Limits of Random Walks via Generalized Gradient Structures

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The Agenda

The ABCs of gradient structures

Limits of random walks

Summary

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The ABCs of gradient structures

Limits of random walks

Summary

Generalized Gradient Flows

$$\dot{\rho} = -\nabla_g \mathscr{E}(\rho)$$

$$\updownarrow$$

$\partial_t \rho + \mathbf{div}\, j = 0$	Continuity Equation
$j = \partial_\xi \mathsf{R}^*(\rho, \xi)$	Force-Flux Relation
$\xi = -\,\mathbf{grad}\, D\mathscr{E}(\rho)$	Energy-Force Relation

$\mathscr{E} \doteq$ **driving energy**

$\mathsf{R}^* \doteq$ **dual dissipation potential**

$\mathsf{R} \doteq$ **dissipation potential**

Force-Flux Relation

$$\Leftrightarrow \quad \partial_j \mathsf{R}(\rho, j) = \xi$$

Generalized Gradient Flows

$\partial_t \rho + \mathbf{div}\, j = 0$	Continuity Equation
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Legendré duality $\quad j = \partial_\xi \mathsf{R}^*(\rho, \xi) \quad \Leftrightarrow \quad \langle \xi, j \rangle = \mathsf{R}(\rho, j) + \mathsf{R}^*(\rho, \xi)$

Chain rule $\quad -\dfrac{d}{dt}\mathscr{E}(\rho) = -\, \langle D\mathscr{E}(\rho), \partial_t \rho \rangle$

Continuity equation $\quad = \langle D\mathscr{E}(\rho), \mathbf{div}\, j \rangle = -\, \langle \mathbf{grad}\, D\mathscr{E}(\rho), j \rangle$

Energy-Dissipation Balance

$$\mathscr{I}(\rho, j) := \int_0^T \mathsf{R}(\rho_t, j_t) + \overbrace{\mathsf{R}^*(\rho_t, -\, \mathbf{grad}\, D\mathscr{E}(\rho_t))}^{=:\, \mathscr{D}(\rho_t) \quad \text{Fisher information}}\, dt + \mathscr{E}(\rho_T) - \mathscr{E}(\rho_0) = 0$$

Generalized Gradient Flows

$$\partial_t \rho + \textbf{div}\, j = 0$$ **Continuity Equation**

$$j = \partial_\xi \mathsf{R}^*(\rho, \xi)$$ **Force-Flux Relation**

$$\xi = -\,\textbf{grad}\, D\mathscr{E}(\rho)$$ **Energy-Force Relation**

Energy-Dissipation Balance

Fisher information

$$\mathscr{I}(\rho, j) := \int_0^T \mathsf{R}(\rho_t, j_t) + \overbrace{\mathsf{R}^*(\rho_t, -\,\textbf{grad}\, D\mathscr{E}(\rho_t))}^{=:\,\mathscr{D}(\rho_t)}\, dt + \mathscr{E}(\rho_T) - \mathscr{E}(\rho_0) = 0$$

It usually happens that the differential equations for a given phenomenon are known first,
and only later is the Lagrangian function found,
from which the differential equations can be obtained.

Methods of Theoretical Physics, Morse and Feshbach, 1953

Generalized Gradient Flows

$$\partial_t \rho + \textbf{div}\, j = 0$$ Continuity Equation

$$j = \partial_\xi \mathsf{R}^*(\rho, \xi)$$ Force-Flux Relation

$$\xi = -\,\textbf{grad}\, D\mathscr{E}(\rho)$$ Energy-Force Relation

Energy-Dissipation Balance

$$0 \le \mathscr{I}(\rho, j) := \int_0^T \mathsf{R}(\rho_t, j_t) + \mathscr{D}(\rho_t)\, dt + \mathscr{E}(\rho_T) - \mathscr{E}(\rho_0) = 0$$

Variational Principle

PDE $\longrightarrow$ Optimization

$$(\mathfrak{X}, \mathsf{R}, \mathscr{E})\text{-}\textbf{(GGF)} \quad :\Leftrightarrow \quad \mathscr{I}(\rho, j) = 0$$

$$\Leftrightarrow \quad (\rho, j) \in \textbf{argmin}\left\{ \mathscr{I}(\mu, \ell) : (\mu, \ell) \in \textbf{CE} \right\}$$

