

Measure-valued Proximal Recursions for Learning and Control

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Dissertation Defense, March 15, 2024

Measure-valued Optimization Problems

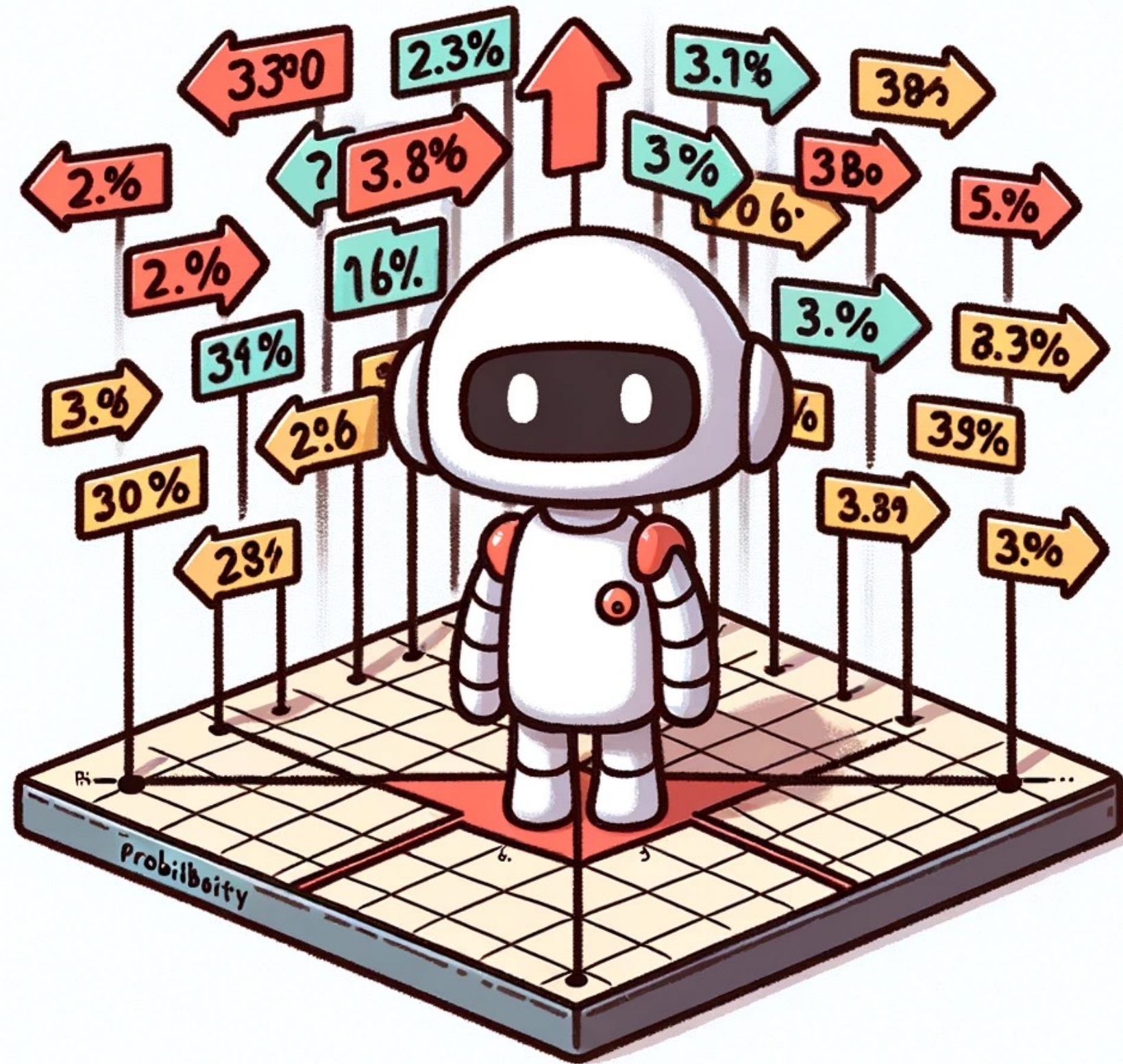
$$\mu^{\text{opt}} = \arg \inf_{\mu} F(\mu)$$

Measure-valued Optimization Problems

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

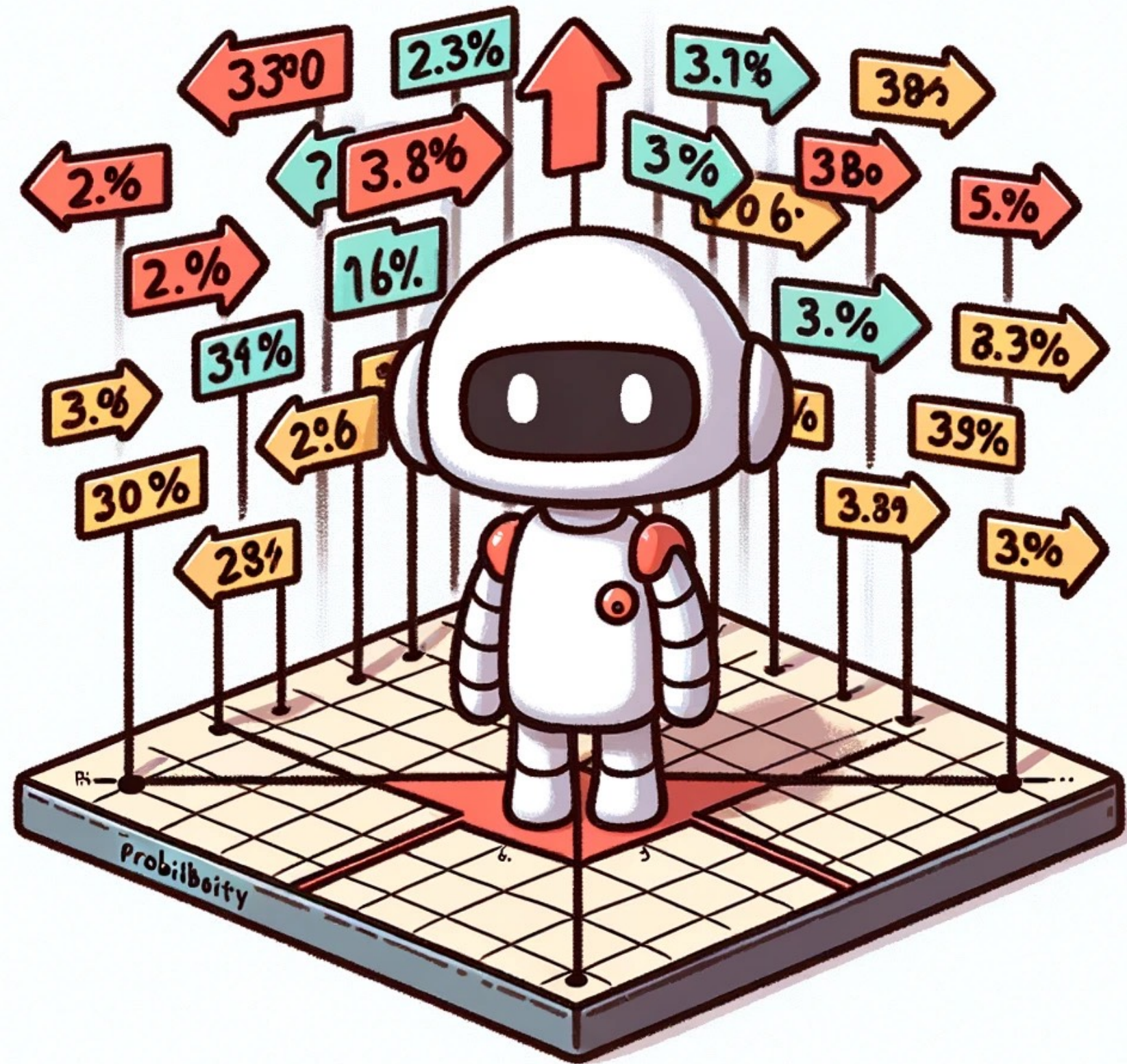
Manifold of probability measures supported on \mathbb{R}^d with finite second moments

