

# Measure-valued Proximal Recursions for Learning and Control

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# Measure-valued Optimization Problems

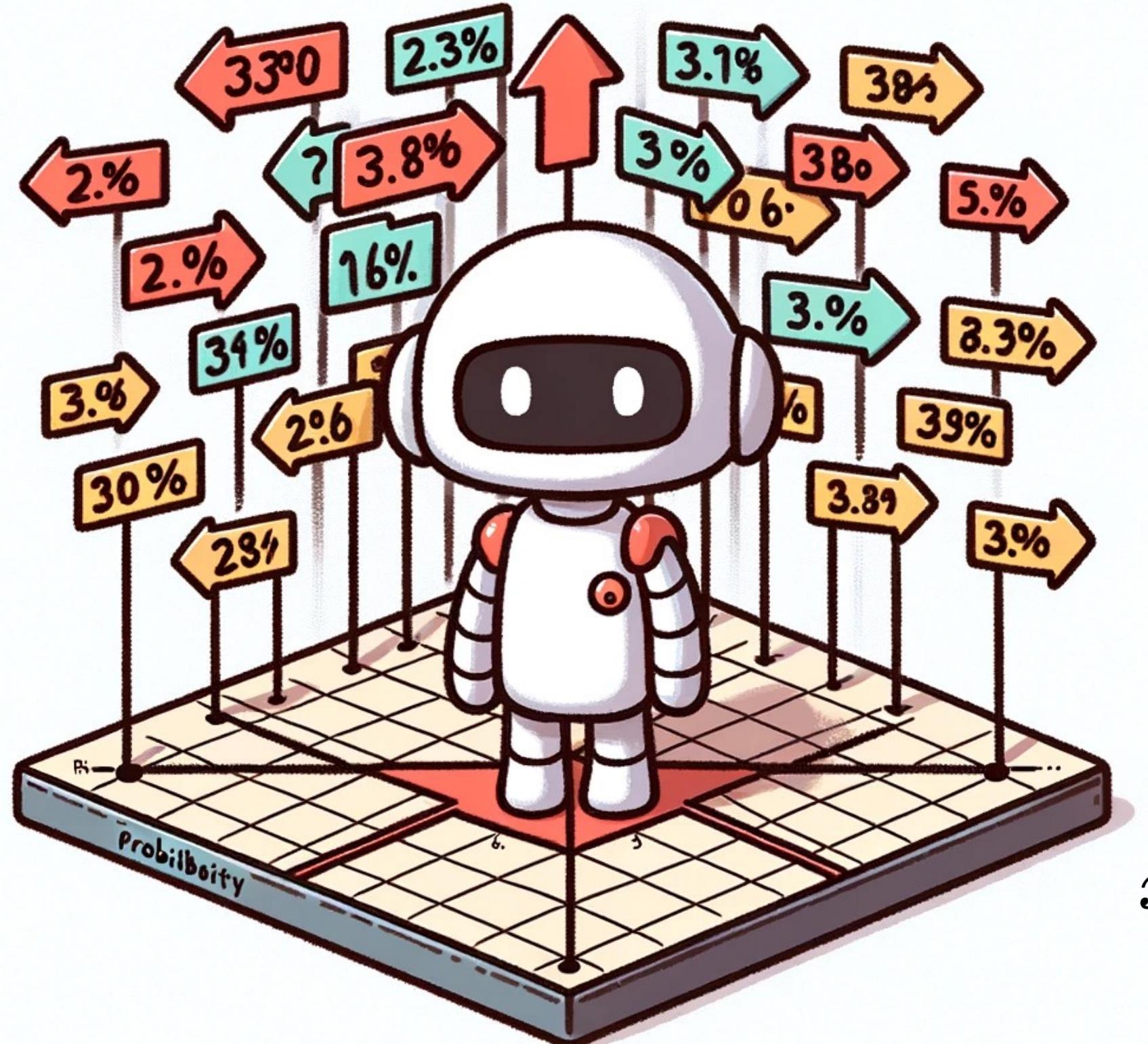
$$\mu^{\text{opt}} = \arg \inf_{\mu} F(\mu)$$

# Measure-valued Optimization Problems

$$\mu^{\text{opt}} = \arg \inf_{\mu \in \mathcal{P}_2(\mathbb{R}^d)} F(\mu)$$

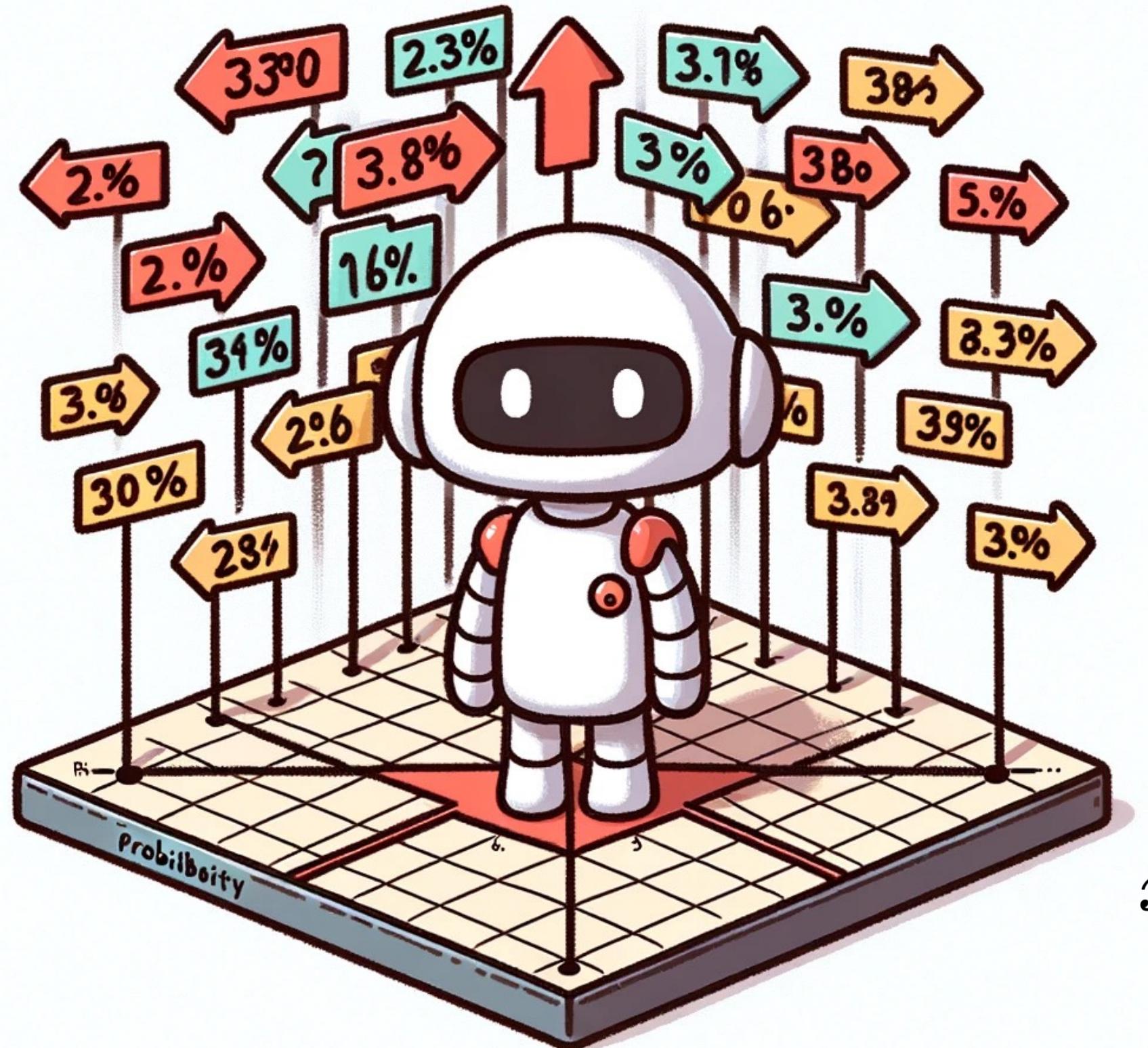
Manifold of probability measures supported on  $\mathbb{R}^d$  with finite second moments

# Probability Distribution



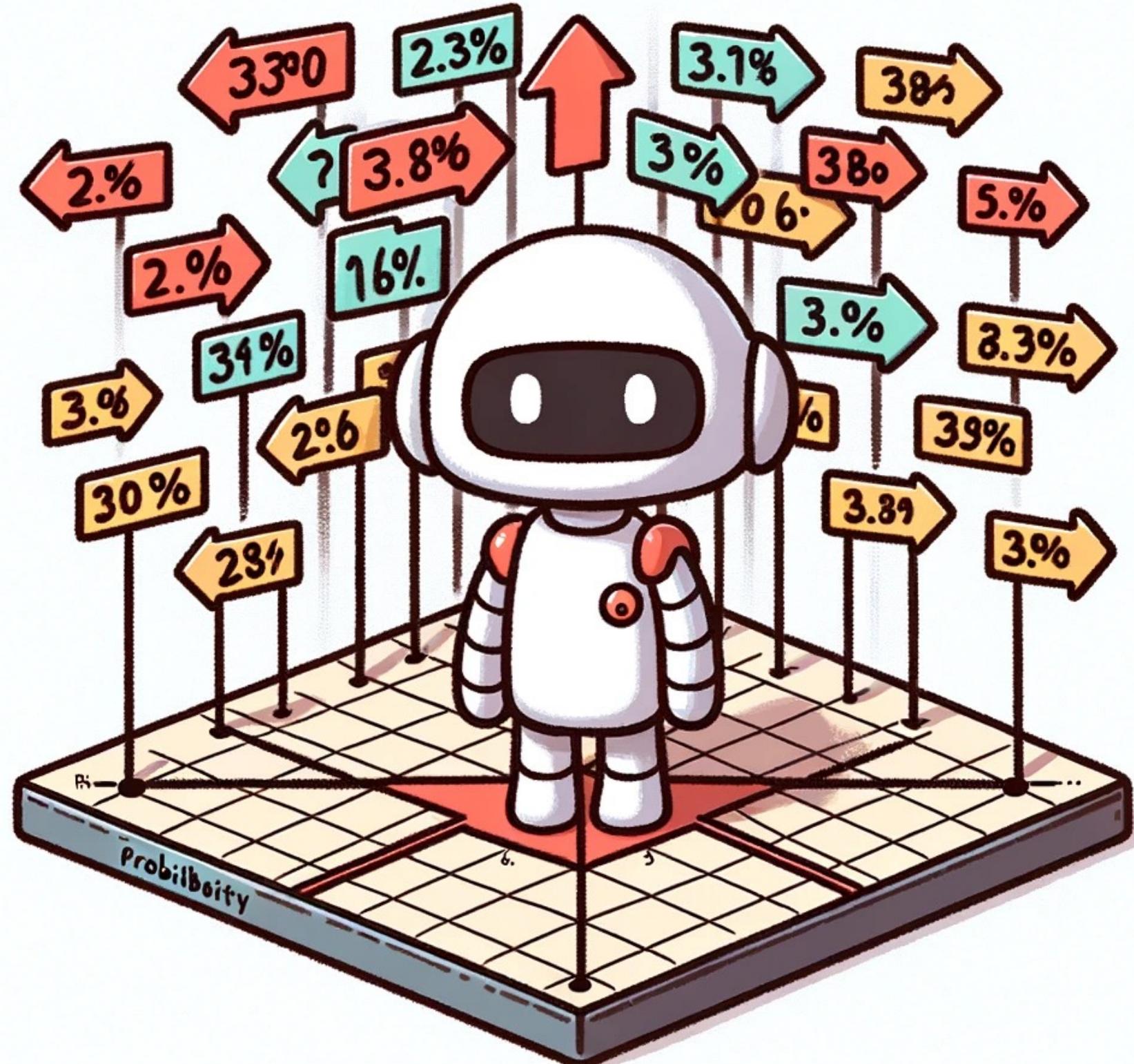
$$x(t) = \begin{pmatrix} x \\ y \\ \theta \end{pmatrix} \in \mathcal{X} \equiv \mathbb{R}^2 \times \mathbb{S}^1$$

# Probability Distribution



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# Probability Distribution

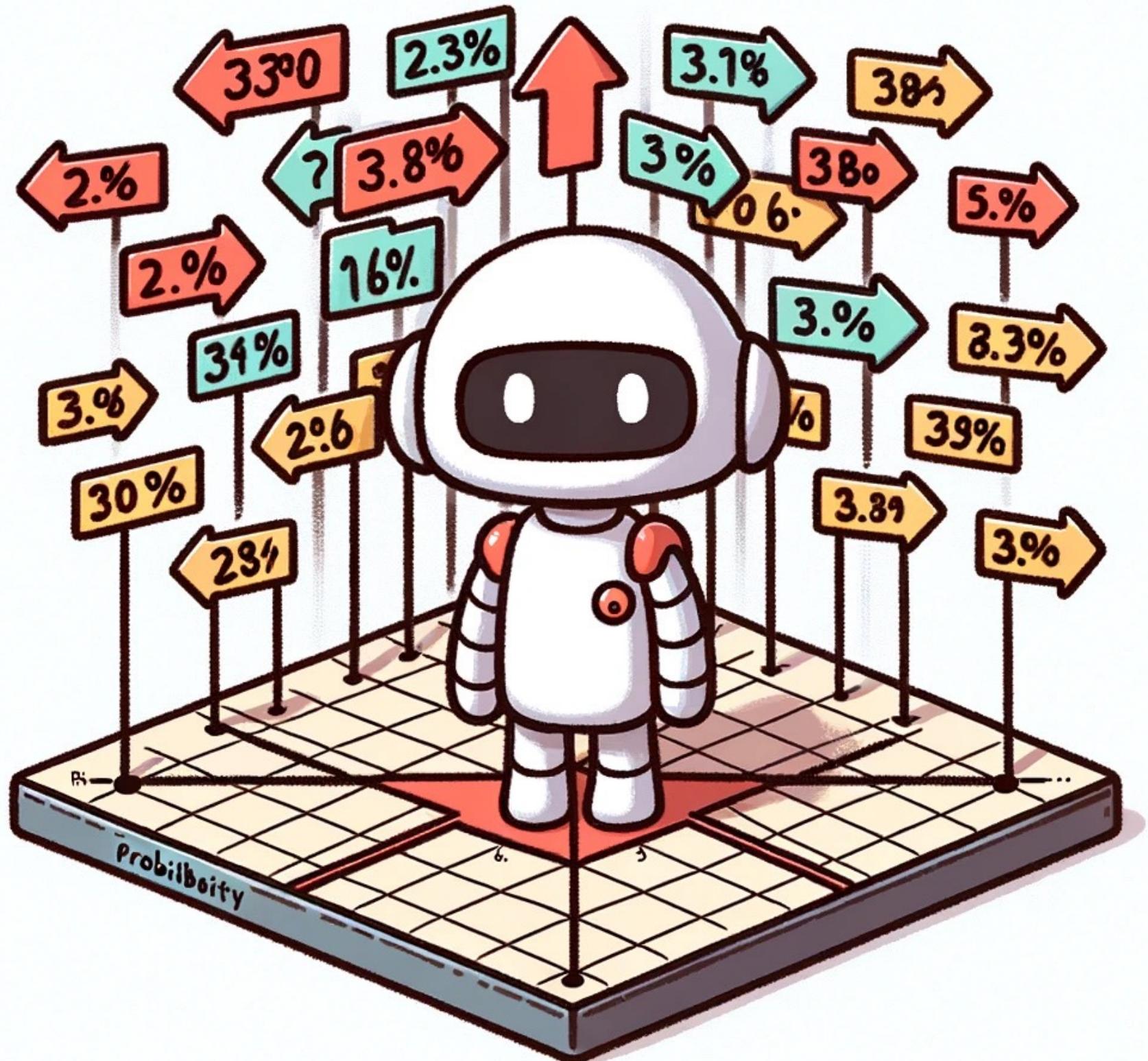


$$x(t) = \begin{pmatrix} x \\ y \\ \theta \end{pmatrix} \in \mathcal{X} \equiv \mathbb{R}^2 \times \mathbb{S}^1$$
$$\rho(x, t) : \mathcal{X} \times [0, \infty) \rightarrow \mathbb{R}_{\geq 0}$$

$$\int_{\mathcal{X}} d\mu = \int_{\mathcal{X}} \rho dx = 1 \quad \text{for all } t \in [0, \infty)$$

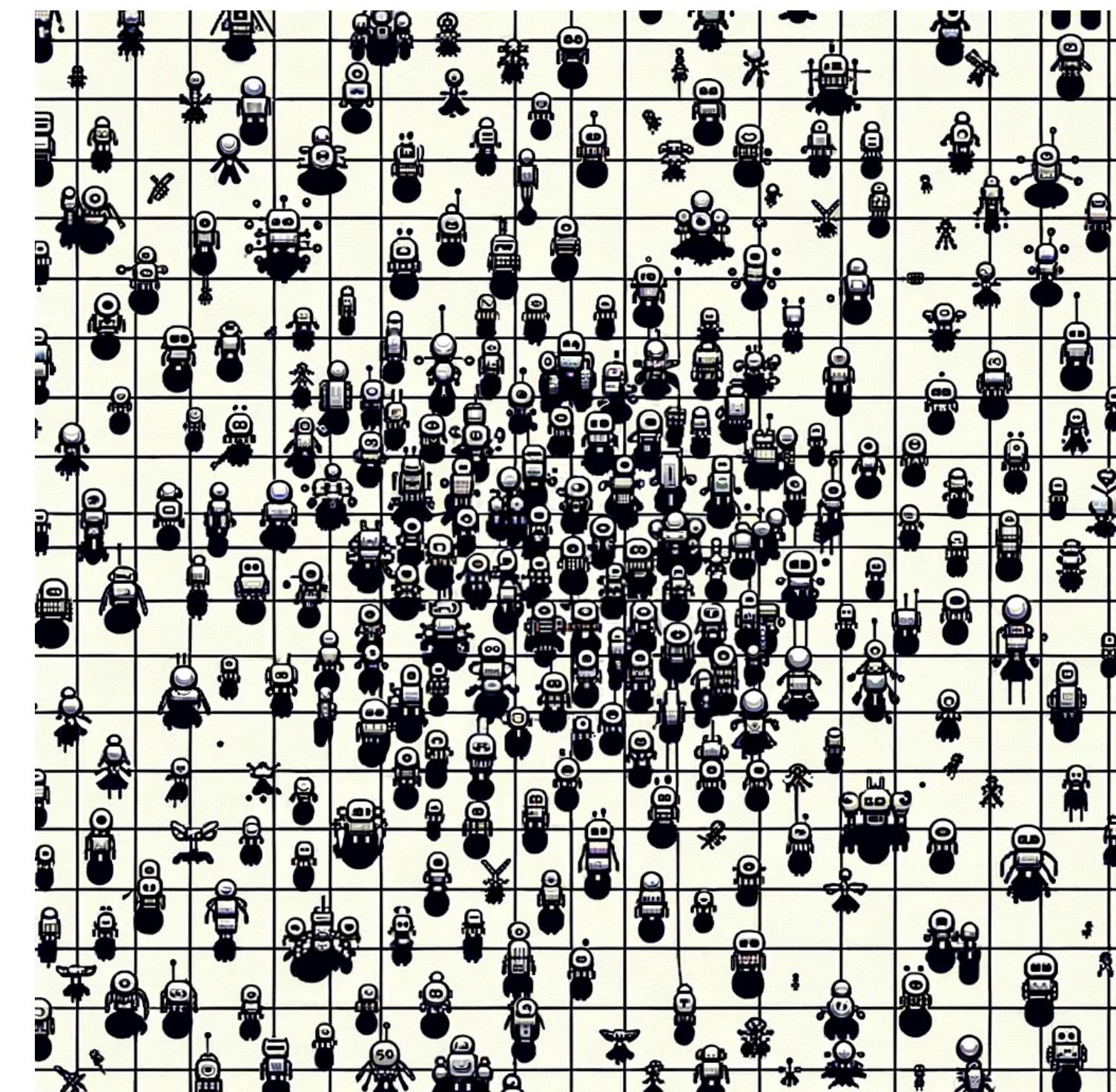
measure      Density function

# Probability Distribution



$$x(t) = \begin{pmatrix} x \\ y \\ \theta \end{pmatrix} \in \mathcal{X} \equiv \mathbb{R}^2 \times \mathbb{S}^1$$

# Population Distribution



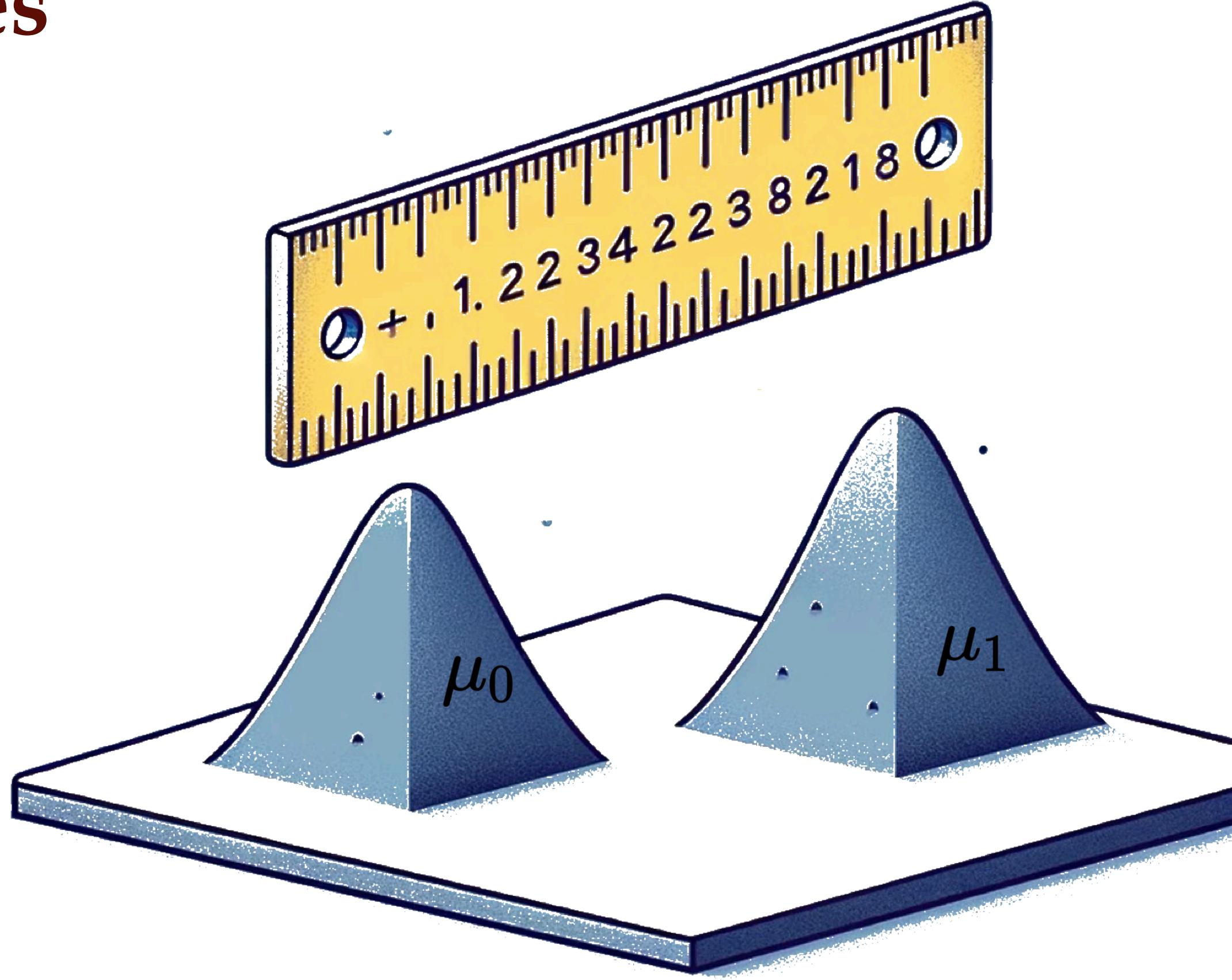
# Geometry on the Space of Prob. Measures

2-Wasserstein distance **metric**

$$W_2(\mu_0, \mu_1) := \left( \inf_m \int_{\mathcal{X} \times \mathcal{Y}} c(\mathbf{x}, \mathbf{y}) dm(\mathbf{x}, \mathbf{y}) \right)^{1/2}$$

subject to  $\int_{\mathcal{Y}} dm = \mu_0(\, d\mathbf{x}), \quad \int_{\mathcal{X}} dm = \mu_1(\, d\mathbf{y})$

Ground cost, e.g.,  $\frac{1}{2} \|\mathbf{x} - \mathbf{y}\|_2^2$



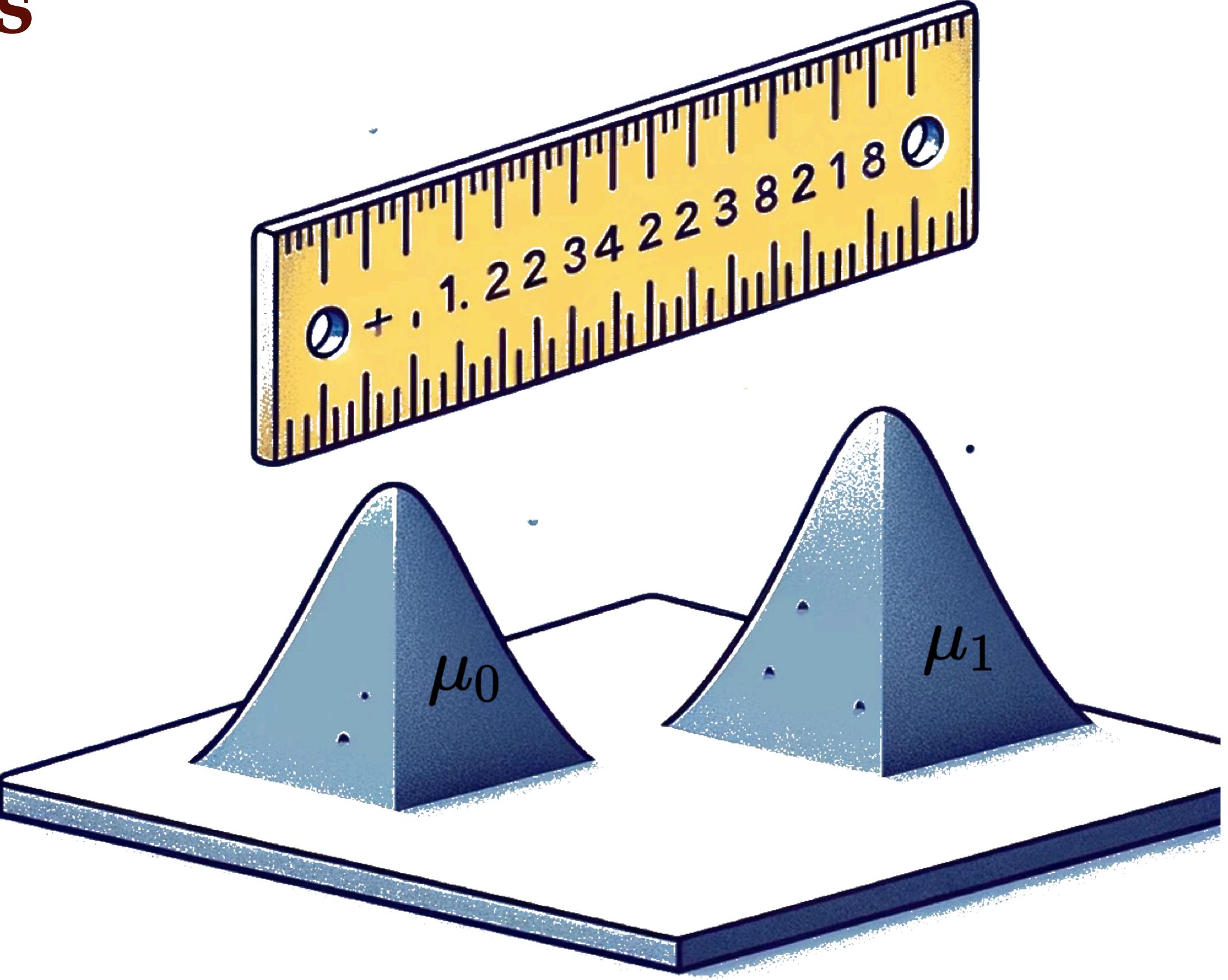
# Geometry on the Space of Prob. Measures

2-Wasserstein distance **metric**

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subject to  $\int_{\mathcal{Y}} dm = \mu_0(\, d\mathbf{x}), \quad \int_{\mathcal{X}} dm = \mu_1(\, d\mathbf{y})$

Ground cost, e.g.,  
 $\frac{1}{2} \|\mathbf{x} - \mathbf{y}\|_2^2$



Sinkhorn divergence:

$$W_\varepsilon(\mu_0, \mu_1) := \left( \inf_m \int_{\mathcal{X} \times \mathcal{Y}} \{c(\mathbf{x}, \mathbf{y}) + \varepsilon \log m\} dm(\mathbf{x}, \mathbf{y}) \right)^{1/2}, \quad \varepsilon > 0$$

subject to  $\int_{\mathcal{Y}} dm = \mu_0(\, d\mathbf{x}), \quad \int_{\mathcal{X}} dm = \mu_1(\, d\mathbf{y})$

# Connection with Wasserstein Gradient Flows

$$\frac{\partial \mu}{\partial t} = -\nabla^{W_2} F(\mu) := \nabla \cdot \left( \mu \nabla \frac{\delta F}{\delta \mu} \right) \quad (\star)$$

Wasserstein gradient

Minimizer of  $\arg \inf_{\mu \in \mathcal{P}_2(\mathbb{R}^d)} F(\mu)$        $\longleftrightarrow$       Stationary solution of  $(\star)$

Transient solution of  $(\star)$        $\rightsquigarrow$       Discrete time-stepping realizing  
grad. descent of  $\arg \inf_{\mu \in \mathcal{P}_2(\mathbb{R}^d)} F(\mu)$

Wasserstein proximal recursion à la Jordan-Kinderlehrer-Otto (JKO) scheme

# Gradient Flows

## Gradient Flow in $\mathcal{X}$

---

$$\frac{dx}{dt} = -\nabla f(x), \quad x(0) = x_0$$

Recursion:

$$\begin{aligned} x_k &= x_{k-1} - h \nabla f(x_k) \\ &= \arg \min_{x \in \mathcal{X}} \left\{ \frac{1}{2} \|x - x_{k-1}\|_2^2 + h f(x) \right\} \\ &=: \text{prox}_{h f}^{\|\cdot\|_2}(x_{k-1}) \end{aligned}$$

Convergence:

$$x_k \rightarrow x(t = kh) \quad \text{as} \quad h \downarrow 0$$

## Gradient Flow in $\mathcal{P}_2(\mathcal{X})$

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$$\frac{\partial \mu}{\partial t} = -\nabla^W F(\mu), \quad \mu(x, 0) = \mu_0$$

Recursion:

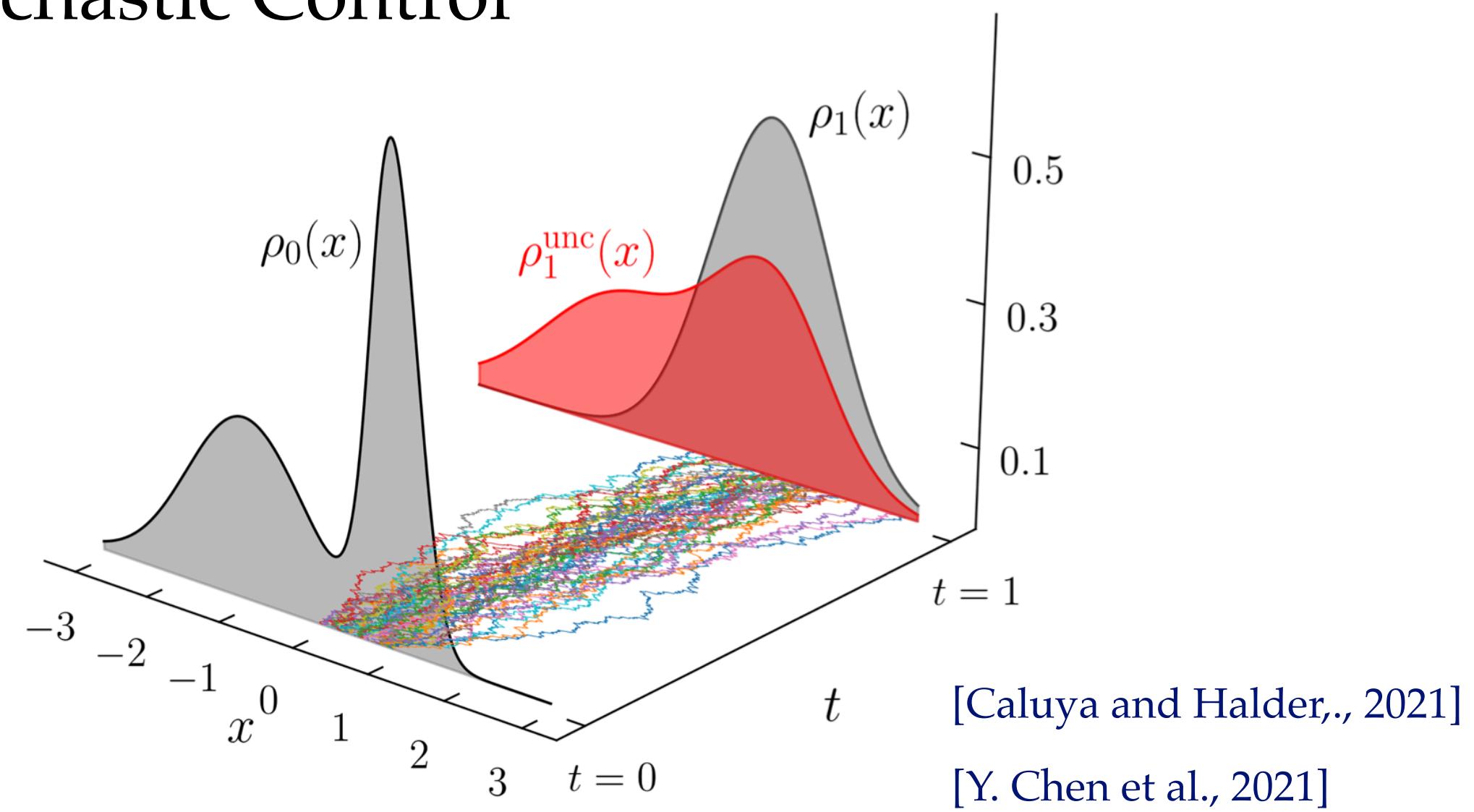
$$\begin{aligned} \mu_k &= \mu(\cdot, t = kh) \\ &= \arg \min_{\mu \in \mathcal{P}_2(\mathcal{X})} \left\{ \frac{1}{2} W^2(\mu, \mu_{k-1}) + h F(\mu) \right\} \\ &=: \text{prox}_{h F}^W(\mu_{k-1}) \end{aligned}$$

Convergence:

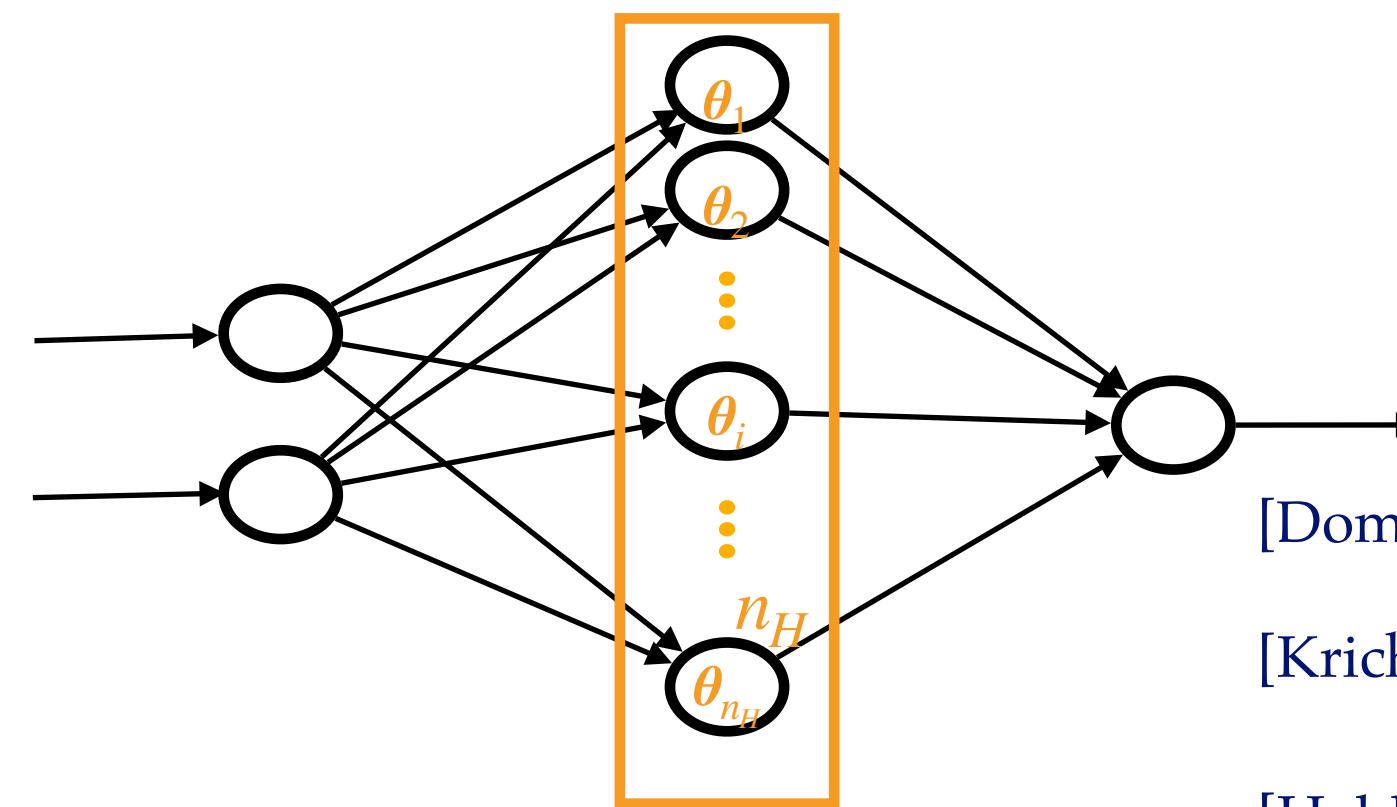
$$\mu_k \rightarrow \mu(\cdot, t = kh) \quad \text{as} \quad h \downarrow 0$$

# Motivating Applications

## Stochastic Control



## Stochastic learning



[Domingo-Enrich et al., 2020]

[Krichene, et al., 2020]

[Halder et al., 2020]

## Stochastic Modeling

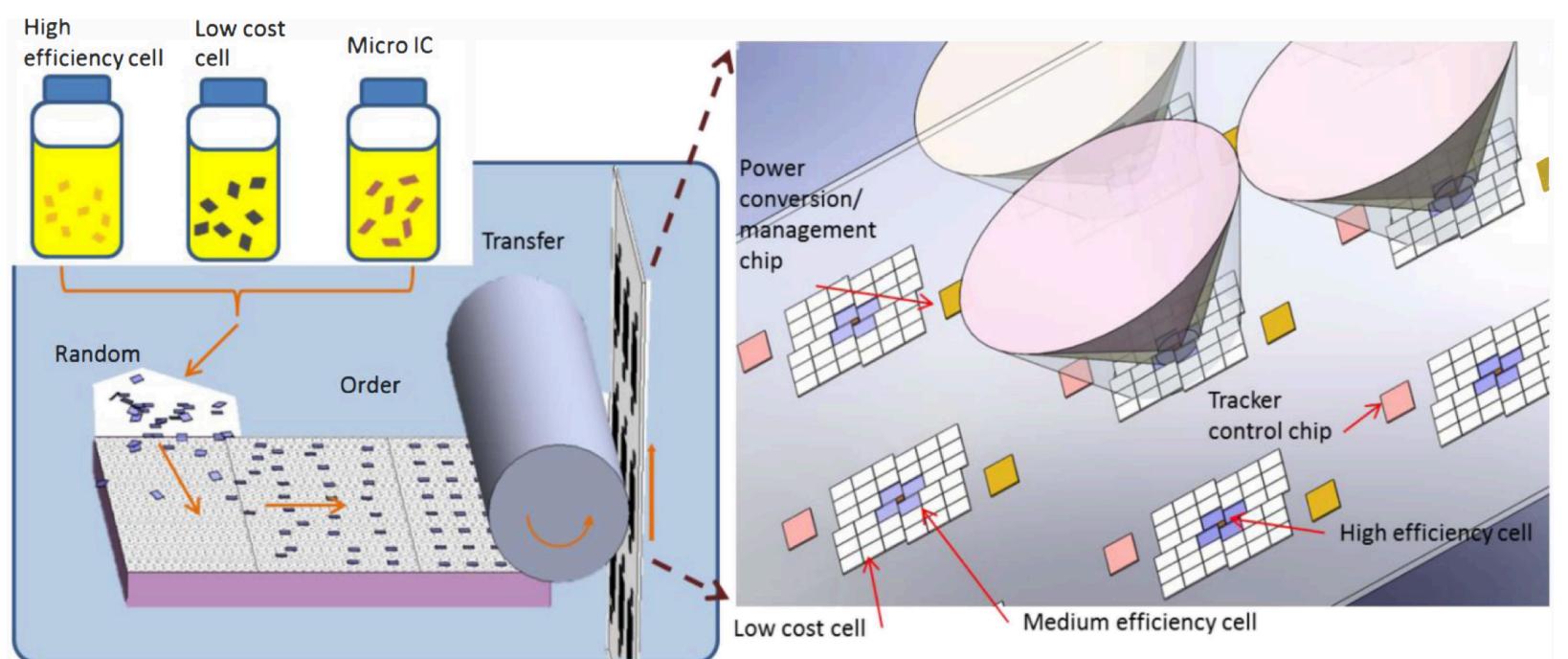


Image credit: PARC

## Generative AI

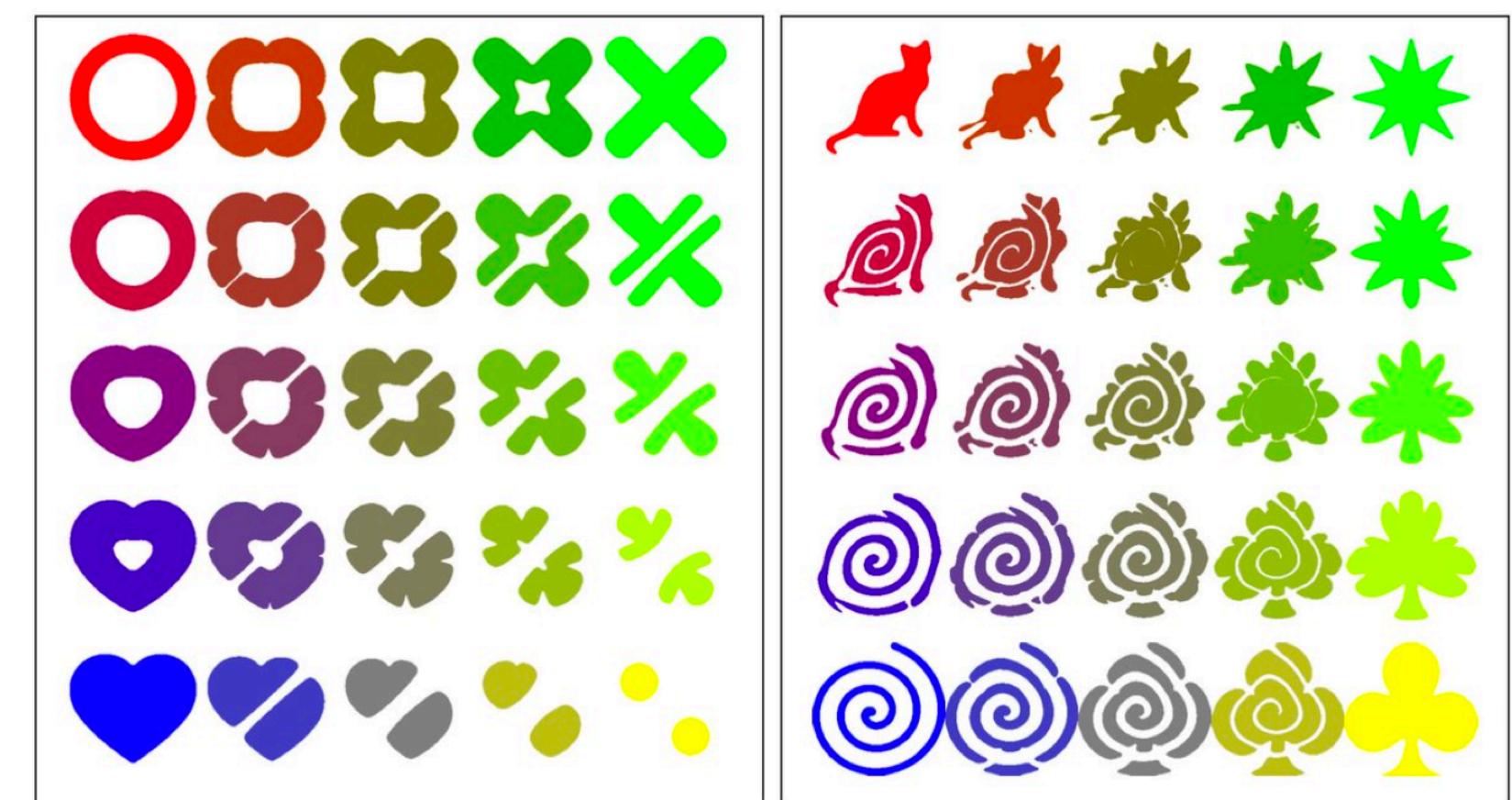


Image credit: G. Pyre

# Contributions

## Part I: Optimal Stochastic Control of Generalized Schrödinger Bridge in

The Control-affine Case Knowing the Model Structure [I. Nodzoi, A. Halder, CDC 22]

The Control Non-affine Case Knowing the Model Structure [I. Nodzoi, et. al., ACC 23]

The Control Non-affine Case not Knowing the Model Structure [I. Nodzoi, et. al., IEEE TCST 23]

## Part II: Stochastic Modeling and Solving of Chiplet Population Dynamics

A Controlled Mean Field Model for Chiplet Population Dynamics [I. Nodzoi, et. al., IEEE LCSS 23]

## Part III: Stochastic Learning

Centralized Computing: Mean Field Learning [A. Teter, I. Nodzoi, A. Halder, TMLR 23]

Distributed Computing: Wasserstein Consensus ADMM [I. Nodzoi, A. Halder, arXiv]

## **Part I: Optimal Stochastic Control of Generalized Schrödinger Bridge**

# Stochastic Control

$$\inf_{\mathbf{u} \in \mathcal{U}} \mathbb{E}_{\mu^u} \left\{ \int_0^T \frac{1}{2} \|\mathbf{u}(\mathbf{x}, t)\|_2^2 dt \right\}$$

subject to

$$d\mathbf{x} = \mathbf{f}(t, \mathbf{x}, \mathbf{u})dt + \sqrt{2\beta^{-1}}\mathbf{g}(t, \mathbf{x}, \mathbf{u})dw$$

$$\mathbf{x}(t=0) \sim \mu_0(\mathbf{x}), \quad \mathbf{x}(t=T) \sim \mu_T(\mathbf{x})$$

Control affine

$$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + \mathbf{B}(t)\mathbf{u}(\mathbf{x}, t)dt + \sqrt{2\epsilon}\mathbf{B}(t)dw$$

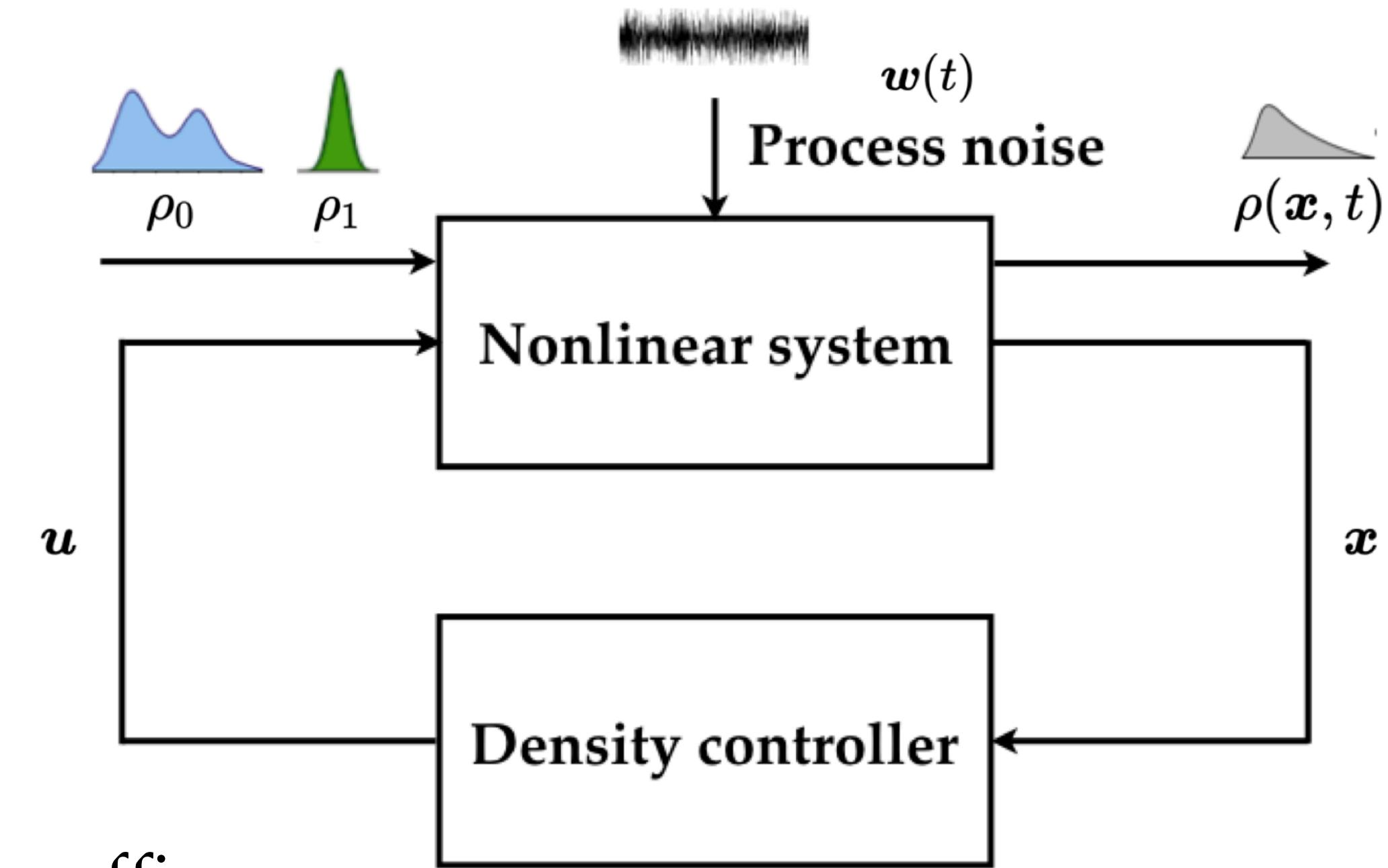
Case study: Nonuniform Noisy Kuramoto Oscillators

Control non-affine

$$d\mathbf{x} = \mathbf{f}(t, \mathbf{x}, \mathbf{u})dt + \sqrt{2\beta^{-1}}\mathbf{g}(t, \mathbf{x}, \mathbf{u})dw$$

Case study: Controlled Self-assembly

$\begin{cases} \text{Model-based} \\ \text{Model-free} \end{cases}$



# Stochastic Control/ Control-affine

## Conditions for Optimality

$$\frac{\partial}{\partial t} \rho^{\text{opt}} + \nabla \cdot \left( \rho^{\text{opt}} (f + \mathbf{B}(t)^\top \nabla \psi) \right) = \epsilon \left\langle \mathbf{D}(t), \text{Hess} (\rho^{\text{opt}}) \right\rangle$$

Controlled FPK PDE

$$\frac{\partial \psi}{\partial t} + \frac{1}{2} \left\| \mathbf{B}(t)^\top \nabla \psi \right\|_2^2 + \langle \nabla \psi, f \rangle = -\epsilon \langle \mathbf{D}(t), \text{Hess} (\psi) \rangle$$

HJB PDE

$$\mathbf{u}^{\text{opt}}(\mathbf{x}, t) = \mathbf{B}(t)^\top \nabla \psi(\mathbf{x}, t)$$

Optimal policy

$$\rho^{\text{opt}}(\mathbf{x}, 0) = \rho_0(\mathbf{x}), \quad \rho^{\text{opt}}(\mathbf{x}, T) = \rho_T(\mathbf{x})$$

Boundary conditions

# Stochastic Control/ Control-affine

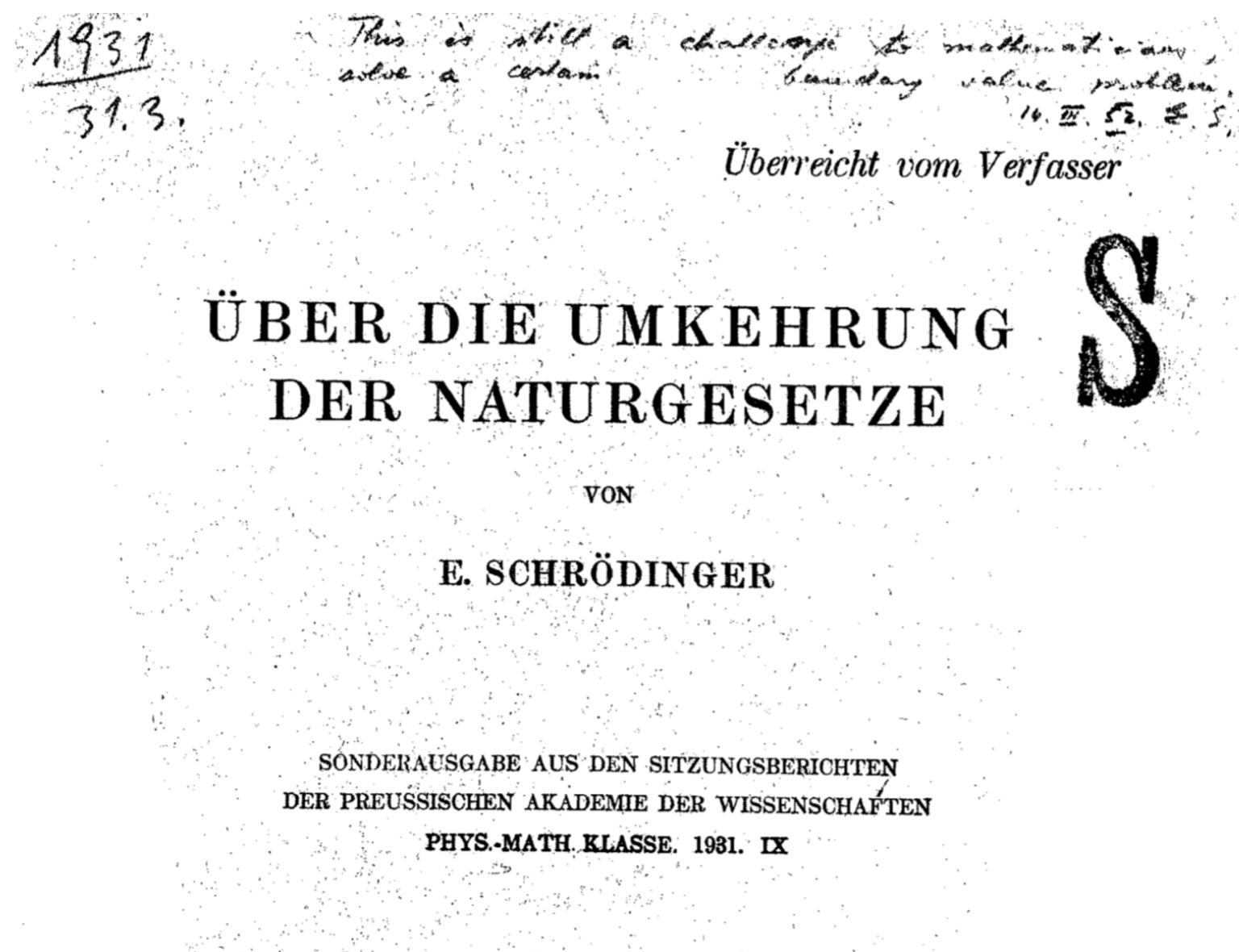
Hopf-Cole a.k.a. Fleming's logarithmic transform:

$$(\rho^{\text{opt}}, \psi) \mapsto (\widehat{\varphi}, \underline{\varphi})$$

Schrödinger factors

$$\varphi(x, t) = \exp\left(\frac{\psi(x, t)}{2\epsilon}\right)$$

$$\hat{\varphi}(x, t) = \rho^{\text{opt}}(x, t) \exp\left(-\frac{\psi(x, t)}{2\epsilon}\right)$$

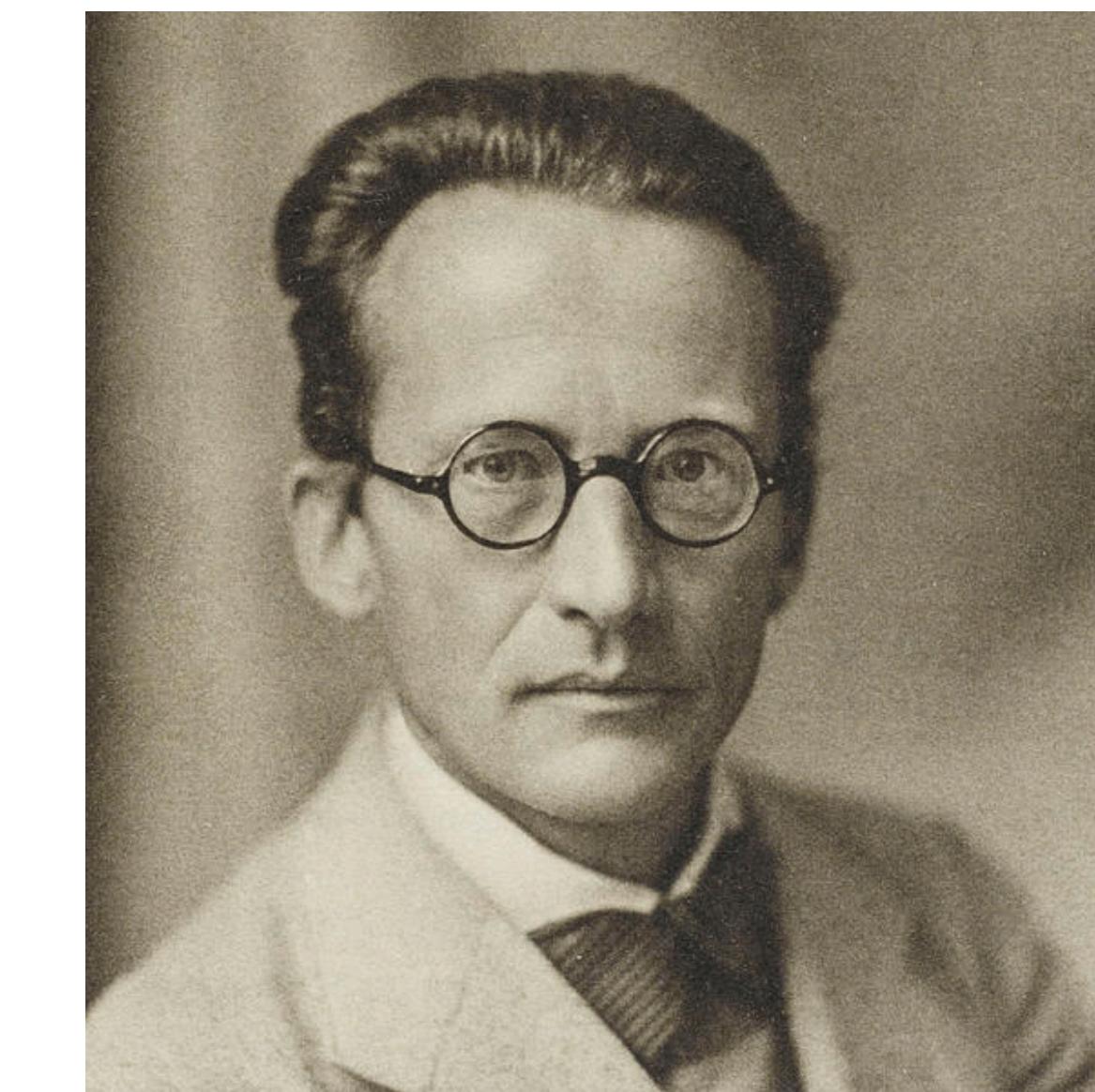


Sur la théorie relativiste de l'électron  
et l'interprétation de la mécanique quantique

PAR  
E. SCHRÖDINGER

## I. — Introduction

J'ai l'intention d'exposer dans ces conférences diverses idées concernant la mécanique quantique et l'interprétation qu'on en donne généralement à l'heure actuelle ; je parlerai principalement de la théorie quantique relativiste du mouvement de l'électron. Autant que nous pouvons nous en rendre compte aujourd'hui, il semble à peu près sûr que la mécanique quantique de l'électron, sous sa forme idéale, que nous ne possédons pas encore, doit former un jour la base de toute la physique. A cet intérêt tout à fait général, s'ajoute, ici à Paris, un intérêt particulier : vous savez tous que les bases de la théorie moderne de l'électron ont été posées à Paris par votre célèbre compatriote Louis de BROGLIE.



# Stochastic Control/ Control-affine

2 coupled nonlinear PDEs → boundary-coupled linear PDEs!!

$$\frac{\partial \varphi}{\partial t} = - \langle \nabla \varphi, f \rangle - \epsilon \langle D(t), \text{Hess}(\varphi) \rangle$$

Forward Fokker-Planck PDE

$$\frac{\partial \hat{\varphi}}{\partial t} = - \nabla \cdot (\hat{\varphi} f) + \epsilon \langle D(t), \text{Hess}(\hat{\varphi}) \rangle$$

Backward Fokker-Planck PDE

Initial and Terminal conditions

$$\varphi(x, 0)\hat{\varphi}(x, 0) = \rho_0(x)$$

$$\varphi(x, T)\hat{\varphi}(x, T) = \rho_T(x)$$

Optimal controlled joint state PDF:

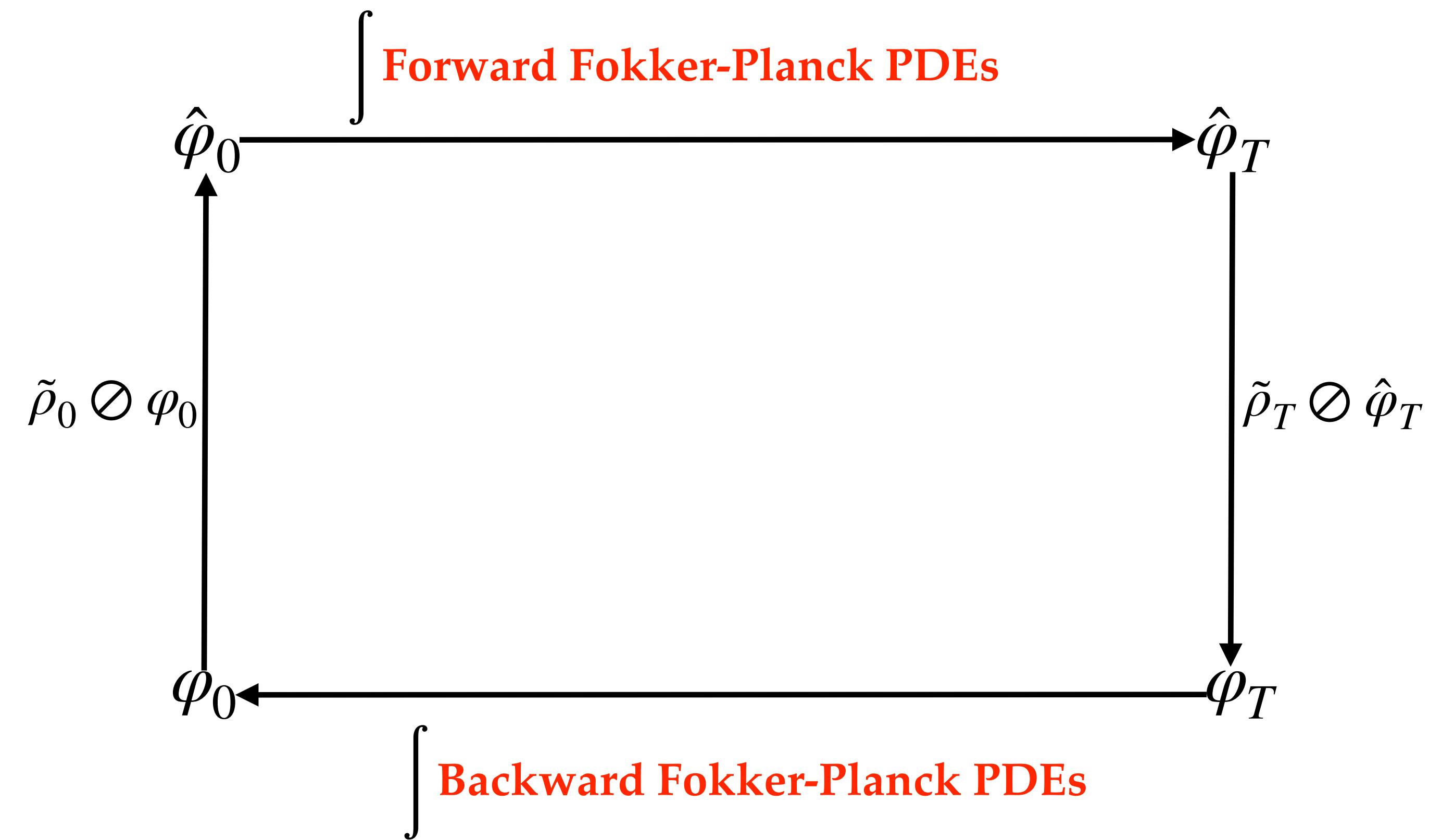
$$\rho^{\text{opt}}(x, t) = \varphi(x, t)\hat{\varphi}(x, t)$$

Optimal control:

$$u^{\text{opt}}(x, t) = 2\epsilon B(t)^T \nabla \log \varphi$$

# Stochastic Control/ Control-affine

Fixed Point Recursion Over Pair  $(\varphi, \hat{\varphi})$

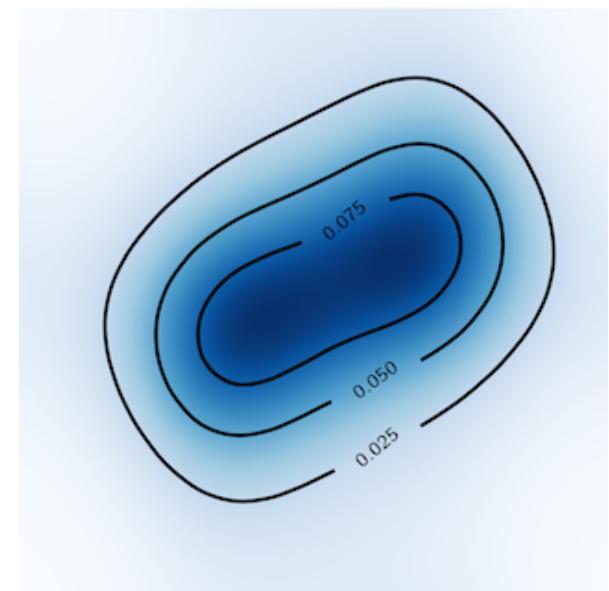


# Stochastic Control/ Control-affine: Nonuniform Noisy Kuramoto Oscillators

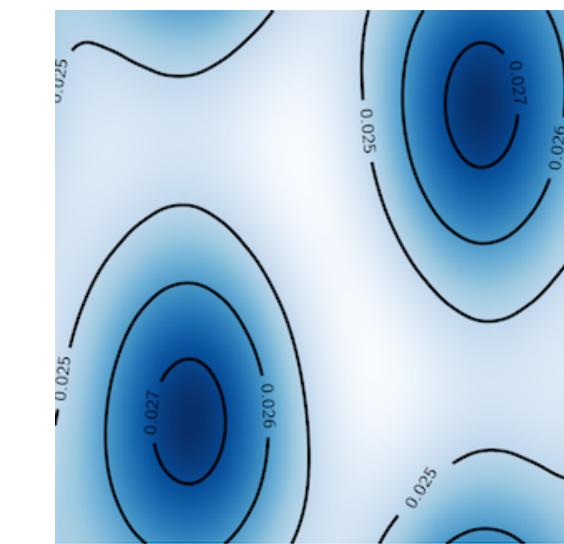
## First order Case Study

$$\inf_{u \in \mathcal{U}} \quad \mathbb{E}_{\mu^u} \left[ \int_0^T \frac{1}{2} u^2 \, dt \right],$$

$$d\theta = (-\nabla_\theta V(\theta) + Su) \, dt + \sqrt{2} S d\omega$$



$\theta(t = 0) \sim \mu_0$  (Desynchronized)



$\theta(t = T) \sim \tilde{\mu}_T$  (Synchronized)

# Stochastic Control/ Control-affine: Nonuniform Noisy Kuramoto Oscillators

Uncontrolled forward-backward Kolmogorov PDEs:

$$\frac{\partial \hat{\phi}}{\partial t} = \nabla_{\xi} \cdot \left( \hat{\phi} \Upsilon \nabla_{\xi} \tilde{V} \right) + \Delta_{\xi} \hat{\phi}$$

Forward Fokker-Planck PDE

$$\frac{\partial \varphi}{\partial t} = \left\langle \nabla_{\xi} \varphi, \Upsilon \nabla_{\xi} \tilde{V} \right\rangle - \Delta_{\xi} \varphi$$

Backward Fokker-Planck PDE

Initial and Terminal conditions

$$\hat{\phi}_0(\xi) \varphi_0(\xi) = \rho_0(S\xi) \left( \prod_{i=1}^n \sigma_i \right)$$

$$\hat{\phi}_T(\xi) \varphi_T(\xi) = \rho_T(S\xi) \left( \prod_{i=1}^n \sigma_i \right)$$

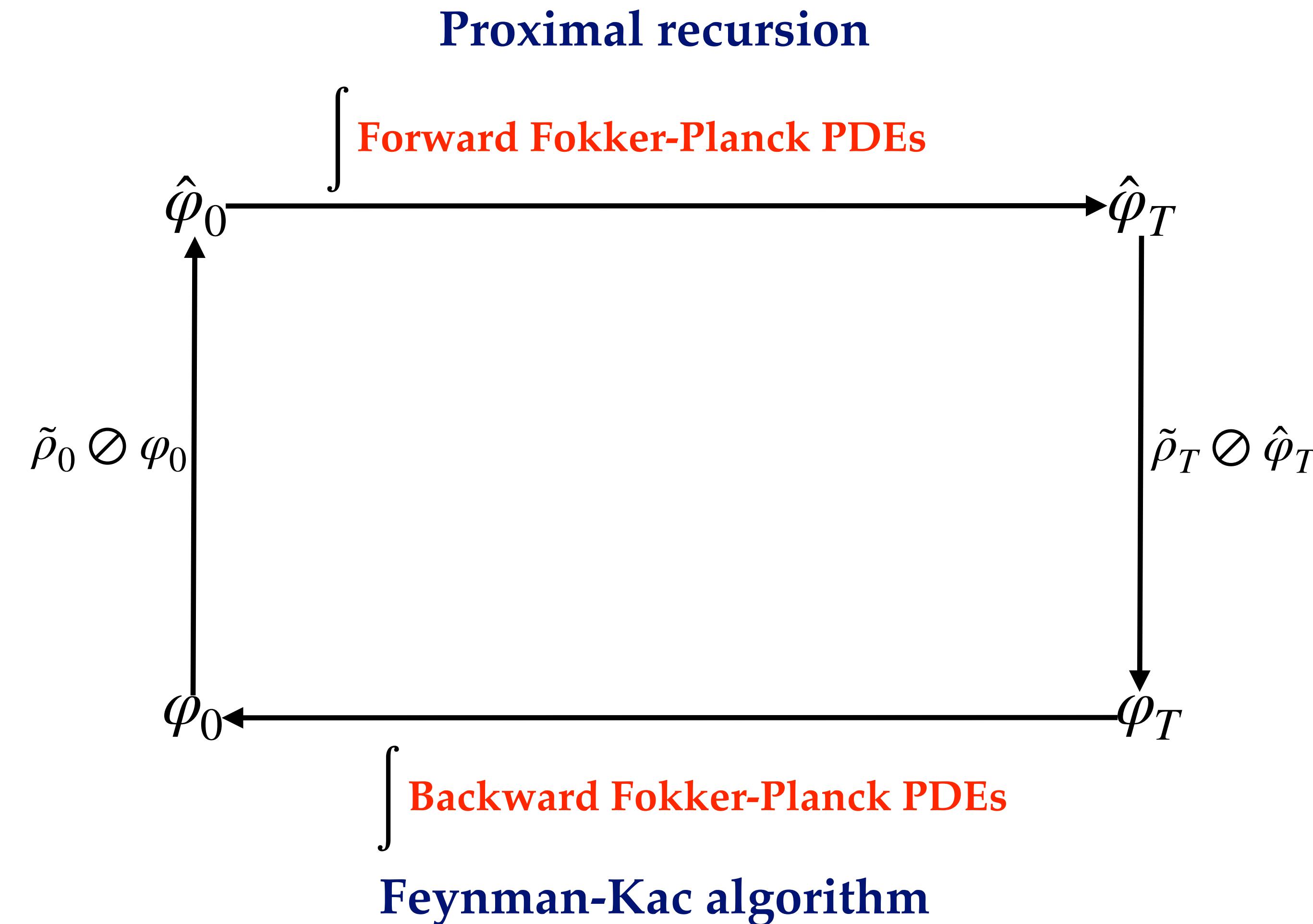
Optimal controlled joint state PDF:

$$\rho^{\text{opt}}(\theta, t) = \hat{\phi}(S^{-1}\theta, t) \varphi(S^{-1}\theta, t) / \left( \prod_{i=1}^n \sigma_i \right)$$

