Nonlinear SPDE models of particle systems

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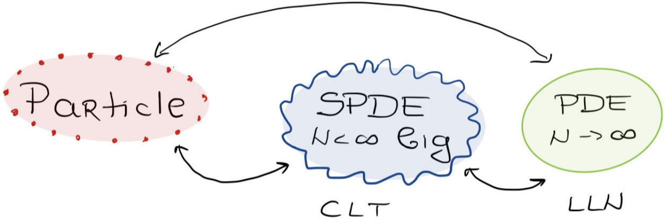
Outlook

- Introduction Interacting particle systems
- Modeling / applications: agent based modeling (ABM)
- Well-posedness of the nonlinear SPDE model – for independent particles
- Numerical analysis ?
- Simulations

Interacting particle systems

- Problem: describe interacting particle system
- Q: How large is the system?
  - N small —— particle description
  - $N \to \infty$ —— hydrodynamics/mean-field limit: PDE
  - $N < \infty$ but large —— fluctuating hydrodynamics: SPDE



Independent Brownian particles
[D96, K73]

- Non-interacting Brownian particles $dX_i = dB_i, i = 1, \dots N$ on $\mathbb{T}^d$
- Goal: empirical density $\rho^N(x,t) = \frac{1}{N}\sum_{i=1}^N \delta(x - B_i(t))$
- Dean-Kawasaki SPDE

$$\partial_t \mu^N = \frac{1}{2}\Delta\mu^N + \frac{1}{\sqrt{N}}\nabla\cdot(\sqrt{\mu^N}\xi) \qquad (DK)$$

- Q: Relation between ρ^N and μ^N: starting with ρ^N can we derive (DK)?

Relation between the empirical density and DK
[D96, K73]

- Empirical density $\rho^N(x,t) = \frac{1}{N}\sum_{i=1}^N \delta(x - B_i(t)) = \frac{1}{N}\sum_{i=1}^N \rho_i(x,t)$
- Ito's formula for ρ_i

$$d\rho_i = \frac{1}{2}\Delta\rho_i dt + \nabla \cdot (\rho_i dB_i)$$

- After summation we obtain almost closed equation

$$d\rho^N = \frac{1}{2}\Delta\rho^N dt + \frac{1}{\sqrt{N}}\sum_i \nabla \cdot (\rho_i dB_i)$$

- What to do with the noise term?

Relation between the empirical density and DK

- Empirical density $\rho^N(x,t) = \frac{1}{N}\sum_{i=1}^N \delta(x - B_i(t)) = \frac{1}{N}\sum_{i=1}^N \rho_i(x,t)$
- Almost closed equation

$$d\rho = \frac{1}{2}\Delta\rho dt + \frac{1}{\sqrt{N}}\sum_{i=1}^N \nabla\cdot(\rho_i dB_i)$$

- What to do with the noise term?

$$\tilde{\eta}(x,t) := \sum_{i=1}^N \nabla\cdot(\dot{B}_i(t)\rho_i(x,t))$$

- Compute correlation function

$$\left\langle \tilde{\eta}(x,t)\tilde{\eta}(y,t')\right\rangle = 2\delta(t-t')\sum_{i=1}^N \nabla_x\nabla_y(\rho_i(x,t)\rho)_i(y,t))$$

- Consider statistically the same noise term

$$\eta(x,t) = \nabla\cdot(\xi(x,t)\rho^{1/2}(x,t))$$

- Dean-Kawasaki

$$\partial_t\mu^N = \frac{1}{2}\Delta\mu^N + \frac{1}{\sqrt{N}}\nabla\cdot(\sqrt{\mu^N}\xi) \qquad (DK)$$

Weakly interacting particles
[D96, K73]

- Particle system

$$dX_i = N^{-1} \sum_{j \neq i} \nabla U(X_i - X_j)dt + dB_i$$

- DK equation

$$\partial_t \mu^N = \frac{1}{2}\Delta \mu^N + \nabla \cdot (\mu^N \nabla U * \mu^N) + N^{-1/2} \nabla \cdot (\sqrt{\mu^N} \xi)$$

- Hydrodynamic limit [McK66, Szn91]

$$\partial_t \mu = \frac{1}{2}\Delta \mu - \nabla \cdot (\mu \nabla U * \mu)$$

- Fluctuations

$$\sqrt{\mu^N - \mu} \to \text{ Gaussian}$$

- Quantifying fluctuations — via semi-discretization [CFIR23]

$$d_{-j}(\mu_h^N - \mu_h, \mu^N - \mu) \lesssim h^{p+1} + e^{-Nh^d} + N^{-j/2}$$

Application: Agent Based Modeling

- Agents: humans, molecules, particles, cells, amoeba ...
- Move randomly in space $X(t)$
- Interact when they are close

  $\Rightarrow$ change of type: opinion, status, ... $Y(t)$

- Examples: infection/disease spreading, historical processes, opinion dynamics, protein complex formation

Schematic of the typical elements of an agent-based model

https://medium.com/arupcitymodelling/

Model formulation

[CFG+18, CHZ+18, HCDjWS21]

- N agents —— very big, but finite —— "mesoscale"
- every agent at time t: $(X_i(t), Y_i(t))_{i=1}^N =: X(t)$
- **position in D**: $X_i(t) \in D \subset \mathbb{R}^d$

$$dX_i(t) = -(\nabla V(X_i(t)) + \nabla U_i(X))dt + \sigma dB_i(t)$$

landscape $V : D \to \mathbb{R}$: attractivity of the environment

interaction potential $U_i : D^N \to \mathbb{R}, X(t) \mapsto \sum_{j \neq i} u(\|X_i(t) - X_j(t)\|)$

