \ell \sqrt{\eta_\ell(a(t))} dB_\ell(t),$$

where the $(B_\ell)_\ell$ are independent one-dimensional Wiener processes.

Soon to come

Stochastic system of reaction-diffusion equations

Stochastic system of reaction-diffusion equations

On the torus $\mathbb{T}^d$, we consider the system

$$da_i - \operatorname{div}(\kappa_i \nabla a_i)\, dt = f_i(a)dt + \sqrt{\nu}\sigma_i^\alpha(a)dB_\alpha(t),$$

with initial data

$$a_i(0) = a_{i0}, \quad a_{i0} \colon \mathbb{T}^d \to \mathbb{R}_+,$$

for $i = 1, \ldots, 4$, where

$$f_i(a) = (-1)^i (a_1 a_3 - a_2 a_4).$$

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The diffusion coefficients κ_i are positive constants, ν is a small constant (remember the factor N^{-1} in the second-order expansion).

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System

$$da_i - \mathrm{div}\,(\kappa_i \nabla a_i)\,dt = f_i(a)dt + \sqrt{\nu}\sigma_i^{\alpha}(a)dB_{\alpha}(t).$$

Finite number of independent one-dimensional Wiener processes $\{B_{\alpha}; 1 \leq \alpha \leq d_W\}$.

Stochastic system of reaction-diffusion equations

Coefficients $\sigma_i^\alpha(a)$ of the type

$$\sigma_i^1(a) = (-1)^i \sqrt{a_1 a_3}, \quad \sigma_i^2(a) = (-1)^i \sqrt{a_2 a_4}, \quad \sigma_i^\alpha = 0,\ \forall \alpha \geq 3.$$

However, we need the cancellation condition

$$a_i = 0 \Rightarrow \sigma_i^\alpha(a) = 0,\ \forall i, \alpha \tag{1}$$

to ensure that the solutions stay non-negative, so asymptotic structure only: for $\alpha \in \mathbb{N} \setminus \{0\}$, $\sigma_i^\alpha \colon \mathbb{R}^d \to \mathbb{R}$ is a smooth function satisfying (1) and the growth condition

$$\forall i,\ \sum_\alpha |\sigma_i^\alpha(a)|^2 \leq (a_1 a_3 + a_2 a_4). \tag{2}$$

Global existence of regular solutions

Suppose that the initial data a_{i0} are smooth: $a_{i0} \in C^\infty(\mathbb{T}^d)$.

Central question: does the system

$$da_i - \operatorname{div}(\kappa_i \nabla a_i)\, dt = f_i(a)dt + \sqrt{\nu}\sigma_i^\alpha(a) dB_\alpha(t),$$

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admit global smooth solutions?

This question is related to the following topics:

1. Global existence for deterministic systems of reaction-diffusion equations,
2. Maximum principle, L^∞-estimates for parabolic scalar equations.

Global existence of smooth solutions for the (deterministic) four-species quadratic reaction-diffusion system

A variety of approaches:

1. De Giorgi's iteration scheme, based on truncation of the entropy [Goudon, Vasseur 2010, d=1,2], [Caputo, Goudon, Vasseur, 2017].
2. Maximum principle, gain of regularity in parabolic equations, interpolation [Kanel 1990], [Souplet 2018], [Fellner, Morgan, Tang, 2020][3].

[3] does not use the entropic structure

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L^∞-estimates in parabolic SPDEs

Here also, there is a variety of approaches

1. De Giorgi's iteration scheme [Dareiotis, Gerencsér, 2017], [Hsu, Wang, Wang, 2017], [Qiu, 2020],
2. Moser's approach by iterative estimates on the L^p-norms [Denis, Matoussi, Stoica, 2005], [Wang, 2018], [Dareiotis, Gess, 2019],
3. in [Debussche, de Moor, Hofmanová, 2015], the "Da Prato - Debussche" trick is used, and estimates separately given on the stochastic convolution and deterministic parabolic equations (the latter exploiting in particular the theory [Ladyženskaja, Solonnikov, Ural′ceva, 1968], where truncations as in De Giorgi's approach are used at some point).
4. Duality and Boccardo-Gallouët estimates [Leocata, Vovelle, 2023].

Some elementary facts

(on the deterministic system)

Some elementary facts

Case of equal diffusions: $\kappa_i = \kappa$ for all i

Add up the four equations

$$\partial_t a_i - \kappa \Delta a_i = (-1)^i (a_1 a_3 - a_2 a_4), \quad 1 \leq i \leq 4,$$

to obtain

$$\partial_t z - \kappa \Delta z = 0 \quad z = \sum_{i=1}^{4} a_i.$$

Maximum principle on z and $a_i \geq 0$ imply the uniform bound $\|a_i(t)\|_{L^\infty(\mathbb{T}^d)} \lesssim 1$.