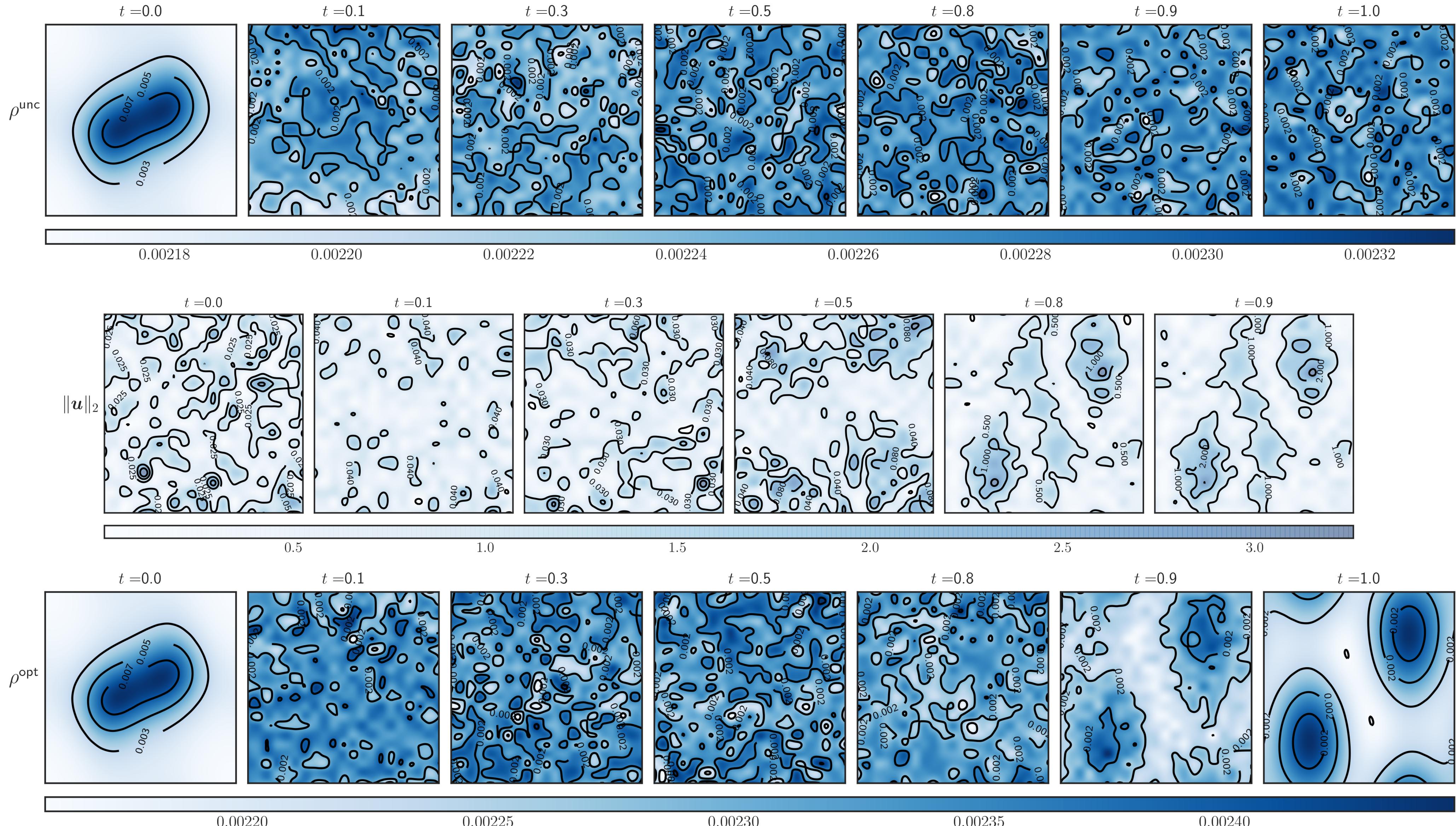
Optimal control:  $\boldsymbol{u}^{\text{opt}}(\theta, t) = S \nabla_{\theta} \log \varphi(S^{-1}\theta, t)$

# Stochastic Control/ Control-affine: Nonuniform Noisy Kuramoto Oscillators

Fixed Point Recursion Over Pair  $(\varphi, \hat{\varphi})$

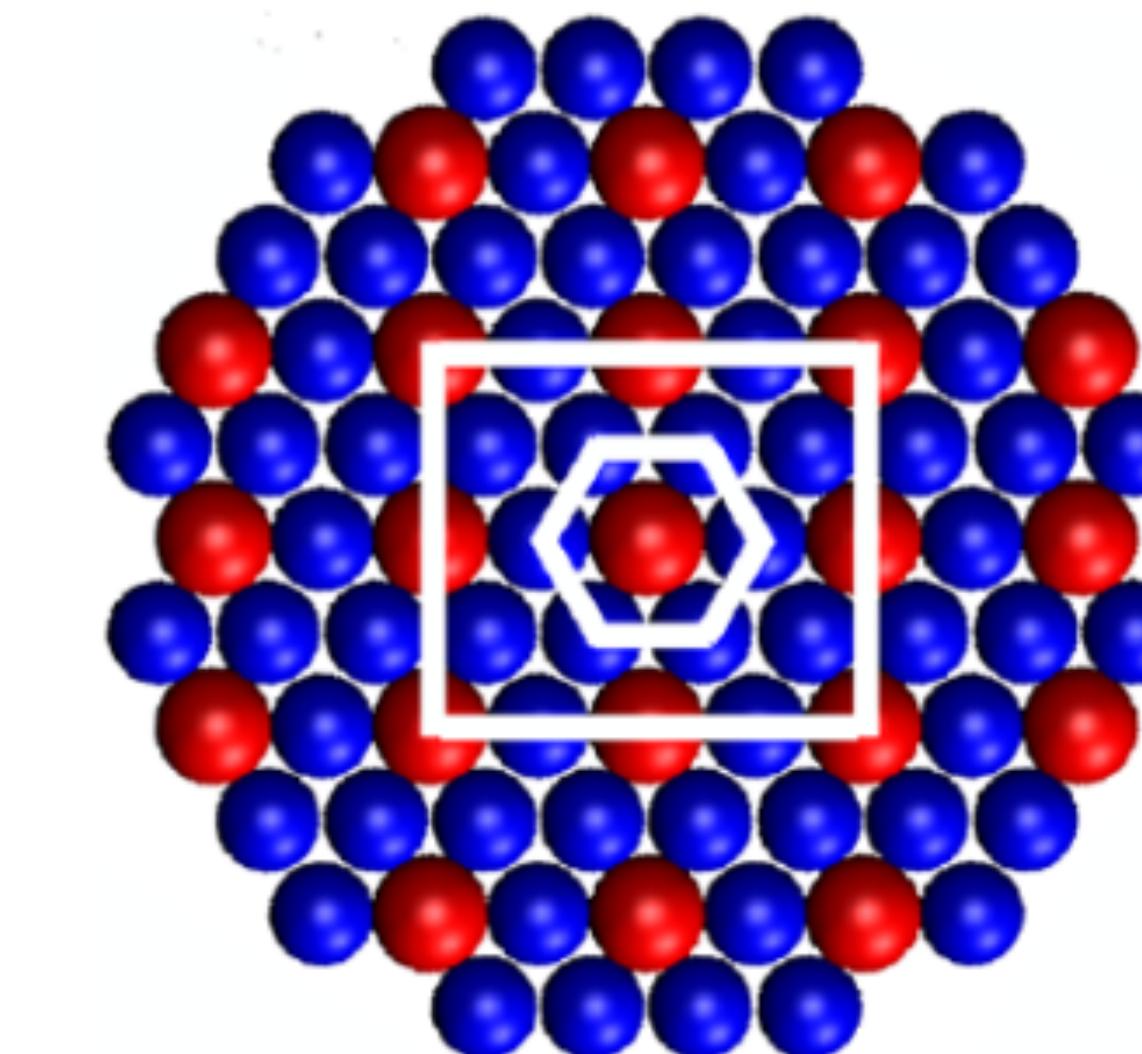
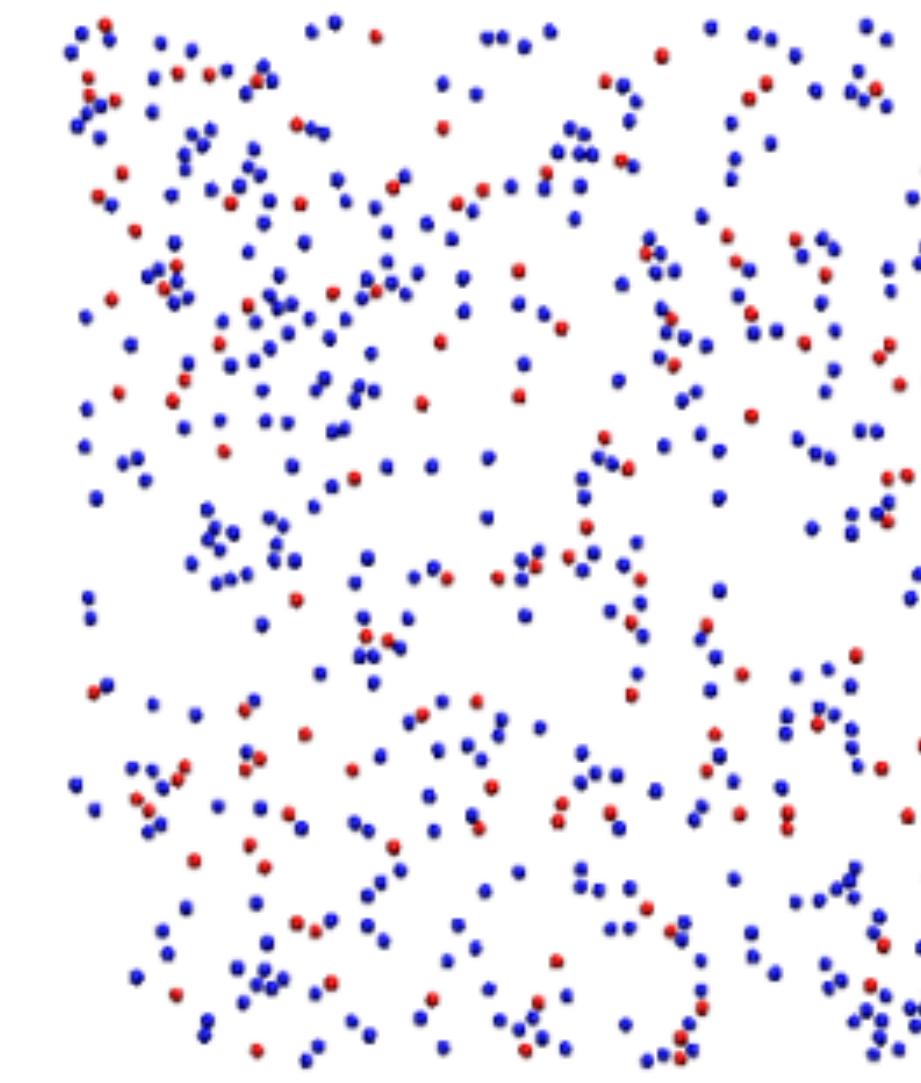


# Stochastic Control/ Control-affine: Nonuniform Noisy Kuramoto Oscillators



# Stochastic Control / Control Non-affine

Controlled Self-assembly



Dispersed particles

Ordered structure

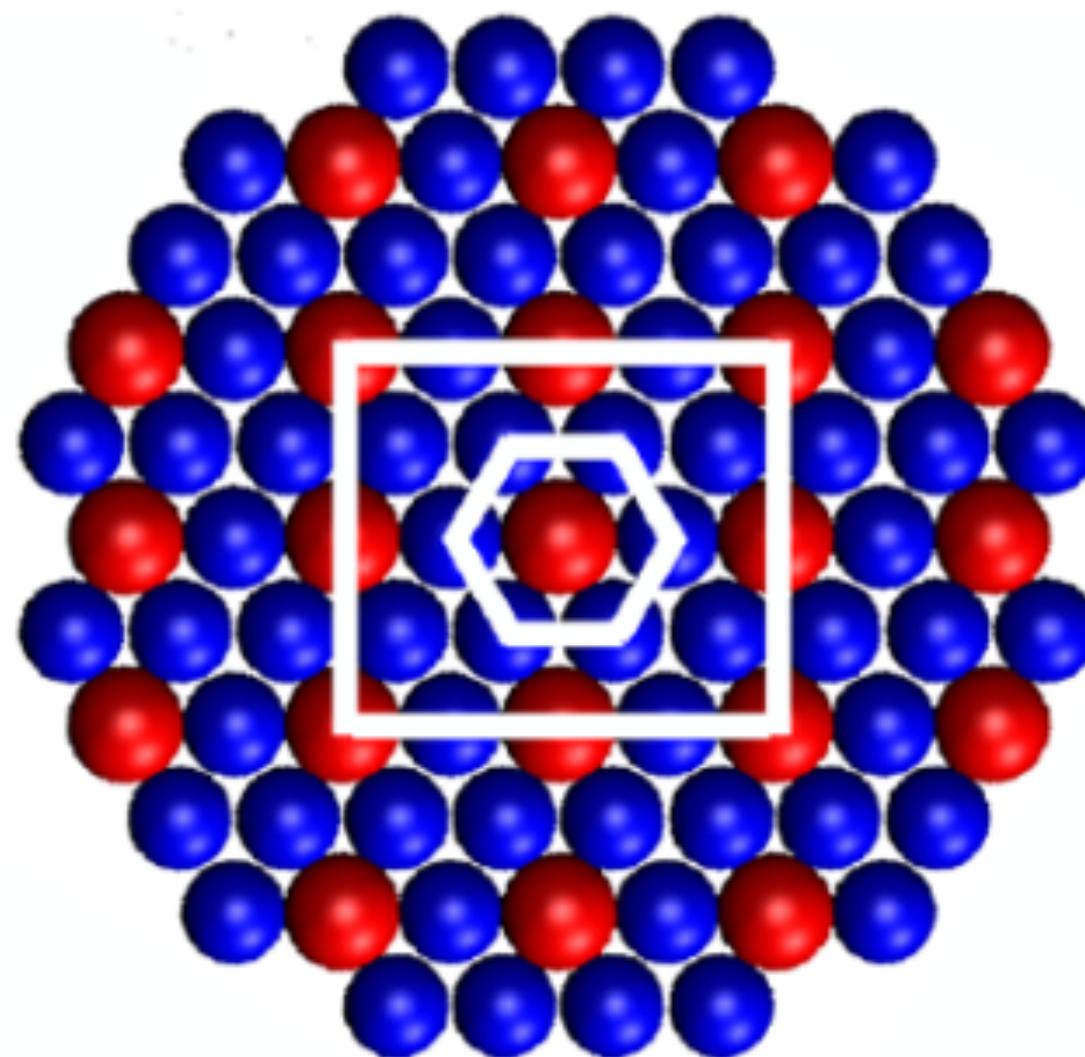
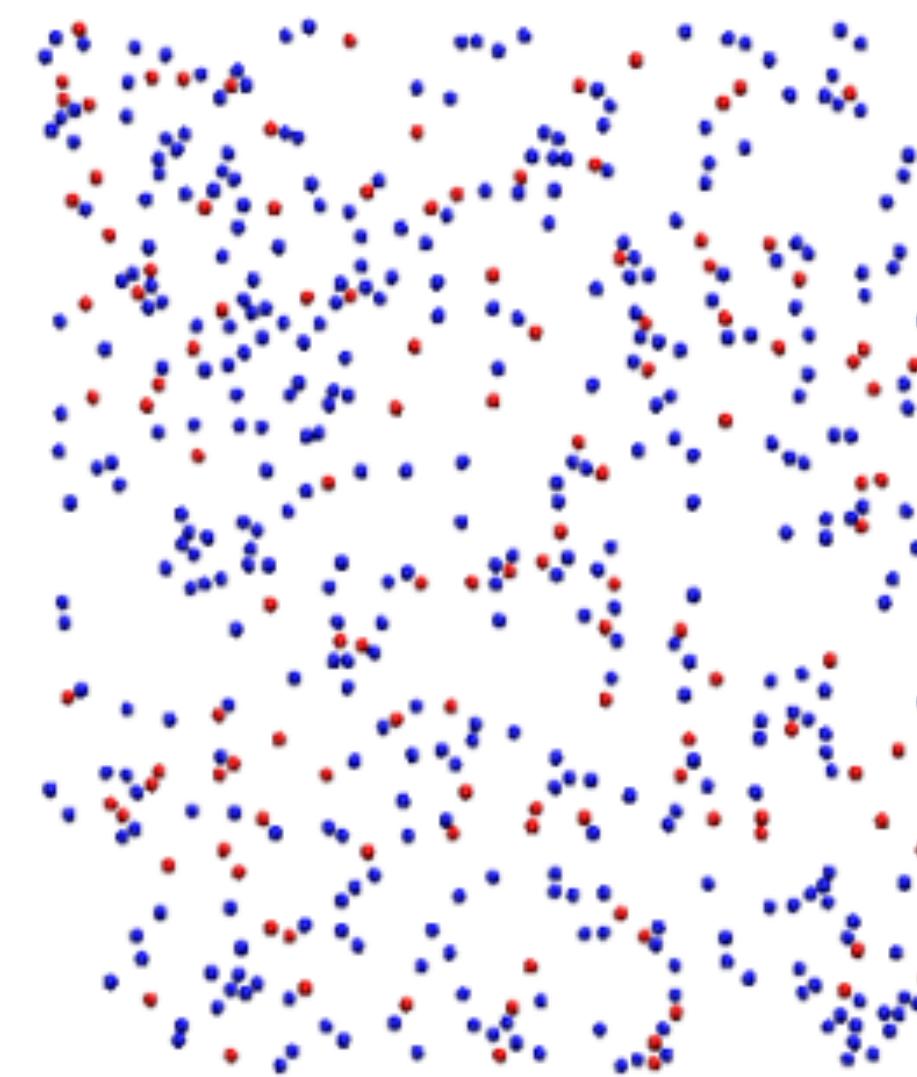
Applications:

Precision (e.g., sub nm scale) manufacturing of materials with advanced electrical, magnetic or optical properties

Two controlled colloidal SA case studies: (1) model-based, (2) data-driven

# Stochastic Control / Control Non-affine

## Controlled Self-assembly Case Study 1: Model Based



Dispersed particles

Ordered structure

Typical state variable:  $\langle C_6 \rangle \in (0,6)$

Average number of hexagonally close packed neighboring particles in 2D assembly  $\rightsquigarrow$  measure of crystallinity order

Typical control variable:  $u$

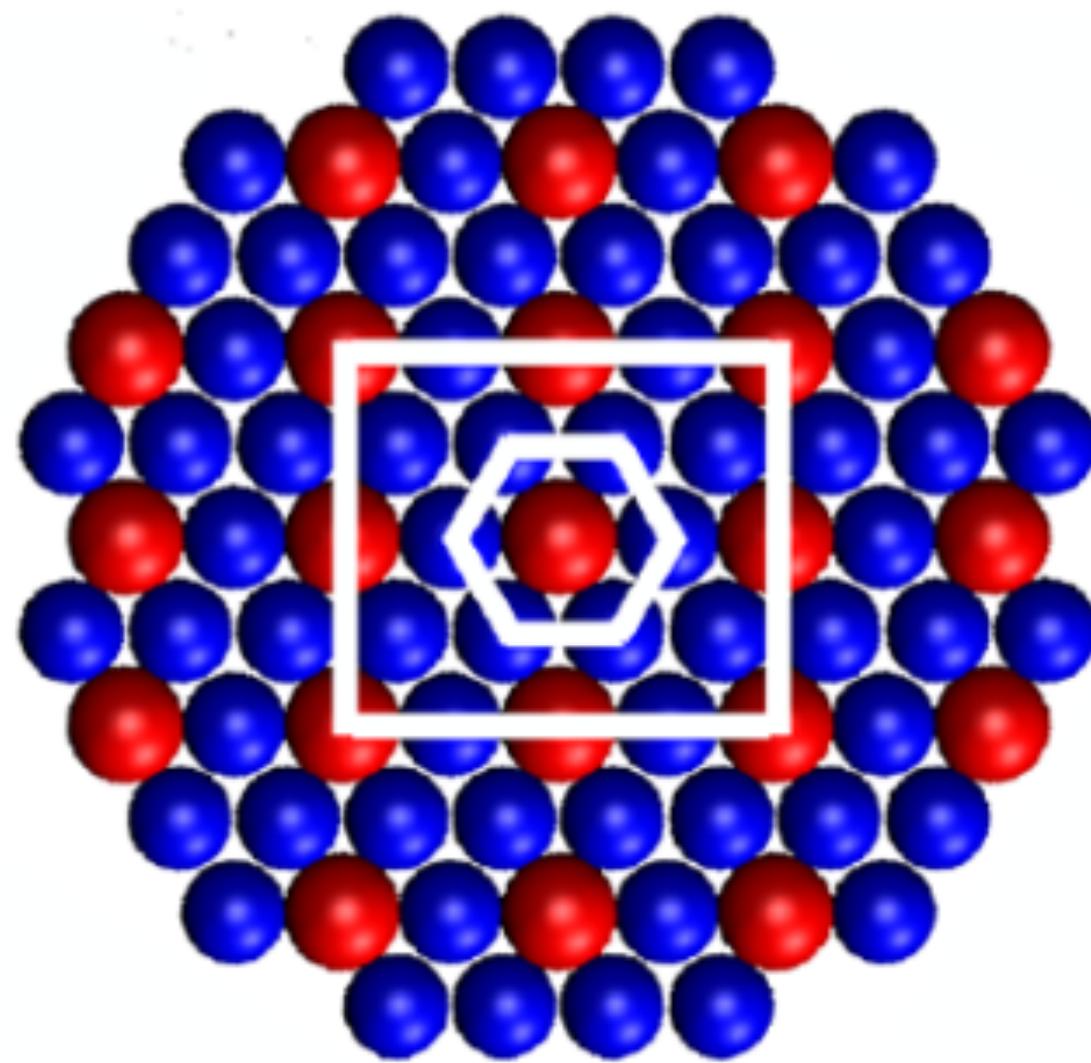
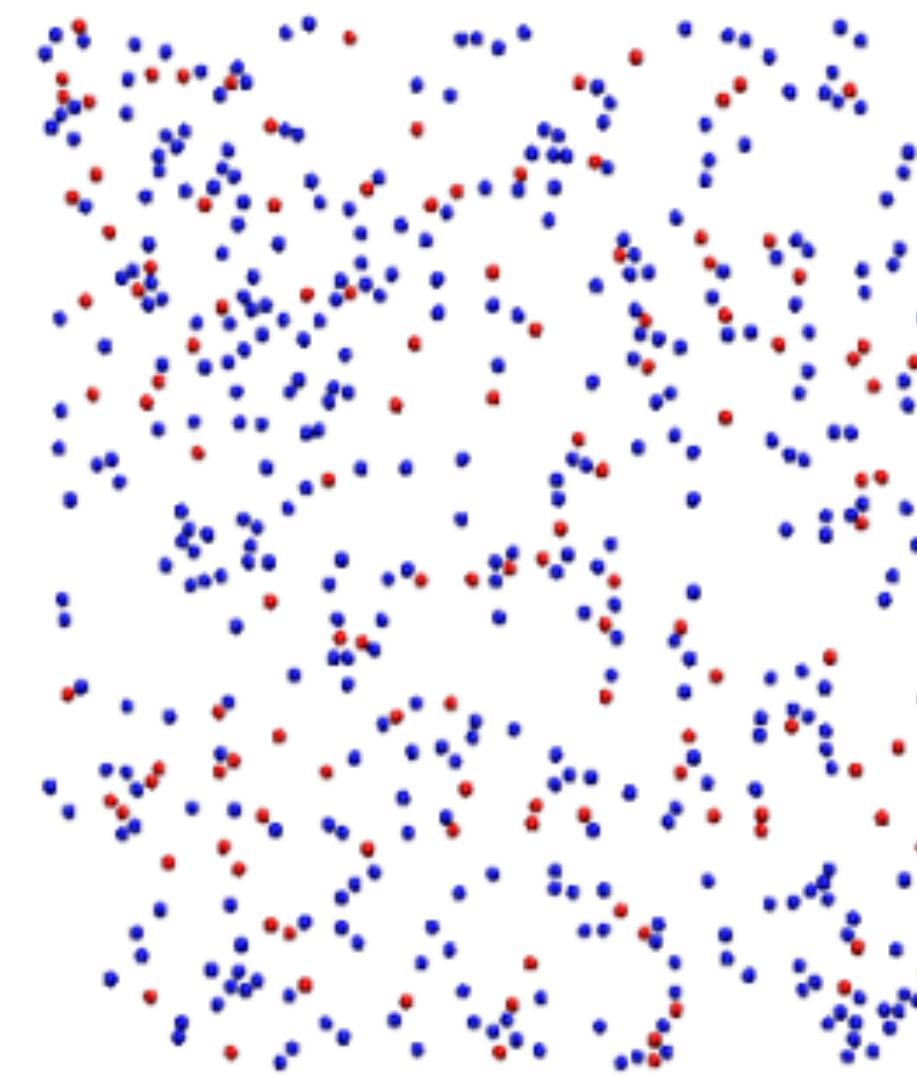
Electric field voltage

Technical challenge:

Nonlinear+ noisy molecular dynamics  $\rightsquigarrow \langle C_6 \rangle$  is a controlled stochastic process

# Stochastic Control / Control Non-affine

## Controlled Self-assembly Case Study 2: Data Driven



Dispersed particles

Ordered structure

Technical challenge:

Difficult to deduce first principle physics-based controlled dynamics over  $(\langle C_{10} \rangle, \langle C_{12} \rangle)$

Typical state variable:  $(\langle C_{10} \rangle, \langle C_{12} \rangle) \in [0,1]^2$

Steinhart bond order parameters  
useful for distinguishing  
between BCC and FCC structures

Typical control variable:  $u$

$(u_1, u_2) = (\text{temperature}, \text{pressure})$

# Stochastic Control / Control Non-affine

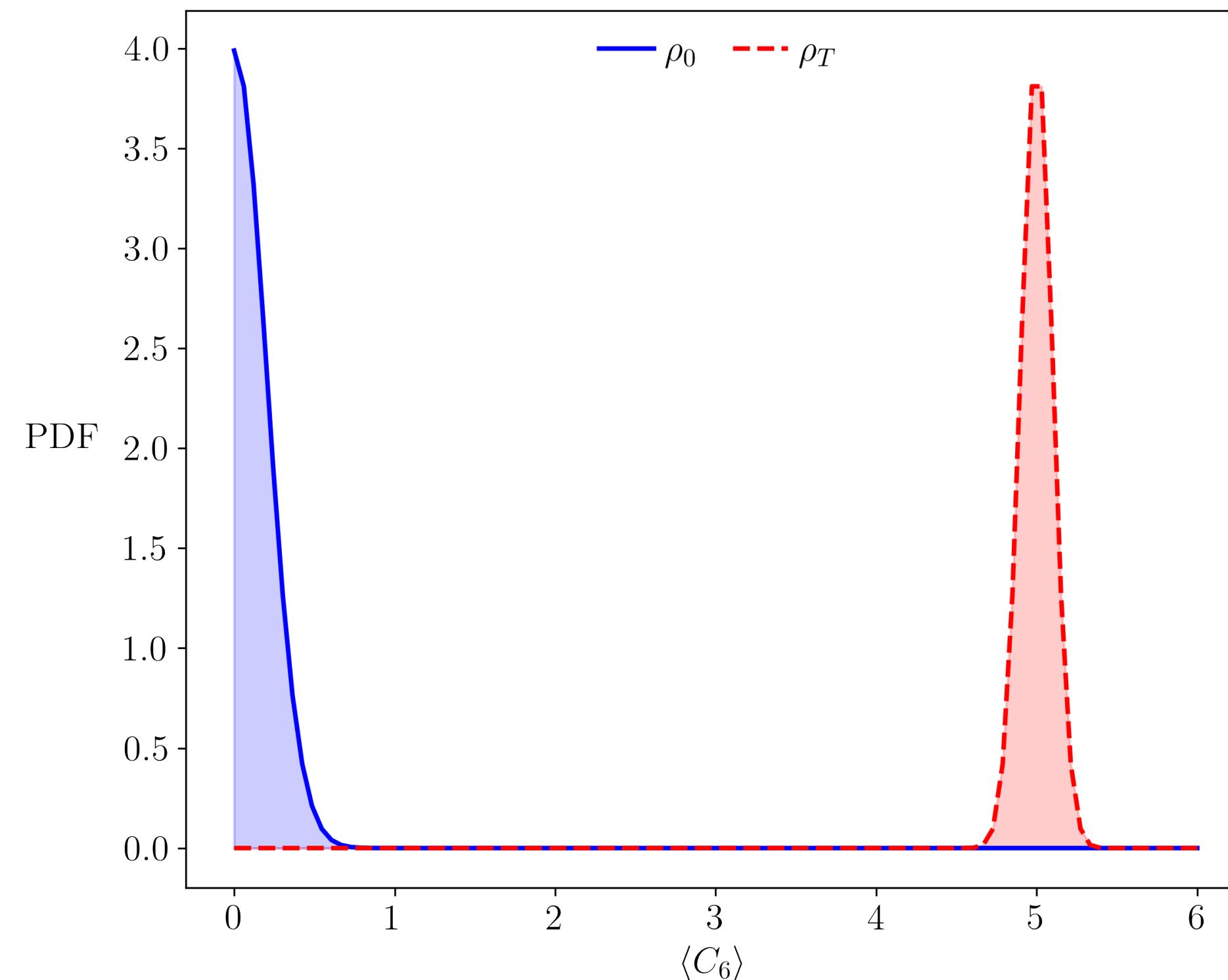
Intuition for Case Study 1:

$\langle C_6 \rangle \approx 0 \Leftrightarrow$  Crystalline disorder

$\langle C_6 \rangle \approx 5 \Leftrightarrow$  Crystalline order



Steer the PDF of the stochastic state  $\langle C_6 \rangle$  from disordered at  $t = t_0 \equiv 0$  to ordered at  $t = T \equiv 200$  s



Typical prescribed finite horizon for controlled self-assembly

Endpoint PDF constraints:  $\langle C_6 \rangle(t = t_0) \sim \rho_0$  (given)

$\langle C_6 \rangle(t = T) \sim \rho_T$  (given)

Control policy to accomplish  
the PDF steering:

$$u = \pi(\langle C_6 \rangle, t)$$

Underdetermined

# Stochastic Control / Control Non-affine

## Case 1: Minimum Effort Self-assembly

Proposed formulation:

$$\inf_{u \in \mathcal{U}} \mathbb{E}_{\mu^u} \left[ \int_0^T \frac{1}{2} u^2 dt \right],$$

drift landscape	diffusion landscape	free energy landscape
$D_1(x^u, u) := \frac{\partial}{\partial x} D_2(x^u, u) - \frac{\partial}{\partial x} F(x^u, u) \frac{D_2(x^u, u)}{k_B \theta}$		
either from model or learnt from MD simulation data		

subject to  $dx^u = D_1(x^u, u) dt + \sqrt{2D_2(x^u, u)} dw,$

$\curvearrowleft \langle C_6 \rangle$        $\curvearrowleft$  standard Wiener process

$$x^u(t=0) \sim d\mu_0 = \rho_0 dx^u, \quad x^u(t=T) \sim d\mu_T = \rho_T dx^u$$

# Stochastic Control / Control Non-affine

## Case 1: Minimum Effort Self-assembly

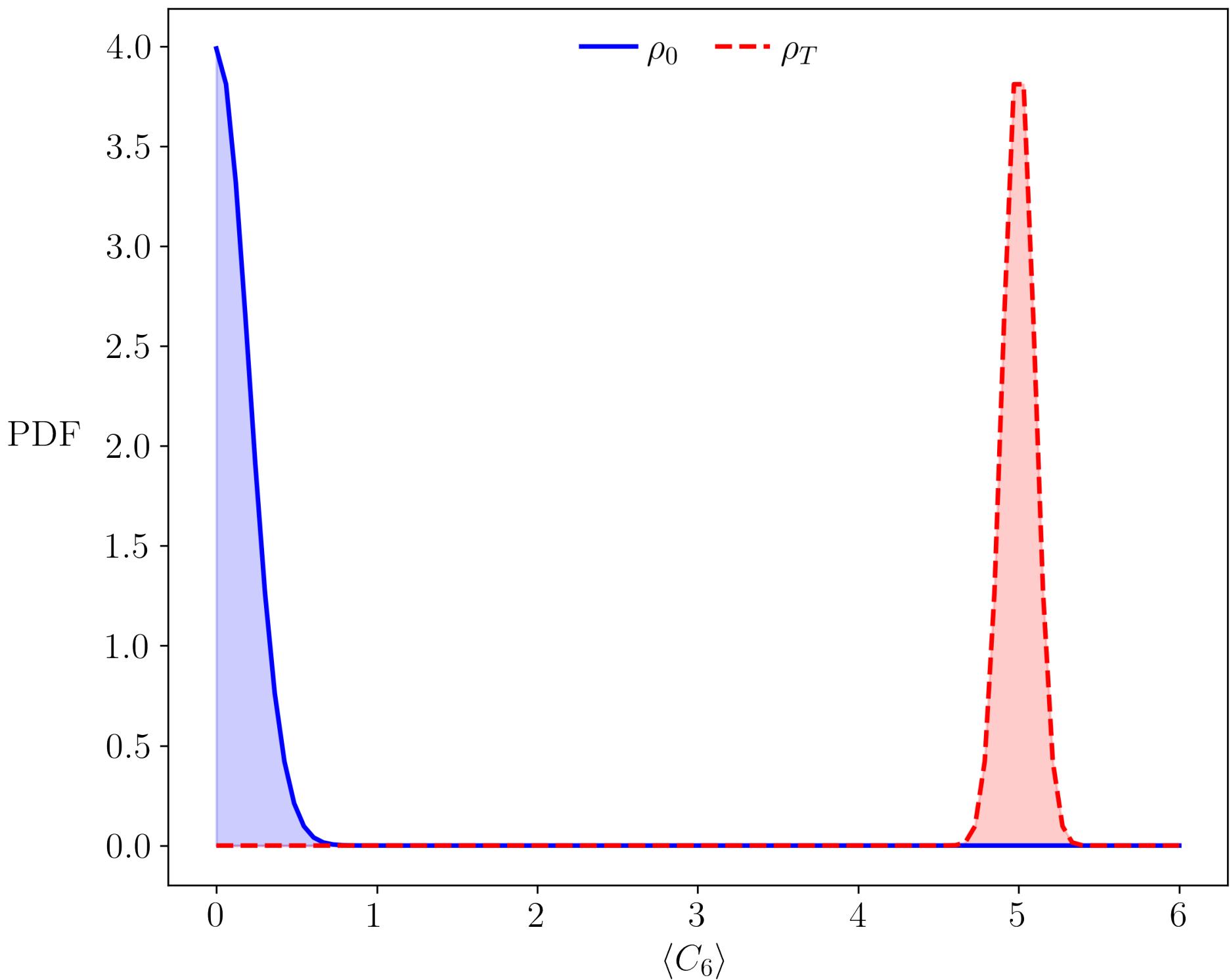
**Equivalent formulation:**

$$\inf_{(\rho^u, u)} \int_0^T \int_{\mathbb{R}} \frac{1}{2} u^2(x^u, t) \rho^u(x^u, t) dx^u dt$$

subject to  $\frac{\partial \rho^u}{\partial t} = - \frac{\partial}{\partial x^u} (D_1 \rho^u) + \frac{\partial^2}{\partial x^{u2}} (D_2 \rho^u)$

$$\rho^u(x^u, t = 0) = \rho_0, \quad \rho^u(x^u, t = T) = \rho_T$$

Guaranteed existence-uniqueness  
for compactly supported  $\rho_0, \rho_T$



# Stochastic Control / Control Non-affine

## Case 1: Conditions for Optimality

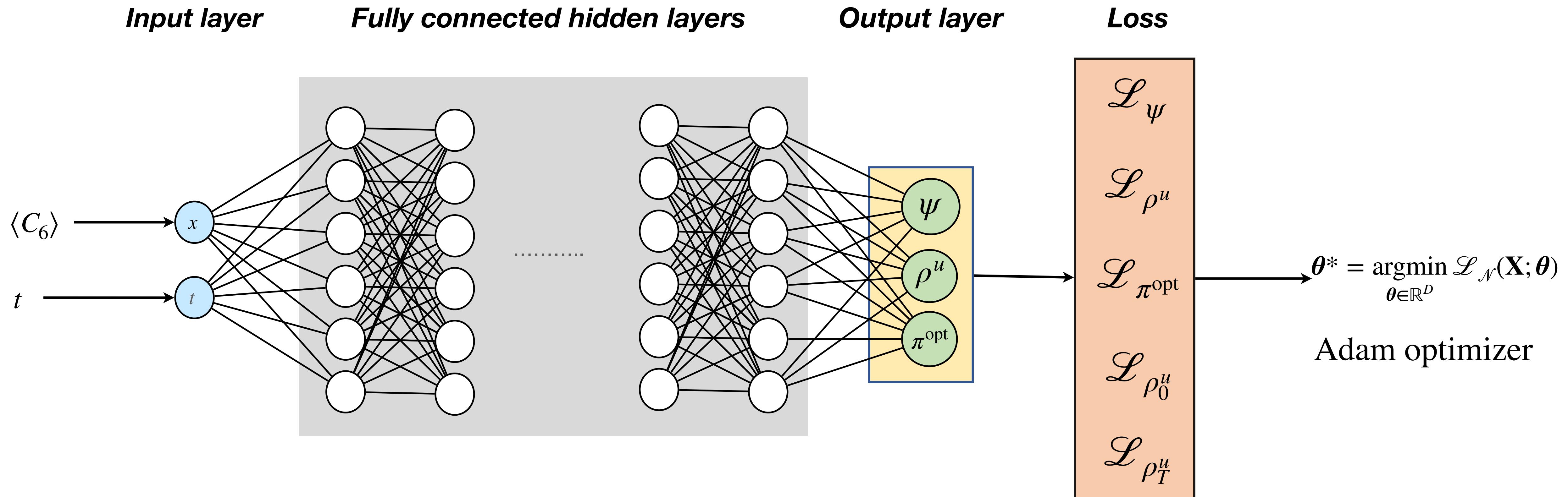
$\frac{\partial \psi}{\partial t} = \frac{1}{2} (\pi^{\text{opt}})^2 - \frac{\partial \psi}{\partial x} D_1 - \frac{\partial^2 \psi}{\partial x^{u2}} D_2$	<b>HJB PDE</b>
$\frac{\partial \rho^u}{\partial t} = - \frac{\partial}{\partial x^u} (D_1 \rho^u) + \frac{\partial^2}{\partial x^{u2}} (D_2 \rho^u)$	<b>Controlled FPK PDE</b>
$\pi^{\text{opt}}(x^u, t) = \frac{\partial \psi}{\partial x^u} \frac{\partial D_1}{\partial u} + \frac{\partial^2 \psi}{\partial x^{u2}} \frac{\partial D_2}{\partial u}$	<b>Optimal policy</b>
$\rho^u(x^u, t = 0) = \rho_0, \quad \rho^u(x^u, t = T) = \rho_T$	<b>Boundary conditions</b>

value function	optimally controlled PDF	optimal policy
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To be solved for the triple:  $\psi(x^u, t), \rho^u(x^u, t), \pi^{\text{opt}}(x^u, t)$