Probability Distribution



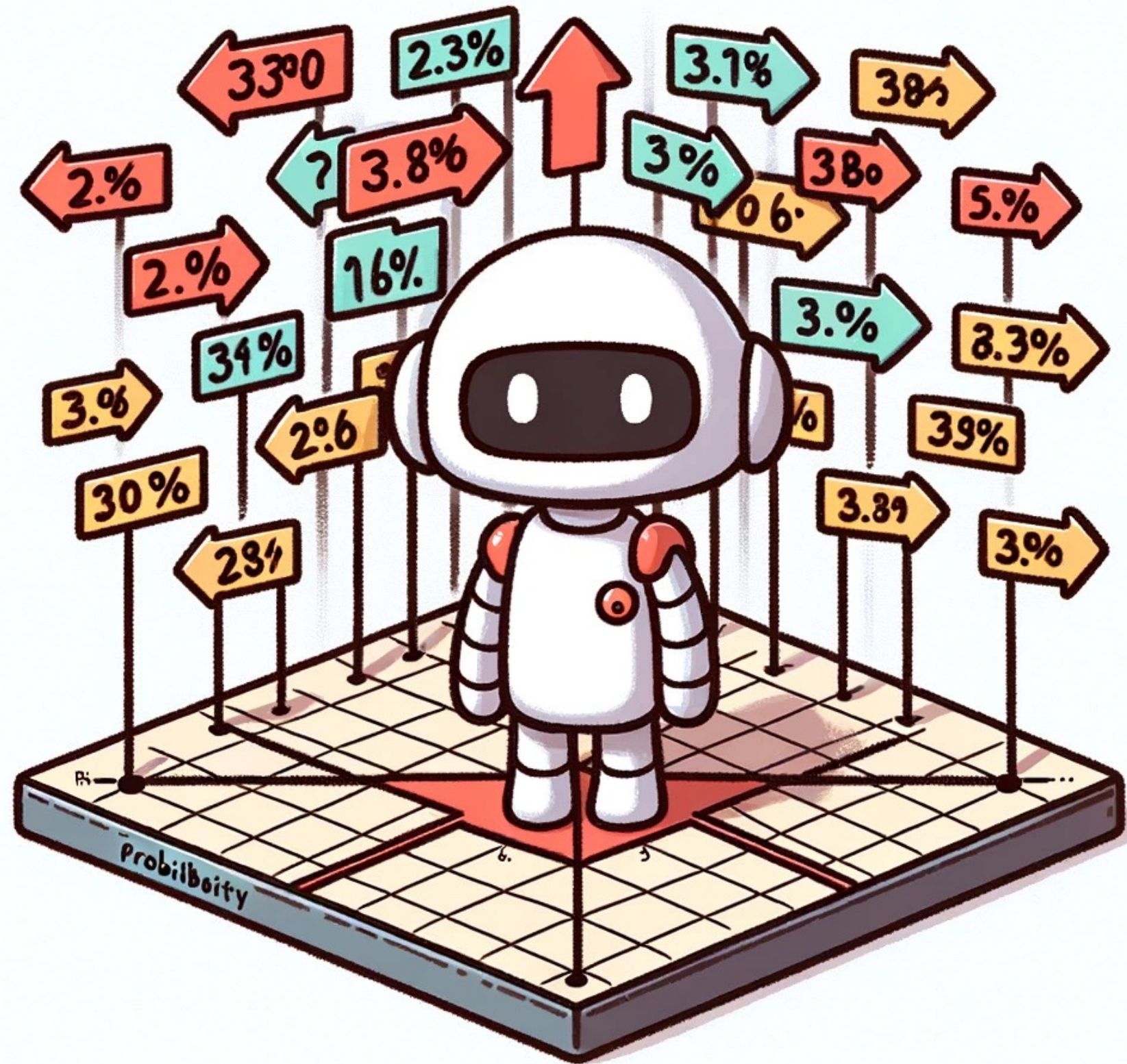
$$x(t) = \begin{pmatrix} x \\ y \\ \theta \end{pmatrix} \in \mathcal{X} \equiv \mathbb{R}^2 \times \mathbb{S}^1$$