Some elementary facts

Conservation of mass

Add up the four equations

$$\partial_t a_i - \mathrm{div}(\kappa_i \nabla a_i) = (-1)^i (a_1 a_3 - a_2 a_4),$$

to obtain

$$\partial_t z - \Delta(Kz) = 0 \quad z = \sum_{i=1}^{4} a_i, \quad K = \sum_{i=1}^{4} \frac{a_i}{z} \kappa_i.$$

In particular,

$$\int_{\mathbb{T}^d} z(x,t)dt = \int_{\mathbb{T}^d} z(x,0)dx,$$

for all t.

Some elementary facts

Entropy estimate

Multiply each equation

$$\partial_t a_i - \operatorname{div}(\kappa_i \nabla a_i) = (-1)^i (a_1 a_3 - a_2 a_4),$$

by $\log(a_i)$ and sum up the result to obtain (after integration):

$$\int_{\mathbb{T}^d} \mathcal{H}(a)(t)dx + \iint_{Q_t} \sum_{i=1}^{4} \kappa_i \frac{|\nabla a_i|^2}{a_i} dxds$$

$$= \int_{\mathbb{T}^d} \mathcal{H}(a)(0)dx - \iint_{Q_t} \sum_{i=1}^{4} (a_1 a_3 - a_2 a_4)(\log(a_1 a_3) - \log(a_2 a_4))dxds,$$

where $\mathcal{H}(a) := \sum_{i=1}^{4} (a_i \log(a_i) - a_i + 1) \geq 0$.

Sooner to come

Main result and main steps of the proof

Main result

Theorem

Assume $d \leq 2$. Let a be a regular solution defined up to the blow-up time τ. There exists a constant $C \geq 0$ depending on d and $(\kappa_i)_{1 \leq i \leq 4}$ only such that, if

$$C\nu \leq 1, \tag{3}$$

then

$$\mathbb{E}\left[\log\left(\log\left(\|a\|_{L^\infty(\mathbb{T}^d \times (0,\tau))}\right)\right)\right] \lesssim 1, \tag{4}$$

and thus $\tau = +\infty$ a.s.

Ingredient 1

Entropy estimate

Remember the deterministic entropy equation

$$\int_{\mathbb{T}^d} \mathcal{H}(a)(t)dx + \iint_{Q_t} \sum_{i=1}^{4} \kappa_i \frac{|\nabla a_i|^2}{a_i} dxds$$

$$= \int_{\mathbb{T}^d} \mathcal{H}(a)(0)dx - \iint_{Q_t} \sum_{i=1}^{4} (a_1 a_3 - a_2 a_4)(\log(a_1 a_3) - \log(a_2 a_4)) dxds,$$

where

$$\mathcal{H}(a) := \sum_{i=1}^{4} (a_i \log(a_i) - a_i + 1).$$

Ingredient 1

Entropy estimate

For the stochastic system, we get

$$\mathbb{E}\left[\int_{\mathbb{T}^d} \mathcal{H}(a)(t)dx\right] + \mathbb{E}\iint_{Q_t} \sum_{i=1}^{4} \kappa_i \frac{|\nabla a_i|^2}{a_i} dxds$$
$$= \mathbb{E}\left[\int_{\mathbb{T}^d} \mathcal{H}(a)(0)dx\right] + \frac{\nu}{2}\mathbb{E}\iint_{Q_t} \sum_{i,\alpha} \frac{|\sigma_i^\alpha(a_i)|^2}{a_i} dxds$$
$$- \mathbb{E}\iint_{Q_t} \sum_{i=1}^{4} (a_1a_3 - a_2a_4)(\log(a_1a_3) - \log(a_2a_4))dxds,$$

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$$- \mathbb{E}\iint_{Q_t} \sum_{i=1}^{4} (a_1a_3 - a_2a_4)(\log(a_1a_3) - \log(a_2a_4))dxds,$$

and after suitable estimates...

Ingredient 1

Entropy estimate

$$\mathbb{E}\left[\int_{\mathbb{T}^d} \mathcal{H}(a)(t)dx\right] + \mathbb{E}\iint_{Q_t} \sum_{i=1}^{4} \kappa_i \frac{|\nabla a_i|^2}{a_i} dxds \lesssim \mathbb{E}\left[\int_{\mathbb{T}^d} \mathcal{H}(a)(0)dx\right]$$

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Taking also into account the martingale term, we get similar estimates on the moments of the entropy and entropy dissipation.

Ingredient 2

An L^2 estimate by duality

Remember the equation for the total mass (in the deterministic case)

$$\partial_t z - \Delta(Kz) = 0 \quad z = \sum_{i=1}^{4} a_i, \quad K = \sum_{i=1}^{4} \frac{a_i}{z} \kappa_i, \tag{5}$$

In (5), the coefficient K is measurable, bounded from above and from below:

$$\min_{1 \le i \le 4} \kappa_i \le K(x,t) \le \max_{1 \le i \le 4} \kappa_i.$$

This allows for an estimate by <u>duality</u>.