- **change process/opinion dynamics**

Markov jump process $Y_i, i \in \{1, \dots, N\}$

interaction rules $\{R_r\}_{r=1}^{N_R}$ – type change: $R_r : T_s + T_{s''} \to T_{s'} + T_{s''}$

network matrix $A_{ij}(t) = 1$ if $\|X_i(t) - X_j(t)\| \leqslant d$

transition rate function $\lambda_i^r = \gamma_r \sum_1^N A_{ij}(t) 1_{s''}(Y_j(t)) 1_s(Y_i(t))$

$$Y_i(t) = Y_i(0) + \sum_r \mathcal{P}_i^r \left(\int_0^t \lambda_i^r(t') dt' \right) v_r$$

Innovation spreading example
[HCDjWS21]

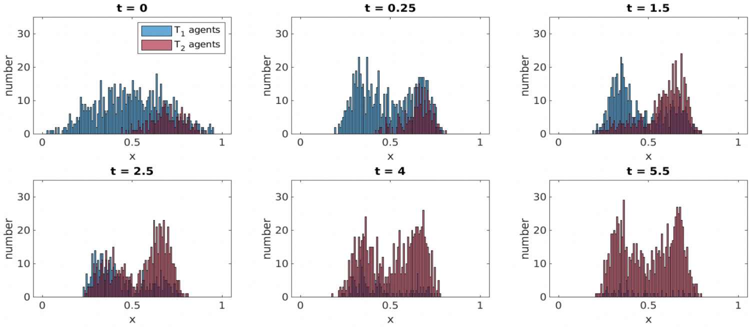
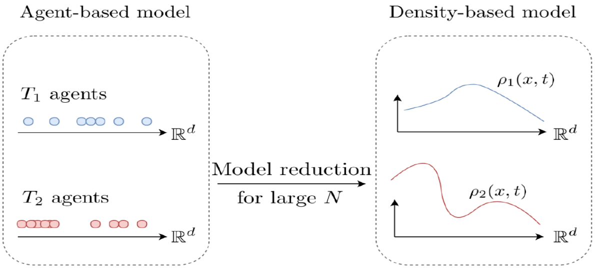


Figure 4: A single realization of the spreading process in a double well landscape on $D = [0, 1]$ with 1000 agents and modeled by the ABM. The empirical density of T_1 agents at time t is given by the blue histogram while the density of type T_2 agents is shown using the red histogram.

$N = 1000$ agents, $D = [0, 1]$, $d_{int} = 0,002$ – interaction just within the well
double well landscape, $N_1 = 800$, initial normal distribution
Interaction rule: $T_1 + T_2 \rightarrow 2T_2$

Model reduction

- Problem: big N is very **expensive**



- Replace the micro-scale model of individual agents by a meso-scale model of stochastic agent densities —— > FHD

- **Agent density** μ_s

$$\partial_t \mu_s = \mathcal{D}\mu_s + \mathcal{I}\mu_s$$

- Diffusion operator: **Dean-Kawasaki equation**

$$\mathcal{D}\mu(x,t) = \frac{\alpha}{2}\Delta\mu + \nabla \cdot (\nabla V \mu) + \frac{1}{\sqrt{N}}\nabla \cdot (\sqrt{\mu}\xi)$$

Simulation and comparison
[HCDjWS21]

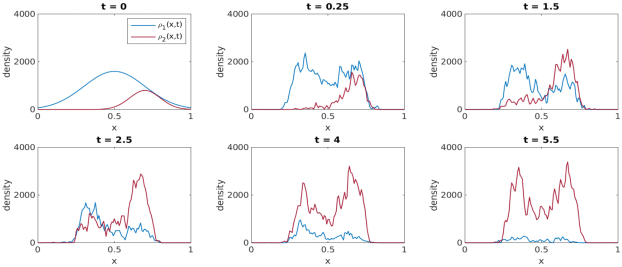


Figure 5: Realization of the innovation spreading process in a double well landscape with 1000 agents (SPDE approach). We plot the number density of non-adopters $\rho_1(x,t)$ and the density of adopters $\rho_2(x,t)$ at a few time instances.

- Error estimates? Choice of parameters? Conservation of properties?

Feedback loop dynamics
[CKDj22]

- Two-way interaction between the agents' spatial movement and their opinion

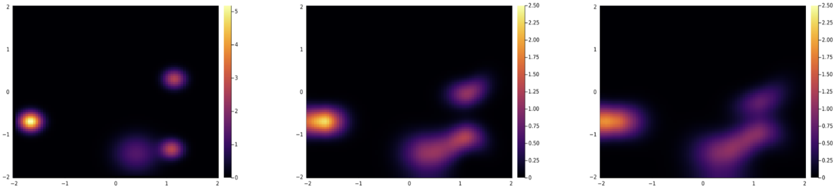
$$\begin{cases} dX_t &= \tilde{U}(X_t, \Theta_t)dt + \sigma_{sp}(X_t, \Theta_t)dB_t^{sp} \\ d\Theta_t &= \tilde{V}(X_t, \Theta_t)dt + \sigma_{op}(X_t, \Theta_t)dB_t^{op} \end{cases}$$

- Agents can interact if they are close enough in space and they attract each other if their opinions are similar

Computation of the limit
[CKDj22]