Probability Distribution



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

Probability Distribution



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

$$\rho(x, t) : \mathcal{X} \times [0, \infty) \rightarrow \mathbb{R}_{\geq 0}$$

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

← measure
← Density function

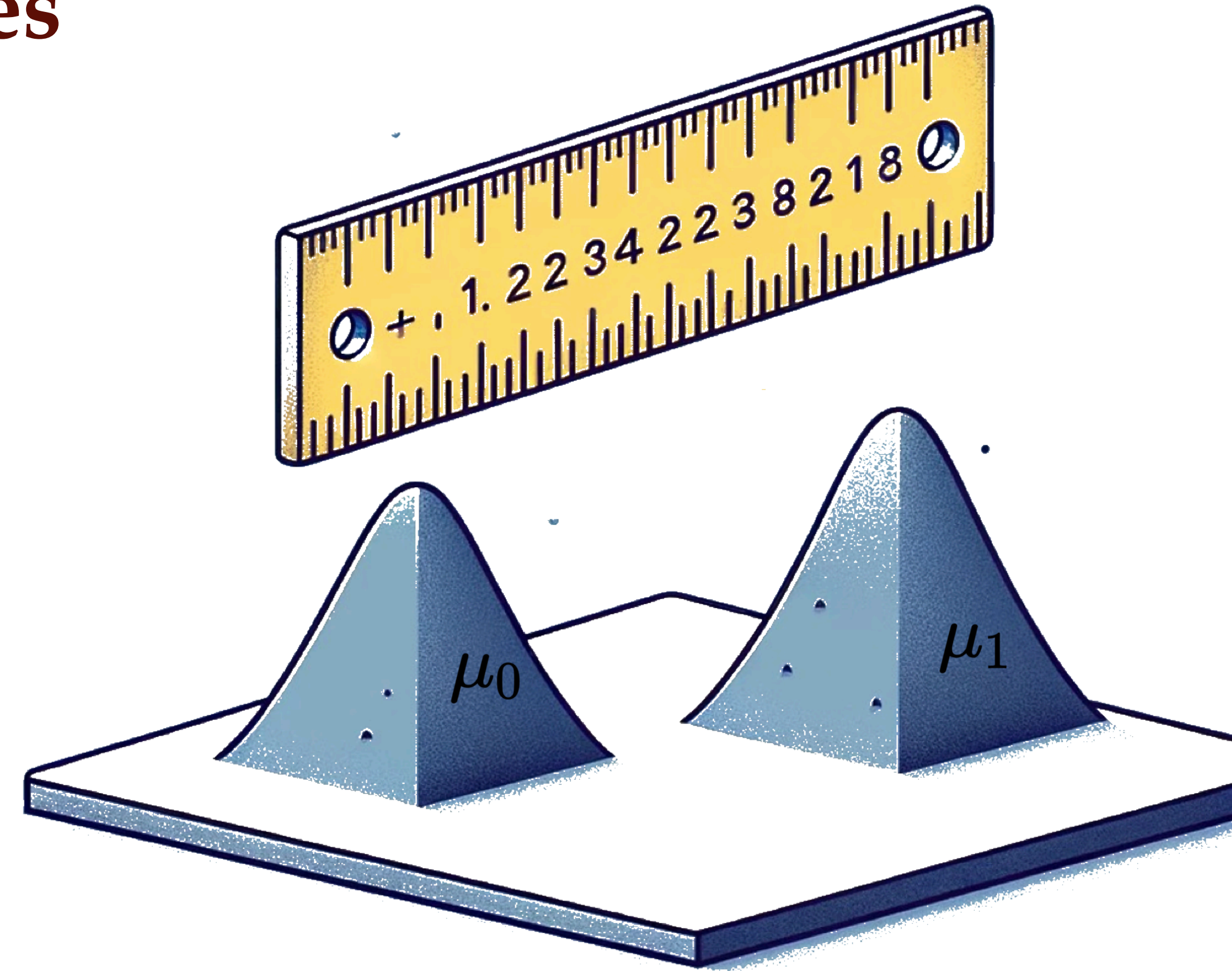
Geometry on the Space of Prob. Measures

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



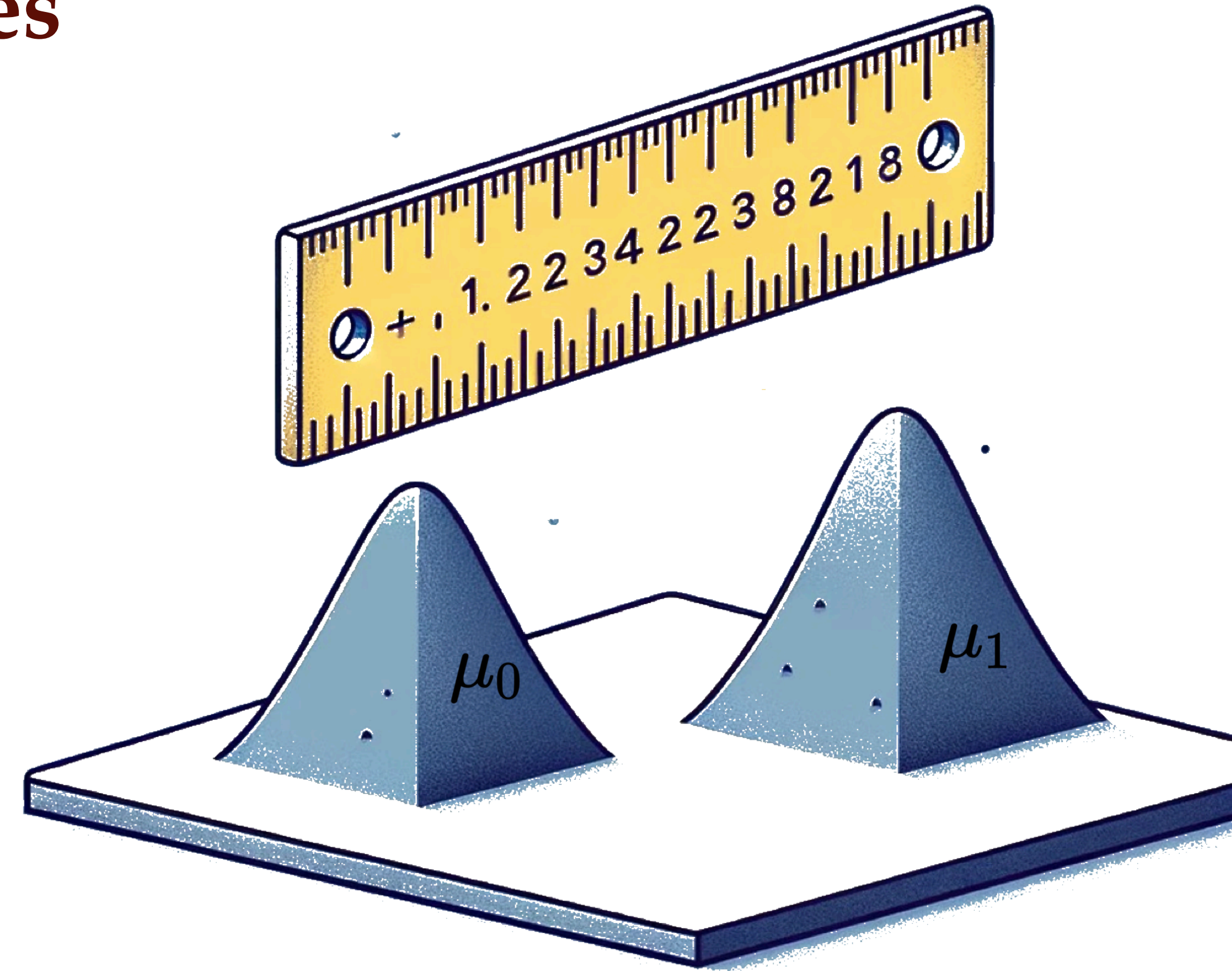
Geometry on the Space of Prob. Measures

2-Wasserstein distance **metric**

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

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



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

Transient solution of (\star) \implies 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}

$$\frac{d\mathbf{x}}{dt} = -\nabla f(\mathbf{x}), \quad \mathbf{x}(0) = \mathbf{x}_0$$

Recursion:

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

Convergence:

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

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

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

Recursion:

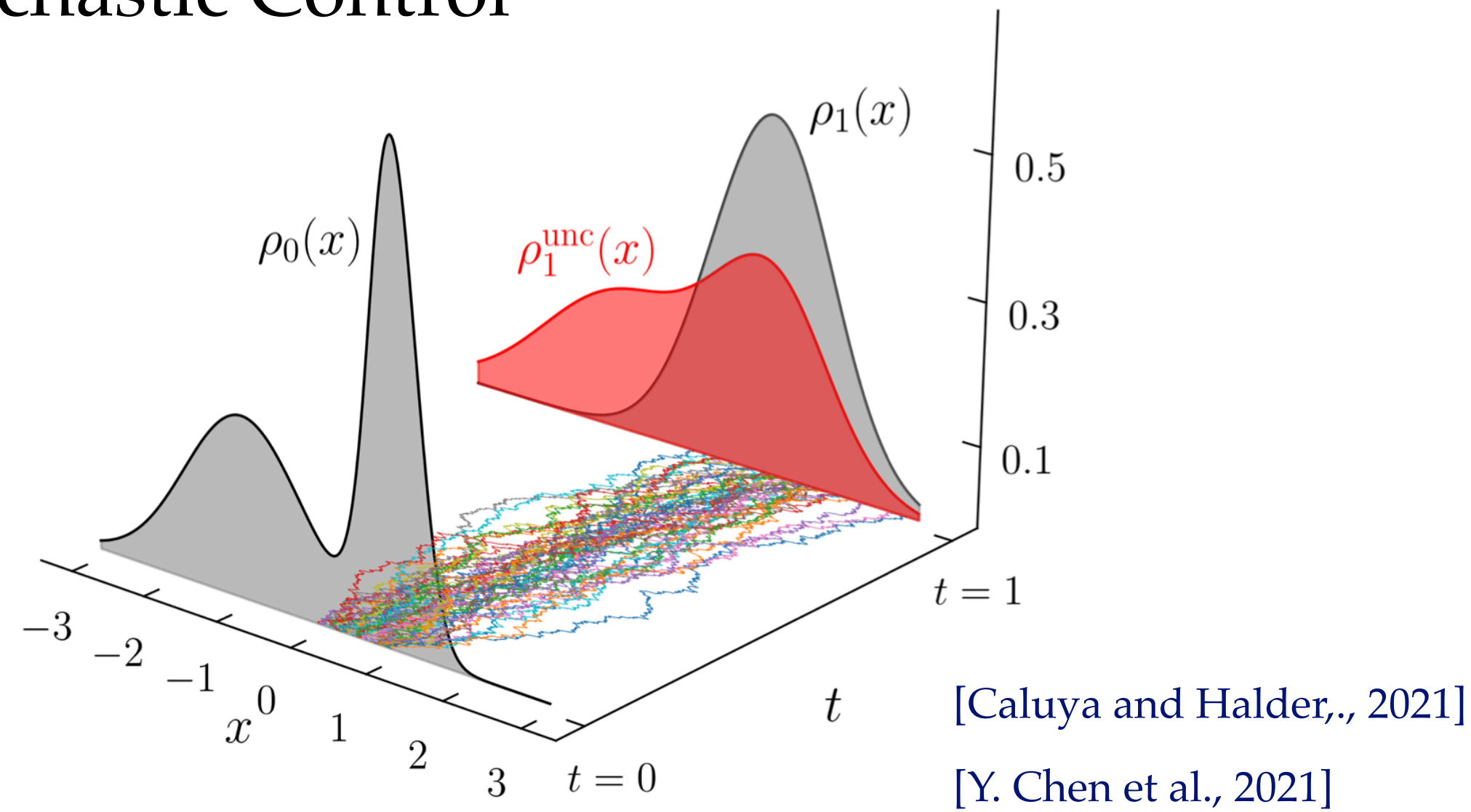
$$\begin{aligned} \mu_k &= \mu(\cdot, t = kh) \\ &= \arg \min_{\mu \in \mathcal{P}_2(\mathcal{X})} \left\{ \frac{1}{2} W^2(\mu, \mu_{k-1}) + hF(\mu) \right\} \\ &=: \text{prox}_{hF}^W(\mu_{k-1}) \end{aligned}$$

Convergence:

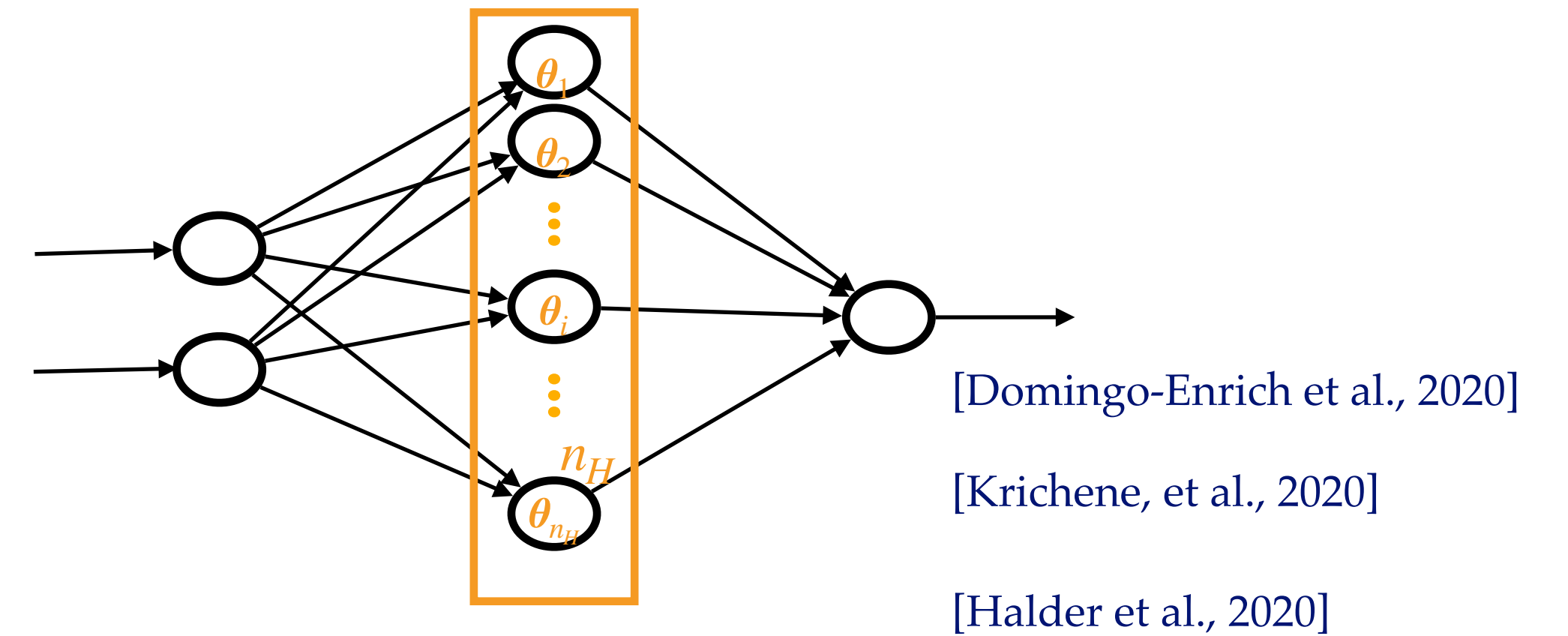
$$\mu_k \rightarrow \mu(\cdot, t = kh) \quad \text{as } h \downarrow 0$$