# Stochastic Control / Control Non-affine

## Case 1: Train Physics Informed Neural Network (PINN) to Learn the Solution of the GSBP



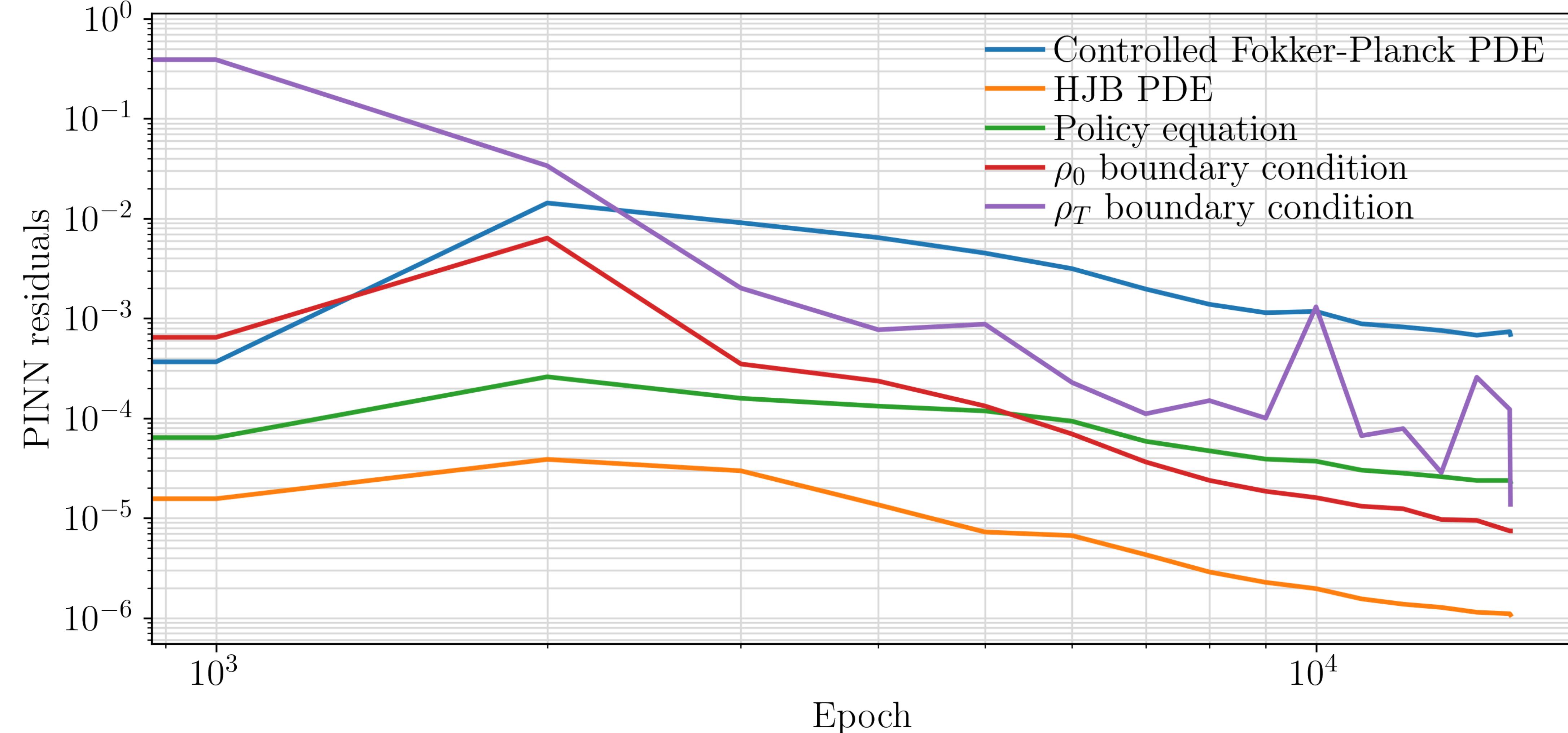
$$\mathcal{L}_{\mathcal{N}} = \mathcal{L}_{\psi} + \mathcal{L}_{\rho^u} + \mathcal{L}_{\pi^{\text{opt}}} + \mathcal{L}_{\rho_0^u} + \mathcal{L}_{\rho_T^u}$$

[Lu Lu, et al, 2021] [Niaki, et al, 2021]

# Stochastic Control / Control Non-affine

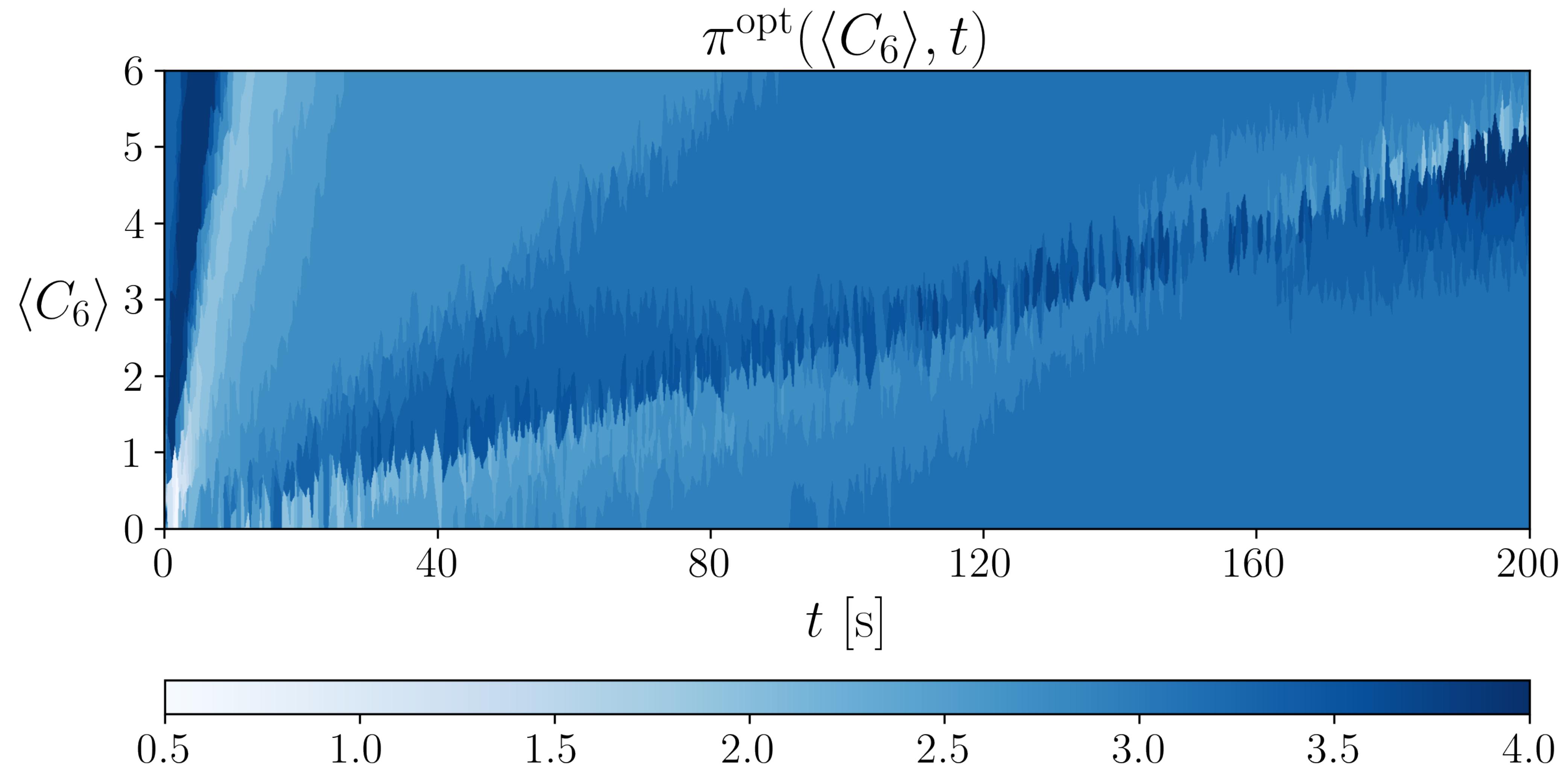
## Case 1: Residual for PINN Training

Benchmark controlled self-assembly system: [Y Xue, et al, *IEEE Trans. Control Sys. Technology*, 2014]



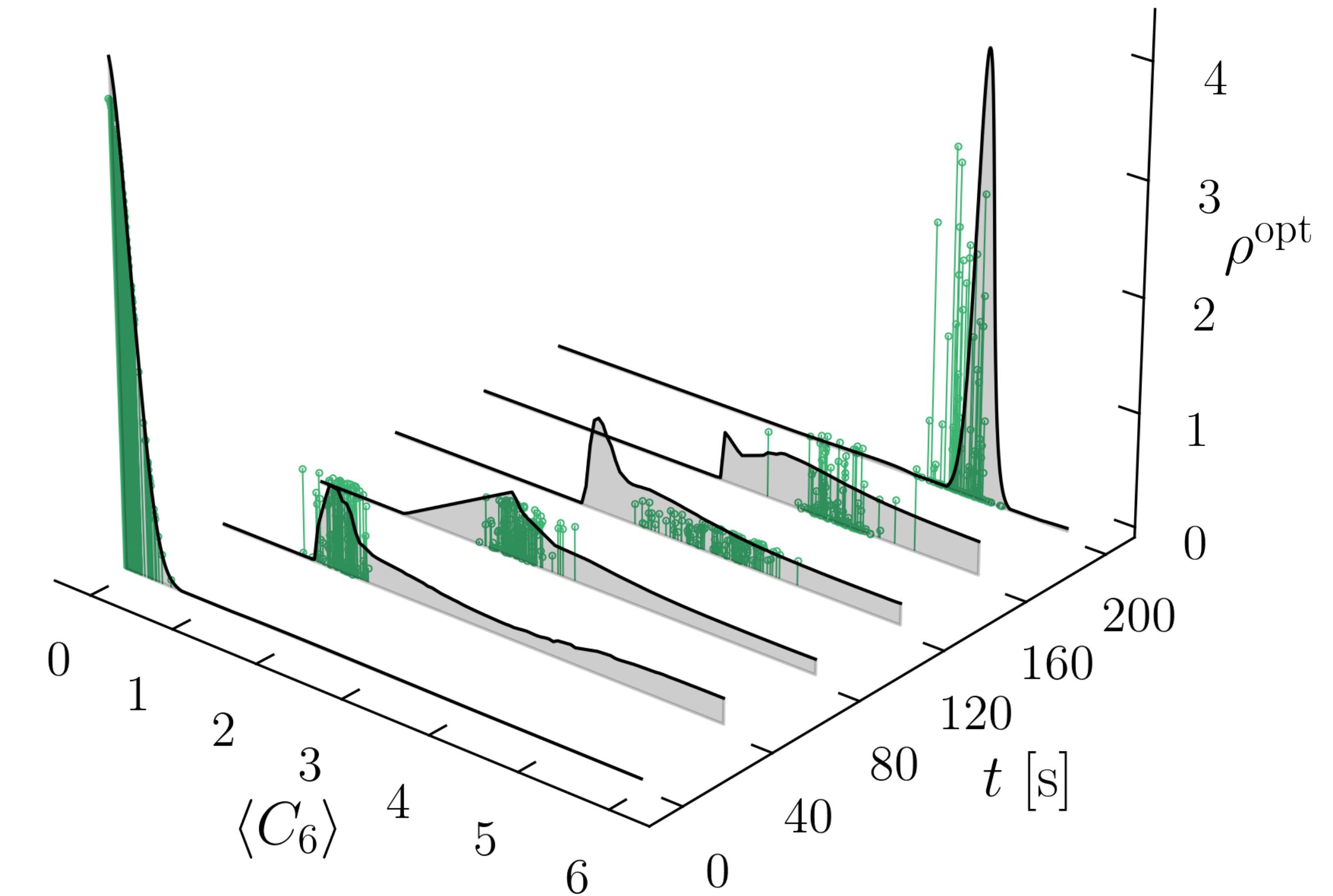
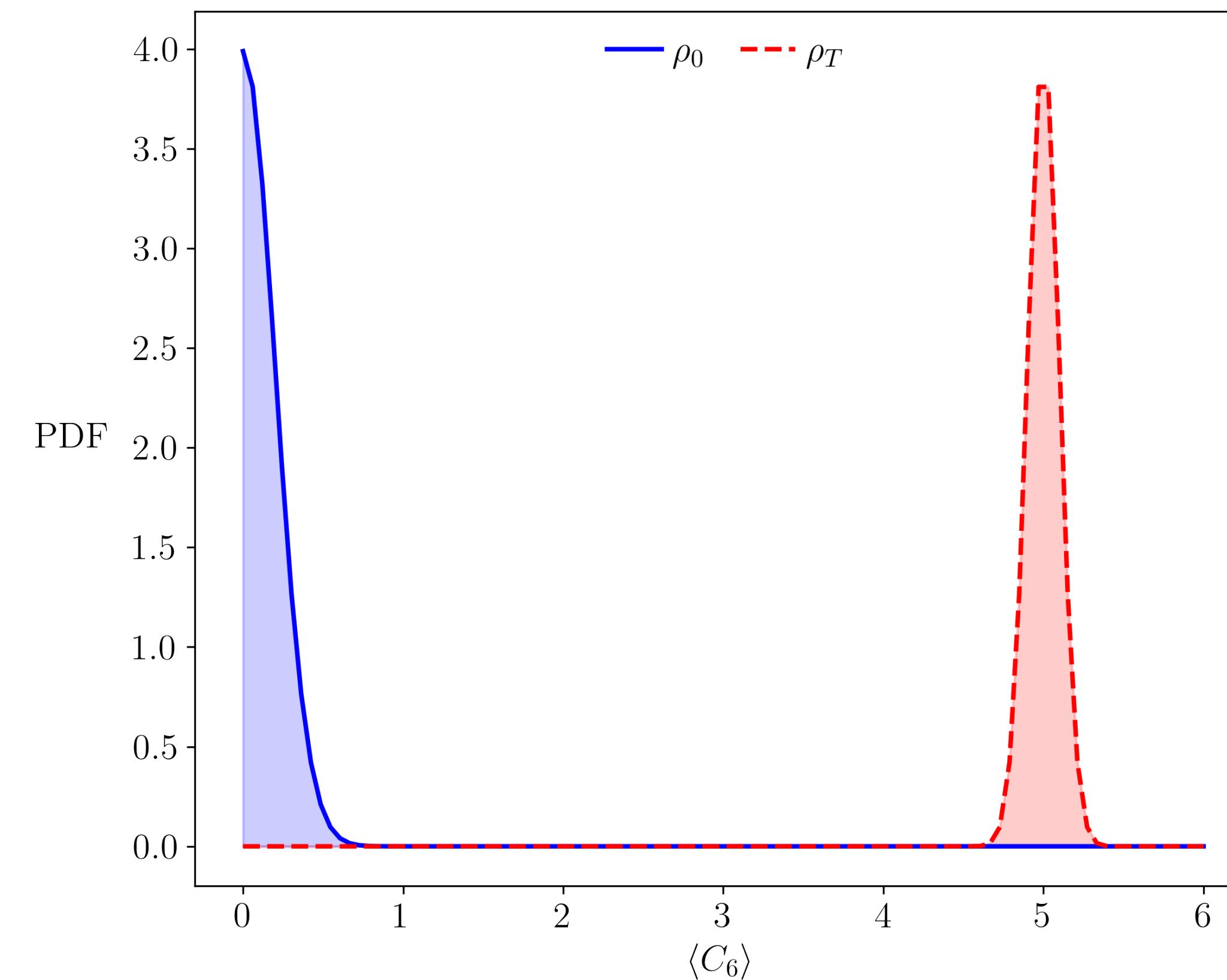
# Stochastic Control / Control Non-affine

## Case 1: Optimal Policy



# Stochastic Control / Control Non-affine

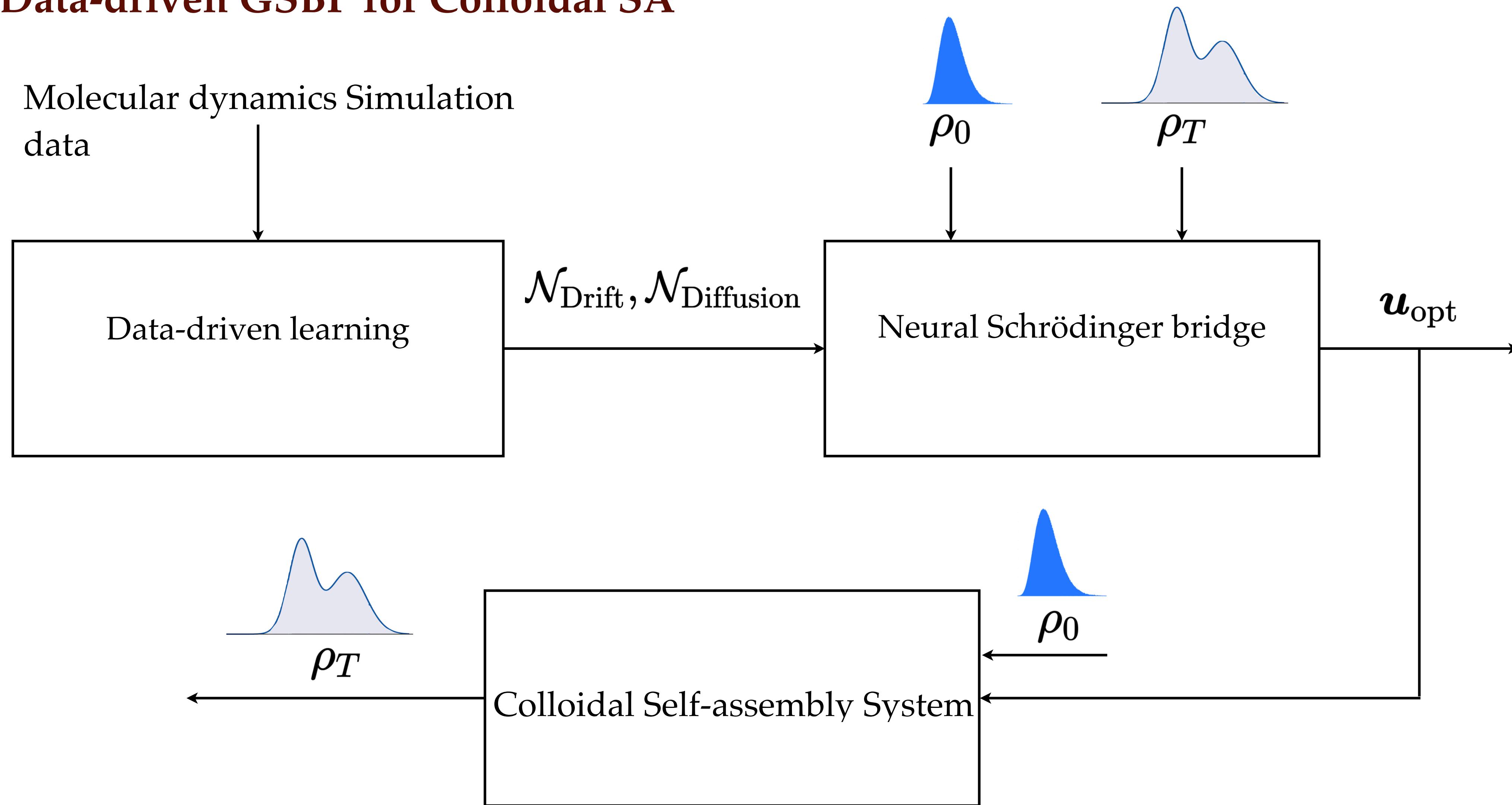
## Case 1: Optimally Controlled State PDFs



... the MSE losses are not appropriate for enforcing the endpoint PDF constraints

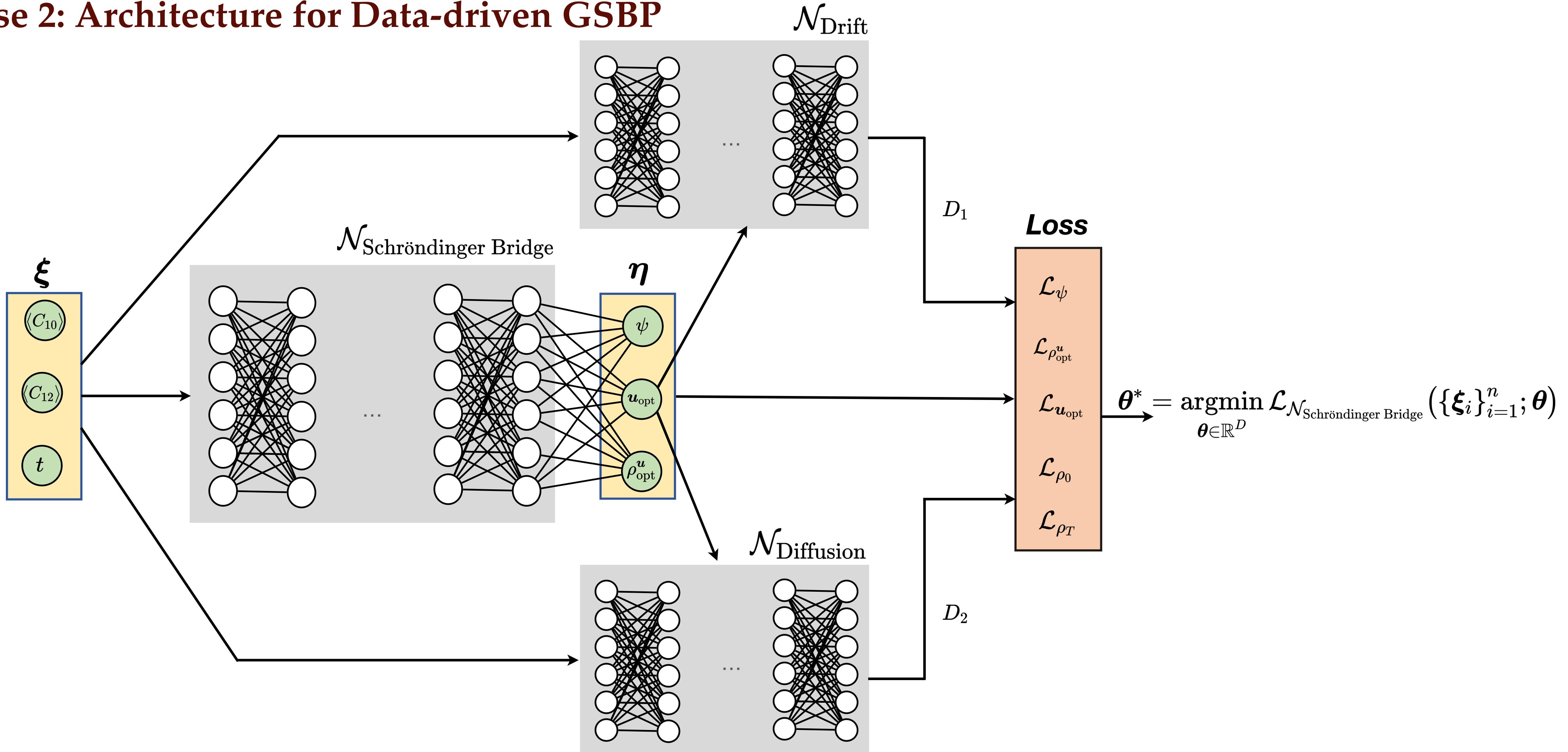
# Stochastic Control / Control Non-affine

## Case 2: Data-driven GSBP for Colloidal SA



# Stochastic Control / Control Non-affine

## Case 2: Architecture for Data-driven GSBP



# Stochastic Control / Control Non-affine

## Case 2: Sinkhorn Losses for Boundary Conditions

$$W_\varepsilon^2(\mu_0, \mu_1) := \inf_{\pi \in \Pi_2(\mu_0, \mu_1)} \int_{\mathbb{R}^n \times \mathbb{R}^n} \{ \|x - y\|_2^2 + \varepsilon \log \pi(x, y)\} d\pi(x, y)$$

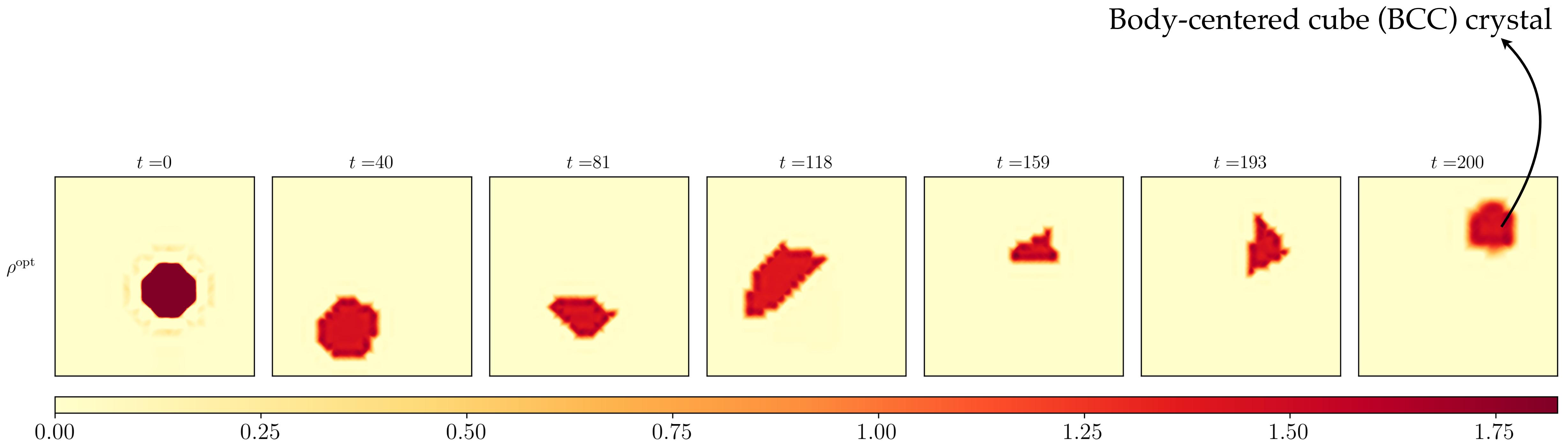
For boundary conditions, use Sinkhorn losses:  $\mathcal{L}_{\rho_i} := W_\varepsilon^2\left(\rho_i, \rho_i^{\text{epoch index}}(\theta)\right)$

Implementation friendly for PINN training:

$$\text{Autodiff}_\theta W_\varepsilon^2\left(\rho_i, \rho_i^{\text{epoch index}}(\theta)\right) \quad \forall i \in \{0, T\}$$

# Stochastic Control / Control Non-affine

## Case 2: Synthesize BCC Crystalline Structure by PDF Steering in $(\langle C_{10} \rangle, \langle C_{12} \rangle)$ Space



Data-driven:

Uses PINN with Sinkhorn losses + the drift-diffusion are themselves NNs

## **Part II: Stochastic Modeling and Solving of Chiplet Population Dynamics**

# Stochastic Modeling

Model dynamics of “chiplet population”: large ensemble of micro/nano sized particles immersed in dielectric fluid

## Motivating applications

Xerographic micro-assembly for printer systems

Manufacturing of photovoltaic solar cells

## Actuation and control

Electric potential generated by very large array of small electrodes



Spatio-temporally non-uniform dielectrophoretic forces on the chiplets

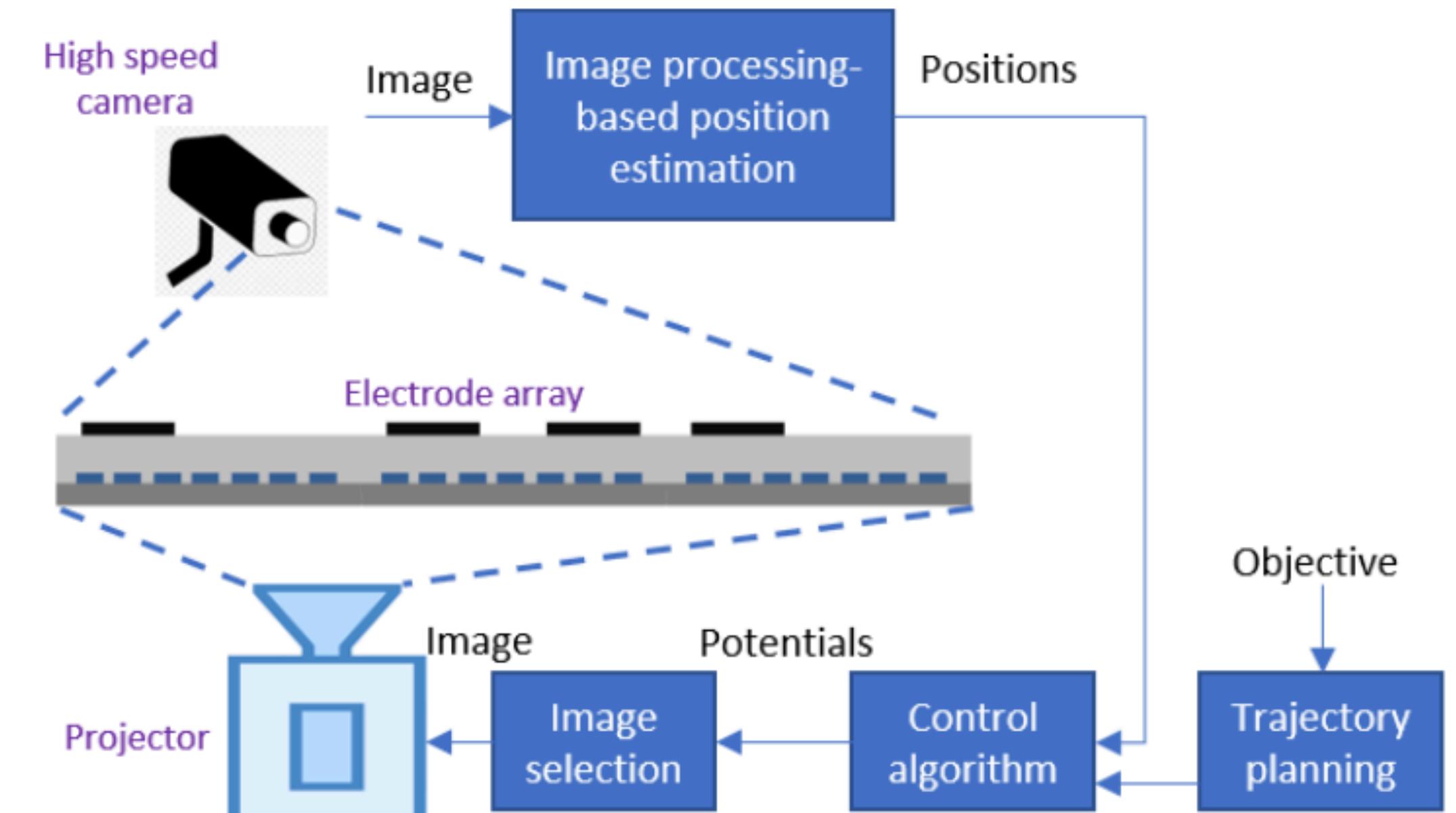


Image credit: PARC

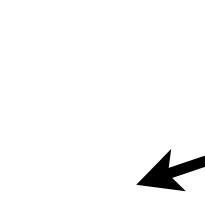
# Stochastic Modeling

Main Idea: derive controlled dynamics in the limit both  
# electrodes and # chiplets  $\rightarrow \infty$

## Derived model

2D position of an individual chiplet:  $\mathbf{x}(t) \in \mathbb{R}^2$

Causal deterministic control policy:  $u : \mathbb{R}^2 \times [0, \infty) \mapsto [u_{\min}, u_{\max}] \subset \mathbb{R}$

Electric voltage  Typically [-400, 400] Volt   
 $u$

At low Reynold's number in dielectric fluid (ignoring small mass of chiplet):

$$\underbrace{\mu \dot{\mathbf{x}}}_{\text{viscous drag force}} = \underbrace{\mathbf{f}^u}_{\text{controlled interaction force}} + \text{noise}$$

At time  $t$ , normalized chiplet population density function (PDF):  $\rho(\mathbf{x}, t) \in \mathcal{P}_2(\mathbb{R}^2)$

The vector field:  $\mathbf{f}^u : \mathbb{R}^2 \times [0, \infty) \times \mathcal{U} \times \mathcal{P}_2(\mathbb{R}^2) \mapsto \mathbb{R}^2$

# Stochastic Modeling

## Derived model: nonlocal Itô SDE

W.l.o.g. viscous coefficient  $\mu = 1$  (else re-scale vector field)

Itô SDE for the  $i$  th chiplet:

$$d\mathbf{x}_i = \mathbf{f}^u(\mathbf{x}_i, t, u, \rho^n)dt + \sqrt{2\beta^{-1}} d\mathbf{w}_i(t) \quad \text{with i.i.d. } \mathbf{x}_{0i} \sim \rho_0 \in \mathcal{P}_2(\mathbb{R}^2) \quad \forall i \in \llbracket n \rrbracket,$$

$\rho^n := \frac{1}{n} \sum_{i=1}^n \delta_{\mathbf{x}_i}$       Standard Wiener process

Non-local vector field:

$$\mathbf{f}^u(\mathbf{x}, t, u, \rho) = -\nabla \left( \int_{\mathbb{R}^2} \phi^u(\mathbf{x}, \mathbf{y}, t) \rho(\mathbf{y}, t) d\mathbf{y} \right) = -\nabla(\rho * \phi^u)$$

Controlled interaction potential      Comma ... not minus      Generalized convolution

# Stochastic Modeling

Derived model: controlled interaction potential  $\phi^u$

Non-local vector field:

$$\mathbf{f}^u(\mathbf{x}, t, u, \rho) = -\nabla \left( \int_{\mathbb{R}^2} \phi^u(\mathbf{x}, \mathbf{y}, t) \rho(\mathbf{y}, t) d\mathbf{y} \right)$$

Controlled interaction potential  $= \phi_{cc}^u(\mathbf{x}, \mathbf{y}, t) + \phi_{ce}^u(\mathbf{x}, \mathbf{y}, t)$

$$\phi_{cc}^u(\mathbf{x}, \mathbf{y}, t) := C_{cc}(\|\mathbf{x} - \mathbf{y}\|_2)(\bar{u}(\mathbf{y}, t) - \bar{u}(\mathbf{x}, t))^2 / 2$$

$$\phi_{ce}^u(\mathbf{x}, \mathbf{y}, t) := C_{ce}(\|\mathbf{x} - \mathbf{y}\|_2)(u(\mathbf{y}, t) - \bar{u}(\mathbf{x}, t))^2 / 2$$

Capacitances (in practice, from COMSOL electrostatic simulation)

$$\bar{u}(\mathbf{x}, t) := \frac{\int_{\mathbb{R}^2} C_{ce}(\|\mathbf{x} - \mathbf{y}\|_2) u(\mathbf{y}, t) \rho(\mathbf{y}, t) d\mathbf{y}}{\int_{\mathbb{R}^2} C_{ce}(\|\mathbf{x} - \mathbf{y}\|_2) \rho(\mathbf{y}, t) d\mathbf{y}}$$

# Stochastic Modeling

## Consistency guarantee for the mean field limit

**Theorem.** The random empirical measure  $\rho^n \rightarrow \rho$  a.s. in the limit  $n \uparrow \infty$

where  $\rho$  solves the nonlinear McKean-Vlasov-Fokker-Planck-Kolmogorov IVP

$$\begin{aligned}\frac{\partial \rho}{\partial t} &= -\nabla \cdot (\rho \mathbf{f}^u) + \beta^{-1} \Delta \rho \\ &= \nabla \cdot (\rho \nabla (\rho * \phi^u + \beta^{-1} (1 + \log \rho))) \\ \rho(\cdot, t = 0) &= \rho_0 \in \mathcal{P}(\mathbb{R}^2) \text{ (given).}\end{aligned}$$

# Stochastic Modeling

## Chiplet mean field dynamics as Wass. grad flow

**Theorem.** Define “energy functional”  $\Phi(\rho) := \mathbb{E}_\rho[\rho * \phi^u + \beta^{-1} \log \rho]$

Then

$$(i) \quad \frac{\partial \rho}{\partial t} = -\nabla^W \Phi(\rho)$$

(ii)  $\Phi(\cdot)$  is a Lyapunov functional for the mean field dynamics.