Ingredient 2

An L^2 estimate by duality

For the dual equation

$$\partial_t \psi + K\Delta\psi = H, \quad H \text{ given, } \psi(T) = 0, \tag{6}$$

we have the maximal regularity result

$$\|\partial_t \psi\|_{L^2(Q_T)} + \|\Delta\psi\|_{L^2(Q_T)} \lesssim \|H\|_{L^2(Q_T)},$$

from which follows the bound

$$\sup_{t\in[0,T]} \|\psi\|_{L^2(\mathbb{T}^d)} + \|\psi\|_{L^2(0,T;W^{2,2}(\mathbb{T}^d))} \lesssim \|H\|_{L^2(Q_T)},$$

which can be exploited to give in turn an estimate

$$\|z\|_{L^2(Q_t)} \lesssim \|z(0)\|_{L^2(\mathbb{T}^d)}.$$

Ingredient 2

An L^2 estimate by duality

Estimate

$$\|z\|_{L^2(Q_t)} \lesssim \|z(0)\|_{L^2(\mathbb{T}^d)}.$$

Use a similar trick starting from the entropy equation, to obtain a $L^2 \log(L^2)$ estimate. [Desvillettes, Fellner, Pierre, Vovelle 2007, Global existence of weak solutions].

Ingredient 2

An L^2 estimate by duality

For the stochastic system, this idea can still be exploited, by considering the backward stochastic parabolic equation

$$d\psi(t) + K\Delta\psi(t)dt = H(t)dt + q^{\alpha}(t)dB_{\alpha}(t),$$

with terminal condition

$$\psi(T) = 0, \quad x \in \mathbb{T}^d.$$

We use the analysis by [Du, Tang 2012] in particular.

Ingredient 3

De Giorgi's iteration scheme

[Goudon, Vasseur, 2010] Analysis of the decay in ξ of the entropy truncated at level ξ:

$$\mathcal{H}(a;\xi) := \sum_{i=1}^{4} (1 + (a_i - \xi)^+) \log(1 + (a_i - \xi)^+) - (a_i - \xi)^+.$$

Aim: show that the decay is fast enough to get cancellation for a finite $\bar{\xi}$:

$$\mathcal{H}(a;\bar{\xi}) = 0 \Longleftrightarrow \forall i,\ a_i \leq \bar{\xi}.$$

Ingredient 3

Standard De Giorgi's iteration scheme

Analysis of the energy truncated at level ξ:

$$\mathcal{E}(u;\xi) := \int \left|(u-\xi)^+\right|^2 dx,$$

where u solves the parabolic equation

$$\partial_t u - \operatorname{div}(k\nabla u) = f, \quad u|_{t=0} = 0.$$

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where u solves the parabolic equation

$$\partial_t u - \operatorname{div}(k\nabla u) = f, \quad u|_{t=0} = 0.$$

Proposition: if k is measurable and $\lambda \leq k \leq \lambda^{-1}$ for a constant $\lambda > 0$, then, for all $\mu > 1 + \frac{d}{2}$, we have, for all $T > 0$,

$$\|u\|_{L^\infty(Q_T)} \leq C(d,\lambda,\mu,T)\|f\|_{L^\mu(Q_T)}.$$

Ingredient 3

Supremum estimate for stochastic parabolic equations

Let u solve

$$du - \Delta u dt = f dt + g^\alpha dB_\alpha(t), \quad u|_{t=0} = 0.$$

Proposition: for all $\mu > 1 + \frac{d}{2}$, we have, for all $T > 0$, for all $p \geq 1$,

$$\mathbb{E}\left[\|u\|^p_{L^\infty(Q_T)}\right] \\ \leq C(d, \lambda, \mu, T, P)\left(\|f\|_{L^\mu(\Omega\times Q_T)} + \||g|_{\ell^2}\|_{L^{2\mu}(\Omega\times Q_T)}\right)^p. \quad (7)$$

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Proof: [Dareiotis, Gess, 2019] (Moser's technique), [Hsu, Wang, Wang, 2017] (where $\mu = +\infty$, and deterministic bound on the data, De Giorgi's technique & exponential martingale inequalities).

Ingredient 3

Proof

[Leocata, Vovelle, 2023] Extension of [Hsu, Wang, Wang, 2017] (any admissible exponent μ) by De Giorgi's approach.

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Alternative proof by duality and Boccardo-Gallouët estimates:
Proposition [Boccardo, Gallouët, 1989]: let ψ solve

$$\partial_t \psi + \Delta \psi = 0 \text{ in } \mathbb{T}^d \times (0, T),$$

with terminal condition $\psi(T) = \phi \in L^1(\mathbb{T}^d)$. For any exponent

$$1 \leq r < p_F := \frac{d+2}{d}$$

we have

$$\|\psi\|_{L^r(Q_T)} \leq C(d, r) \|\phi\|_{L^1(\mathbb{T}^d)}.$$

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Remark: $p_F' = 1 + \frac{d}{2}$ (threshold for L^∞ estimate).

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Adaptation to the stochastic case: use a backward SPDE again!.

Open questions

1. Case $d \geq 3$ of course. Other boundary conditions.
2. Space-time white noise.
3. Large-time behaviour and, for possibly different stochastic systems of reaction-diffusion equations, study of pattern formation [Hausenblas, Randrianasolo, Thalhammer, 2020].

Thanks for your attention!

Welcome to the cocktail-dinner! Santé ! Kanpai !