Motivating Applications

Stochastic Control



Stochastic learning



Stochastic Modeling

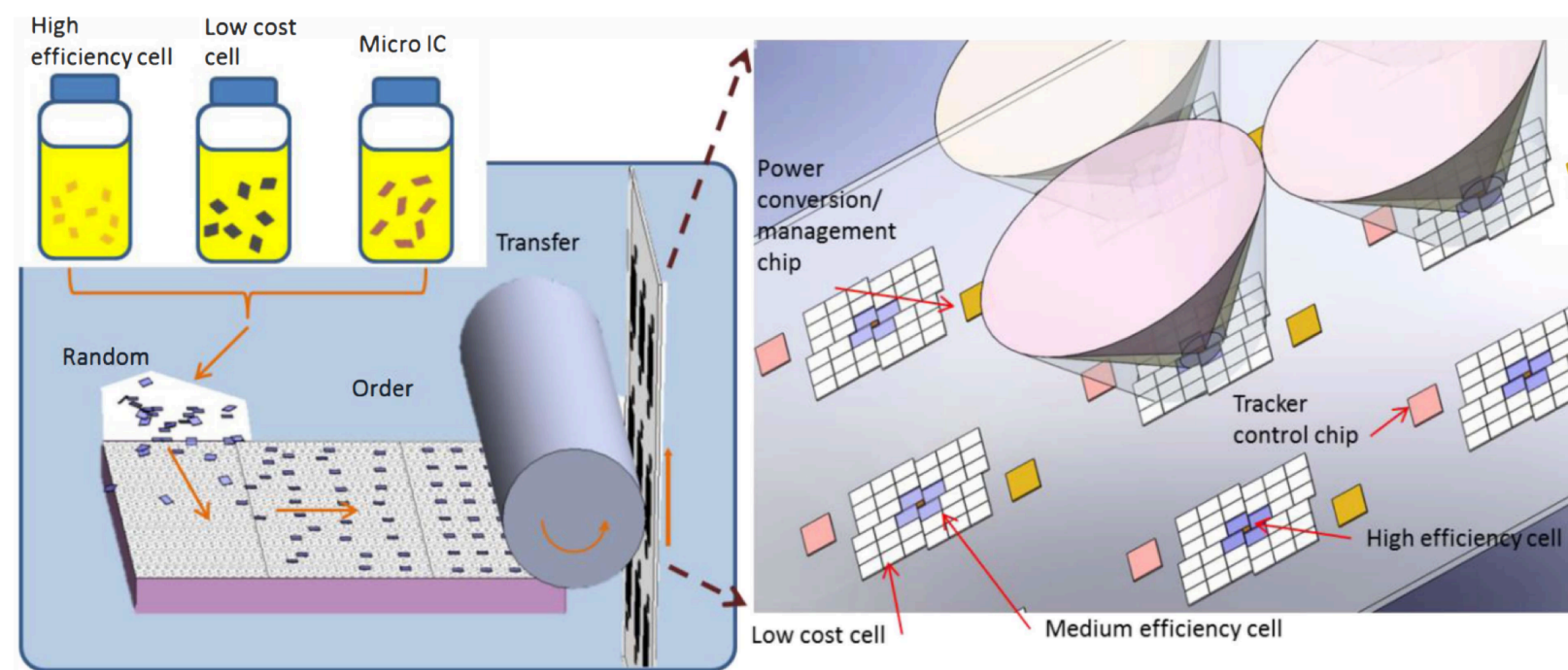


Image credit: PARC

Generative AI

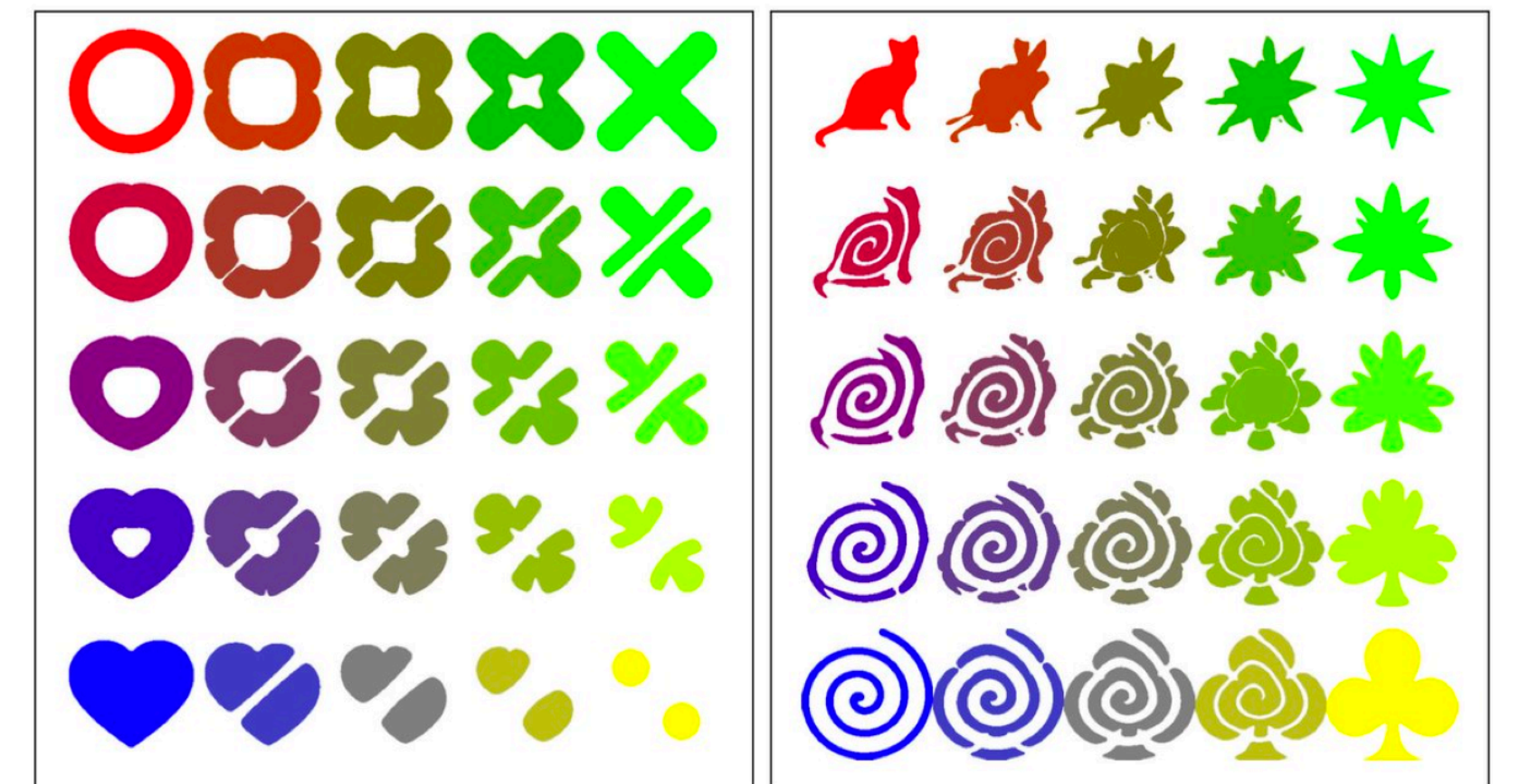


Image credit: G. Pyre

Contributions

Part I: Optimal Stochastic Control of Generalized Schrödinger Bridge in

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

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

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

Part III: Stochastic Learning

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

Distributed Computing: Wasserstein Consensus ADMM [I. Nadozi, 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