The Agenda

The ABCs of gradient structures

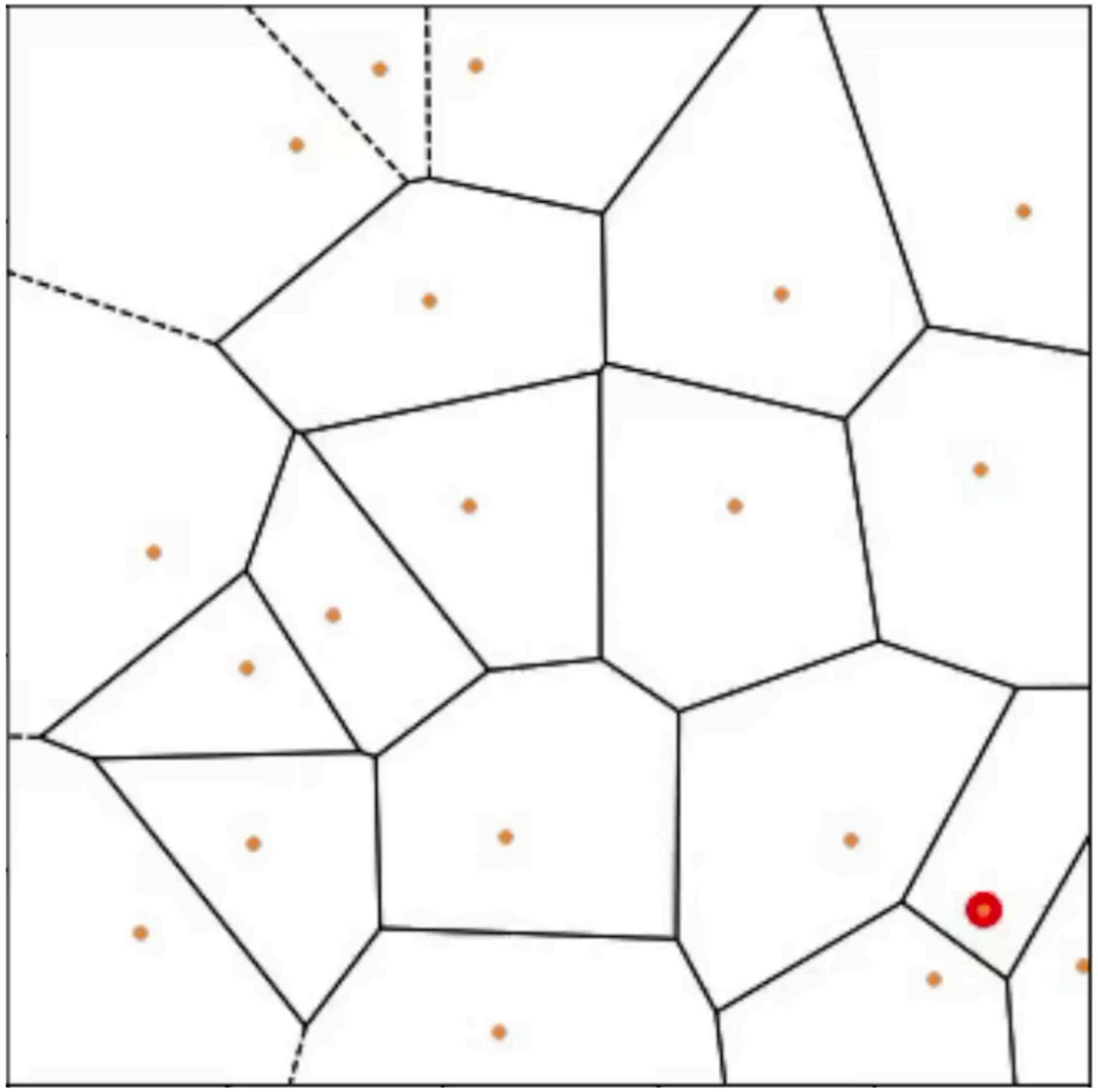
Limits of random walks

Summary

Random Walks on Tessellations

Tessellation: $\mathscr{T}_h = (V_h, E_h)$

$$\partial_t \rho_K^h = \sum_{L \sim K} \left(\kappa_{LK}^h \, \rho_L^h - \kappa_{KL}^h \, \rho_K^h \right)$$



Questions:

- What assumptions about the *tessellations* and *transition intensities* lead to a *diffusive* limit?
- What is the impact of these assumptions on the limiting process?