# Stochastic Modeling

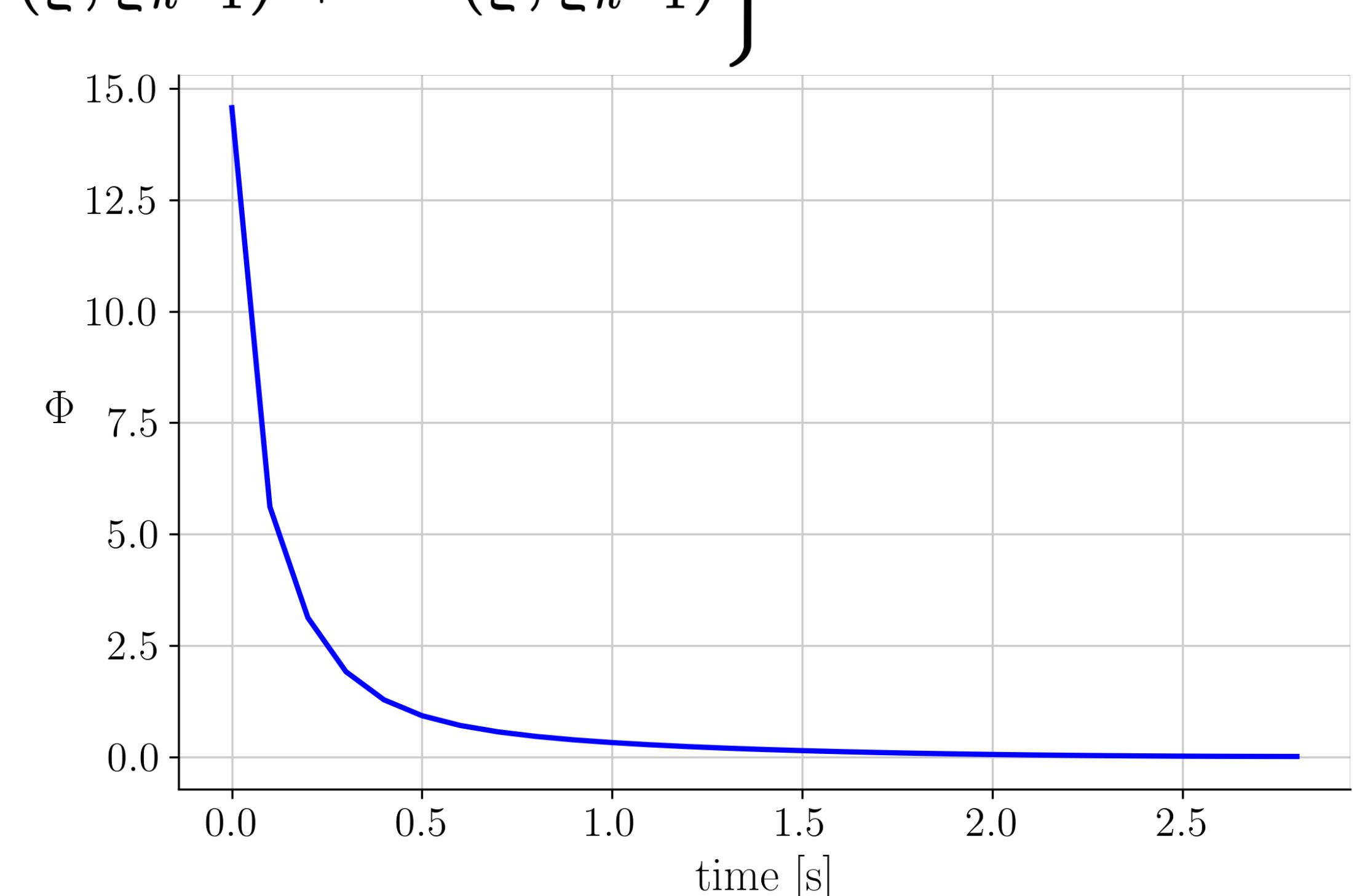
## Wasserstein proximal recursion

**Theorem.** Let  $\widehat{\Phi}(\varrho, \varrho_{k-1}) := \mathbb{E}_\varrho [\varrho_{k-1} * \phi^u + \beta^{-1} \log \varrho]$ ,  $\varrho, \varrho_{k-1} \in \mathcal{P}_2(\mathbb{R}^2)$   $\forall k \in \mathbb{N}$

Then the proximal recursion

$$\begin{aligned}\varrho_k &= \text{prox}_{\tau\widehat{\Phi}}^W(\varrho_{k-1}) \\ &:= \arg \inf_{\varrho \in \mathcal{P}_2(\mathbb{R}^2)} \left\{ \frac{1}{2} W^2(\varrho, \varrho_{k-1}) + \tau \widehat{\Phi}(\varrho, \varrho_{k-1}) \right\}\end{aligned}$$

approximates the transient solutions of the mean  
field nonlinear PDE IVP



## **Part III: Stochastic Learning**

# Stochastic Learning / Centralized Computing

## Centralized Computing Can Become Intensive: Mean Field SGD Dynamics in NN Classification

Free energy functional  $F(\rho) := R(\hat{f}(x, \rho))$

For quadratic loss:

$$F(\mu) = F_0 + \int_{\mathbb{R}^p} V(\theta) d\mu(\theta) + \int_{\mathbb{R}^{2p}} U(\theta, \tilde{\theta}) d\mu(\theta) d\mu(\tilde{\theta})$$

depend on activation functions of the NN

Neuronal population measure dynamics:

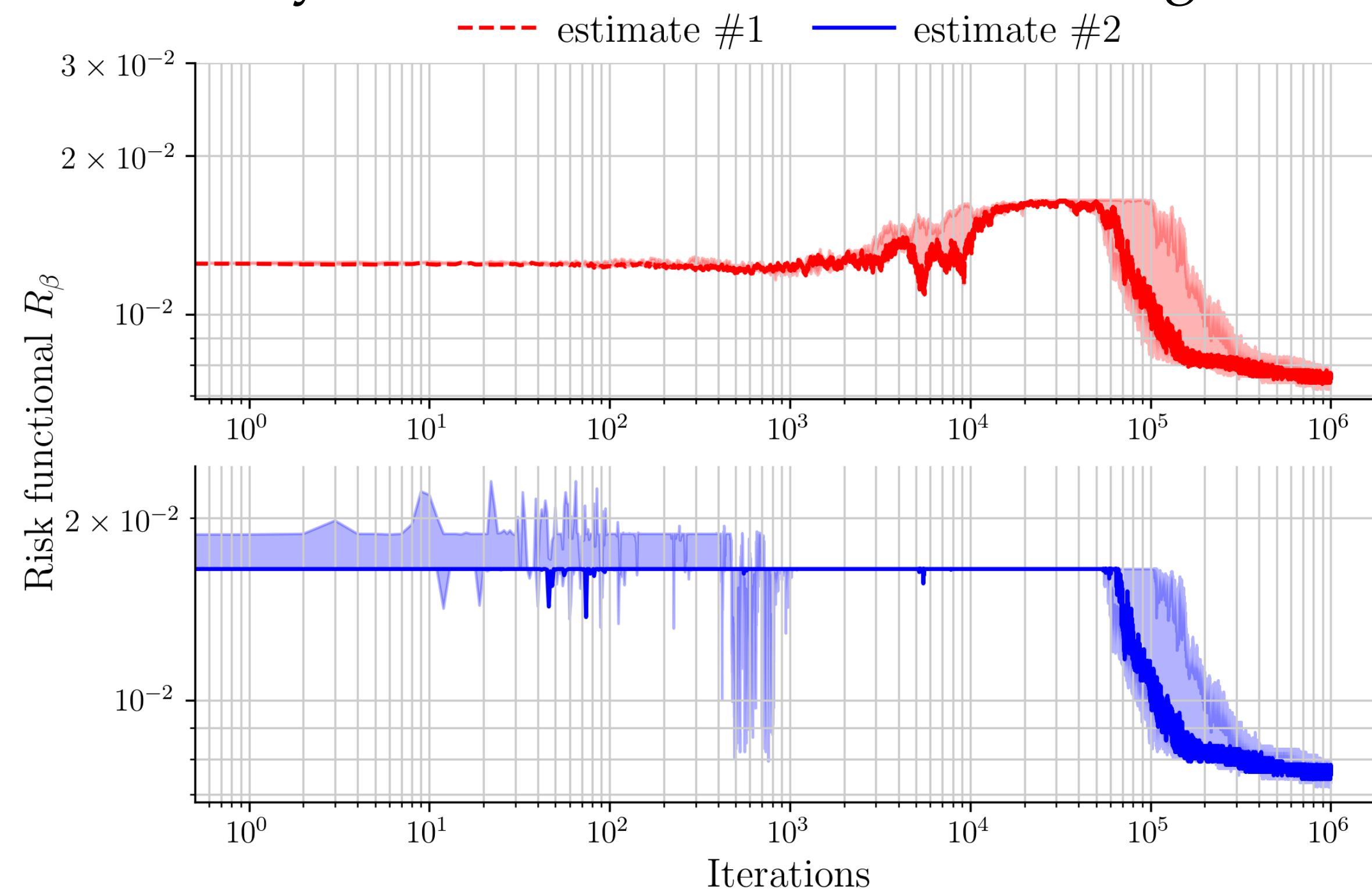
$$\frac{\partial \mu}{\partial t} = \nabla \cdot \left( \mu \nabla \frac{\delta F}{\delta \mu} \right) =: -\nabla^{W_2} F(\mu)$$

Wasserstein proximal recursion:  $\mu_{k+1} = \text{prox}_{hF}^W(\mu_k)$

# Stochastic Learning / Centralized Computing

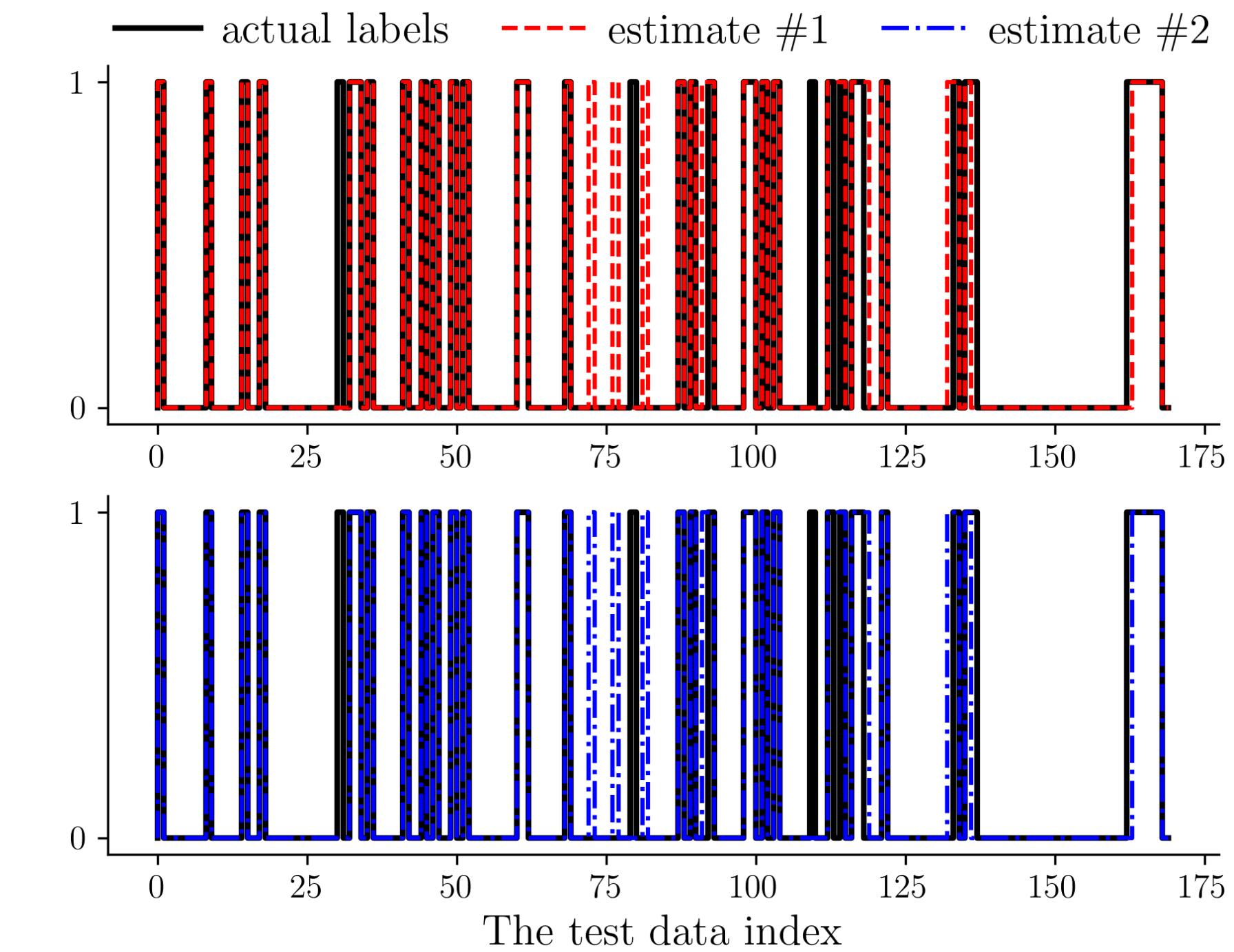
## Centralized Computing Can Become Intensive: Mean Field SGD Dynamics in NN Classification

Case study: Wisconsin Breast Cancer (Diagnostic) Data Set



CPU: 3.4 GHz 6 core intel i5 8GB RAM ( $\approx 33$  hrs runtime)

GPU: Jetson TX2 NVIDIA Pascal GPU 256 CUDA cores, 64 bit NVIDIA Denver + ARM Cortex A57 CPUs ( $\approx 2$  hrs runtime)



Classification accuracy for the WBDC dataset		
$\beta$	Estimate #1	Estimate #2
0.03	91.17%	92.35%
0.05	92.94%	92.94%
0.07	78.23%	92.94%

# Stochastic Learning/ Distributed Computing

## Our Present Work: Distributed Algorithm

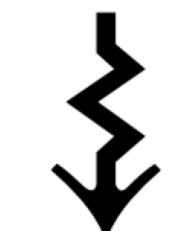
$$\arg \inf_{\mu \in \mathcal{P}_2(\mathbb{R}^d)} F_1(\mu) + F_2(\mu) + \dots + F_n(\mu)$$

# Stochastic Learning/ Distributed Computing

## Our Present Work: Distributed Algorithm

Main idea:

$$\arg \inf_{\mu \in \mathcal{P}_2(\mathbb{R}^d)} F_1(\mu) + F_2(\mu) + \dots + F_n(\mu)$$

 re-write

$$\arg \inf_{(\mu_1, \dots, \mu_n, \zeta) \in \mathcal{P}_2^{n+1}(\mathbb{R}^d)} F_1(\mu_1) + F_2(\mu_2) + \dots + F_n(\mu_n)$$

subject to  $\mu_i = \zeta$  for all  $i \in [n]$

# Stochastic Learning/ Distributed Computing

## Our Present Work: Distributed Algorithm

Main idea:

$$\arg \inf_{\mu \in \mathcal{P}_2(\mathbb{R}^d)} F_1(\mu) + F_2(\mu) + \dots + F_n(\mu)$$

↓ re-write

$$\arg \inf_{(\mu_1, \dots, \mu_n, \zeta) \in \mathcal{P}_2^{n+1}(\mathbb{R}^d)} F_1(\mu_1) + F_2(\mu_2) + \dots + F_n(\mu_n)$$

subject to  $\mu_i = \zeta$  for all  $i \in [n]$

Define Wasserstein augmented Lagrangian:

$$L_\alpha(\mu_1, \dots, \mu_n, \zeta, \nu_1, \dots, \nu_n) := \sum_{i=1}^n \left\{ F_i(\mu_i) + \frac{\alpha}{2} W^2(\mu_i, \zeta) + \int_{\mathbb{R}^d} \nu_i(\theta) (\mathrm{d}\mu_i - \mathrm{d}\zeta) \right\}$$

regularization  $> 0$

Lagrange multipliers

# Stochastic Learning/ Distributed Computing

## Proposed Consensus ADMM

$$\mu_i^{k+1} = \arg \inf_{\mu_i \in \mathcal{P}_2(\mathbb{R}^d)} L_\alpha(\mu_1, \dots, \mu_n, \zeta^k, \nu_1^k, \dots, \nu_n^k)$$

$$\zeta^{k+1} = \arg \inf_{\zeta \in \mathcal{P}_2(\mathbb{R}^d)} L_\alpha(\mu_1^{k+1}, \dots, \mu_n^{k+1}, \zeta, \nu_1^k, \dots, \nu_n^k)$$

$$\nu_i^{k+1} = \nu_i^k + \alpha(\mu_i^{k+1} - \zeta^{k+1})$$

where  $i \in [n], k \in \mathbb{N}_0$

Define

$$\nu_{\text{sum}}^k(\boldsymbol{\theta}) := \sum_{i=1}^n \nu_i^k(\boldsymbol{\theta}), \quad k \in \mathbb{N}_0$$

and simplify the recursions to

$$\mu_i^{k+1} = \text{prox}_{\frac{1}{\alpha}(F_i(\cdot) + \int \nu_i^k d(\cdot))}^W(\zeta^k)$$

$$\zeta^{k+1} = \arg \inf_{\zeta \in \mathcal{P}_2(\mathbb{R}^d)} \left\{ \left( \sum_{i=1}^n W^2(\mu_i^{k+1}, \zeta) \right) - \frac{2}{\alpha} \int_{\mathbb{R}^d} \nu_{\text{sum}}^k(\boldsymbol{\theta}) d\zeta \right\}$$

$$\nu_i^{k+1} = \nu_i^k + \alpha(\mu_i^{k+1} - \zeta^{k+1})$$

# Stochastic Learning/ Distributed Computing

## Discrete Version of the Proposed ADMM

Outer layer ADMM

$$\boxed{\begin{aligned}\boldsymbol{\mu}_i^{k+1} &= \text{prox}_{\frac{1}{\alpha}(F_i(\boldsymbol{\mu}_i) + \langle \boldsymbol{\nu}_i^k, \boldsymbol{\mu}_i \rangle)}^W(\boldsymbol{\zeta}^k) \\ &= \arg \inf_{\boldsymbol{\mu}_i \in \Delta^{N-1}} \left\{ \min_{\boldsymbol{M} \in \Pi_N(\boldsymbol{\mu}_i, \boldsymbol{\zeta}^k)} \frac{1}{2} \langle \mathbf{C}, \boldsymbol{M} \rangle + \frac{1}{\alpha} (F_i(\boldsymbol{\mu}_i) + \langle \boldsymbol{\nu}_i^k, \boldsymbol{\mu}_i \rangle) \right\} \\ \boldsymbol{\zeta}^{k+1} &= \arg \inf_{\boldsymbol{\zeta} \in \Delta^{N-1}} \left\{ \left( \sum_{i=1}^n \min_{\boldsymbol{M}_i \in \Pi_N(\boldsymbol{\mu}_i^{k+1}, \boldsymbol{\zeta})} \frac{1}{2} \langle \mathbf{C}, \boldsymbol{M}_i \rangle \right) - \frac{2}{\alpha} \langle \boldsymbol{\nu}_{\text{sum}}^k, \boldsymbol{\zeta} \rangle \right\} \\ \boldsymbol{\nu}_i^{k+1} &= \boldsymbol{\nu}_i^k + \alpha (\boldsymbol{\mu}_i^{k+1} - \boldsymbol{\zeta}^{k+1})\end{aligned}}$$

Euclidean distance matrix

Inner layer ADMM

where  $N$  is the number of samples

# Stochastic Learning/ Distributed Computing

$$\mu_i^{k+1} = \text{prox}_{\frac{1}{\alpha}(F_i(\cdot) + \int \nu_i^k d(\cdot))}^W(\zeta^k)$$

Split free energy functionals:

$$\Phi_i(\mu_i) := F_i(\mu_i) + \int_{\mathbb{R}^d} \nu_i^k d\mu_i$$

$\therefore$  Distributed Wasserstein prox  $\approx$  time updates of

$$\frac{\partial \tilde{\mu}_i}{\partial t} = -\nabla^W \Phi_i(\tilde{\mu}_i)$$

**Examples:**

$\Phi_i(\cdot) = F_i(\cdot) + \int \nu_i^k d(\cdot)$	PDE	Name
$\int_{\mathbb{R}^d} (V(\boldsymbol{\theta}) + \nu_i^k(\boldsymbol{\theta})) d\mu_i(\boldsymbol{\theta})$	$\frac{\partial \tilde{\mu}_i}{\partial t} = \nabla \cdot (\tilde{\mu}_i (\nabla V + \nabla \nu_i^k))$	Liouville equation
$\int_{\mathbb{R}^d} (\nu_i^k(\boldsymbol{\theta}) + \beta^{-1} \log \mu_i(\boldsymbol{\theta})) d\mu_i(\boldsymbol{\theta})$	$\frac{\partial \tilde{\mu}_i}{\partial t} = \nabla \cdot (\tilde{\mu}_i \nabla \nu_i^k) + \beta^{-1} \Delta \tilde{\mu}_i$	Fokker-Planck equation
$\int_{\mathbb{R}^d} \nu_i^k(\boldsymbol{\theta}) d\mu_i(\boldsymbol{\theta}) + \int_{\mathbb{R}^{2d}} U(\boldsymbol{\theta}, \boldsymbol{\sigma}) d\mu_i(\boldsymbol{\theta}) d\mu_i(\boldsymbol{\sigma})$	$\frac{\partial \tilde{\mu}_i}{\partial t} = \nabla \cdot (\tilde{\mu}_i (\nabla \nu_i^k + \nabla (U \circledast \tilde{\mu}_i)))$	Propagation of chaos equation
$\int_{\mathbb{R}^d} \left( \nu_i^k(\boldsymbol{\theta}) + \frac{\beta^{-1}}{m-1} \mathbf{1}^\top \mu_i^m \right) d\mu_i(\boldsymbol{\theta}), m > 1$	$\frac{\partial \tilde{\mu}_i}{\partial t} = \nabla \cdot (\tilde{\mu}_i \nabla \nu_i^k) + \beta^{-1} \Delta \tilde{\mu}_i^m$	Porous medium equation

# Stochastic Learning/ Distributed Computing

$\mu_i$  update  $\rightsquigarrow$  Outer Consensus (Sinkhorn) ADMM

Example:  $\Phi(\mu) := \langle \mathbf{a}, \mu \rangle, \mathbf{a} \in \mathbb{R}^N \setminus \{\mathbf{0}\}, \mu, \zeta \in \Delta^{N-1}, \Gamma := \exp(-\mathbf{C}/2\varepsilon), \varepsilon > 0$

$$\text{prox}_{\frac{1}{\alpha}\Phi}^{W_\varepsilon}(\zeta) = \exp\left(-\frac{1}{\alpha\varepsilon}\mathbf{a}\right) \odot \left(\Gamma^\top \left( \zeta \oslash \left( \Gamma \exp\left(-\frac{1}{\alpha\varepsilon}\mathbf{a}\right) \right) \right)\right)$$

# Stochastic Learning/ Distributed Computing

## $\zeta$ update $\rightsquigarrow$ Inner (Euclidean) ADMM

**Theorem.** Consider the convex problem

$$\begin{aligned} (\mathbf{u}_1^{\text{opt}}, \dots, \mathbf{u}_n^{\text{opt}}) &= \arg \min_{(\mathbf{u}_1, \dots, \mathbf{u}_n) \in \mathbb{R}^{nN}} \sum_{i=1}^n \langle \boldsymbol{\mu}_i^{k+1}, \log(\boldsymbol{\Gamma} \exp(\mathbf{u}_i/\varepsilon)) \rangle \\ \text{subject to } \sum_{i=1}^n \mathbf{u}_i &= \frac{2}{\alpha} \boldsymbol{\nu}_{\text{sum}}^k. \end{aligned}$$

Then

$$\boldsymbol{\zeta}^{k+1} = \exp(\mathbf{u}_i^{\text{opt}}/\varepsilon) \odot \left( \boldsymbol{\Gamma} \left( \boldsymbol{\mu}_i^{k+1} \oslash \left( \boldsymbol{\Gamma} \exp(\mathbf{u}_i^{\text{opt}}/\varepsilon) \right) \right) \right) \in \Delta^{N-1} \forall i \in [n]$$

# Stochastic Learning/ Distributed Computing

## $\zeta$ update $\rightsquigarrow$ Inner (Euclidean) ADMM

**Theorem.** Let  $f_i(\mathbf{u}_i) := \langle \boldsymbol{\mu}_i^{k+1}, \log(\Gamma \exp(\mathbf{u}_i/\varepsilon)) \rangle$ ,  $\mathbf{u}_i \in \mathbb{R}^N$ , for all  $i \in [n]$ ,

Then the following Euclidean ADMM solves

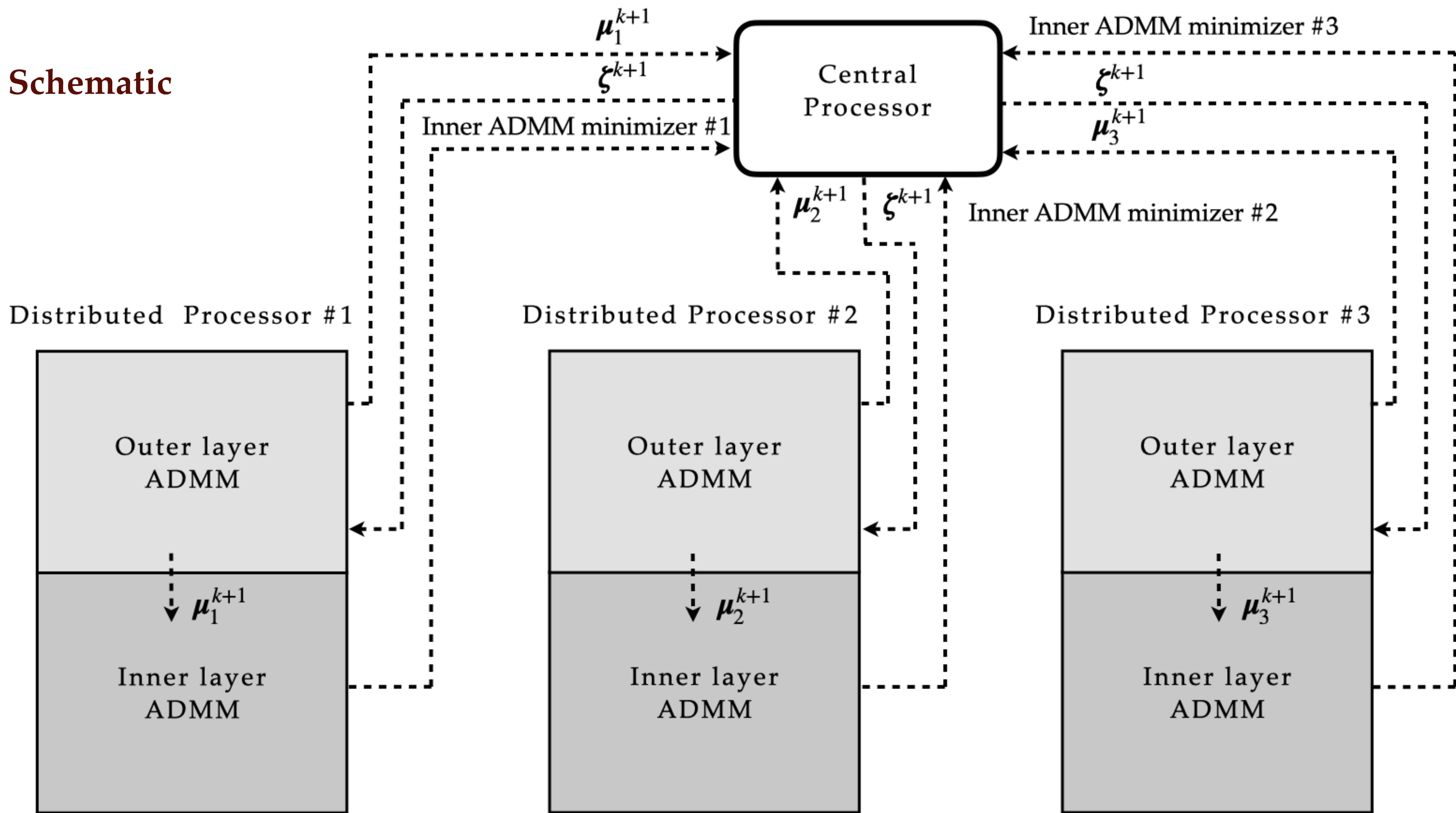
$$\begin{aligned}\mathbf{u}_i^{\ell+1} &= \text{prox}_{\frac{1}{\tau}f_i}^{\|\cdot\|_2} \left( \mathbf{z}_i^\ell - \tilde{\boldsymbol{\nu}}_i^\ell \right) \\ \mathbf{z}_i^{\ell+1} &= \left( \mathbf{u}_i^{\ell+1} - \frac{1}{n} \sum_{i=1}^n \mathbf{u}_i^{\ell+1} \right) + \left( \tilde{\boldsymbol{\nu}}_i^\ell - \frac{1}{n} \sum_{i=1}^n \tilde{\boldsymbol{\nu}}_i^\ell \right) + \frac{2}{n\alpha} \boldsymbol{\nu}_{\text{sum}}^k \\ \tilde{\boldsymbol{\nu}}_i^{\ell+1} &= \tilde{\boldsymbol{\nu}}_i^\ell + (\mathbf{u}_i^{\ell+1} - \mathbf{z}_i^{\ell+1})\end{aligned}$$

**Theorem.**

Guaranteed convergence for inner layer ADMM under some constraints on hyper-parameters

# Stochastic Learning/ Distributed Computing

## Overall Schematic



# Stochastic Learning/ Distributed Computing

## Centralized computation:

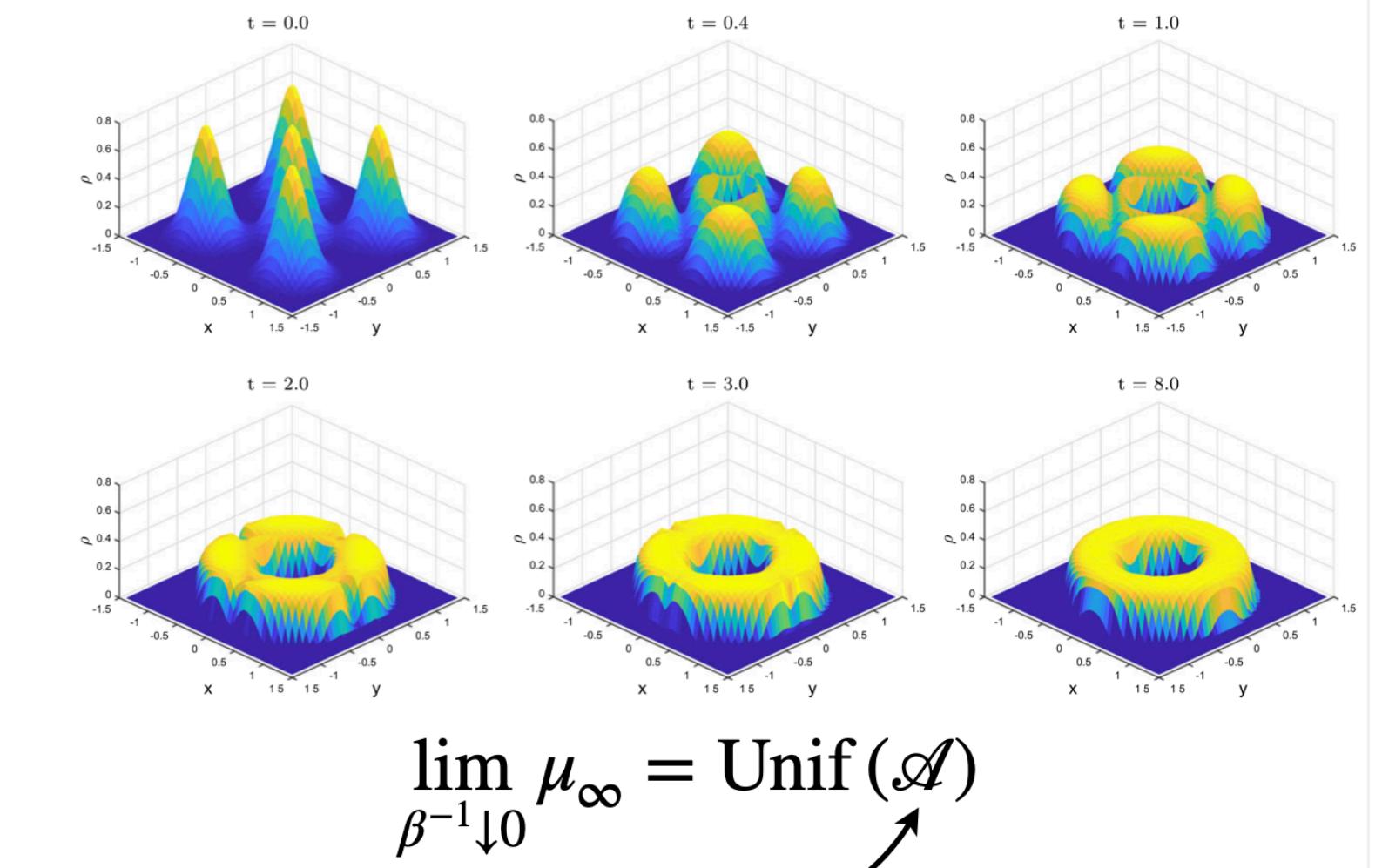
Carrillo, Craig, Wang and Wei, FOCM, 2021