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

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

Control affine

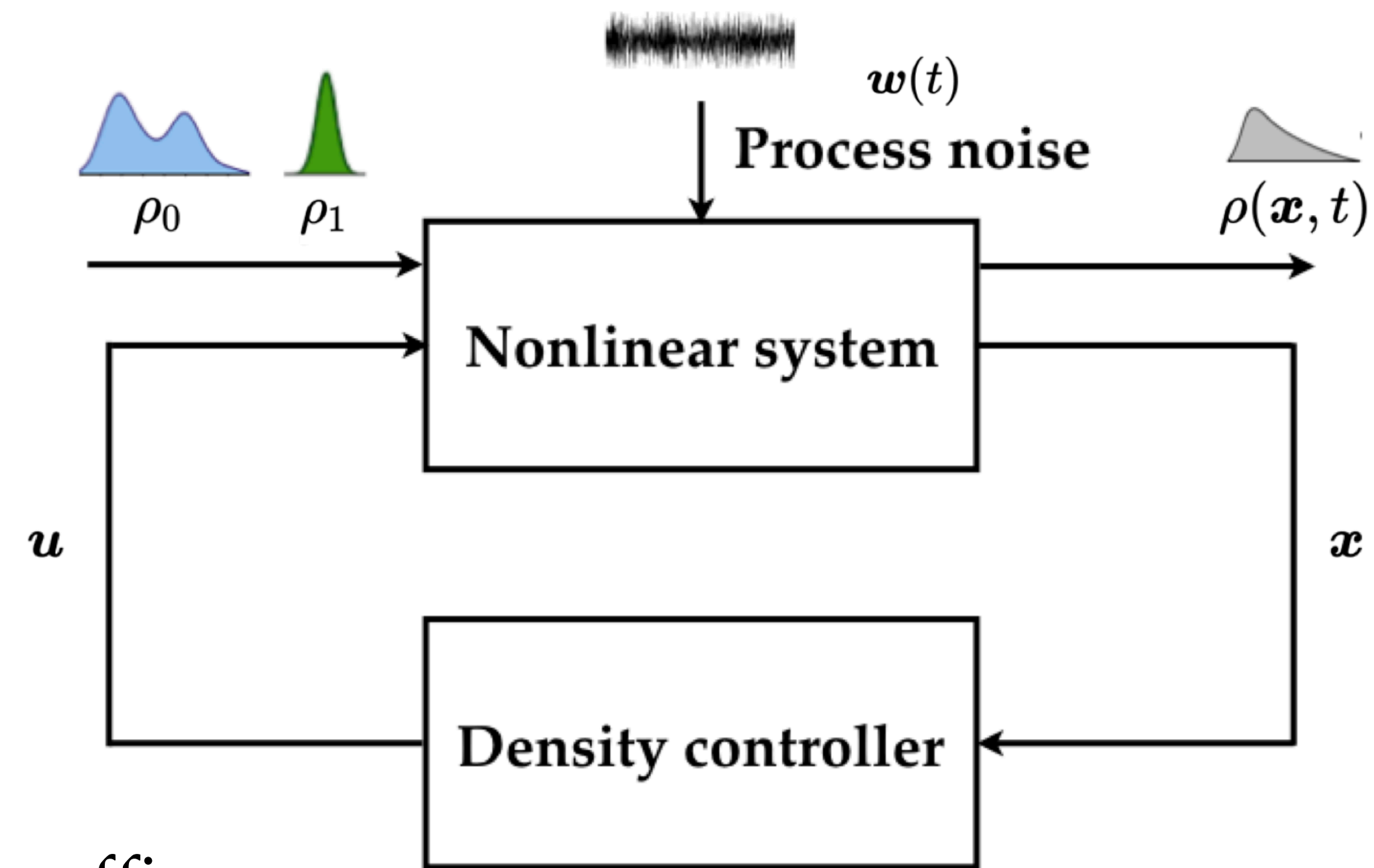
$$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + \mathbf{B}(t)\mathbf{u}(\mathbf{x}, t)dt + \sqrt{2\epsilon}\mathbf{B}(t)d\mathbf{w}$$

Case study: Nonuniform Noisy Kuramoto Oscillators

Control non-affine

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

Case study: Controlled Self-assembly $\left\{ \begin{array}{l} \text{Model-based} \\ \text{Model-free} \end{array} \right.$



Stochastic Control/ Control-affine

Conditions for Optimality

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

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

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

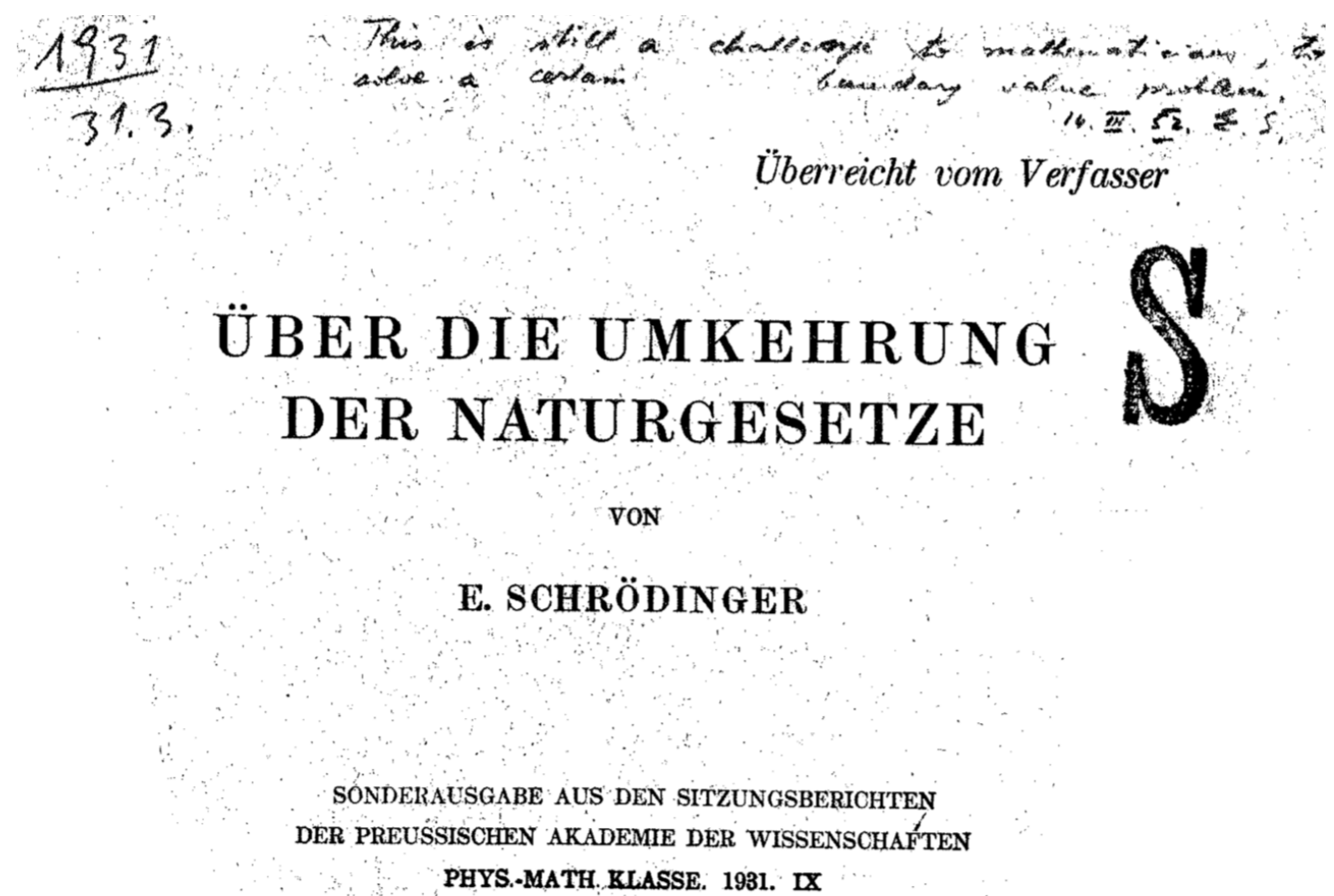
$$\rho^{\text{opt}}(\mathbf{x}, 0) = \rho_0(\mathbf{x}), \quad \rho^{\text{opt}}(\mathbf{x}, T) = \rho_T(\mathbf{x}) \quad \text{Boundary conditions}$$

Stochastic Control/ Control-affine

Hopf-Cole a.k.a. Fleming's logarithmic transform: $(\rho^{\text{opt}}, \psi) \mapsto (\underbrace{\hat{\varphi}}, \underbrace{\varphi})$
Schrödinger factors

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

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



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!!