Markov Jump Process

$$\partial_t \rho + \mathbf{div}\, j = 0$$
$$j = \partial_\xi \mathsf{R}^*(\rho, \xi)$$
$$\xi = -\,\mathbf{grad}\, D\mathscr{E}(\rho)$$

Tessellation: $\mathscr{T}_h = (V_h, E_h)$

$$\partial_t \rho_K^h = \sum_{L \sim K} \left(\kappa_{LK}^h \, \rho_L^h - \kappa_{KL}^h \, \rho_K^h \right)$$

Gradient flow $\Longleftrightarrow$ Detailed balance $\exists\, \pi^h : \quad \vartheta_{KL}^h := \kappa_{KL}^h \pi_K^h$ **symmetric**

Flux: $j = j_{KL}$, $\quad$ $\mathbf{grad}\, \varphi(K, L) = \varphi_L - \varphi_K$, $\quad$ $\mathbf{div}\, j(K) = \sum_{L \sim K} \left(j_{KL} - j_{LK} \right)$

Driving energy: $\mathscr{E}_h(\rho) = \frac{1}{2} \mathbf{Ent}(\rho \,|\, \pi^h)$ **Relative Entropy** $\quad u_K = \frac{\rho_K}{\pi_K^h}$

Dual dissipation potential: $\mathsf{R}_h^*(\rho, \xi) = \sum_{KL \in E^h} 2\left(\cosh(\xi_{KL}/2) - 1 \right) \sqrt{u_K u_L}\, \vartheta_{KL}^h$

Markov Jump Process

$$\partial_t\rho + \textbf{div}\, j = 0$$
$$j = \partial_\xi \mathsf{R}^*(\rho,\xi)$$
$$\xi = -\,\textbf{grad}\, D\mathscr{E}(\rho)$$

Tessellation: $\mathscr{T}_h = (V_h, E_h)$

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Flux: $j = j_{KL}$, **grad** $\varphi(K,L) = \varphi_L - \varphi_K$, **div** $j(K) = \sum_{L\sim K}\left(j_{KL} - j_{LK}\right)$

Energy-Dissipation Balance

$$\mathscr{I}_h(\rho^h, j^h) := \int_0^T \mathsf{R}_h(\rho_t^h, j_t^h) + \mathscr{D}_h(\rho_t^h)\,dt + \mathscr{E}_h(\rho_T^h) - \mathscr{E}_h(\rho_0^h) = 0$$

Fisher information: $\mathscr{D}_h(\rho) = \frac{1}{2}\sum_{KL\in E^h}\left(\textbf{grad}\sqrt{u}\,(K,L)\right)^2 \vartheta_{KL}^h$

Discrete-to-Continuum Limit

$\mathscr{T}_h = (V^h, E^h)$ **Discrete world**

$\rho^h \in \mathscr{P}(V^h), \;\; j^h \in \mathscr{M}(E^h)$

$(\rho^h, j^h) \in \mathbf{CE}_h : \mathscr{I}_h(\rho^h, j^h) = 0$

$\Omega \subset \mathbb{R}^d$ **Continuous world**

$\rho \in \mathscr{P}(\Omega), \;\; j \in \mathscr{M}(\Omega; \mathbb{R}^d)$

$(\rho, j) \in \mathbf{CE} : \mathscr{I}_0(\rho, j) = 0$

$\Omega \subset \mathbb{R}^d$ **Intermediate world**

$$\hat{\rho}^h = \sum_{K \in V^h} \rho^h_K 1_K, \;\; \hat{j}^h = \sum_{KL \in E^h} j^h_{KL} \sigma^h_{KL}$$

$(\hat{\rho}^h, \hat{j}^h) \in \mathbf{CE} : \widehat{\mathscr{I}}_h(\hat{\rho}^h, \hat{j}^h) = 0$

Compactness: $(\hat{\rho}^h, \hat{j}^h) \rightharpoonup^* (\rho, j)$

Liminf inequality:

$$\mathscr{I}_0(\rho, j) \le \liminf_{h \to 0} \widehat{\mathscr{I}}_h(\hat{\rho}^h, \hat{j}^h)$$