- McKean–Vlasov-type PDE for the limiting measure

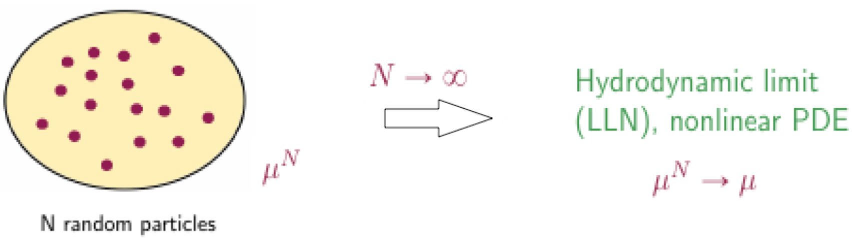
$$\partial_t \mu_t(z,\eta) = -\operatorname{div}_z\left(\mu_t(z,\eta)\cdot U(z,\eta,\mu_t)\right) - \operatorname{div}_\eta\left(\mu_t(z,\eta)\cdot V(z,\eta,\mu_t)\right)$$
$$+\frac{1}{2}\sum_{i,j=1}^{d}\frac{\partial^2}{\partial z_i \partial z_j}\left(\mu_t(z,\eta)\cdot\sigma_{sp}(z,\eta,\mu_t)\cdot\sigma_{sp}(z,\eta,\mu_t)^\top\right)_{i,j}$$
$$+\frac{1}{2}\frac{\partial^2}{\partial\eta^2}\left(\mu_t(z,\eta)\sigma_{op}(z,\eta,\mu_t)^2\right)$$



(a) $t=0$ (b) $t=0.5$ (c) $t=1$

Figure 7. Empirical density of agents in mean-field limit given by Equation (20) at initial time $t=0$, intermediate time $t=0.5$, and final time $t=1$.

What can we say about the empirical density?



interacting particle systems

How to include finite size effects? In applications: $N < \infty$!

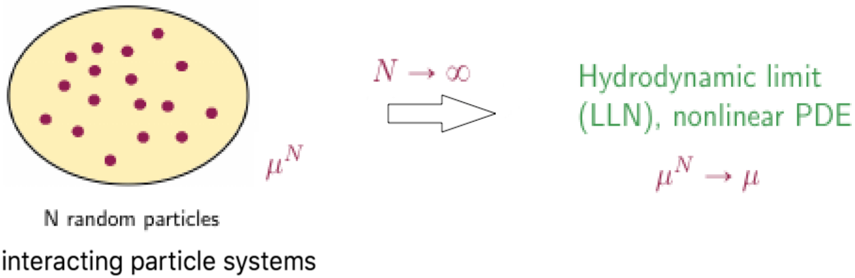
Linear fluctuations (CLT):

linearize around PDE $\rightsquigarrow$ linear Gaussian SPDE

$$\mu^N \simeq \mu + \frac{1}{\sqrt{N}}\nu \qquad d\nu = \frac{1}{2}\Delta \nu dt + \nabla \cdot (\sqrt{\mu} dW)$$

Problem: Violates "physical" constraints
(positivity, conservation of mass) — could be controlled (IC, N)

Wish list



How to include finite size effects? In applications: $N < \infty$!

Goal: Find nonlinear SPDE models. Wish list:

- preserve "physical" constraints (positivity, conservation laws)
- preserve dynamical properties (metastability, condensation, . . .)
- control the approximation error
- rigorous numerical analysis

Reliable nonlinear SPDE approximation of particle systems/ABM

DK - Ill-posedness vs. Triviality
[KLvR19]

- Diffusive DK

$$d\mu^N = \frac{1}{2}\Delta\mu^N dt + \frac{1}{\sqrt{N}}\nabla\cdot(\sqrt{\mu^N}dW), \qquad \mu_0 = \frac{1}{N}\sum_{i=1}^{N}\delta_{x^i}$$

- Difficulties: regularity, square-root, super-criticality
- **Existing literature:** Konarovskyi, Lehmann, von Renesse [KLvR19,KLvR20]
  Gess, Fehrman [FG19,FG20, FG22,...]
  Cornalba, Shardlow, Zimmer, Fischer, Raithel [CFIR23,CF21,CSZ20,CZS19]
  Martini, Mayorcas [MM22]
- **measure-valued martingale solution:** μ^N is a solution to the MP iff

$$M_t^f := \langle \mu_t^N, f\rangle - \frac{1}{2}\int_0^t \langle \mu_s^N, \Delta f\rangle\, ds \quad \forall f \in C_c^\infty(\mathbb{R}^d)$$

is a martingale with quadratic variation

$$[M^f, M^f]_t = \frac{1}{N}\int_0^t \langle \mu_s^N, |\nabla f|^2\rangle\, ds$$

- Still problems: sensitivity, approximation

Approximation of DK
[Dj, Kremp, Perkowski 22]

We replace the square root with

$$f(x) = f_{\delta_N}(x) = \begin{cases} \frac{1}{\sqrt{\delta_N}} x & |x| \leqslant \delta_N/2, \\ \text{smooth} & \delta_N/2 \leqslant |x| \leqslant \delta_N, \\ \operatorname{sign}(x)\sqrt{|x|} & |x| \geqslant \delta_N. \end{cases}$$

$$f \in C^1(\mathbb{R}), \quad \|f'\|_{L^\infty} \leqslant \frac{C_N}{\delta_N}, \quad |f'(x)| \lesssim \frac{1}{\sqrt{x}}, \text{ for all } x > 0$$

and

$$|f(x)| \lesssim \sqrt{|x|}, \quad |f(x)^2 - x| \lesssim \delta, \text{ for all } x \geqslant 0.$$