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

Forward Fokker-Planck PDE

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

Backward Fokker-Planck PDE

Initial and Terminal conditions

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

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

Optimal controlled joint state PDF:

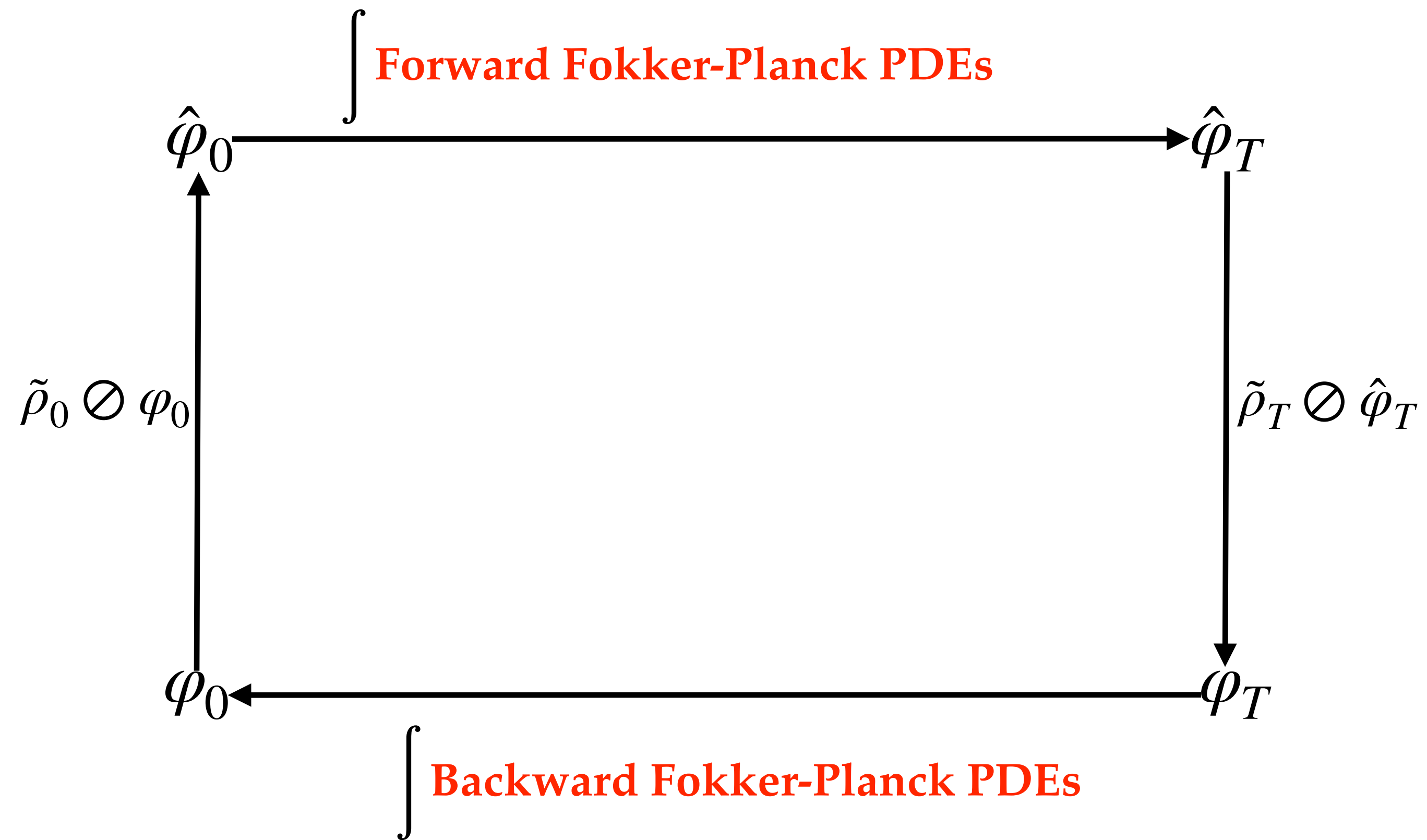
$$\rho^{\text{opt}}(\mathbf{x}, t) = \varphi(\mathbf{x}, t) \hat{\varphi}(\mathbf{x}, t)$$

Optimal control:

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

Stochastic Control/ Control-affine

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

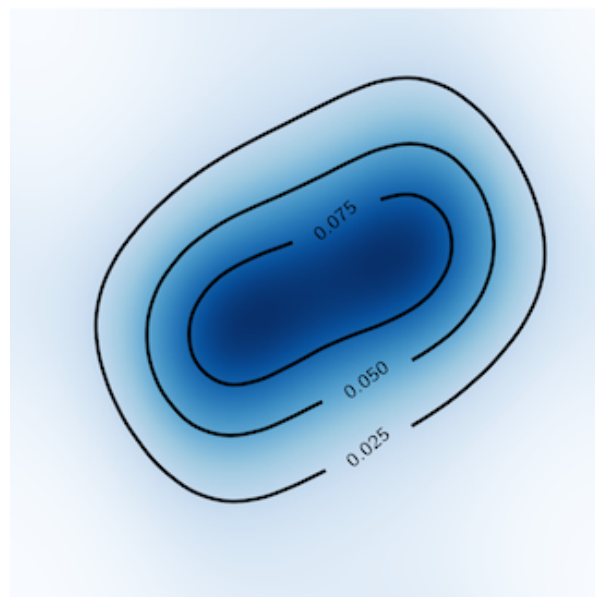


Stochastic Control/ Control-affine: Nonuniform Noisy Kuramoto Oscillators

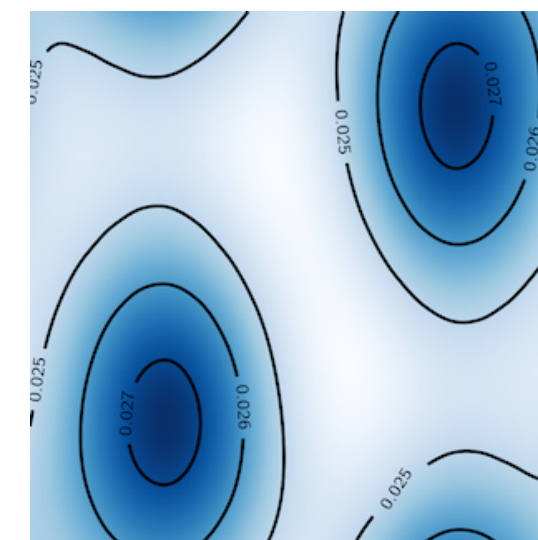
First order Case Study

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

$$d\boldsymbol{\theta} = (-\nabla_{\boldsymbol{\theta}} V(\boldsymbol{\theta}) + S\mathbf{u}) dt + \sqrt{2}Sd\mathbf{w}$$



$\boldsymbol{\theta}(t = 0) \sim \mu_0$ (Desynchronized)



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

Stochastic Control/ Control-affine: Nonuniform Noisy Kuramoto Oscillators

Uncontrolled forward-backward Kolmogorov PDEs:

$$\frac{\partial \hat{\varphi}}{\partial t} = \nabla_{\xi} \cdot \left(\hat{\varphi} \Upsilon \nabla_{\xi} \tilde{V} \right) + \Delta_{\xi} \hat{\varphi} \quad \text{Forward Fokker-Planck PDE}$$

$$\frac{\partial \varphi}{\partial t} = \left\langle \nabla_{\xi} \varphi, \Upsilon \nabla_{\xi} \tilde{V} \right\rangle - \Delta_{\xi} \varphi \quad \text{Backward Fokker-Planck PDE}$$