Chain rule: $\mathscr{I}_0(\rho, j) \ge 0$

Variational Convergence

Liminf inequality: $$\mathscr{I}_0(\rho, j) \leq \liminf_{h\to 0} \mathscr{I}_h(\rho^h, j^h)$$

Recall: $$\mathscr{I}_h(\rho^h, j^h) := \int_0^T \mathsf{R}_h(\rho_t^h, j_t^h) + \boxed{\mathscr{D}_h(\rho_t^h)}\, dt + \mathscr{E}_h(\rho_T^h) - \mathscr{E}_h(\rho_0^h)$$

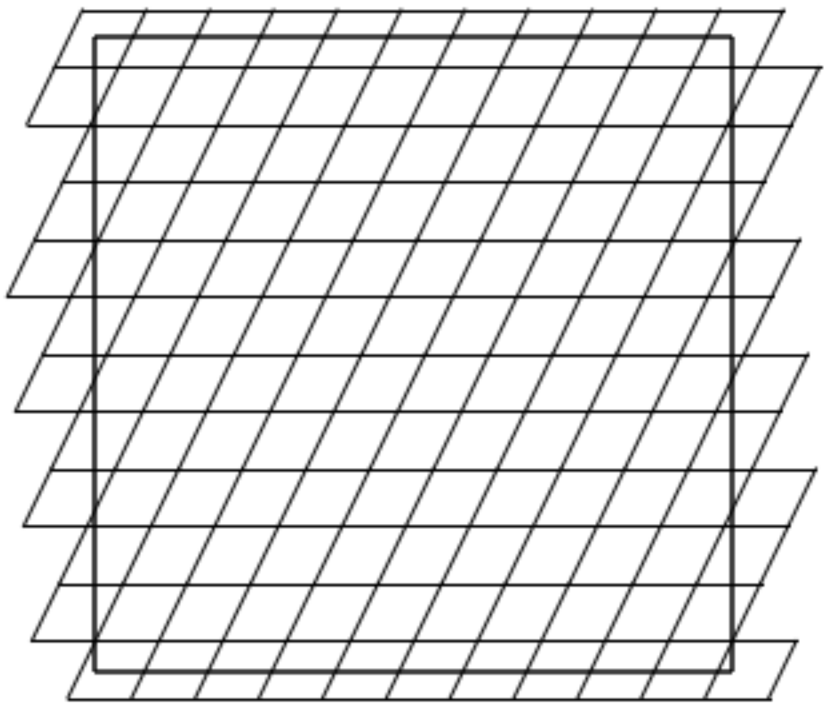
$$\mathscr{D}_h(\rho^h) = \frac{1}{2}\sum_{KL\in E^h}\left(\textbf{grad}\sqrt{u^h}\,(K,L)\right)^2 \vartheta_{KL}^h, \qquad u_K^h = \frac{\rho_K^h}{\pi_K^h}$$

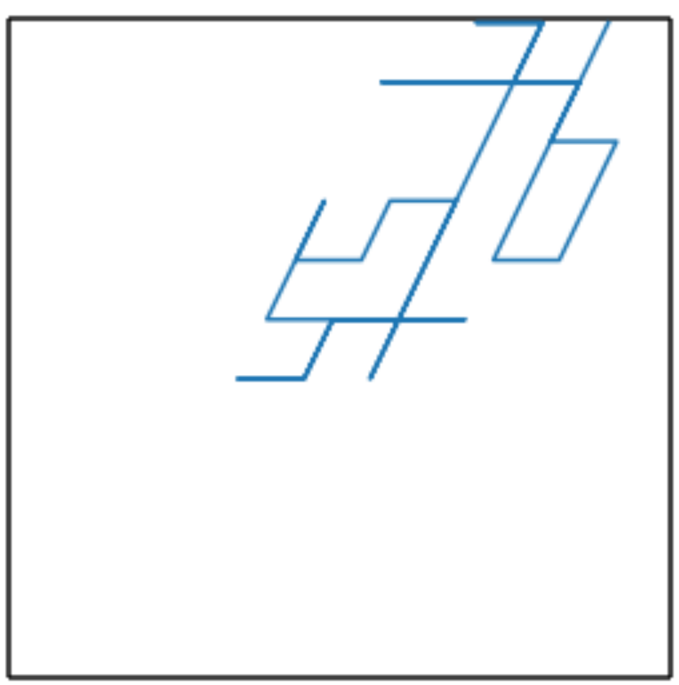
Γ-convergence result: $$\Gamma\text{-}\lim_{h\to 0}\mathscr{D}_h(\rho^h) = \mathscr{D}_0(\rho) := \frac{1}{2}\int_\Omega \left\langle \nabla\sqrt{u}, \overbrace{\mathbb{T}}^{\text{Diffusion tensor}}\nabla\sqrt{u}\right\rangle d\pi$$