### Experiment #1 Aggregation-drift-diffusion nonlinear PDE

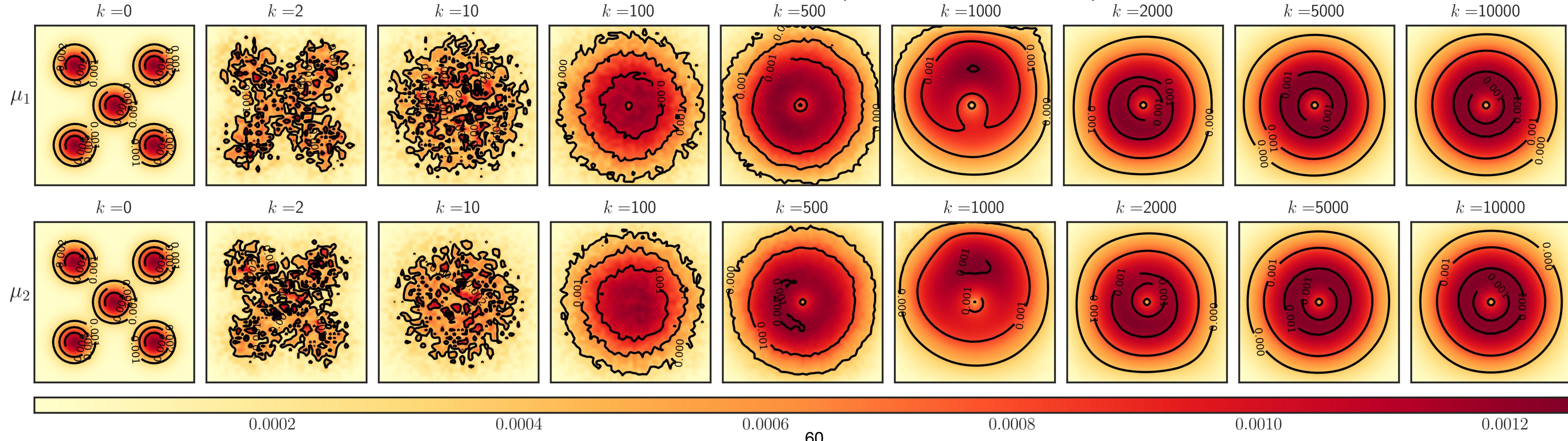
$$\frac{\partial \mu}{\partial t} = \underbrace{\nabla \cdot (\mu \nabla (U * \mu))}_{i=1} + \underbrace{\nabla \cdot (\mu \nabla V) + \beta^{-1} \Delta \mu^2}_{i=2}$$

$$U(\mathbf{x}) = \frac{1}{2} \|\mathbf{x}\|_2^2 - \ln \|\mathbf{x}\|_2$$

$$V(\mathbf{x}) = -\frac{1}{4} \ln \|\mathbf{x}\|_2$$



Distributed computation:  $F_1(\mu) = \langle \mathbf{U}_k \mu, \mu \rangle$     $F_2(\mu) = \langle \mathbf{V}_k + \beta^{-1} \log \mu, \mu \rangle$



# Stochastic Learning/ Distributed Computing

Centralized computation:

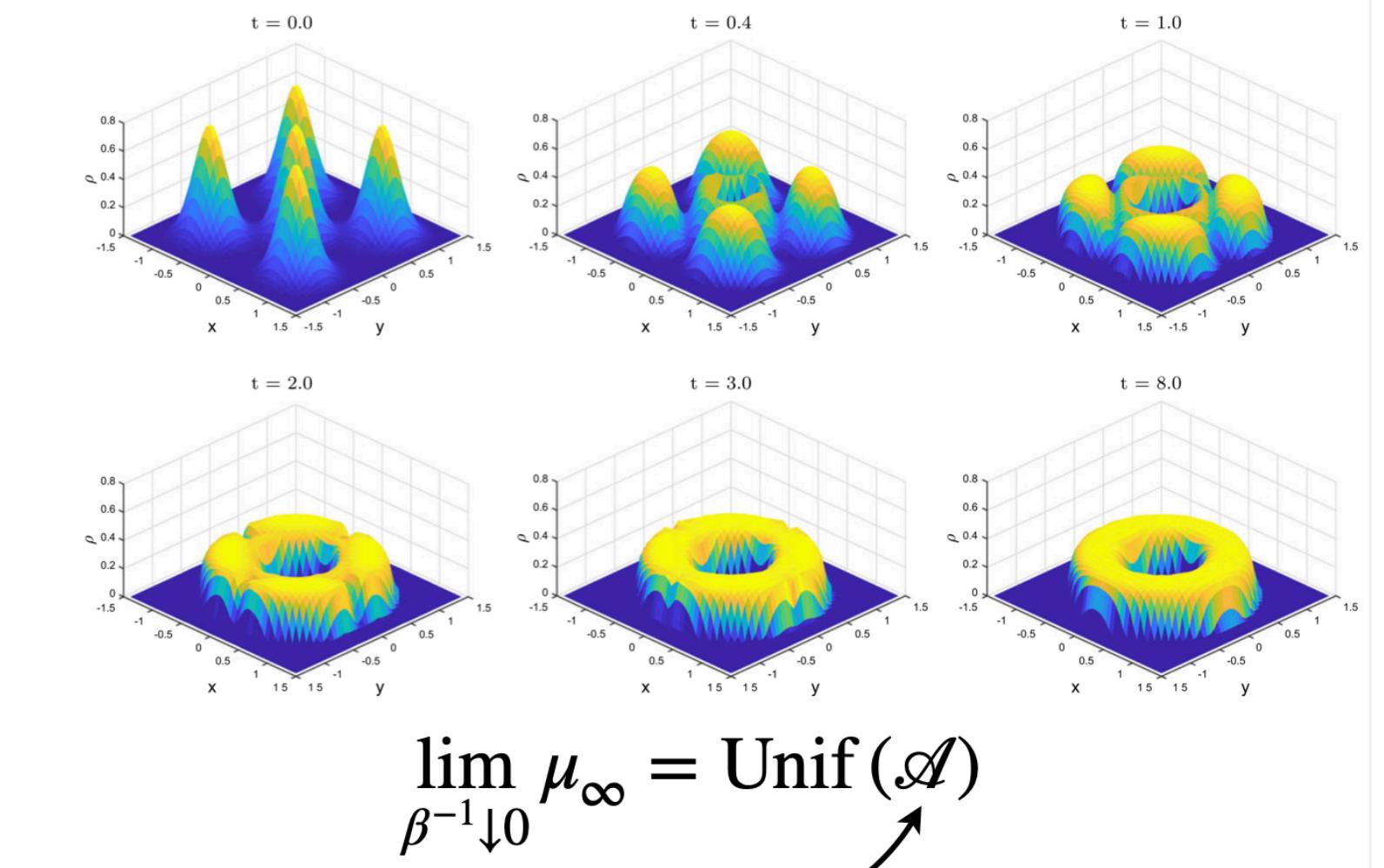
Carrillo, Craig, Wang and Wei, FOCM, 2021

## Experiment #1 Aggregation-drift-diffusion nonlinear PDE

$$\frac{\partial \mu}{\partial t} = \underbrace{\nabla \cdot (\mu \nabla (U * \mu))}_{i=1} + \underbrace{\nabla \cdot (\mu \nabla V) + \beta^{-1} \Delta \mu^2}_{i=2}$$

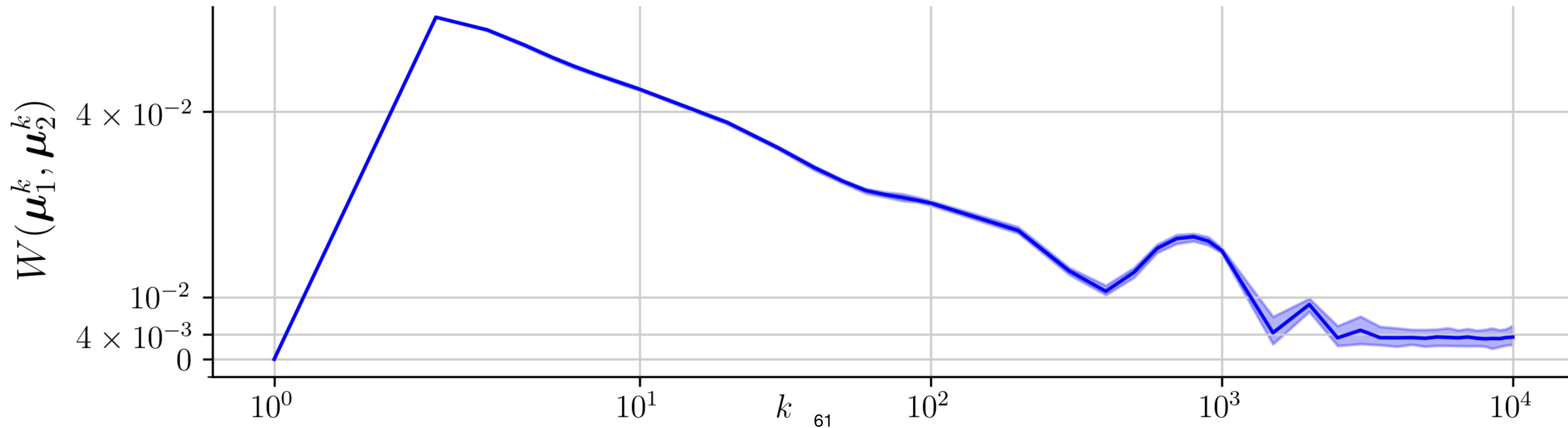
$$U(\mathbf{x}) = \frac{1}{2} \|\mathbf{x}\|_2^2 - \ln \|\mathbf{x}\|_2$$

$$V(\mathbf{x}) = -\frac{1}{4} \ln \|\mathbf{x}\|_2$$



Annulus with inner radius  $1/2$  and outer radius  $\sqrt{5}/2$

Distributed computation:  $F_1(\mu) = \langle \mathbf{U}_k \mu, \mu \rangle$     $F_2(\mu) = \langle \mathbf{V}_k + \beta^{-1} \log \mu, \mu \rangle$



# Stochastic Learning/ Distributed Computing

**Experiment #2** Wasserstein barycenter

$$\arg \inf_{\mu \in \mathcal{P}_2(\mathcal{X})} \sum_{i=1}^n w_i W^2(\mu, \xi_i)$$

# Stochastic Learning/ Distributed Computing

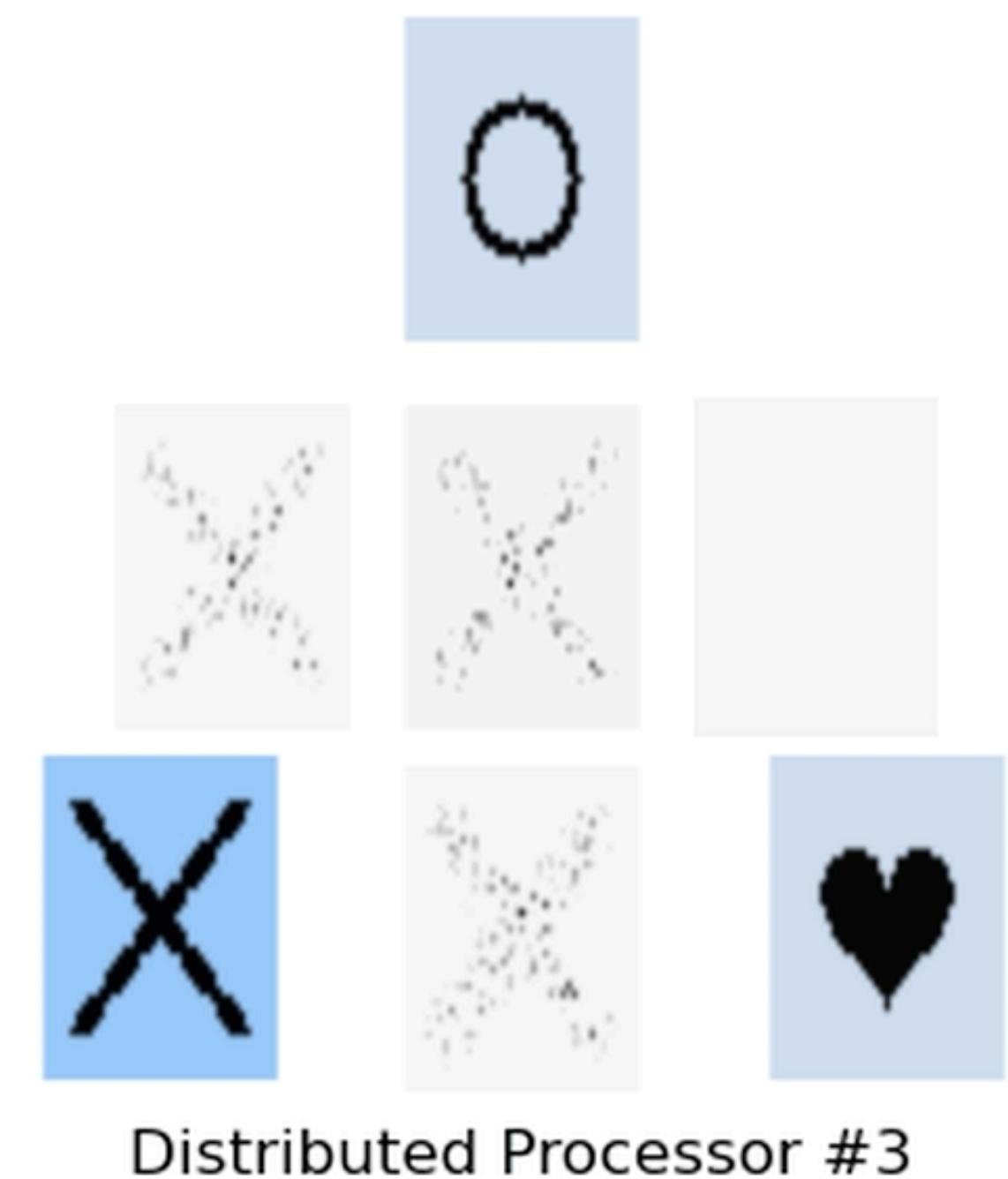
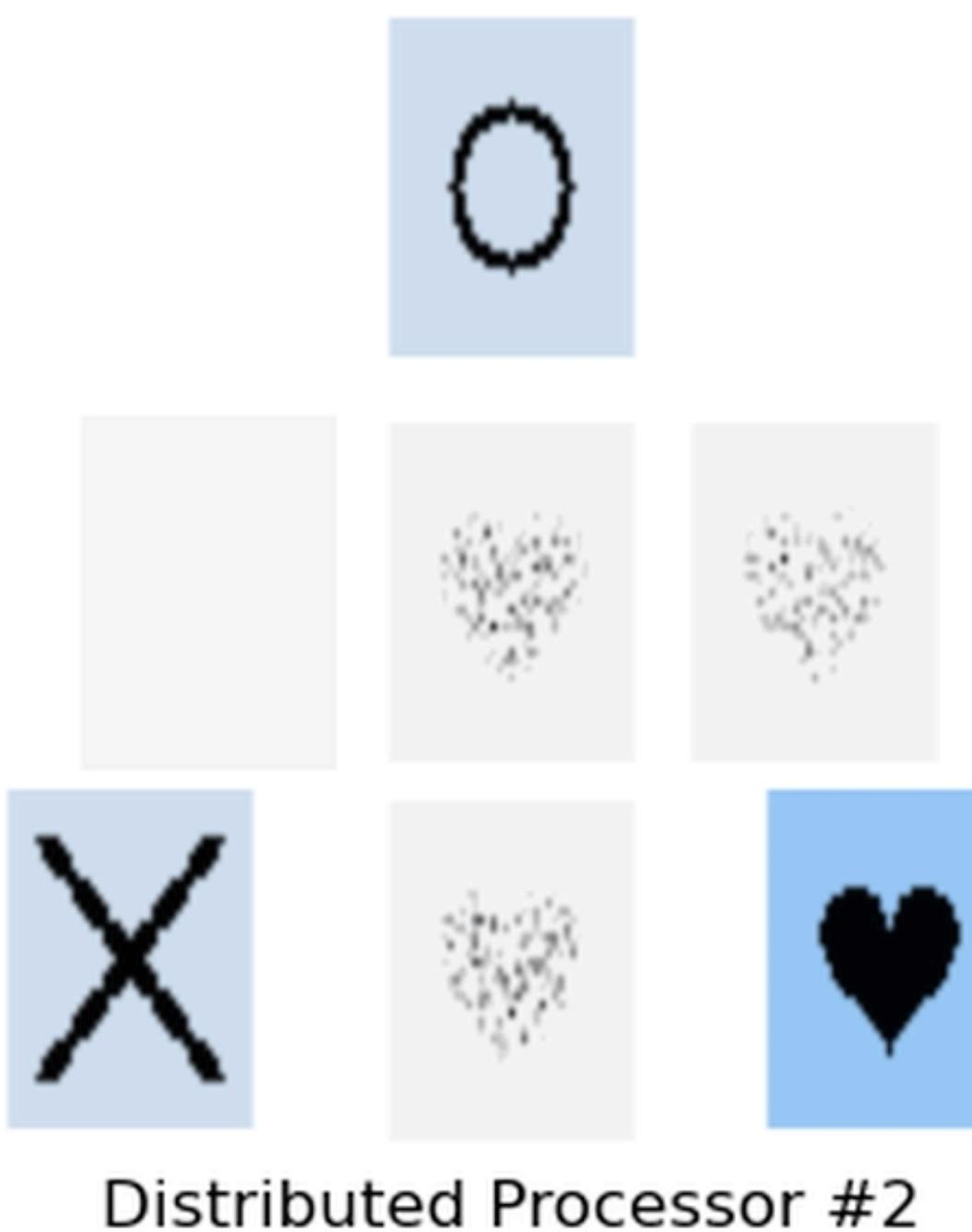
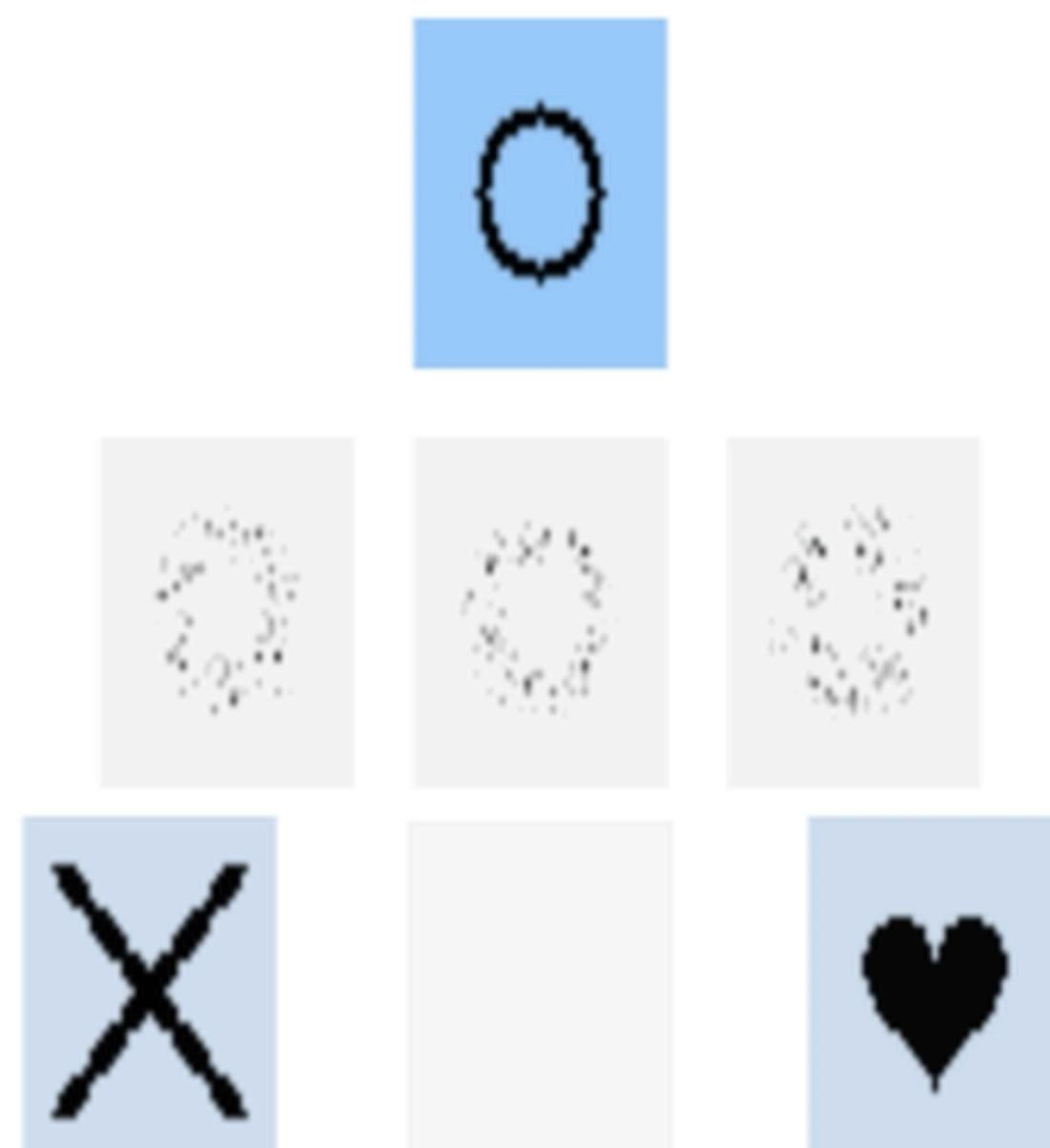
**Experiment #2** Wasserstein barycenter

$$\arg \inf_{\mu \in \mathcal{P}_2(\mathcal{X})} \sum_{i=1}^n w_i W^2(\mu, \xi_i)$$



# Stochastic Learning/ Distributed Computing

## Experiment #2 Wasserstein barycenter



# Thank You

## Acknowledgment:



1923278, 2112754, 2112755



UNIVERSITY OF CALIFORNIA  
**SANTA CRUZ**

Regent's Fellowship

BSOE Dissertation Year Fellowship

# **Backup Slides**

# Stochastic Control/ Control-affine: Nonuniform Noisy Kuramoto Oscillators

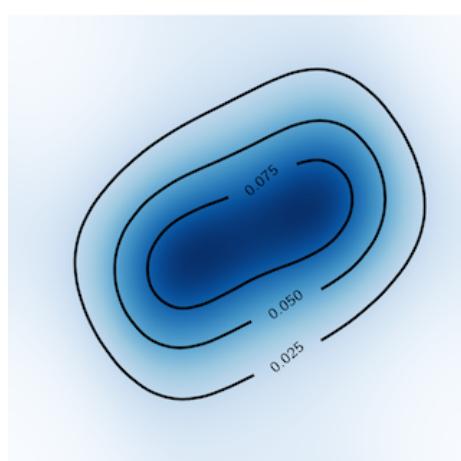
## First order Case Study

$$\inf_{u \in \mathcal{U}} \mathbb{E}_{\mu^u} \left[ \int_0^T \frac{1}{2} u^2 dt \right],$$

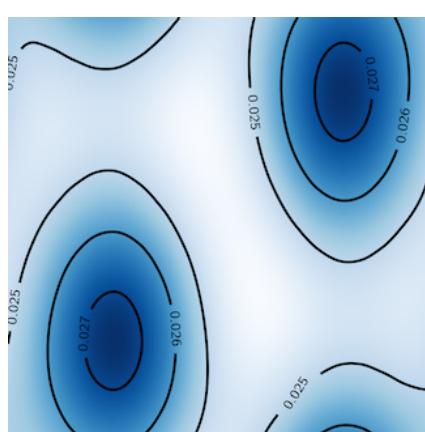
$$\inf_{u \in \mathcal{U}} \mathbb{E}_{\mu^u} \left[ \int_0^T \frac{1}{2} u^2 dt \right],$$

Change of variables

$$d\theta = (-\nabla_\theta V(\theta) + Su) dt + \sqrt{2} S dw \xrightarrow{\theta \mapsto \xi := S^{-1}\theta} d\xi = (u - \Upsilon \nabla_\xi \tilde{V}(\xi)) dt + \sqrt{2} dw$$



$\theta(t = 0) \sim \mu_0$  (Desynchronized)



$\theta(t = T) \sim \tilde{\mu}_T$  (Synchronized)

$\xi(t = 0) \sim \tilde{\mu}_0$  (Desynchronized)

$\xi(t = T) \sim \tilde{\mu}_T$  (Synchronized)

# Stochastic Control/ Control-affine: Nonuniform Noisy Kuramoto Oscillators

First order

$$d\theta = (-\nabla_{\theta} V(\theta) + Su) dt + \sqrt{2} S dw$$

Second order

$$\begin{pmatrix} d\theta \\ d\omega \end{pmatrix} = \begin{pmatrix} \omega \\ -M^{-1} \nabla_{\theta} V(\theta) - M^{-1} \Gamma \omega + M^{-1} Su \end{pmatrix} dt + \begin{pmatrix} 0_{n \times 1} \\ \sqrt{2} M^{-1} S dw \end{pmatrix}$$

Potential function

$$V(\theta) := \sum_{i < j} k_{ij}(1 - \cos(\theta_i - \theta_j - \varphi_{ij})) - \sum_{i=1}^n P_i \theta_i$$

Coupling  $> 0$

Phase difference  $\in [0, \pi/2)$

Linear coeff.  $> 0$

Positive diagonal matrices

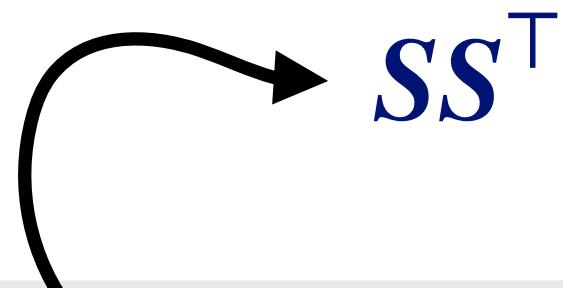
$$M, \Gamma, S$$

# Stochastic Control/ Control-affine: Nonuniform Noisy Kuramoto Oscillators

$$\inf_{(\rho, u)} \int_0^T \int_{\mathcal{X}} \|u(x, t)\|_2^2 \rho(x, t) \, dx dt$$

First order,  $\mathcal{X} \equiv \mathbb{T}^n$

$$\text{s.t } \frac{\partial \rho}{\partial t} = - \nabla_{\theta} \cdot \left( \rho (S u - \nabla_{\theta} V) \right) + \langle D, \text{Hess} (\rho) \rangle$$

$$SS^{\top}$$


Second order,  $\mathcal{X} \equiv \mathbb{T}^n \times \mathbb{R}^n$

$$\text{s.t } \frac{\partial \rho}{\partial t} = \nabla_{\omega} \cdot \left( \rho (M^{-1} \nabla_{\theta} V(\theta) + M^{-1} \Gamma \omega - M^{-1} S u + M^{-1} D M^{-1} \nabla_{\omega} \log \rho) - \langle \omega, \nabla_{\theta} \rho \rangle \right)$$

Initial and Terminal conditions  $\rho(x, t = 0) = \rho_0, \quad \rho(x, t = T) = \rho_T$

# Stochastic Control/ Control-affine: Nonuniform Noisy Kuramoto Oscillators

## The Second Order Case

**Uncontrolled forward-backward Kolmogrov PDEs**

$$\frac{\partial \hat{\varphi}}{\partial t} = - \left\langle \boldsymbol{\eta}, \nabla_{\boldsymbol{\xi}} \hat{\varphi} \right\rangle + \nabla_{\boldsymbol{\eta}} \cdot \left( \hat{\varphi} \left( \widetilde{\mathbf{Y}} \nabla_{\boldsymbol{\xi}} \mathbf{U}(\boldsymbol{\xi}) + \nabla_{\boldsymbol{\eta}} \mathbf{F}(\boldsymbol{\eta}) \right) \right) + \Delta_{\boldsymbol{\eta}} \hat{\varphi}$$

$$\frac{\partial \varphi}{\partial t} = - \left\langle \boldsymbol{\eta}, \nabla_{\boldsymbol{\xi}} \varphi \right\rangle + \left\langle \widetilde{\mathbf{Y}} \nabla_{\boldsymbol{\xi}} \mathbf{U}(\boldsymbol{\xi}) + \nabla_{\boldsymbol{\eta}} \mathbf{F}(\boldsymbol{\eta}), \nabla_{\boldsymbol{\eta}} \varphi \right\rangle - \Delta_{\boldsymbol{\eta}} \varphi$$

**Optimal controlled joint state PDF:**  $\rho^{\text{opt}}(\boldsymbol{\theta}, \boldsymbol{\omega}, t) = \hat{\varphi} \left( (\mathbf{I}_2 \otimes \mathbf{M} \mathbf{S}^{-1}) \begin{pmatrix} \boldsymbol{\theta} \\ \boldsymbol{\omega} \end{pmatrix}, t \right) \varphi \left( (\mathbf{I}_2 \otimes \mathbf{M} \mathbf{S}^{-1}) \begin{pmatrix} \boldsymbol{\theta} \\ \boldsymbol{\omega} \end{pmatrix}, t \right) \left( \prod_{i=1}^n \frac{m_i^2}{\sigma_i^2} \right)$

**Optimal control:**  $\mathbf{u}^{\text{opt}} \left( (\mathbf{I}_2 \otimes \mathbf{M} \mathbf{S}^{-1}) \begin{pmatrix} \boldsymbol{\theta} \\ \boldsymbol{\omega} \end{pmatrix}, t \right) = (\mathbf{I}_2 \otimes \mathbf{S} \mathbf{M}^{-1}) \nabla_{\boldsymbol{\theta}} \log \varphi \left( (\mathbf{I}_2 \otimes \mathbf{M} \mathbf{S}^{-1}) \begin{pmatrix} \boldsymbol{\theta} \\ \boldsymbol{\omega} \end{pmatrix}, t \right)$

**Initial and Terminal conditions**

$$\hat{\varphi}_0(\boldsymbol{\xi}) \varphi_0(\boldsymbol{\xi}) = \rho_0 \left( (\mathbf{I}_2 \otimes \mathbf{S} \mathbf{M}^{-1}) \begin{pmatrix} \boldsymbol{\xi} \\ \boldsymbol{\eta} \end{pmatrix} \right) \left( \prod_{i=1}^n \frac{\sigma_i^2}{m_i^2} \right)$$

$$\hat{\varphi}_T(\boldsymbol{\xi}) \varphi_T(\boldsymbol{\xi}) = \rho_T \left( (\mathbf{I}_2 \otimes \mathbf{S} \mathbf{M}^{-1}) \begin{pmatrix} \boldsymbol{\xi} \\ \boldsymbol{\eta} \end{pmatrix} \right) \left( \prod_{i=1}^n \frac{\sigma_i^2}{m_i^2} \right)$$

# Stochastic Control/ Control-affine/ Nonuniform Noisy Kuramoto Oscillators

## Proximal recursion

$$\hat{\phi}_k = \text{prox}_{h\Psi}^d(\hat{\phi}_{k-1}) := \arg \inf_{\hat{\phi}} \frac{1}{2} \left( d(\hat{\phi}, \hat{\phi}_{k-1}) \right)^2 + h\Psi(\hat{\phi})$$

Distance      Step size      Energy-like functional

**First order:**  $d \equiv W_\Gamma \quad \Psi(\hat{\phi}) \equiv \int_{\prod_{i=1}^n [0, 2\pi/\sigma_i)} (\tilde{V} + \log \hat{\phi}) \hat{\phi} d\xi$

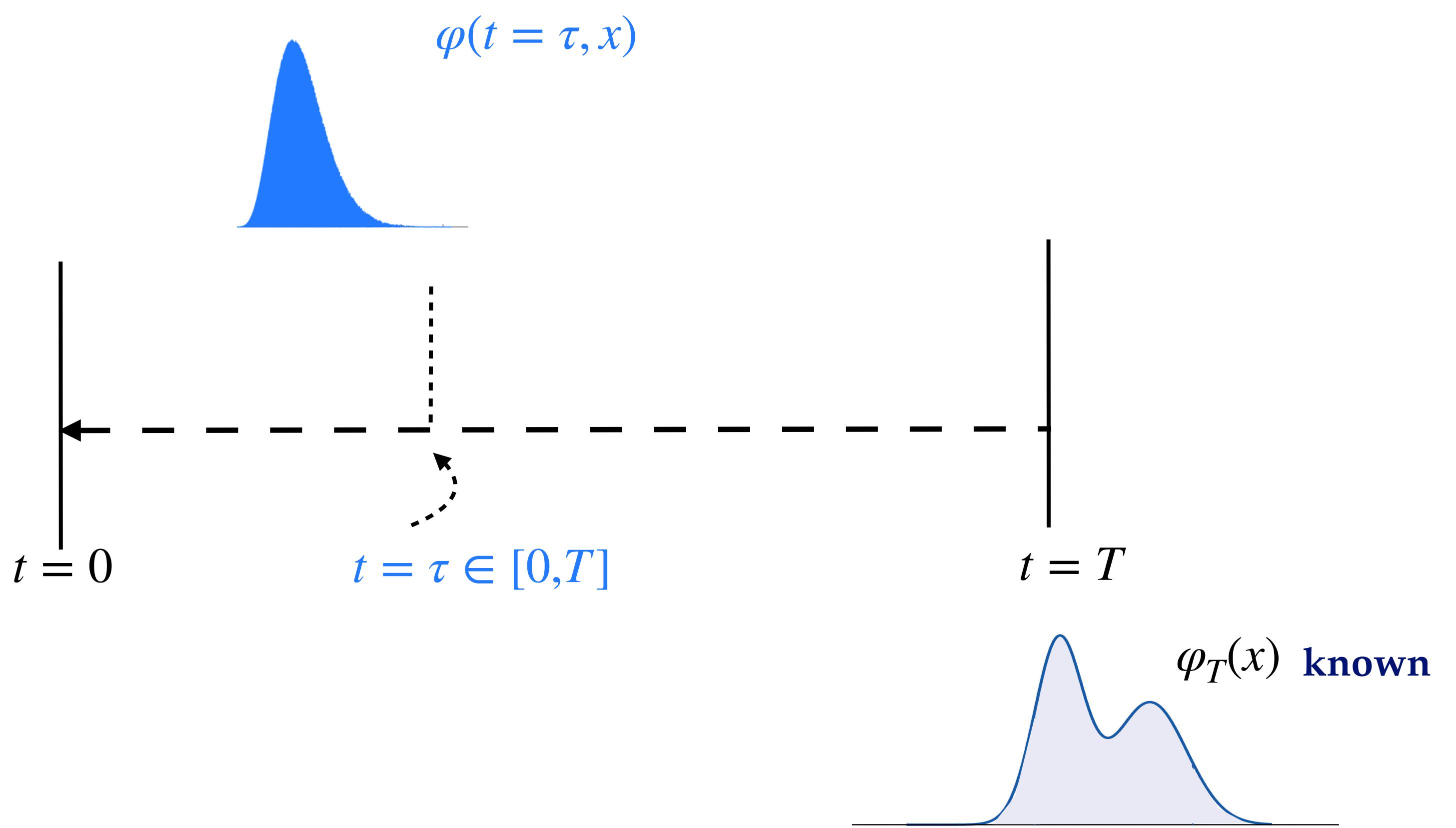
**Second order:**  $d \equiv W_{h,\tilde{\Gamma}}$

$$\Psi(\hat{\phi}) \equiv \int \left( \prod_{i=1}^n [0, 2\pi m_i/\sigma_i) \right) \times \mathbb{R}^n (F + \log \hat{\phi}) \hat{\phi} d\xi d\eta$$