Initial and Terminal conditions

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

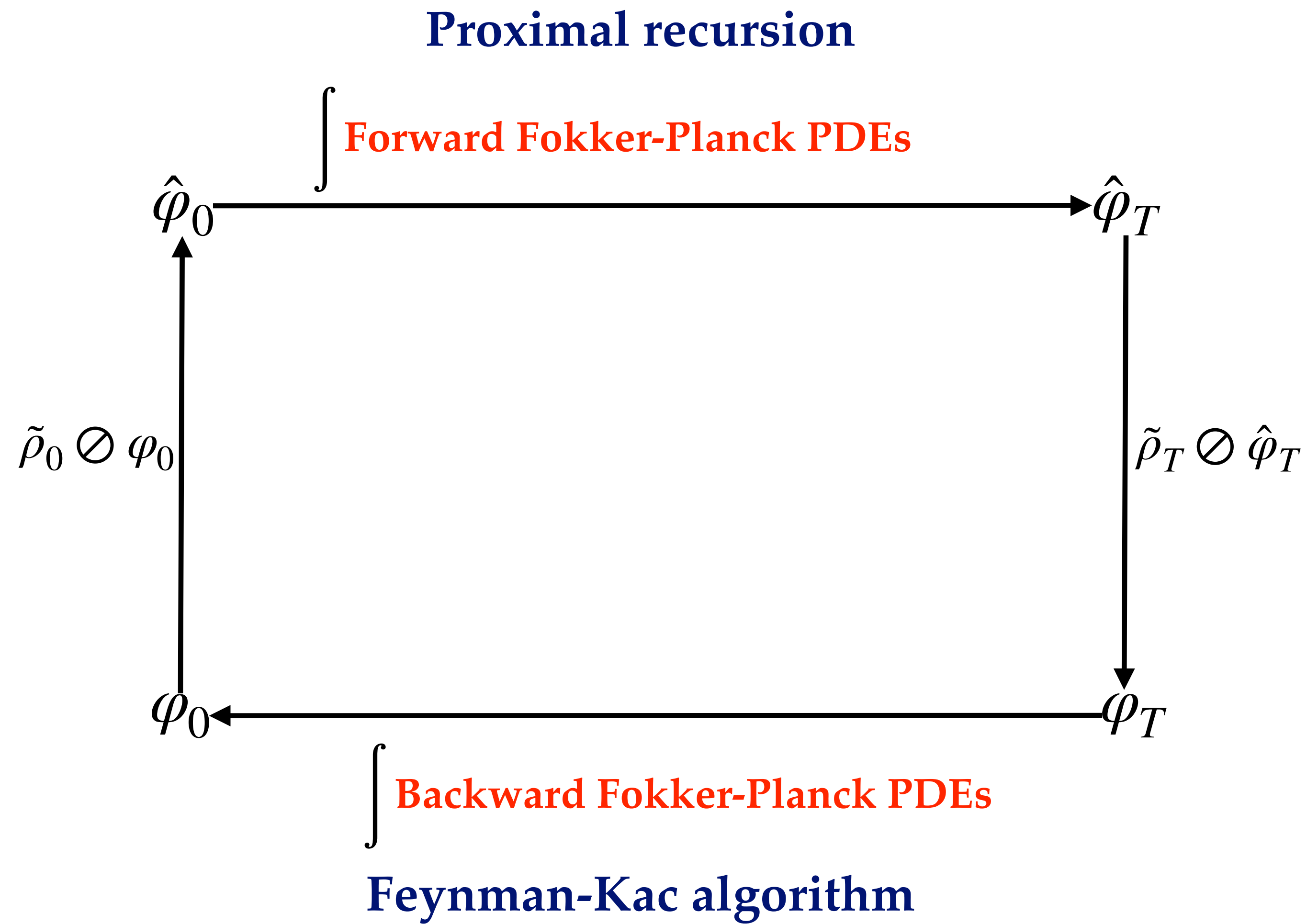
$$\hat{\varphi}_T(\xi) \varphi_T(\xi) = \rho_T(\mathbf{S}\xi) \left(\prod_{i=1}^n \sigma_i \right)$$

Optimal controlled joint state PDF: $\rho^{\text{opt}}(\boldsymbol{\theta}, t) = \hat{\varphi}(\mathbf{S}^{-1}\boldsymbol{\theta}, t) \varphi(\mathbf{S}^{-1}\boldsymbol{\theta}, t) / \left(\prod_{i=1}^n \sigma_i \right)$

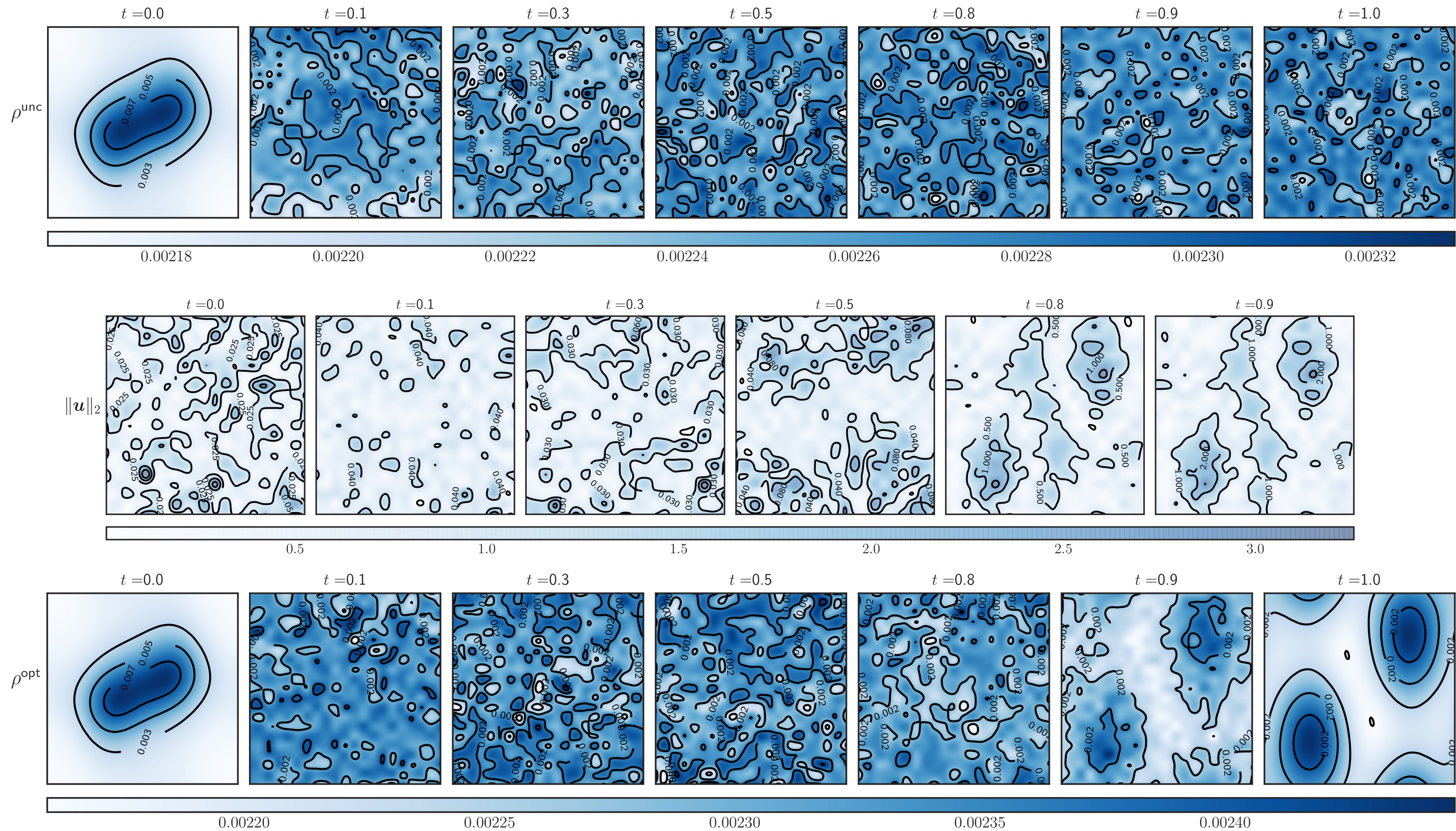
Optimal control: $\mathbf{u}^{\text{opt}}(\boldsymbol{\theta}, t) = \mathbf{S} \nabla_{\boldsymbol{\theta}} \log \varphi (\mathbf{S}^{-1}\boldsymbol{\theta}, t)$