$$\mathbb{T}^h := \sum_{KL\in E^h}\theta_{KL}^h (x_L - x_K)\otimes(x_L - x_K)1_K \rightharpoonup^* \mathbb{T}$$

$\left\{\begin{array}{l}\textbf{Uniformly bounded}\\ \textbf{Uniformly elliptic}\end{array}\right.$

Example: Tilted Tessellation





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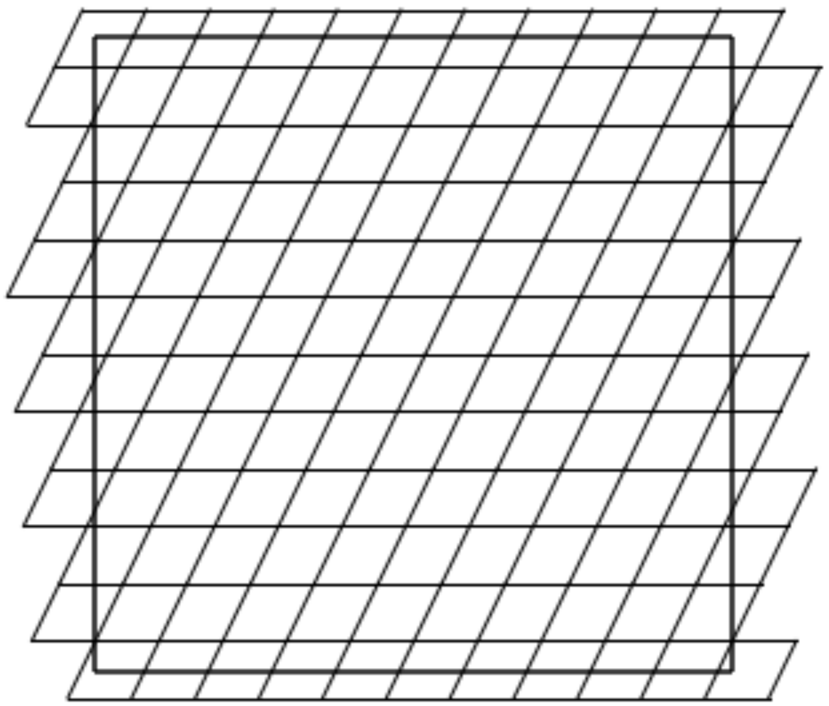
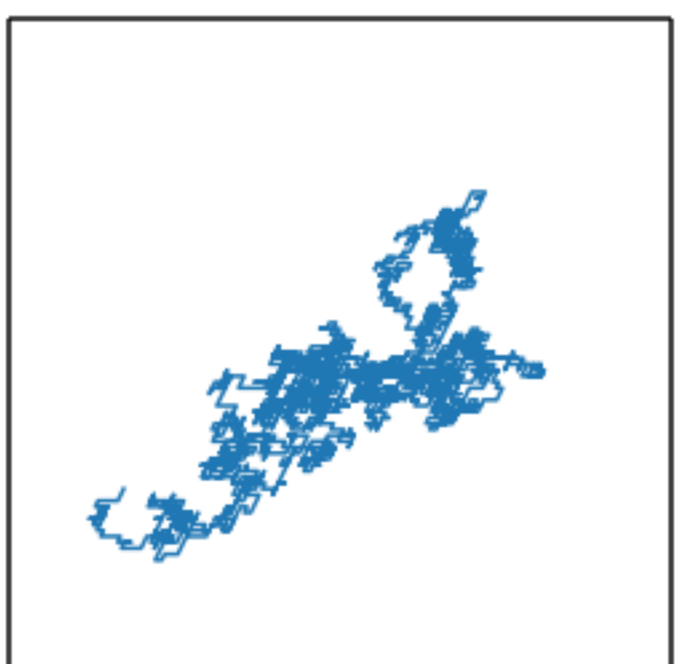