Approximate equation

$$d\tilde{\mu}_t^N = \frac{1}{2}\Delta\tilde{\mu}_t^N dt + \frac{1}{\sqrt{N}}\nabla\cdot(f(\tilde{\mu}_t^N)dW_t^N)$$

$$\tilde{\mu}_0^N = \rho^N * \mu_0^N \in L^2(\mathbb{T}^d) \qquad \rho^N \text{ appropriate mollifier}$$

Truncated noise

$$W_t^N(x) := \sum_{|k|\leqslant M_N} e_k(x)B_t^k := \sum_{|k|\leqslant M_N} \exp(2\pi i k\cdot x)B_t^k$$

Approximated DK - notion of the solution

- "Assumptions": $f:\mathbb{R}\to\mathbb{R}$, $\|f'\|_\infty \leqslant L$, $f(0)=0$

$$d\tilde{\mu}_t^N = \frac{1}{2}\Delta\tilde{\mu}_t^N dt + \frac{1}{\sqrt{N}}\nabla\cdot(f(\tilde{\mu}_t^N)dW_t^N)$$

$$\tilde{\mu_0}^N \in L^2$$

Definition

A stochastic process $(\tilde{\mu}_t)_{t\geqslant 0}$ with paths in $L^2([0,T],H^1(\mathbb{T}^d))\cap C([0,T],L^2(\mathbb{T}^d))$ is a solution for the initial condition $\tilde{\mu}_0\in L^2(\mathbb{T}^d)$, if for all $\varphi\in H^1(\mathbb{T}^d)$,

$$\begin{aligned}\langle\tilde{\mu}_t,\varphi\rangle &= \langle\tilde{\mu}_0,\varphi\rangle - \int_0^t \frac{1}{2}\langle\nabla\tilde{\mu}_s,\nabla\varphi\rangle ds + \sum_{k\in\mathbb{Z}^d}\int_0^t \langle\nabla(f(\tilde{\mu}_t)\phi_k),\varphi\rangle\cdot dB_s^k \\ &= \langle\tilde{\mu}_0,\varphi\rangle - \sum_{i=1}^d\int_0^t \frac{1}{2}\langle\partial_i\tilde{\mu}_s,\partial_i\varphi\rangle ds + \sum_{i=1}^d\sum_{k\in\mathbb{Z}^d}\int_0^t \langle\partial_i(f(\tilde{\mu}_t)\phi_k),\varphi\rangle dB_s^{k,i}.\end{aligned}$$

Remark

- The well-posedness result can be generalized to ($b = \frac{1}{\sqrt{N}} f$)

$$du_t = \frac{1}{2}\Delta u_t dt + \nabla \cdot (b(u_t) dW_t)$$

- Noise $W_t(x) := \sum_{k \in \mathbb{Z}^d} \phi_k(x) B_t^k$ such that

$$C_1^W := \sum_{k \in \mathbb{Z}^d} \|\phi_k\|_\infty^2 < \infty \quad \text{and} \quad C_2^W := \sum_{k \in \mathbb{Z}^d} \|\nabla \phi_k\|_\infty^2 < \infty$$

- Diffusion $b \in C^1(\mathbb{R}, \mathbb{R})$: $\|b'\|_\infty \leqslant L.$

In particular, b has most linear growth: There exist C_1^b, C_2^b such that

$$|b(x)|^2 \leqslant C_1^b |x|^2 + C_2^b, \qquad x \in \mathbb{R}.$$

- Our case: $L^2 = C_1^b = \frac{C_N}{N\delta}$, $C_1^W \leqslant (2M_N + 1)^d$
- Small noise / Stochastic parabolicity (Ito vs Str) $C_1^W \max(L^2, C_1^b) < 1$
- Coercivity assumption $\frac{C_N (2M_N+1)^d}{N\delta_N} < 1$

Approximated DK - well-posedness result

$$d\tilde{\mu}_t^N = \frac{1}{2}\Delta\tilde{\mu}_t^N dt + \frac{1}{\sqrt{N}}\nabla \cdot (f(\tilde{\mu}_t^N) dW_t^N)$$
$$\tilde{\mu}_0^N \in L^2$$

- the variational theory cannot be applied directly
- **Idea:** transform the equation, by applying $(1-\Delta)^{-1/2}$, use the variational approach and conclude from there together with a-priori bounds the well-posedness result

Lemma (Dj, Kremp, Perkowski 22)

Under previous assumptions, there exists a unique probabilistically strong solution $v \in L^2([0,T], H^1) \cap C([0,T], L^2)$ to

$$d\langle v_t, \varphi\rangle = -\frac{1}{2}\langle \nabla v_t, \nabla\varphi\rangle dt + \frac{1}{\sqrt{N}} \sum_{|k| \leqslant M_N} \langle G_k(v_t), \varphi\rangle dB_t^k$$

for all $\varphi \in H^1$ with $G_k(v) := (1-\Delta)^{-1/2}\nabla(f((1-\Delta)^{1/2}v)\phi_k)$ and initial condition $v_0 \in L^2$.