# Stochastic Control/ Control-affine/ Nonuniform Noisy Kuramoto Oscillators

## Feynman-Kac Path Integral

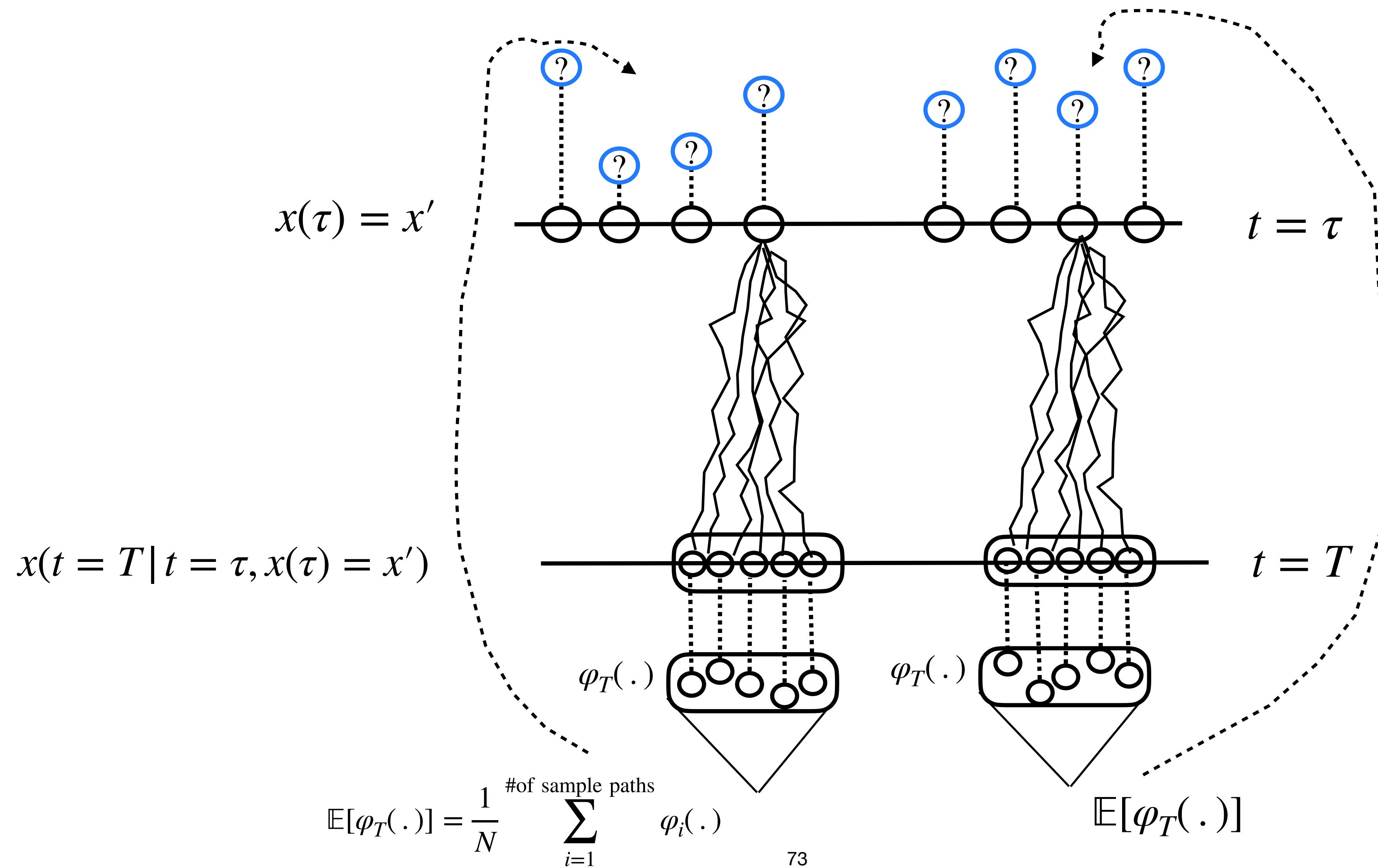
$$\frac{\partial \varphi}{\partial t} = L_{\text{Backward}} \varphi$$



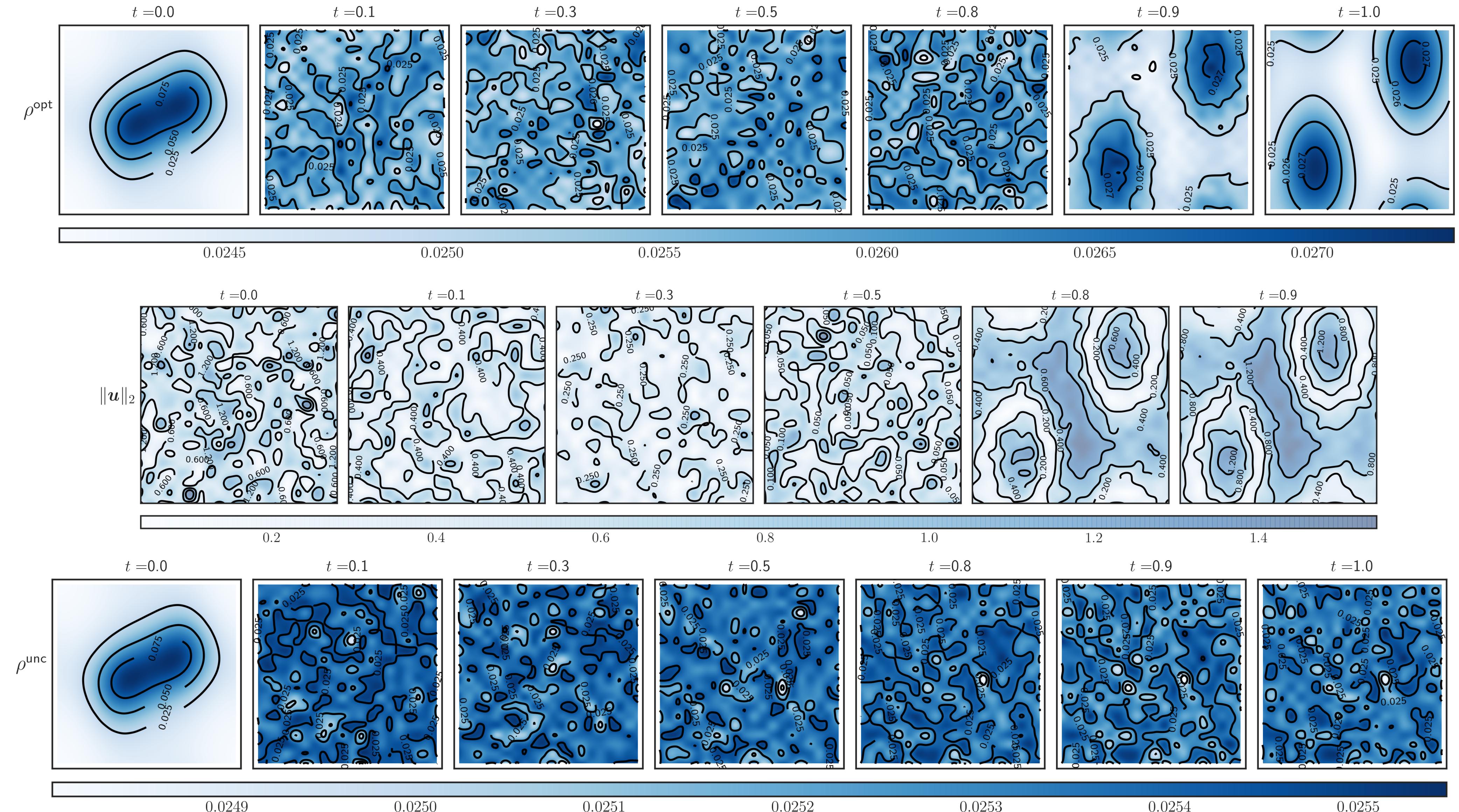
# Stochastic Control/ Control-affine/ Nonuniform Noisy Kuramoto Oscillators

## Feynman-Kac Path Integral

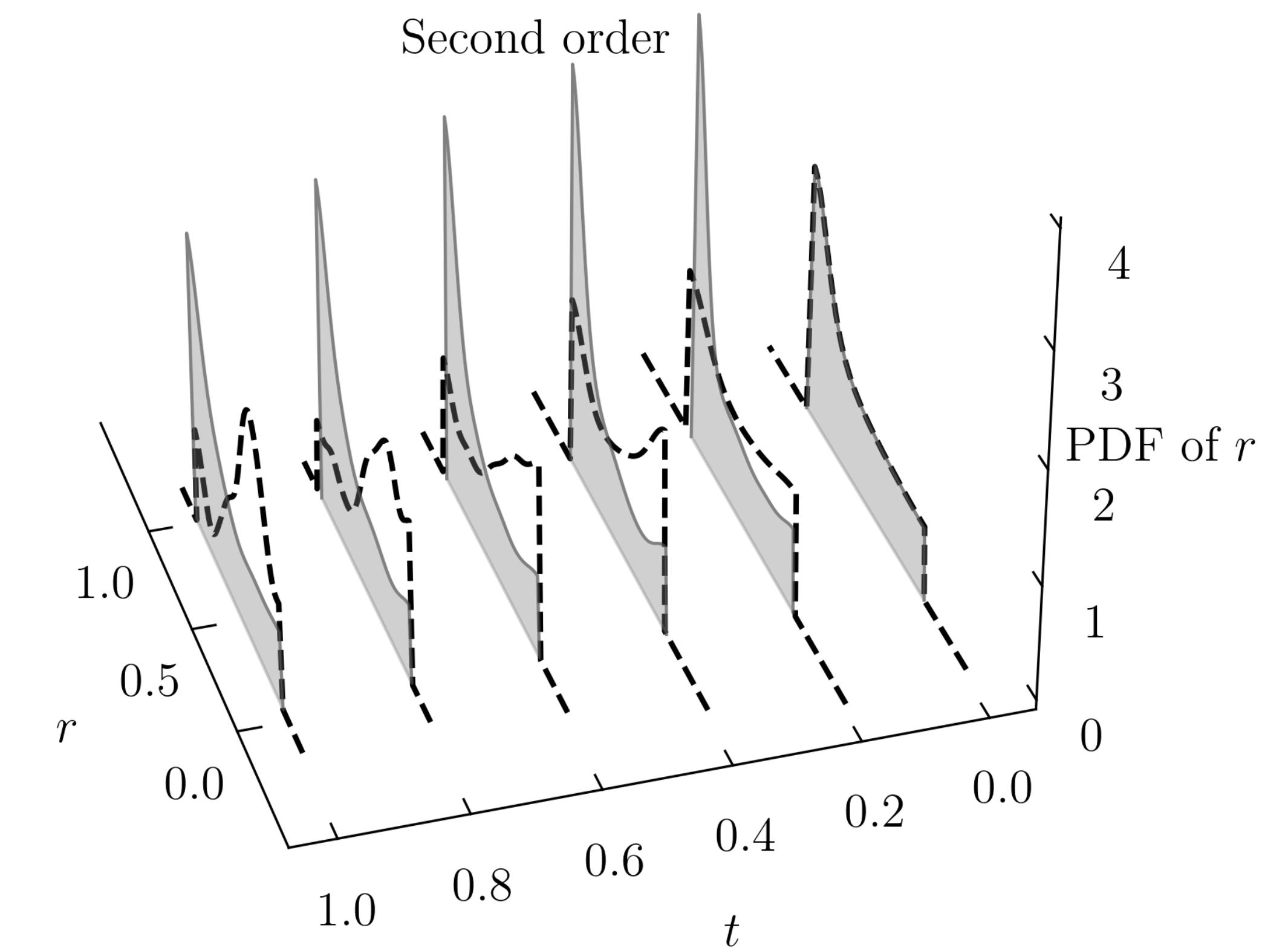
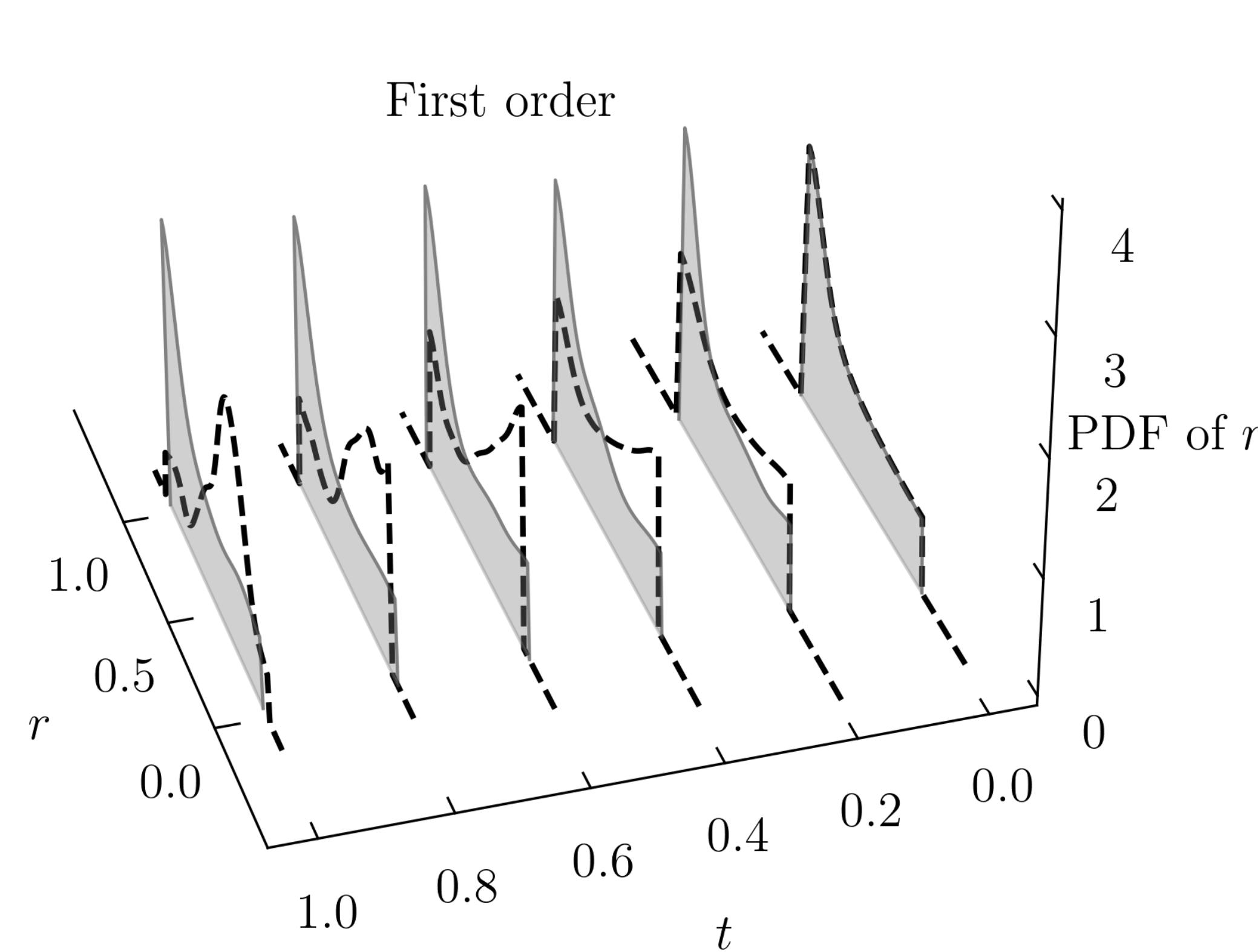
$\varphi(t = \tau, x')$



# Stochastic Control/ Control-affine/ Nonuniform Noisy Kuramoto Oscillators



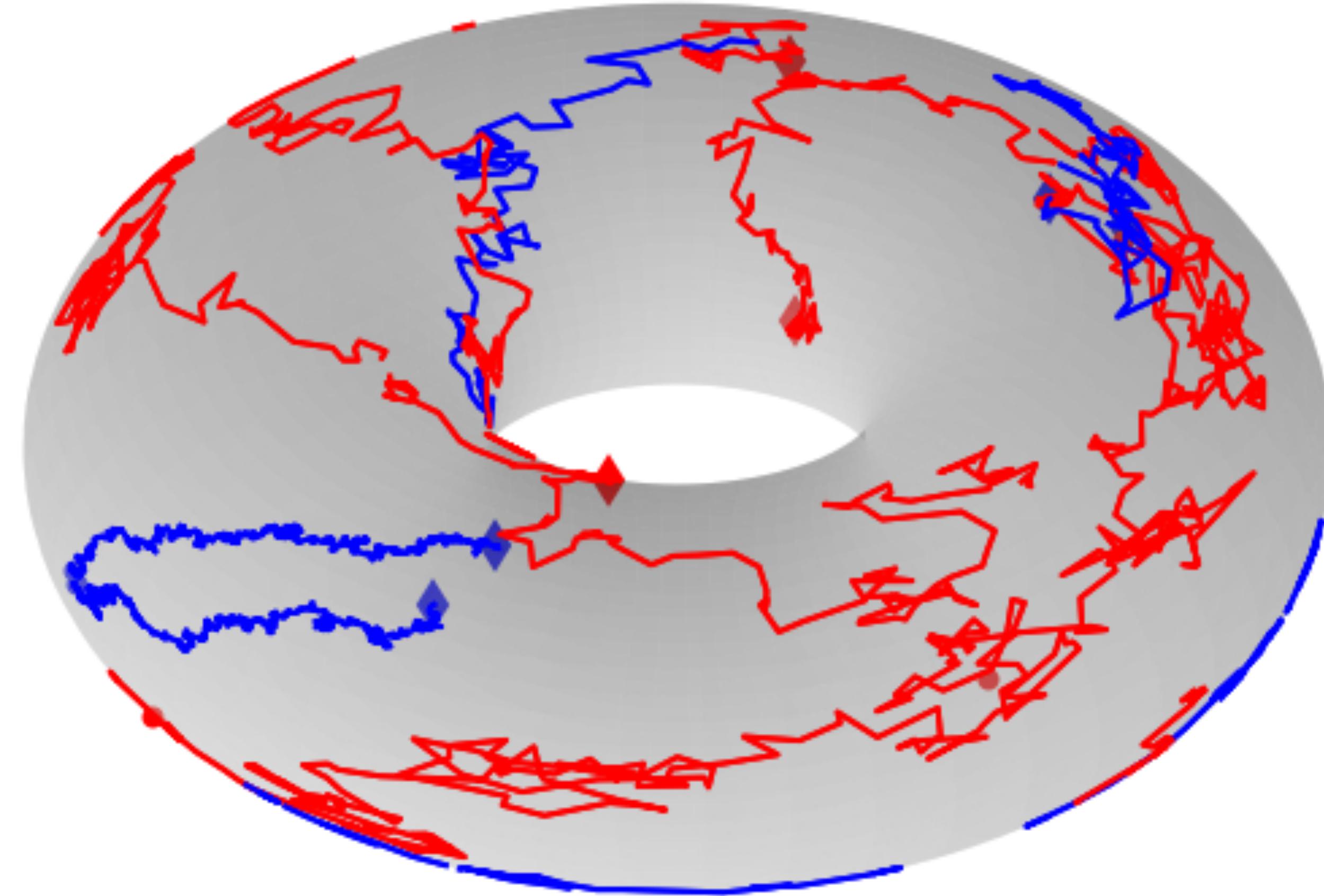
# Stochastic Control/ Control-affine/ Nonuniform Noisy Kuramoto Oscillators



PDF of order parameter  $r := \frac{1}{n} \sqrt{\left( \sum_{i=1}^n \cos \theta_i \right)^2 + \left( \sum_{i=1}^n \sin \theta_i \right)^2}$

# Stochastic Control/ Control-affine/ Nonuniform Noisy Kuramoto Oscillators

Optimally Controlled Sample Paths



# Stochastic Control/ Control Non-affine

**Case1: Solve via PINN**

**Loss term for HJB PDE**

$$\mathcal{L}_\psi = \frac{1}{n} \sum_{i=1}^n \left( \frac{\partial \psi}{\partial t} \Big|_{x_i} - \frac{1}{2} (\pi^{\text{opt}})^2 \Big|_{x_i^u} + \frac{\partial \psi}{\partial x^u} D_1 \Big|_{x_i^u} + \frac{\partial^2 \psi}{\partial x^{u2}} D_2 \Big|_{x_i^u} \right)^2$$

**Loss term for FPK PDE**

$$\mathcal{L}_{\rho^u} = \frac{1}{n} \sum_{i=1}^n \left( \frac{\partial \rho^u}{\partial t} \Big|_{x_i^u} + \frac{\partial}{\partial x^u} (D_1 \rho^u) \Big|_{x_i^u} - \frac{\partial^2}{\partial x^{u2}} (D_2 \rho^u) \Big|_{x_i^u} \right)^2$$

**Loss term for policy equation**

$$\mathcal{L}_{\pi^{\text{opt}}} = \frac{1}{n} \sum_{i=1}^n \left( \pi^{\text{opt}} \Big|_{x_i^u} - \frac{\partial \psi}{\partial x^u} \frac{\partial D_1}{\partial u} \Big|_{x_i^u} - \frac{\partial^2 \psi}{\partial x^{u2}} \frac{\partial D_2}{\partial u} \Big|_{x_i^u} \right)^2$$

**Loss term for initial condition**

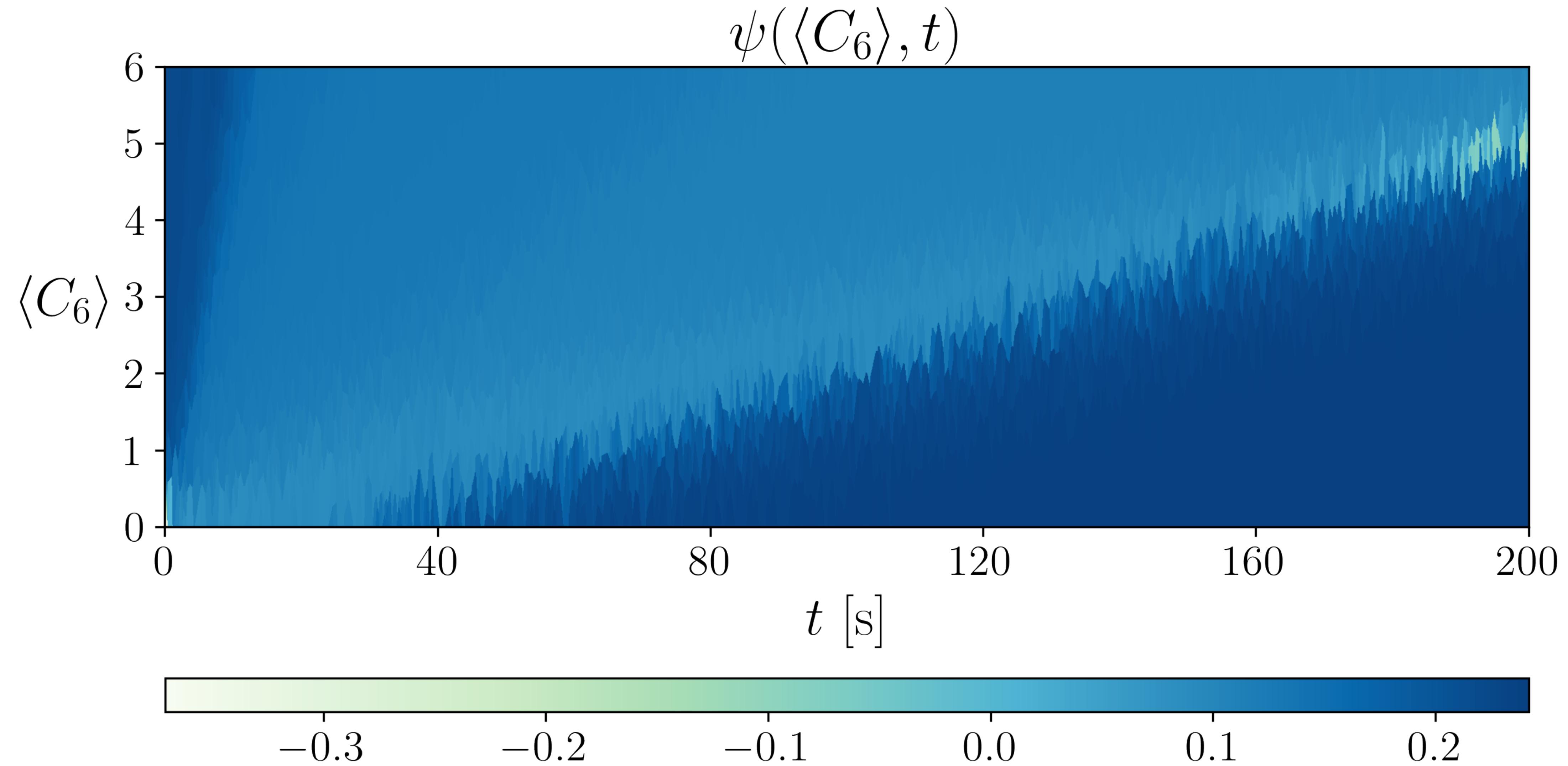
$$\mathcal{L}_{\rho_0^u} = \frac{1}{n} \sum_{i=1}^n \left( \rho^u \Big|_{t=0} - \rho_0^u(x) \right)^2$$

**Loss term for terminal condition**

$$\mathcal{L}_{\rho_T^u} = \frac{1}{n} \sum_{i=1}^n \left( \rho^u \Big|_{t=T} - \rho_T^u(x) \right)^2$$

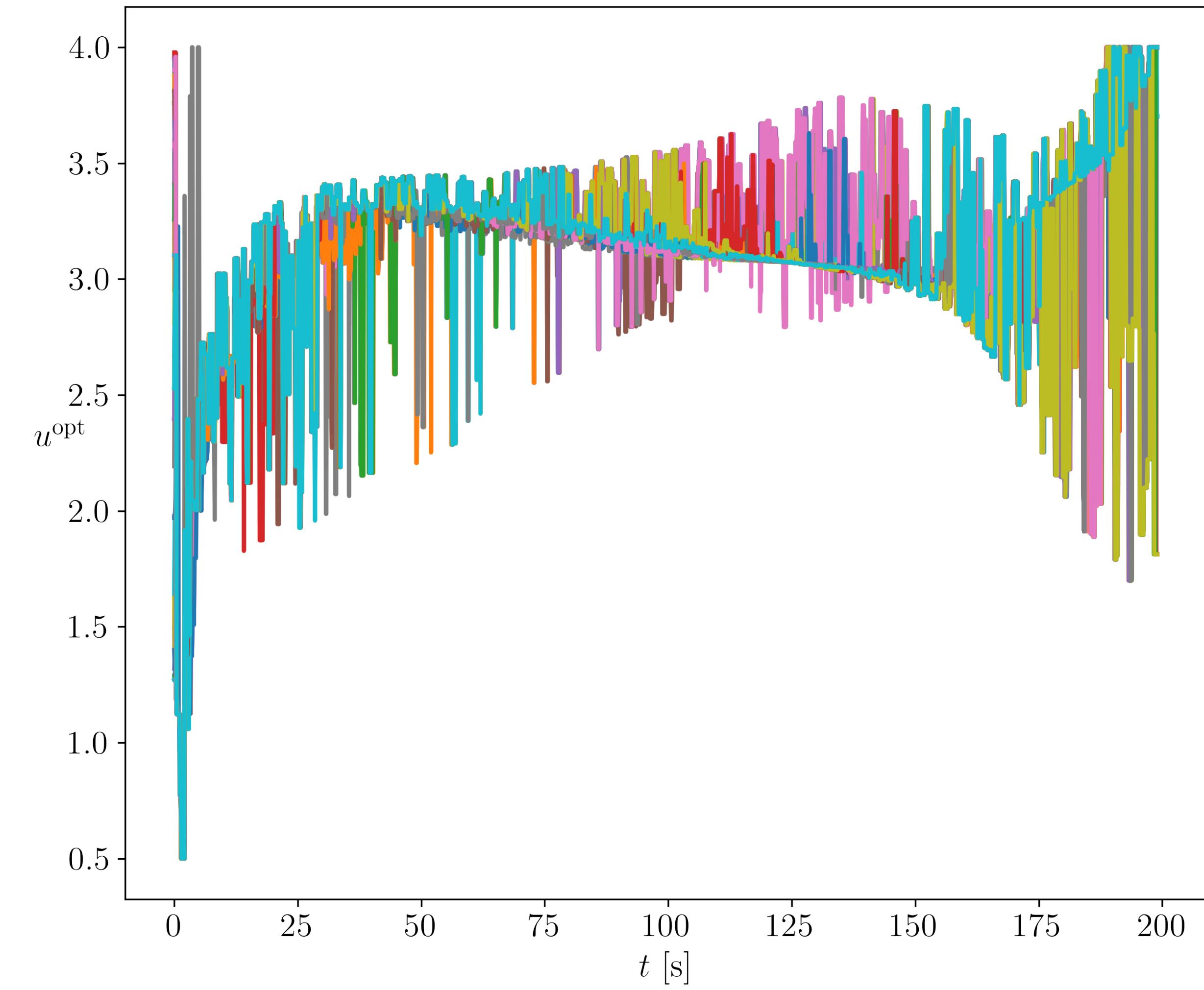
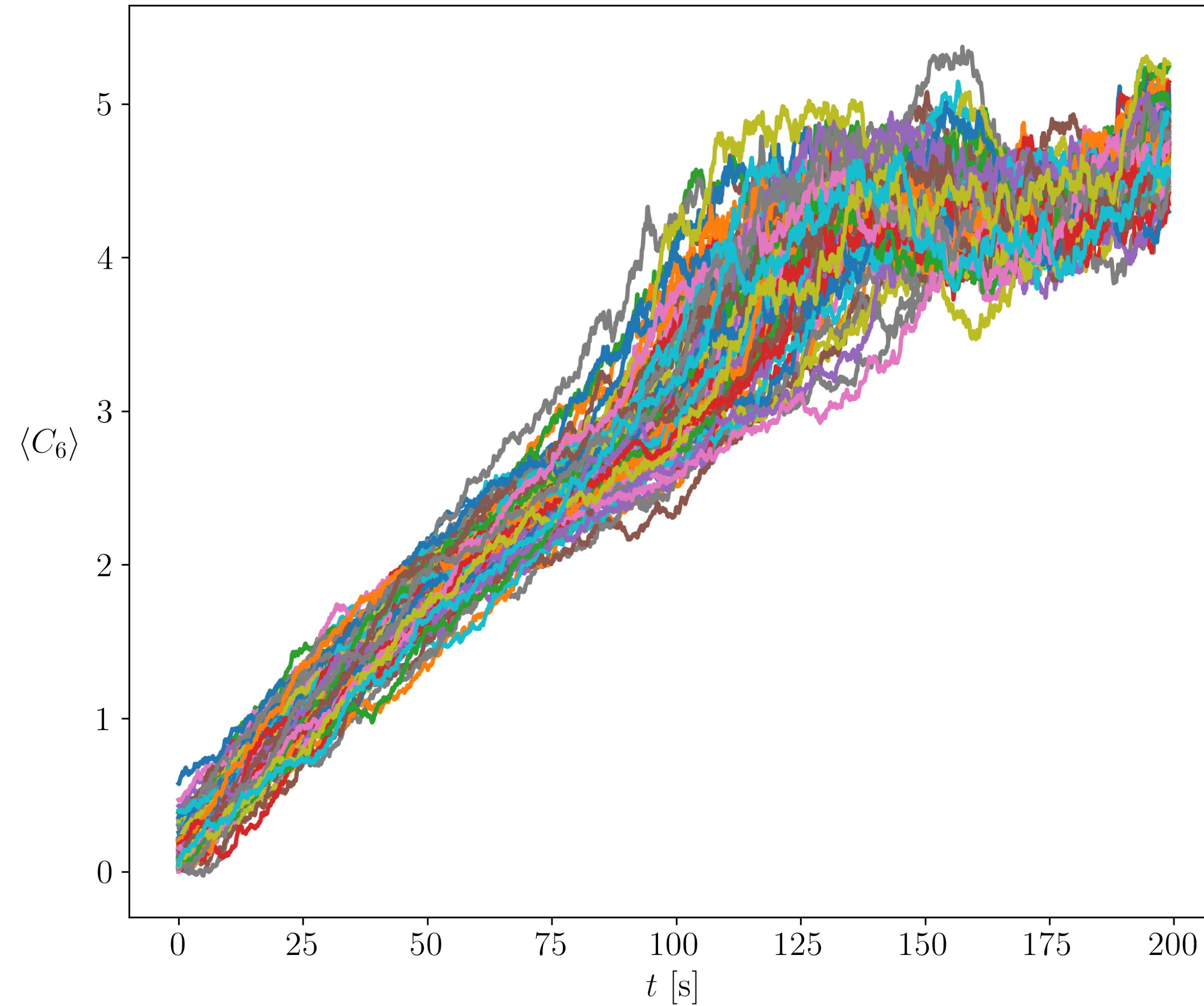
# Stochastic Control/ Control Non-affine

## Case 1: Value Function



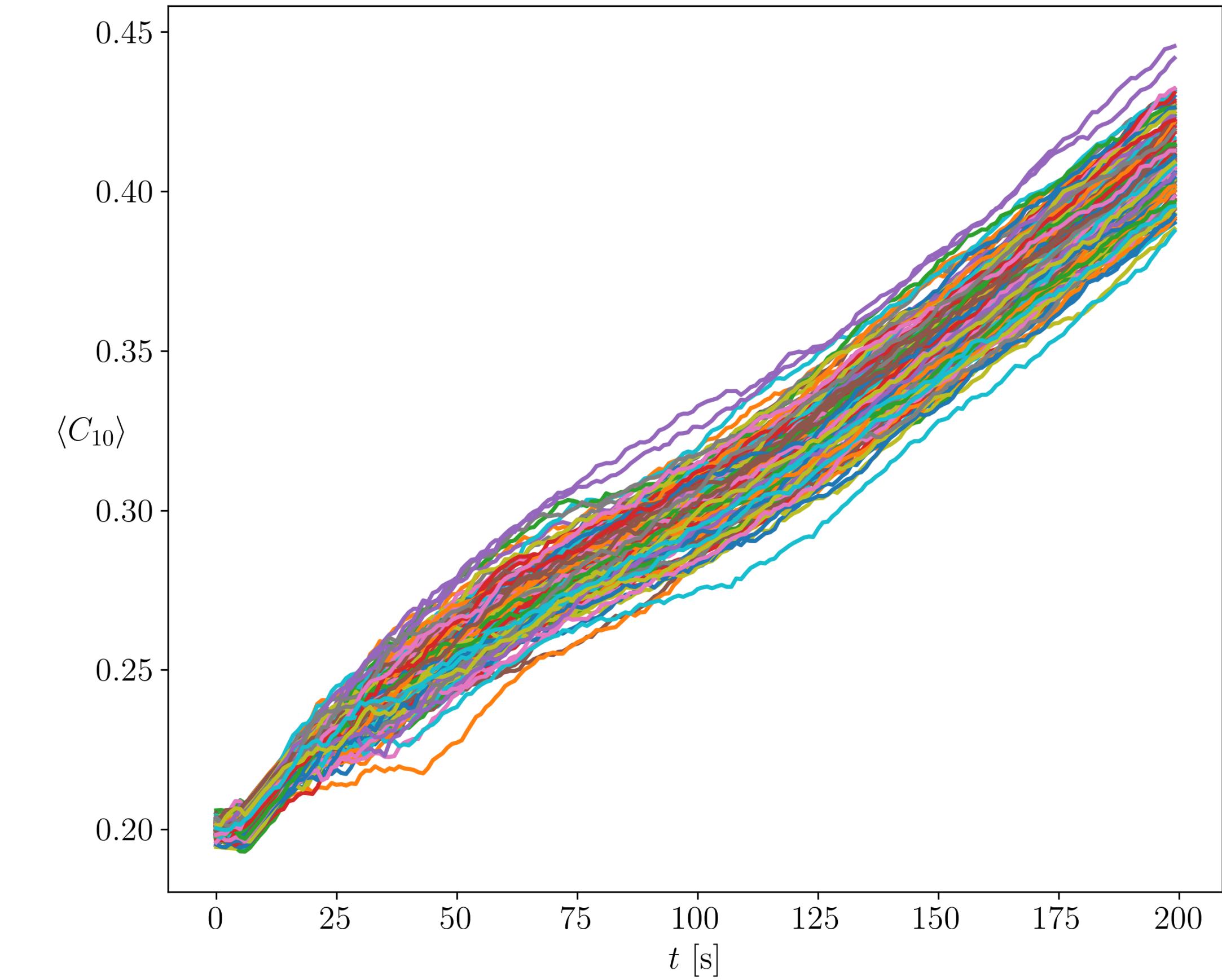
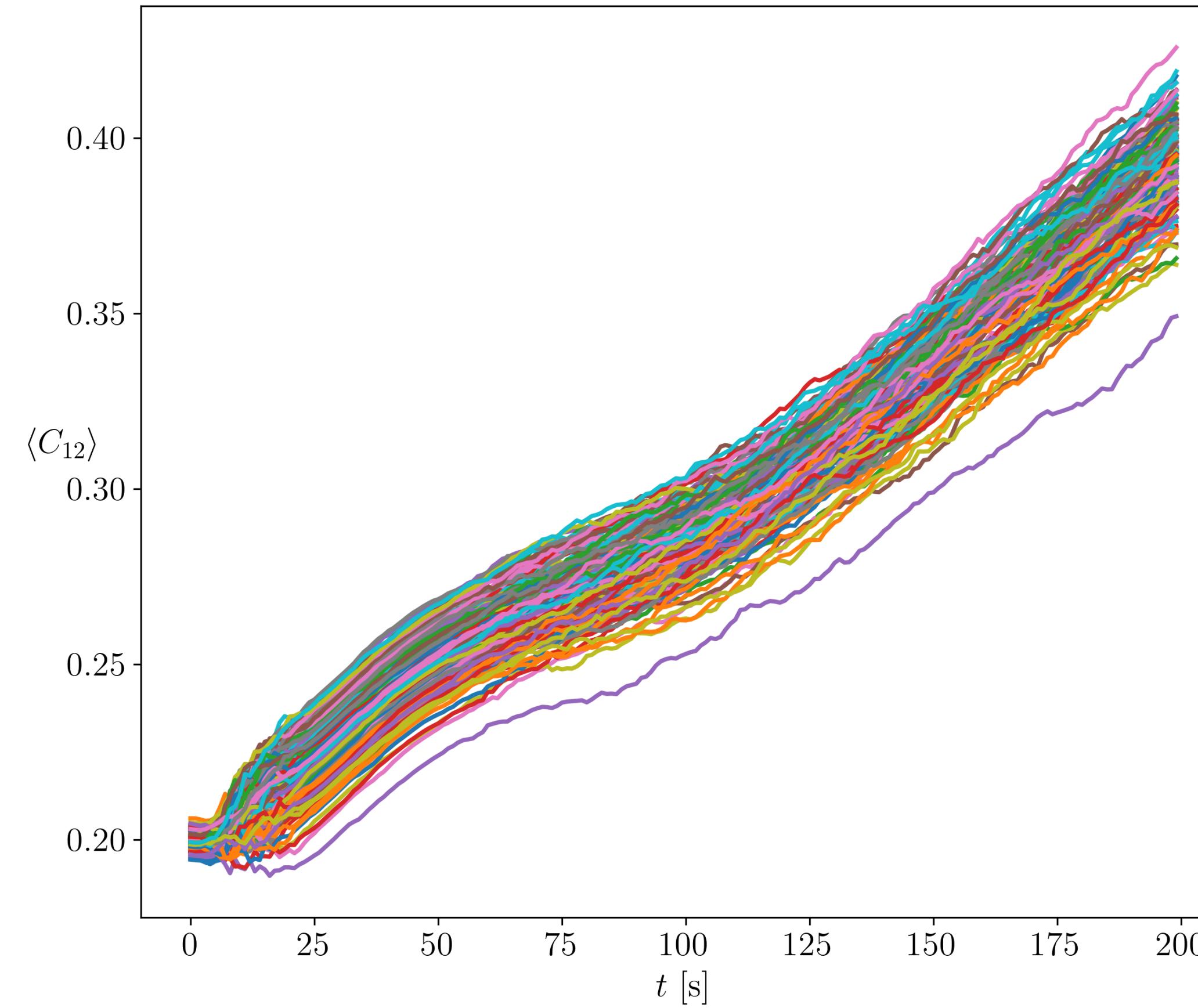
# Stochastic Control/ Control Non-affine