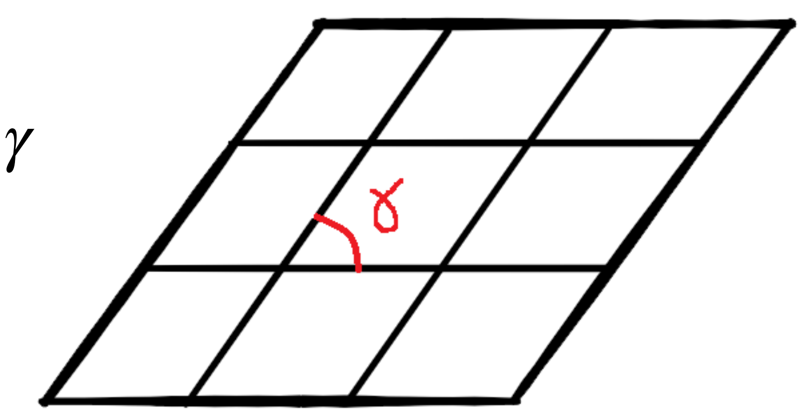


Diffusion tensor:

$$\mathbb{T}^h := \sum_{KL \in E^h} \theta^h_{KL}(x_L - x_K) \otimes (x_L - x_K) 1_K$$

$$\mathbb{T}^h \rightharpoonup^* \mathbb{T} = \begin{pmatrix} 1 + \alpha^4 & \alpha^2(1 - \alpha^2) \\ \alpha^2(1 - \alpha^2) & (1 - \alpha^2)^2 \end{pmatrix}$$

$\alpha = \cos\gamma$



Random Walks on Tessellations

Result: Let $(\rho^h)_{h>0}$ be a family of discrete solutions satisfying

$$\sup_{h>0} \mathscr{E}_h(\rho_0^h \,|\, \pi^h) < \infty, \qquad \lim_{h\to 0} \mathbf{Ent}(\hat{\rho}_0^h \,|\, \hat{\pi}^h) = \mathbf{Ent}(\rho_0 \,|\, \pi)$$

Under *some* assumptions, there is a *unique* pair $(\rho, j) \in$ **CE**

and a s.p.d. diffusion tensor $\mathbb{T} \in L^\infty(\Omega; \mathbb{R}^{d\times d})$ such that

$$\mathscr{I}_0(\rho, j) = \int_0^T \mathsf{R}(\rho_t, j_t) + \mathscr{D}(\rho_t)\, dt + \mathbf{Ent}(\rho_T \,|\, \pi) - \mathbf{Ent}(\rho_0 \,|\, \pi) = 0$$

Dissipation potential

$$\mathsf{R}(\rho, j) = \frac{1}{2}\int_\Omega \left|\frac{dj}{d\rho}\right|_{\mathbb{T}^{-1}}^2 d\rho$$

Fisher information

$$\mathscr{D}(\rho) = \frac{1}{2}\int_\Omega \left|\nabla\sqrt{u}\right|_{\mathbb{T}}^2 d\pi$$

In particular,

$$\partial_t \rho_t = \mathbf{div}\big(\mathbb{T}\nabla\rho_t - \rho_t \mathbb{T}\nabla \log \pi\big) \quad \text{in distributions}$$

Hraivoronska, T. (2023), Hraivoronska, Schlichting, T. (2024)

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Stochastic interpretation

$\exists$ a probability space: $X^h \to X$ in distribution, where

$$dX_t = \mathbb{T}(X_t)\, \nabla \log \pi(X_t)\, dt + \sqrt{2\mathbb{T}(X_t)} \circ dB_t$$

Hraivoronska, T. (2023), Hraivoronska, Schlichting, T. (2024)

Wrapping things up

Physics

PDEs $\longrightarrow$ Optimization

$$\partial_t\rho + \mathbf{div}\, j = 0$$
$$j = D_\xi \mathsf{R}^*(\rho, \xi)$$
$$\xi = -\,\mathbf{grad}\, D\mathscr{E}(\rho)$$

Energy-Dissipation Identity

$$\mathscr{I}(\rho, j) = 0$$

Diffusive limits

$$\partial_t\rho = \mathbf{div}\,\mathbb{T}(\nabla\rho - \rho\nabla\log\pi)$$

Thank you!