Proof: apply variational theory – coercivity and monotonicity

Approximated DK - well-posedness result

$$d\tilde{\mu}_t^N = \frac{1}{2}\Delta\tilde{\mu}_t^N dt + \frac{1}{\sqrt{N}}\nabla\cdot(f(\tilde{\mu}_t^N)dW_t^N)$$
$$\tilde{\mu}_0^N \in L^2$$

Lemma (A priori energy estimate)

Under the previous assumptions, the following energy bound holds true:

$$\mathbb{E}[\|\tilde{\mu}_t\|_{L^2}^2] + \lambda\int_0^t \mathbb{E}[\|\nabla\tilde{\mu}_s\|_{L^2}^2]ds \leqslant \|\tilde{\mu}_0\|_{L^2}^2 + \frac{C_2^W}{N}t\|\tilde{\mu}_0\|_{L^1}.$$

Proof: Ito's lemma
Caution: be careful about $\|\tilde{\mu}\|_{L^2}^2$

Theorem (Dj, Kremp, Perkowski 22)

Consider the equation

$$d\tilde{\mu}_t^N = \frac{1}{2}\Delta\tilde{\mu}_t^N dt + \frac{1}{\sqrt{N}}\nabla\cdot(f(\tilde{\mu}_t^N)dW_t^N),$$
$$\tilde{\mu}_0^N \in L^2(\mathbb{T}^d),$$

where $f \in C^1(\mathbb{R})$ *satisfies* $\|f'\|_{L^\infty} \lesssim \frac{1}{\sqrt{\delta}}, \quad |f'(x)| \lesssim \frac{1}{\sqrt{x}},$ *for all* $x > 0$ *and*

$$|f(x)| \lesssim \sqrt{|x|}, \quad |f(x)^2 - x| \lesssim \delta, \text{ for all } x \geqslant 0,$$

and where

$$W_t^N(x) := \sum_{|k|\leqslant M_N} e_k(x)B_t^k := \sum_{|k|\leqslant M_N} \exp(2\pi i k\cdot x)B_t^k$$

If $\frac{C_N(2M_N+1)^d}{N\delta_N} < 1$ *holds ("coercivity condition"), where* $C_N > 0$ *is such that* $\|f'\|_\infty^2 \leqslant \frac{C_N}{\delta_N}$*, then equation has a unique strong solution. If* $\tilde{\mu}_0^N \geqslant 0$*, then* $\tilde{\mu}_t^N \geqslant 0$ *and* $\|\tilde{\mu}_t^N\|_{L^1} = \|\tilde{\mu}_0^N\|_{L^1}$ *for all* $t \in [0, T]$.

Approximated DK - well-posedness result

Idea of the proof: Let $\tilde{\mu}_t^N = (1-\Delta)^{1/2} v_t$, then

$$\tilde{\mu}^N \in L^2([0,T], L^2) \cap C([0,T], H^{-1})$$

By the a-priori energy estimate, it follows that almost surely

$$\tilde{\mu}^N \in L^2([0,T], H^1) \qquad \text{and} \qquad \sup_{t\in[0,T]} \mathbb{E}[\|\tilde{\mu}_t^N\|_{L^2}^2] < \infty$$

$\Rightarrow \quad t \mapsto \tilde{\mu}_t^N \in L^2$ is weakly continuous

Together with a.s. continuity of the mapping

$$t \mapsto \|\tilde{\mu}_t^N\|_{L^2}^2$$

$\Rightarrow \tilde{\mu}^N \in C([0,T], L^2)$

Preservation of non-negativity and conservation of mass

Theorem (DjKrempPerkowski22)

Let u^+ and u^- be two solutions with initial conditions $u_0^+, u_0^- \in L^2$, respectively, such that $u_0^+(x) \geqslant u_0^-(x)$ for Lebesgue-almost all $x \in \mathbb{T}^d$. Then

$$\mathbb{P}\big(u_t^+ \geqslant u_t^- \ \mathrm{Leb}\text{-}a.e.\, \forall t \in [0,T]\big) = 1.$$

Idea of the proof:

application of Itô's formula to a suitable C^2 approximation of the map $x \mapsto \max(x,0)^2$, applied to the difference of the solutions

$w_t := u_t^- - u_t^+$

choose $\Phi_p(w_t) \uparrow \|\max(w_t,0)\|_{L^2}^2$, $p \to \infty$

Apply Ito's formula - bound terms, take the expectation, consider the limit

$$\mathbb{E}\left[\|\max(w_s,0)\|_{L^2}^2\right] = 0$$

$$(\mathbb{P} \otimes \mathrm{Leb})(w_t \leqslant 0) = 1, \forall t \geqslant 0$$

Use the continuity of the solution to conclude

Preservation of non-negativity and conservation of mass

Corollary

Assume additionally that $b(0) = 0$. Let u be a solution with initial condition $u_0 \geqslant 0$ almost everywhere. Then $\mathbb{P}(u_t \geqslant 0 \text{ Leb-a.e.} \, \forall t \in [0, T]) = 1$.

Since the zero function is a solution as $f(0) = 0$, with zero initial condition, the result follows directly.

Use the positivity of the solution μ and test with $\varphi = 1 \in C^\infty(\mathbb{T}^d)$.

Preservation of non-negativity and conservation of mass

Corollary

Assume additionally that $b(0) = 0$*. Let* u *be a solution with initial condition* $u_0 \geqslant 0$ *almost everywhere. Then* $\mathbb{P}(u_t \geqslant 0 \text{ Leb-a.e.} \forall t \in [0, T]) = 1$*.*

Since the zero function is a solution as $f(0) = 0$, with zero initial condition, the result follows directly.

Corollary

Let u *be the solution with non-negative initial condition* u_0*. Then almost surely* $\int |u_t|(x)dx = \int |u_0|(x)dx$ *for all* $t \in [0, T]$*.*

Use the positivity of the solution μ and test with $\varphi = 1 \in C^\infty(\mathbb{T}^d)$.