## Case 1: Optimal State and Optimal Control Sample Paths



# Stochastic Control/ Control Non-affine

## Case 2: Closed Loop State Sample Paths



Desired transport from mean  $(0.2, 0.2)$  to  $(0.40, 0.37)$  for BCC structure

# Stochastic Modeling

## Existing state-of-the-art

Several works on modeling the finite population:

[Lu et. al., Appl. Phys. Lett., 2014] [Edward and Bevan, Langmuir, 2014] [Matei et. al., CDC, 2020]

[Matei et. al., CDC, 2021]

[Lefevre et. al., IEEE / ASME Trans. on Mechatronics, 2022]

## How to steer the large finite population toward desired pattern:

Vectorize the positions of all chiplets, then apply MPC [Matei et. al., US Patent 17121411]

Computation does not scale ... need new ideas

# Stochastic Learning/ Distributed Computing

## Discrete Version of the Proposed ADMM

Euclidean distance matrix

$$\mu_i^{k+1} = \text{prox}_{\frac{1}{\alpha}(F_i(\mu_i) + \langle \nu_i^k, \mu_i \rangle)}^W(\zeta^k)$$

$$= \arg \inf_{\mu_i \in \Delta^{N-1}} \left\{ \min_{M \in \Pi_N(\mu_i, \zeta^k)} \frac{1}{2} \langle C, M \rangle + \frac{1}{\alpha} (F_i(\mu_i) + \langle \nu_i^k, \mu_i \rangle) \right\}$$

$$\zeta^{k+1} = \arg \inf_{\zeta \in \Delta^{N-1}} \left\{ \left( \sum_{i=1}^n \min_{M_i \in \Pi_N(\mu_i^{k+1}, \zeta)} \frac{1}{2} \langle C, M_i \rangle \right) - \frac{2}{\alpha} \langle \nu_{\text{sum}}^k, \zeta \rangle \right\}$$

$$\nu_i^{k+1} = \nu_i^k + \alpha (\mu_i^{k+1} - \zeta^{k+1})$$

Outer layer ADMM
Inner layer ADMM

where  $N$  is the number of samples

With Sinkhorn regularization:

Discrete Sinkhorn divergence

$$\mu_i^{k+1} = \text{prox}_{\frac{1}{\alpha}(F_i(\mu_i) + \langle \nu_i^k, \mu_i \rangle)}^{W_\varepsilon}(\zeta^k)$$

$$= \arg \inf_{\mu_i \in \Delta^{N-1}} \left\{ \min_{M \in \Pi_N(\mu_i, \zeta^k)} \left\langle \frac{1}{2} C + \varepsilon \log M, M \right\rangle + \frac{1}{\alpha} (F_i(\mu_i) + \langle \nu_i^k, \mu_i \rangle) \right\}$$

$$\zeta^{k+1} = \arg \inf_{\zeta \in \Delta^{N-1}} \left\{ \left( \sum_{i=1}^n \min_{M_i \in \Pi_N(\mu_i^{k+1}, \zeta)} \left\langle \frac{1}{2} C + \varepsilon \log M_i, M_i \right\rangle \right) - \frac{2}{\alpha} \langle \nu_{\text{sum}}^k, \zeta \rangle \right\}$$

$$\nu_i^{k+1} = \nu_i^k + \alpha (\mu_i^{k+1} - \zeta^{k+1})$$

Outer layer ADMM
Inner layer ADMM

# Stochastic Learning/ Distributed Computing

$\mu_i$  update  $\rightsquigarrow$  Outer Consensus (Sinkhorn) ADMM

Example:

$$G_i(\boldsymbol{\mu}_i) := F_i(\boldsymbol{\mu}_i) + \langle \boldsymbol{\nu}_i^k, \boldsymbol{\mu}_i \rangle, \boldsymbol{\zeta}^k \in \Delta^{N-1}, k \in \mathbb{N}_0$$

$$\boldsymbol{\mu}_i^{k+1} = \text{prox}_{\frac{1}{\alpha}(F_i(\boldsymbol{\mu}_i) + \langle \boldsymbol{\nu}_i^k, \boldsymbol{\mu}_i \rangle)}^{W_\varepsilon}(\boldsymbol{\zeta}^k) = \exp\left(\frac{\boldsymbol{\lambda}_{1i}^{\text{opt}}}{\alpha\varepsilon}\right) \odot \left( \exp\left(-\frac{\mathbf{C}^\top}{2\varepsilon}\right) \exp\left(\frac{\boldsymbol{\lambda}_{0i}^{\text{opt}}}{\alpha\varepsilon}\right) \right)$$

where  $\boldsymbol{\lambda}_{0i}^{\text{opt}}, \boldsymbol{\lambda}_{1i}^{\text{opt}} \in \mathbb{R}^N$  solve

$$\exp\left(\frac{\boldsymbol{\lambda}_{0i}^{\text{opt}}}{\alpha\varepsilon}\right) \odot \left( \exp\left(-\frac{\mathbf{C}}{2\varepsilon}\right) \exp\left(\frac{\boldsymbol{\lambda}_{1i}^{\text{opt}}}{\alpha\varepsilon}\right) \right) = \boldsymbol{\zeta}_k$$

$$\mathbf{0} \in \partial_{\boldsymbol{\lambda}_{1i}^{\text{opt}}} G_i^*(-\boldsymbol{\lambda}_{1i}^{\text{opt}}) - \exp\left(\frac{\boldsymbol{\lambda}_{1i}^{\text{opt}}}{\alpha\varepsilon}\right) \odot \left( \exp\left(-\frac{\mathbf{C}^\top}{2\varepsilon}\right) \exp\left(\frac{\boldsymbol{\lambda}_{0i}^{\text{opt}}}{\alpha\varepsilon}\right) \right)$$

# Stochastic Learning/ Distributed Computing

## $\zeta$ update $\rightsquigarrow$ Inner (Euclidean) ADMM

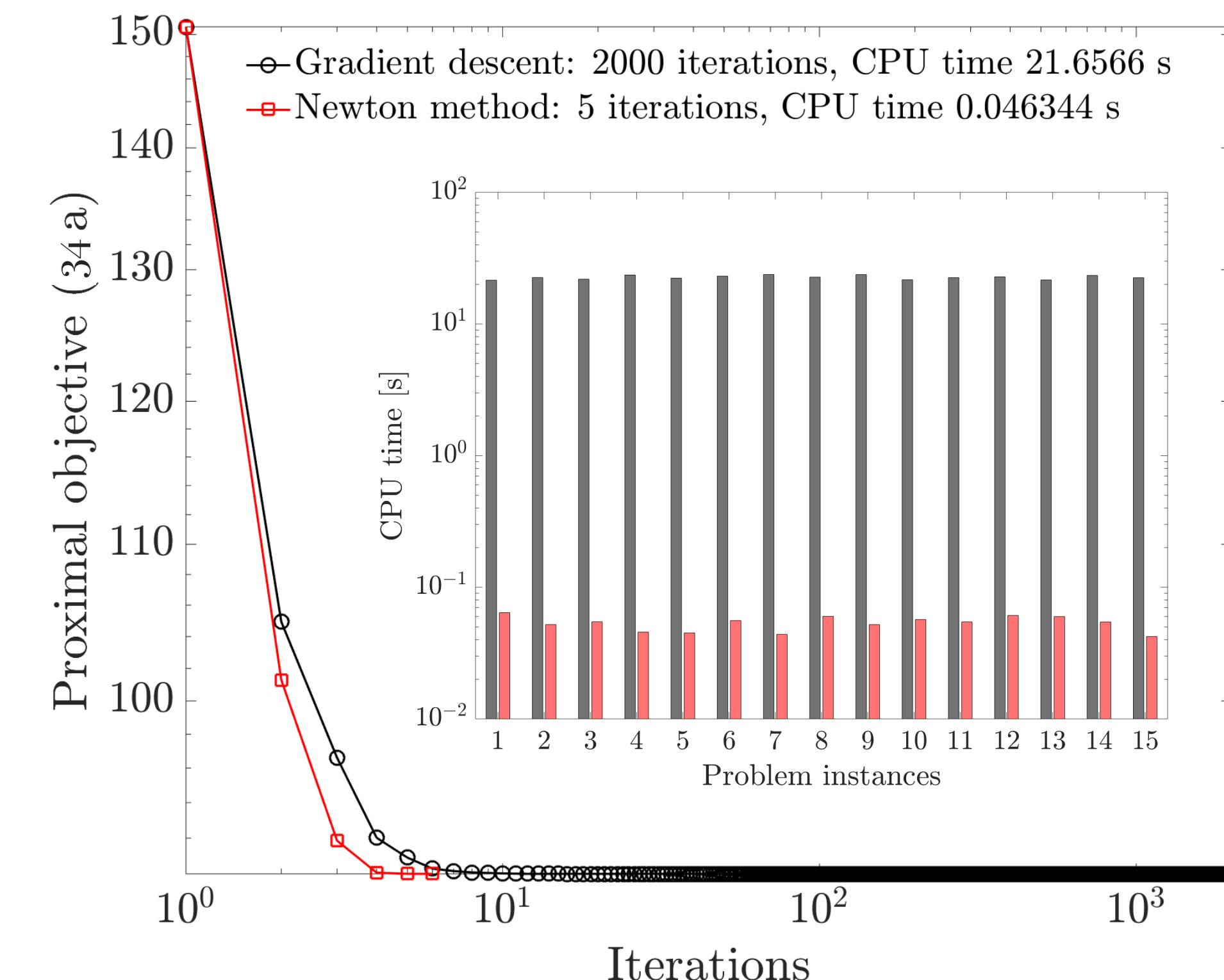
**Theorem.** Let  $f_i(\mathbf{u}_i) := \langle \boldsymbol{\mu}_i^{k+1}, \log(\Gamma \exp(\mathbf{u}_i/\varepsilon)) \rangle$ ,  $\mathbf{u}_i \in \mathbb{R}^N$ , for all  $i \in [n]$ ,

Then the following Euclidean ADMM solves

$$\begin{aligned}\mathbf{u}_i^{\ell+1} &= \text{prox}_{\frac{1}{\tau}f_i}^{\|\cdot\|_2} \left( \mathbf{z}_i^\ell - \tilde{\boldsymbol{\nu}}_i^\ell \right) \\ \mathbf{z}_i^{\ell+1} &= \left( \mathbf{u}_i^{\ell+1} - \frac{1}{n} \sum_{i=1}^n \mathbf{u}_i^{\ell+1} \right) + \left( \tilde{\boldsymbol{\nu}}_i^\ell - \frac{1}{n} \sum_{i=1}^n \tilde{\boldsymbol{\nu}}_i^\ell \right) + \frac{2}{n\alpha} \boldsymbol{\nu}_{\text{sum}}^k \\ \tilde{\boldsymbol{\nu}}_i^{\ell+1} &= \tilde{\boldsymbol{\nu}}_i^\ell + (\mathbf{u}_i^{\ell+1} - \mathbf{z}_i^{\ell+1})\end{aligned}$$

**Theorem.**  
Guaranteed convergence for inner layer ADMM  
under some constraints on hyper-parameters

No analytical solution, use e.g.,  
Newton's method (has structured Hess)



# Stochastic Learning/ Distributed Computing

Centralized computation:

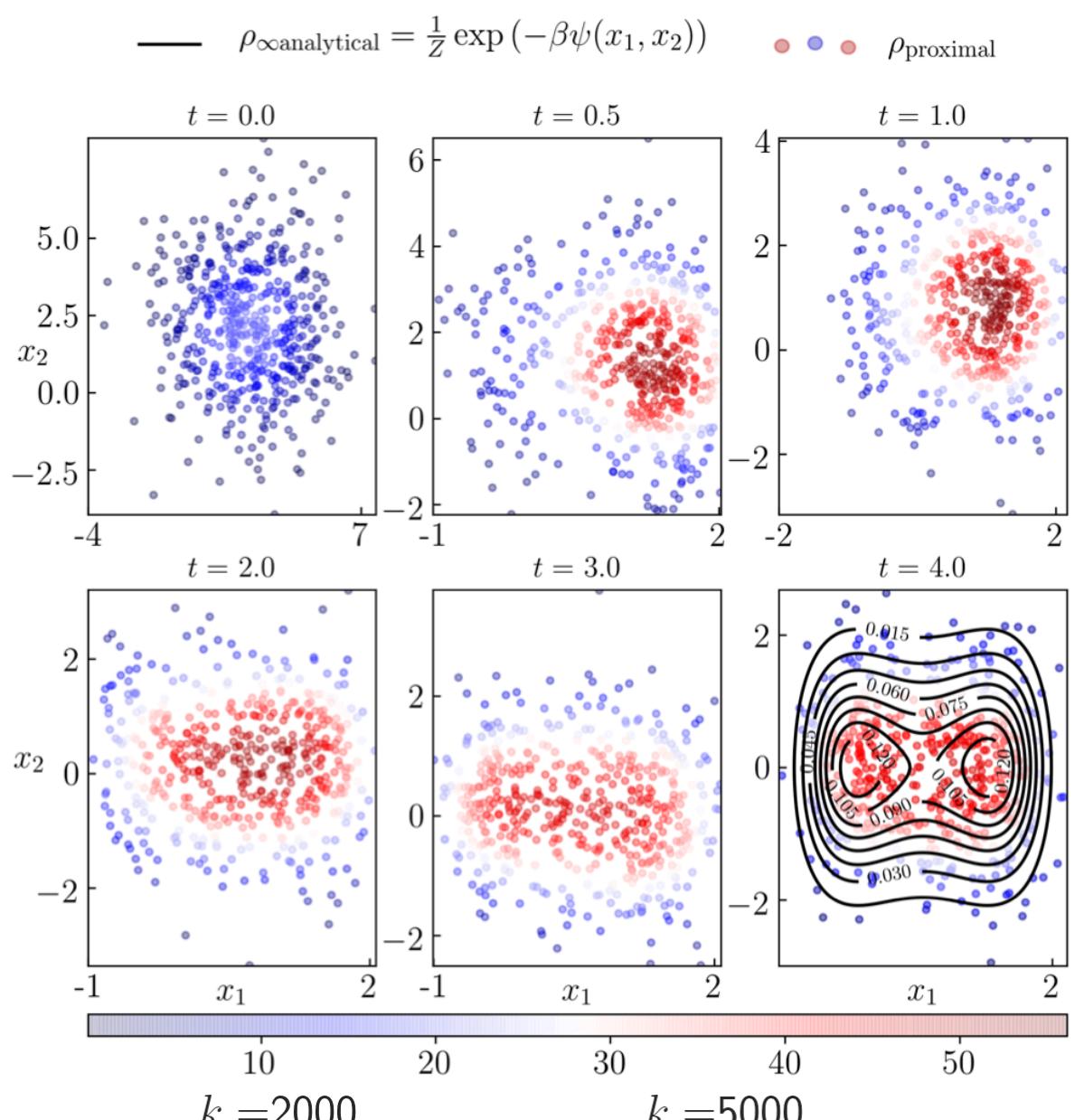
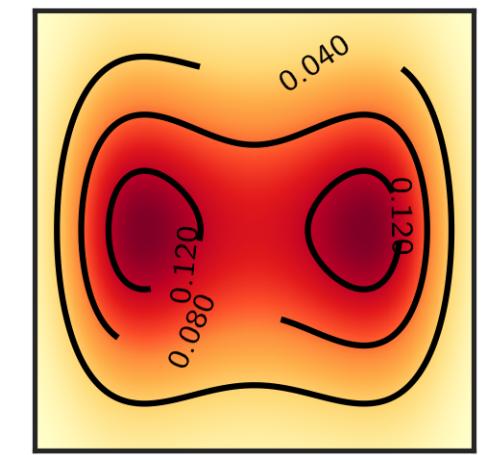
Caluya and Halder, IEEE Trans. Automatic Control, 2019

## Experiment #3 Linear Fokker-Planck-Kolmogorov PDE

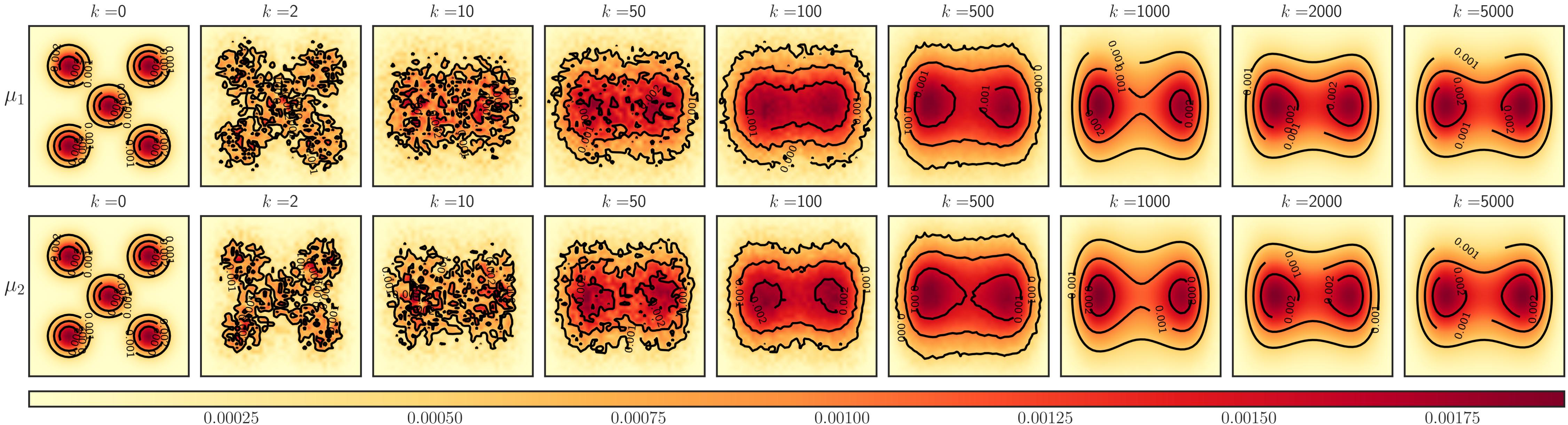
$$\frac{\partial \mu}{\partial t} = \nabla \cdot (\mu \nabla V) + \beta^{-1} \Delta \mu$$

$$V(x_1, x_2) = \frac{1}{4}(1 + x_1^4) + \frac{1}{2}(x_2^2 - x_1^2)$$

$$\mu_\infty \propto \exp(-\beta V(x_1, x_2)) dx_1 dx_2$$



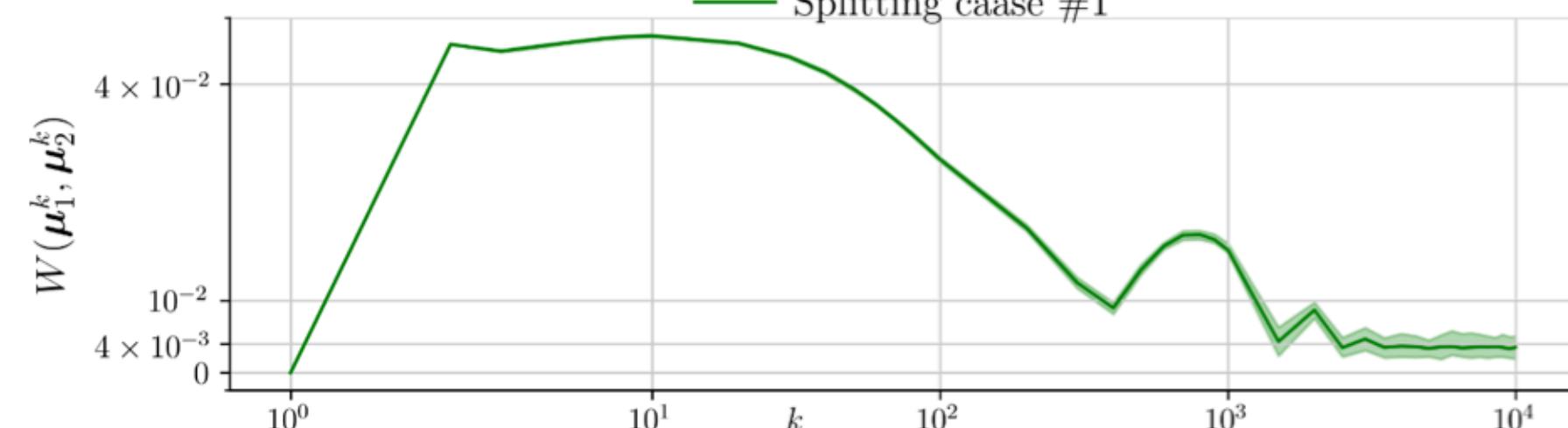
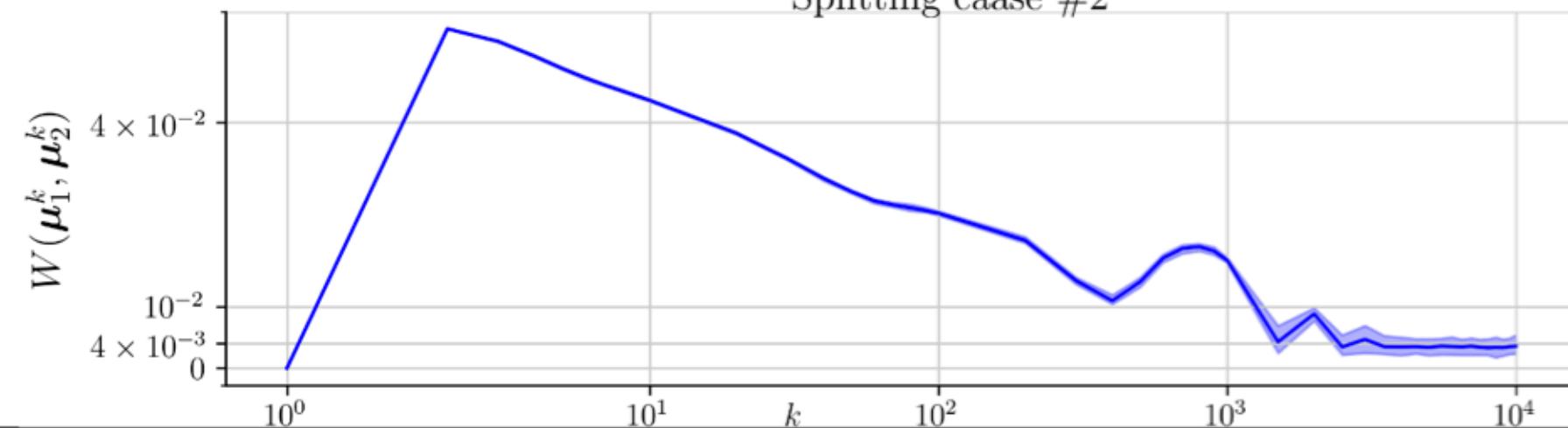
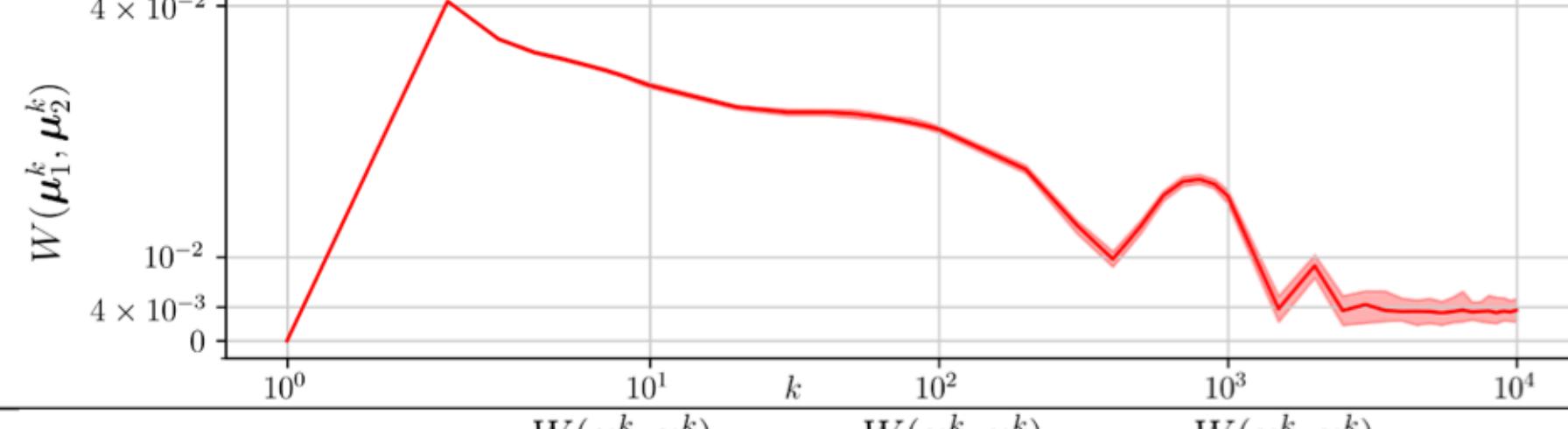
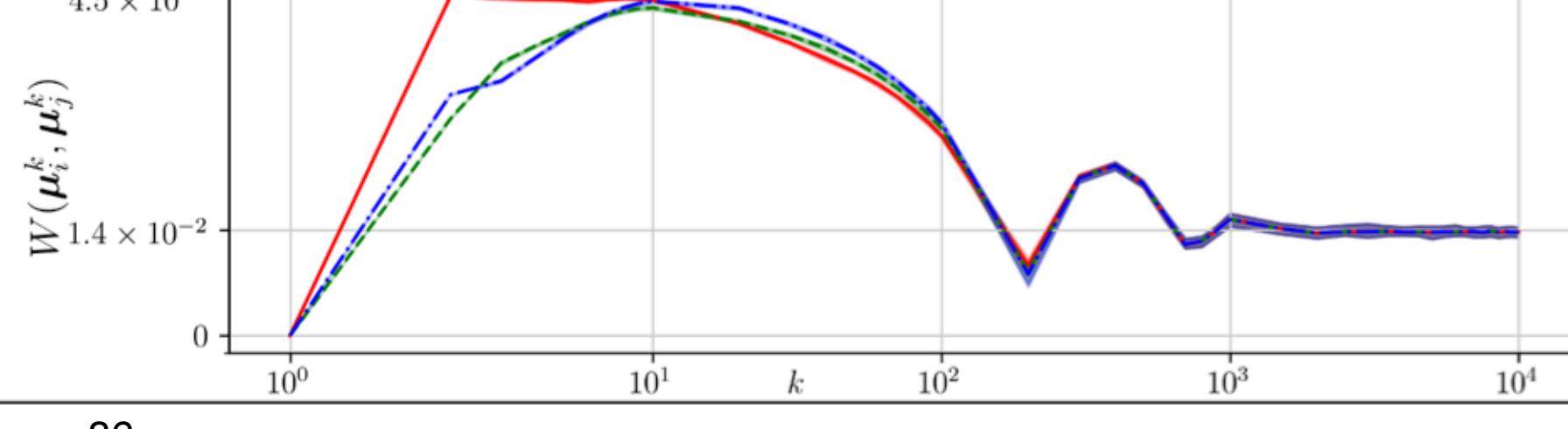
Distributed computation:  $F_1(\mu) = \langle V_k, \mu \rangle$     $F_2(\mu) = \langle \beta^{-1} \log \mu, \mu \rangle$



# Stochastic Learning/ Distributed Computing

Centralized av. runtime = 310.21 s

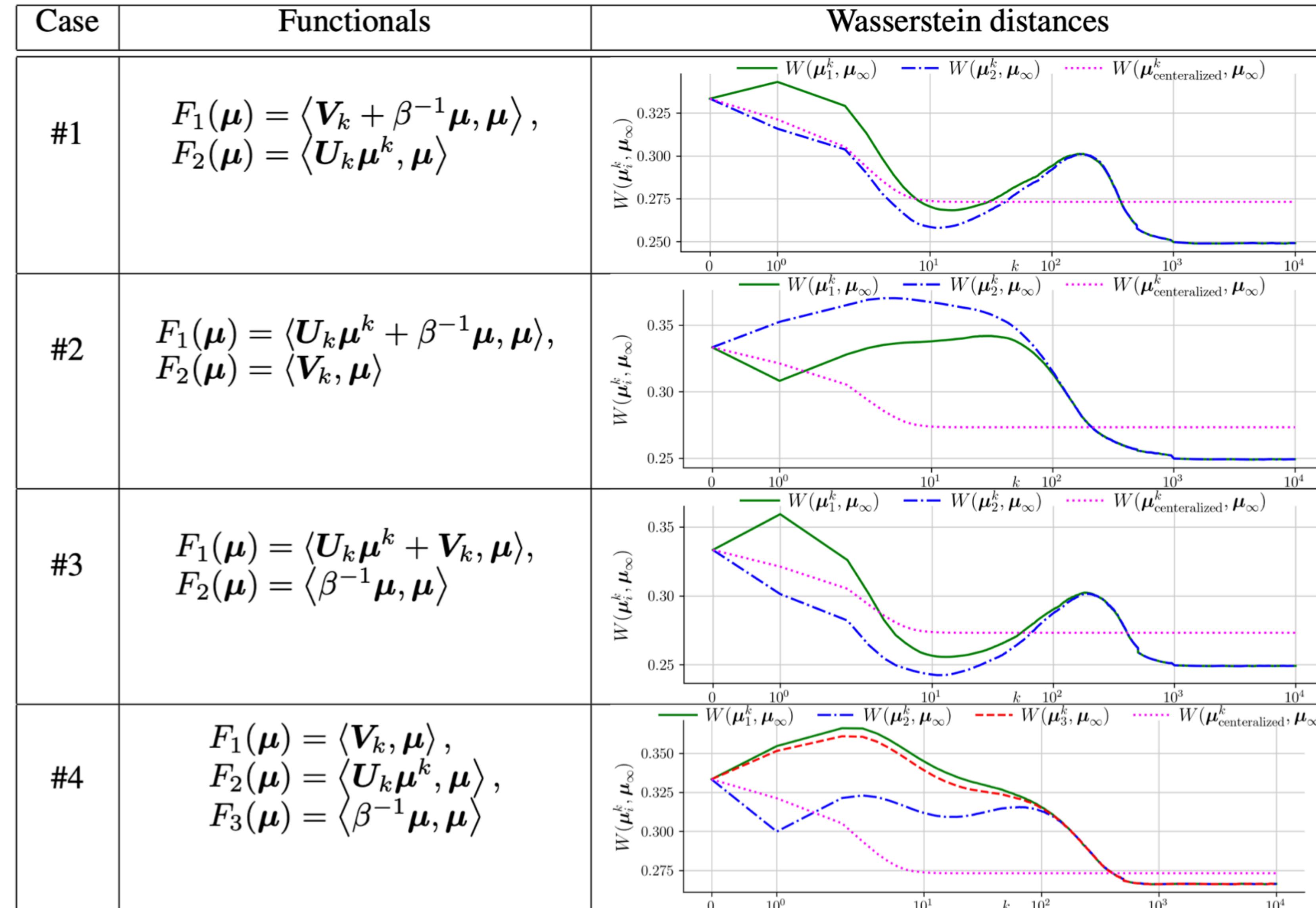
100 run statistics for each of the 4 ways of splitting: ( $B_n - 1$  ways in general)

Splitting case	Functionals	Wasserstein distance
#1	$F_1(\mu) = \langle V_k + \beta^{-1}\mu, \mu \rangle,$ $F_2(\mu) = \langle U_k\mu^k, \mu \rangle$ av. runtime = 294.06 s	 <p>Splitting case #1</p>
#2	$F_1(\mu) = \langle U_k\mu^k + \beta^{-1}\mu, \mu \rangle,$ $F_2(\mu) = \langle V_k, \mu \rangle$ av. runtime = 285.32 s	 <p>Splitting case #2</p>
#3	$F_1(\mu) = \langle U_k\mu^k + V_k, \mu \rangle,$ $F_2(\mu) = \langle \beta^{-1}\mu, \mu \rangle$ av. runtime = 289.87 s	 <p>Splitting case #3</p>
#4	$F_1(\mu) = \langle V_k, \mu \rangle,$ $F_2(\mu) = \langle U_k\mu^k \rangle,$ $F_3(\mu) = \langle \beta^{-1}\mu, \mu \rangle$ av. runtime = 108.99 s	 <p> <span style="color:red">—</span> <math>W(\mu_1^k, \mu_2^k)</math>  <span style="color:green">- - -</span> <math>W(\mu_1^k, \mu_3^k)</math>  <span style="color:blue">- · -</span> <math>W(\mu_2^k, \mu_3^k)</math> </p>

# Stochastic Learning/ Distributed Computing

Centralized is pink dotted (repeated in subplots)

100 run statistics for each of the 4 ways of splitting: ( $B_n - 1$  ways in general)



# Publications

- Alexis Teter, **Iman Nodozi**, and Abhishek Halder. "Proximal Mean Field Learning in Shallow Neural Networks." *Transactions on Machine Learning Research*, 2023.
- **Iman Nodozi**, Charlie Yan, Mira Khare, Abhishek Halder, and Ali Mesbah. "Neural Schrödinger Bridge with Sinkhorn Losses: Application to Data-driven Minimum Effort Control of Colloidal Self-assembly." *IEEE Transactions on Control Systems Technology*, 2023.
- **Iman Nodozi**, Abhishek Halder, and Ion Matei. "A Controlled Mean Field Model for Chiplet Population Dynamics." *IEEE Control Systems Letters*, 2023. Also in 62nd IEEE Conference on Decision and Control (CDC), Singapore, 2023.
- Charlie Yan, **Iman Nodozi**, and Abhishek Halder. "Optimal Mass Transport over the Euler Equation." *Proceedings of the 62nd IEEE Conference on Decision and Control (CDC)*, Singapore, 2023. Invited paper in Session 'Optimal Transport'.
- **Iman Nodozi**, Jared O'Leary, Abhishek Halder, and Ali Mesbah. "A Physics-informed Deep Learning Approach for Minimum Effort Stochastic Control of Colloidal Self-Assembly." *Proceedings of American Control Conference (ACC)*, San Diego, California, USA, 2023. Invited paper in Session 'Learning and Stochastic Optimal Control'.
- **Iman Nodozi**, and Abhishek Halder. "Schrödinger Meets Kuramoto via Feynman-Kac: Minimum Effort Distribution Steering for Noisy Nonuniform Kuramoto Oscillators." *Proceedings of the 61st IEEE Conference on Decision and Control (CDC)*, Cancún, Mexico, 2022.
- **Iman Nodozi**, and Abhishek Halder. "A Distributed Algorithm for Measure-valued Optimization with Additive Objective." *25th International Symposium on Mathematical Theory of Networks and Systems (MTNS)*, Bayreuth, Germany, 2022. Invited paper in Session 'Optimal transport: Theory and applications in networks and systems'.
- Alexis Teter, **Iman Nodozi**, and Abhishek Halder. "Solution of the Probabilistic Lambert's Problem: Optimal Transport Approach."
- Alexis Teter, **Iman Nodozi**, and Abhishek Halder. "Solution of the Probabilistic Lambert Problem: Connections with Optimal Mass Transport, Schrödinger Bridge, and Reaction-Diffusion PDEs."
- **Iman Nodozi**, and Abhishek Halder. "Wasserstein Consensus ADMM."