Entropy estimate

- Goal: weak-error estimate (better than HLim)

$$|\mathbb{E}[F(\tilde{\mu}_t^N)] - \mathbb{E}[F(\mu_t^N)]| \lesssim N^{-1-\frac{1}{d/2+1}}(t + \log(N))$$

- Problem: dependence on $\|\tilde{\mu}_0\|_{L^2}$ — [FG21]

Entropy estimate

- Goal: weak-error estimate (better than HLim)

$$|\mathbb{E}[F(\tilde{\mu}_t^N)] - \mathbb{E}[F(\mu_t^N)]| \lesssim N^{-1-\frac{1}{d/2+1}}(t + \log(N))$$

- Problem: dependence on $\|\tilde{\mu}_0\|_{L^2}$ — [FG21]

Theorem (Entropy estimate - DjKrempPerkowski22)

Consider the initial condition $\tilde{\mu}_0^N := \rho^N * \mu_0^N$ for $\mu_0^N := \frac{1}{N}\sum_{i=1}^N \delta_{x^i}$ and let $(\rho^N)_{N\geqslant 1}$ be a mollifying sequence such that $\tilde{\mu}_0^N \geqslant 0$ and $\|\rho^N * \mu_0^N\|_{L^1} = 1$. Under the coercivity condition, the following entropy estimate holds

$$\sup_{t\in[0,T]} \mathbb{E}\Big[\int \tilde{\mu}_t^N \log(\tilde{\mu}_t^N)\Big] + \lambda \int_0^T \mathbb{E}\Big[\int \frac{|\nabla \tilde{\mu}_t^N|^2}{\tilde{\mu}_t^N}\Big] dt \lesssim \int \tilde{\mu}_0^N \log(\tilde{\mu}_0^N) + \frac{T M_N^{d+2}}{N}, \tag{1}$$

for $\lambda := \frac{1}{4}(1 - \frac{C(2M_N+1)^d}{N\delta_N})$.

Remark: why does it matter

$$\int \tilde{\mu}_0^N \log(\tilde{\mu}_0^N) \lesssim \log(N) \text{ vs } \|\tilde{\mu}_0^N\|_{L^2}^2 \lesssim N^d$$

Initial condition

There exist accurate approximations of Dirac masses with moderately large entropy:

Lemma

Let $\rho \in C_c^\infty(\mathbb{R}^d)$ *with* $\int_{\mathbb{R}^d} \rho(y)dy = 1$*, such that* $\rho \geqslant 0$ *and* ρ *is symmetric in the sense that* $\rho(x) = \rho(-x)$ *for all* $x \in \mathbb{R}^d$*. Define* $\rho^N(y) := \sum_{k\in\mathbb{Z}^d} N^d \rho(N(y+k))$*,* $y \in \mathbb{T}^d$*. Then* $\rho^N \in C^\infty(\mathbb{T}^d)$ *is positive,* $\int_{\mathbb{T}^d} \rho^N(y)dy = 1$*, and with* $\mu_0^N = \sum_{i=1}^N \delta_{x_i}$ *and* $\tilde{\mu}_0^N := \mu^N * \rho^N$ *we have*

$$\tilde{\mu}_0^N \geqslant 0, \qquad \|\tilde{\mu}_0^N\|_{L^1(\mathbb{T}^d)} = 1, \qquad \int \tilde{\mu}_0^N \log(\tilde{\mu}_0^N) \lesssim \log N.$$

Moreover, we have for all $\varphi \in C_b^2(\mathbb{R}^d)$*:*

$$|\langle \mu_0^N, \varphi\rangle - \langle \tilde{\mu}_0^N, \varphi\rangle| \lesssim N^{-2} \|\varphi\|_{C_b^2},$$

where $\|\varphi\|_{C_b^2} := \sum_{j=0}^2 \|D^j\varphi\|_\infty$*.*

Weak error estimate

Theorem (DjKrempPerkowski22)

Let μ^N be the martingale solution of the original Dean-Kawasaki equation with initial condition $\mu_0^N := \frac{1}{N}\sum_{i=1}^N \delta_{x^i}$. Let $\tilde{\mu}_0^N$ be as just constructed and let f and W^N be as before. Assume the coercivity, $\sup_N \frac{C_N(2M_N+1)^d}{N\delta_N} < 1$. Let $\tilde{\mu}^N$ be the solution of the approximate Dean-Kawasaki equation with initial condition $\tilde{\mu}_0^N$.
Then for any $t > 0$, $\varphi \in C^\infty(\mathbb{T}^d)$ and $F(\mu) := \exp(\langle \mu, \varphi \rangle)$ for $\mu \in \mathcal{M}$, the following weak error bound holds:

$$|\mathbb{E}[F(\tilde{\mu}_t^N)] - \mathbb{E}[F(\mu_t^N)]| \lesssim_\varphi N^{-2} + \frac{\delta_N}{N} t + \frac{t}{M_N^2 N} + \frac{M_N^d}{N^2} t + \frac{\log N}{M_N^2 N}.$$

For $M_N = \delta_N^{-1/2}$ and $\delta_N \simeq N^{-\frac{1}{d/2+1}}$ (which is the optimal choice under the coercivity condition) we have

$$|\mathbb{E}[F(\tilde{\mu}_t^N)] - \mathbb{E}[F(\mu_t^N)]| \lesssim_\varphi N^{-1-\frac{1}{d/2+1}}(t + \log(N)).$$

Laplace duality argument

KLvR19

- **Hamilton-Jacobi equation**

$$\partial_t v = \frac{1}{2}\Delta v + \frac{1}{2N}|\nabla v|^2, \quad v_0 = \varphi \in C^\infty(\mathbb{T}^d).$$

- Cole-Hopf transformation $w = e^{\frac{1}{N}v} \quad : \quad \partial_t w = \frac{1}{2}w$
- **Laplace duality argument** [KLvR19] For $F(\mu_t^N) = exp(\langle \mu_t^N, v_{t-t} \rangle)$

$$\mathbb{E}[F(\mu_t^N)] = exp(\langle \mu_0^N, v_t \rangle)$$

- For approximated equation we get

$$d\Big(\exp(\langle \tilde\mu_s^N, v_{t-s}\rangle)\Big)_s = -\frac{1}{\sqrt{N}} \sum_{|k|\leqslant M_N} \exp(\langle \tilde\mu_s^N, v_{t-s}\rangle)\langle f(\tilde\mu_s^N)e_k, \nabla v_{t-s}\rangle dB_s^k$$
$$+ \frac{1}{2N}\exp(\langle \tilde\mu_s^N, v_{t-s}\rangle)\Bigg(\sum_{|k|\leqslant M_N} |\langle f(\tilde\mu_s^N)e_k, \nabla v_{t-s}\rangle|^2 - \langle \tilde\mu_s^N, |\nabla v_{t-s}|^2\rangle\Bigg) ds$$

Proof

$$
\begin{aligned}
|\mathbb{E}[F(\tilde{\mu}_t^N)] - \mathbb{E}[F(\mu_t^N)]| &\leqslant |\exp(\langle \tilde{\mu}_0^N, v_t\rangle) - \exp(\langle \mu_0^N, v_t\rangle)| \\
&+ \frac{1}{2N}\mathbb{E}\Bigg[\int_0^t \exp(\langle \tilde{\mu}_s^N, v_{t-s}\rangle)\Bigg|\sum_{|k|\leqslant M_N} |\langle f(\tilde{\mu}_s^N)e_k, \nabla v_{t-s}\rangle|^2 - \langle \tilde{\mu}_s^N, |\nabla v_{t-s}|^2\rangle\Bigg| ds\Bigg]
\end{aligned}
$$

- Initial condition

$$
|\exp(\langle \tilde{\mu}_0^N, v_t\rangle) - \exp(\langle \mu_0^N, v_t\rangle)| \leqslant |\langle \tilde{\mu}_0^N - \mu_0^N, v_t\rangle| \exp(\|v_t\|_\infty) \lesssim_\varphi N^{-2},
$$

- Split the second term and use assumptions on f

$$
\frac{1}{2N}\Bigg(\sum_{|k|\leqslant M_N} |\langle f(\tilde{\mu}_s^N)e_k, \nabla v_{t-s}\rangle|^2 - \langle \tilde{\mu}_s^N, |\nabla v_{t-s}|^2\rangle\Bigg) = \frac{A_s + C_s}{2N},
$$

- Use entropy estimate

$$
\mathbb{E}\left[\int_0^T \int |\partial_x f(\tilde{\mu}_t^N)|^2\right] \leqslant \mathbb{E}\left[\int_0^T \int \frac{|\partial_x \tilde{\mu}_s|^2}{\tilde{\mu}_s}\right] \leqslant \mathbb{E}\left[\int \tilde{\mu}_0^N \log \tilde{\mu}_0^N\right] + C(M,N)
$$

Proof - last steps

Collecting all the estimates

$$|\mathbb{E}[F(\tilde{\mu}_t^N)] - \mathbb{E}[F(\mu_t^N)]| \lesssim_\varphi N^{-2} + \frac{\delta_N}{N} t + \frac{t}{M_N^2 N} + \frac{M_N^d}{N^2} t + \frac{\log N}{M_N^2 N}.$$

- coercivity assumption $M_N^d \lesssim \delta_N N$
- choose $M_N = \delta_N^{-1/2}$, $\delta_N \simeq N^{-\frac{1}{d/2+1}}$

$$\begin{aligned} |\mathbb{E}[F(\tilde{\mu}_t^N)] - \mathbb{E}[F(\mu_t^N)]| &\lesssim_\varphi N^{-2} + N^{-1-\frac{1}{d/2+1}} (t + \log N) \\ &\lesssim N^{-1-\frac{1}{d/2+1}} (t + \log N). \end{aligned}$$

Numerics for (approximate) DK - outlook

- Problem: positivity preserving scheme for singular (div) SPDE
- Existing work:

  Numerics for singular (div noise) SPDEs [GG19, CS22, CF21, CFIR23]

  Positivity preserving scheme for FHD: [MGPCK22]

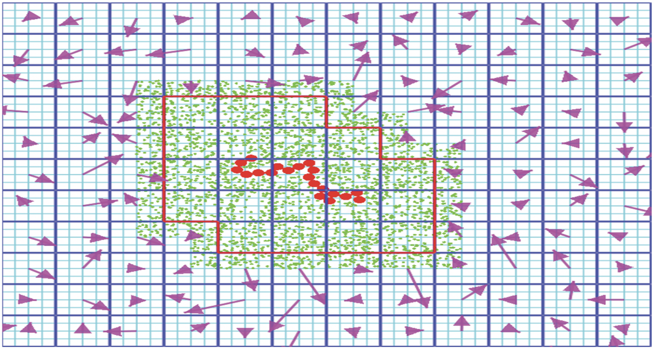
  FHD - computations - finite volume [DVEGB10]

  Positivity preserving schemes for SPDEs: [BCU23]
- How do we measure if the scheme is accurate?

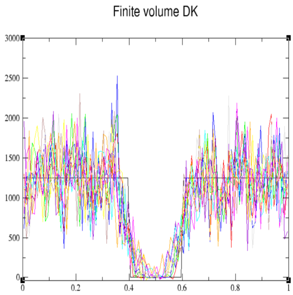
Hybrid method

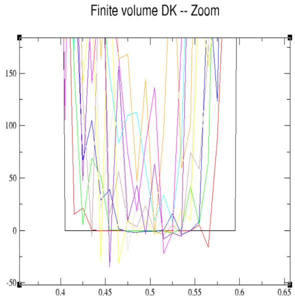
- Work in progress with J. Bell (LBNL)
- Previous work: Bell, Foo, Garcia - for stochastic Burgers' [BFG07]

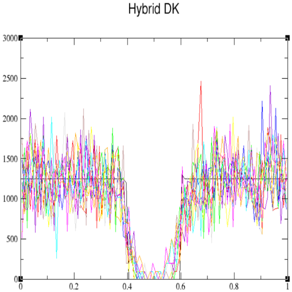
  Donev, Bell, Garcia, Alder - FHD [DBGA10]



Hybrid method for DK







Approximated DK

- Motivation/application: opinion dynamics
- formal SPDE: Dean - Kawasaki equation: non-robust martingale solution

$$d\mu^N = \frac{1}{2}\Delta\mu^N dt + \frac{1}{\sqrt{N}}\nabla\cdot(\sqrt{\mu^N}dW), \quad \mu_0 = \frac{1}{N}\sum_{i=1}^{N}\delta_{x^i}$$

- Modified Dean-Kawasaki equation

$$d\tilde{\mu}_t^N = \frac{1}{2}\Delta\tilde{\mu}_t^N dt + \frac{1}{\sqrt{N}}\nabla\cdot(f_\delta(\tilde{\mu}^N)dW^{M_N})$$

- Well-posedness results
- Preservation of non-negativity and conservation of mass
- Model error estimate:

$$|\mathbb{E}[F(\tilde{\rho}_t^N)] - \mathbb{E}[F(\rho_t^N)]| \leqslant N^{-k} + N^{-1-\frac{1}{d/2+1}}(1+\log N)$$

- Numerical approximation: weak error estimate – in progress
- Outlook: Interacting particles - nonlinear SPDE approximation

Thank you for your attention!

References

Djurdjevac, A., Kremp, H., Perkowski, N. (2022). Weak error analysis for a nonlinear SPDE approximation of the Dean-Kawasaki equation. arXiv:2212.11714

Djurdjevac Conrad, N., Köppl, J., Djurdjevac, A. (2022). Feedback Loops in Opinion Dynamics of Agent-Based Models with Multiplicative Noise. Entropy, 24(10), 13–52.

Helfmann, L., Djurdjevac Conrad, N., Djurdjevac, A., Winkelmann, S., Schütte, C. (2021). From interacting agents to density-based modeling with stochastic PDEs. Comm App Math Comp Sci, 16(1), 1-32.

References

[BFG07] J. Bell, J. Foo, A. Garcia, J. Comput. Phys. 223.1, 2007

[BCU23] C.E. Brehier, D. Cohen, J. Ulander, arXiv:2302.08858, 2023

[CSZ20] F. Cornalba, T. Shardlow, J. Zimmer. Nonlinearity, 2020

[MM22] A. Martini, A. Mayorcas. arXiv preprint arXiv:2207.10711

[CFIR23] F. Cornalba, J Fischer,J. Ingmanns, C. Raithel. arXiv:2303.00429,2023

[CT22] F. Cornalba, T. Shardlow. arXiv:2207.09989, 2022

[CF21] F. Cornalba, J. Fischer. arXiv:2109.06500, 2021

[CSZ19] F. Cornalba, T. Shardlow, J. Zimmer. SIAM J. Math. Anal., 51, 2019

[DFG20] N. Dirr, B. Fehrman, B. Gess. arXiv:2012.02126, 2020

[D96]D. S. Dean. Journal of PhysicsA: Mathematical and General,29(24):L613,1996

[DBGA10] A. Donev,J. Bell,A. Garcia, B. Alder, Multiscale Model Simul 8.3,2010

[DVEGB10] A.Donev, E. Vanden-Eijnden, A. Garcia, J. Bell, Comm App Math Comp Sci 5.2, 2010

References

[FG19] B. Fehrman, B. Gess. Arch. Rational Mech. and Analysis, 2019

[FG20] B. Fehrman, B. Gess. arXiv:1910.11860, 2020

[FG21] B. Fehrman, B. Gess. arXiv:2108.08858, 2021

[GG19] H. Grillmeier, G. Grün. Mathematics of Computation, 88(317), 2019

[K73] K. Kawasaki, Synergetics: Cooperative Phenomena in Multi-Component Systems, 1973

[KLvR19] V. Konarovskyi, T. Lehmann, M. von Renesse. E.Comm.Probab.,2019

[KLvR20] V. Konarovskyi, T. Lehmann, M. von Renesse. J. of Stat.Phys.,2020

[MGPCK22] F. Magaletti, M. Gallo, S. Perez, J. Carillo, S. Kalliadasis. Journal of Computational Physics 463, 2022

[McK66] H. McKean. Proc. Nat. Acad. of Sciences, 1966

[Szn91] A.-S. Sznitman. École d'Été de Prob. de St.-Flour XIX, 1991