Stochastic Control/ Control-affine: Nonuniform Noisy Kuramoto Oscillators

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

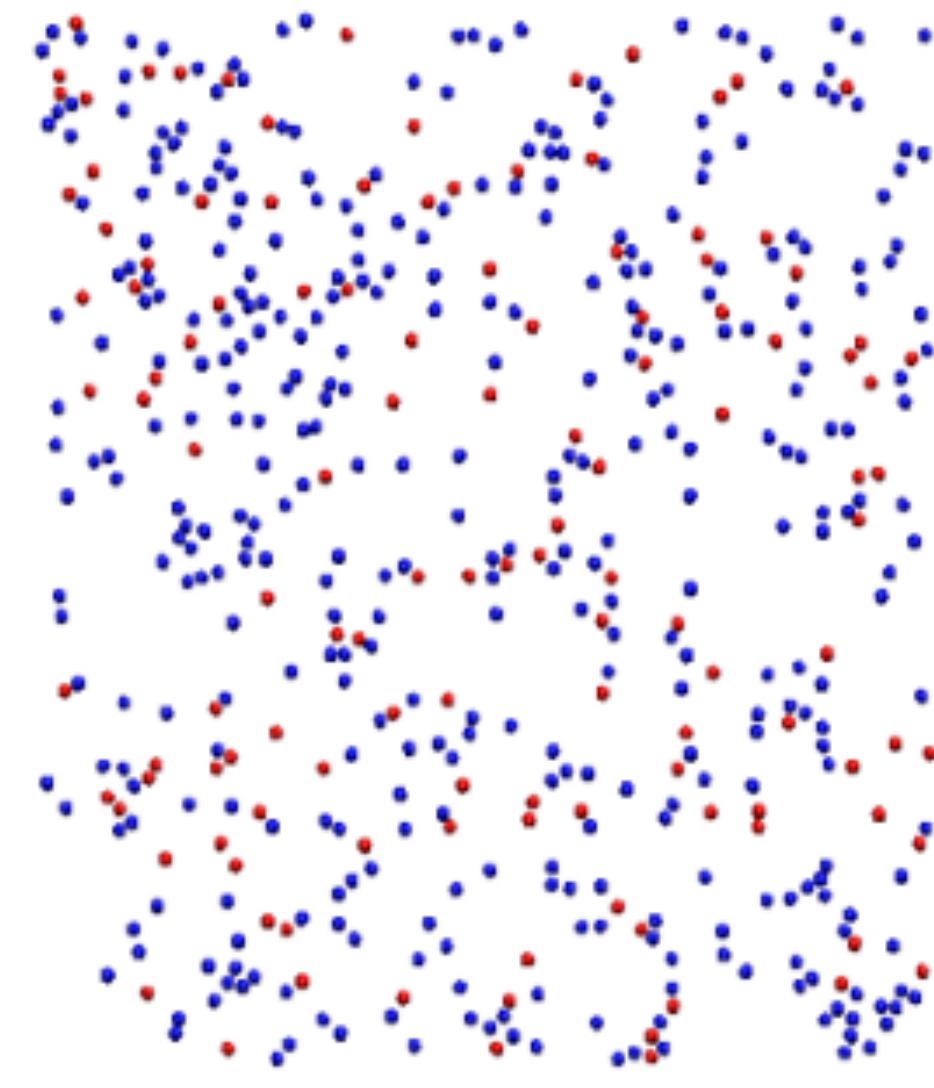


Stochastic Control/ Control-affine: Nonuniform Noisy Kuramoto Oscillators

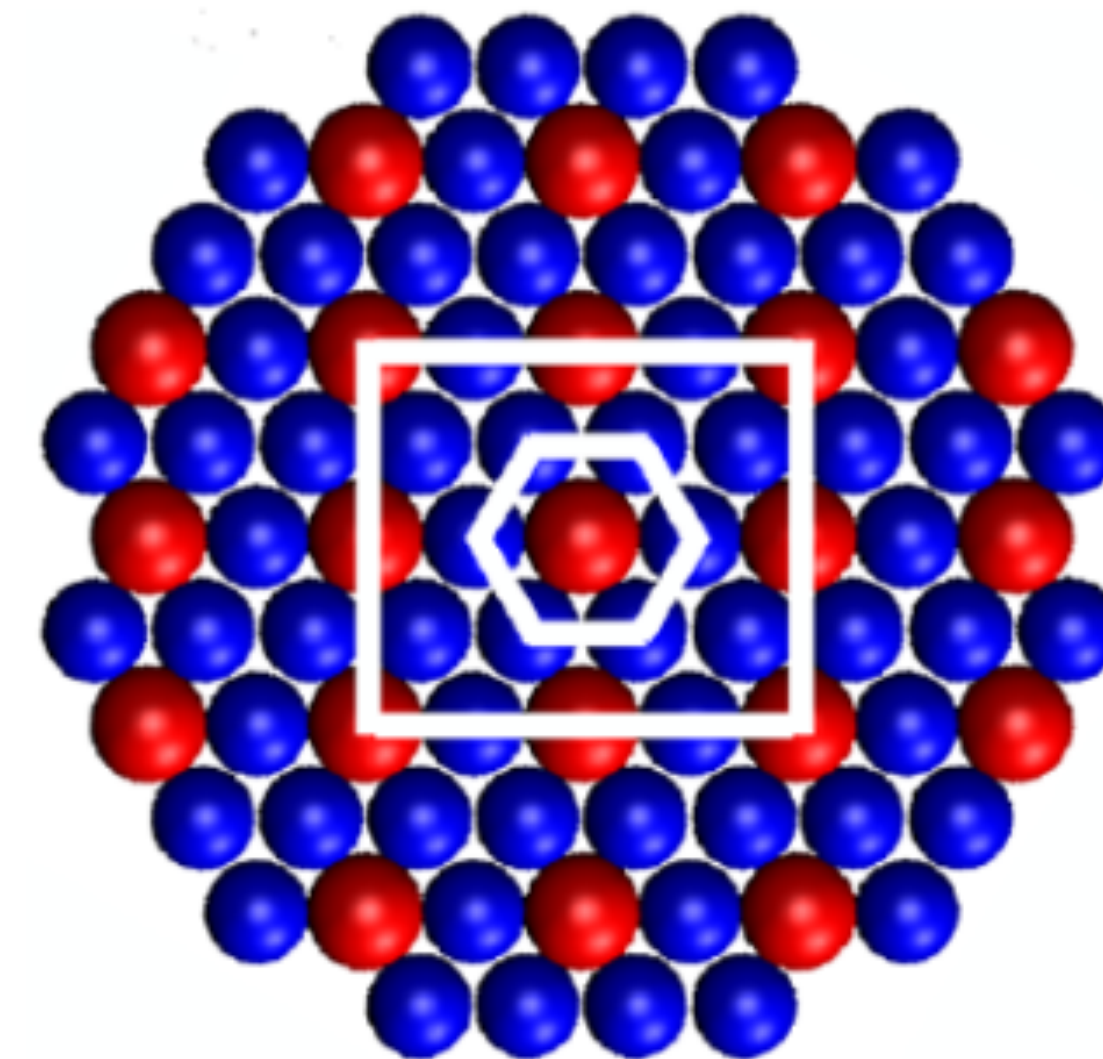


Stochastic Control / Control Non-affine

Controlled Self-assembly



Dispersed particles



Ordered structure

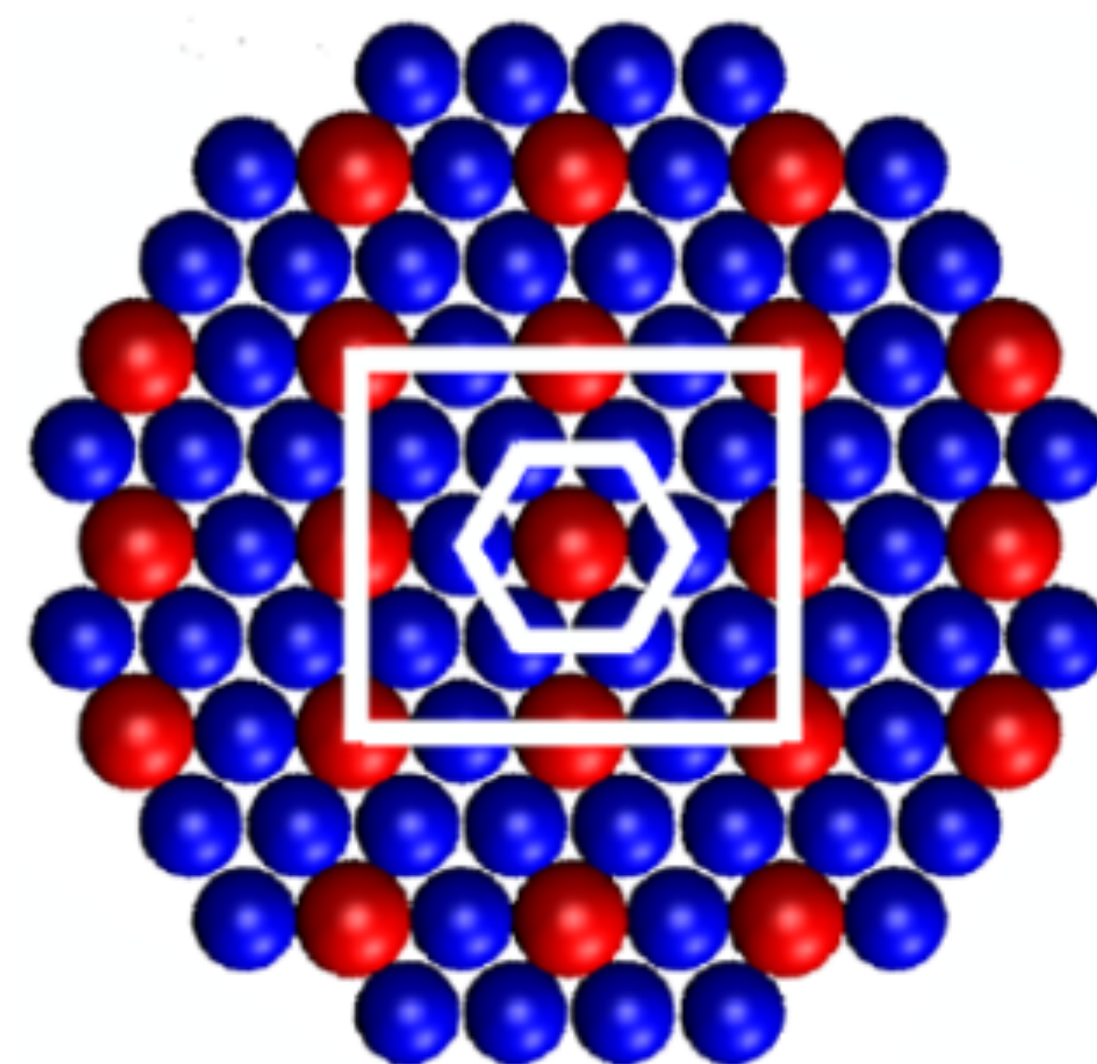
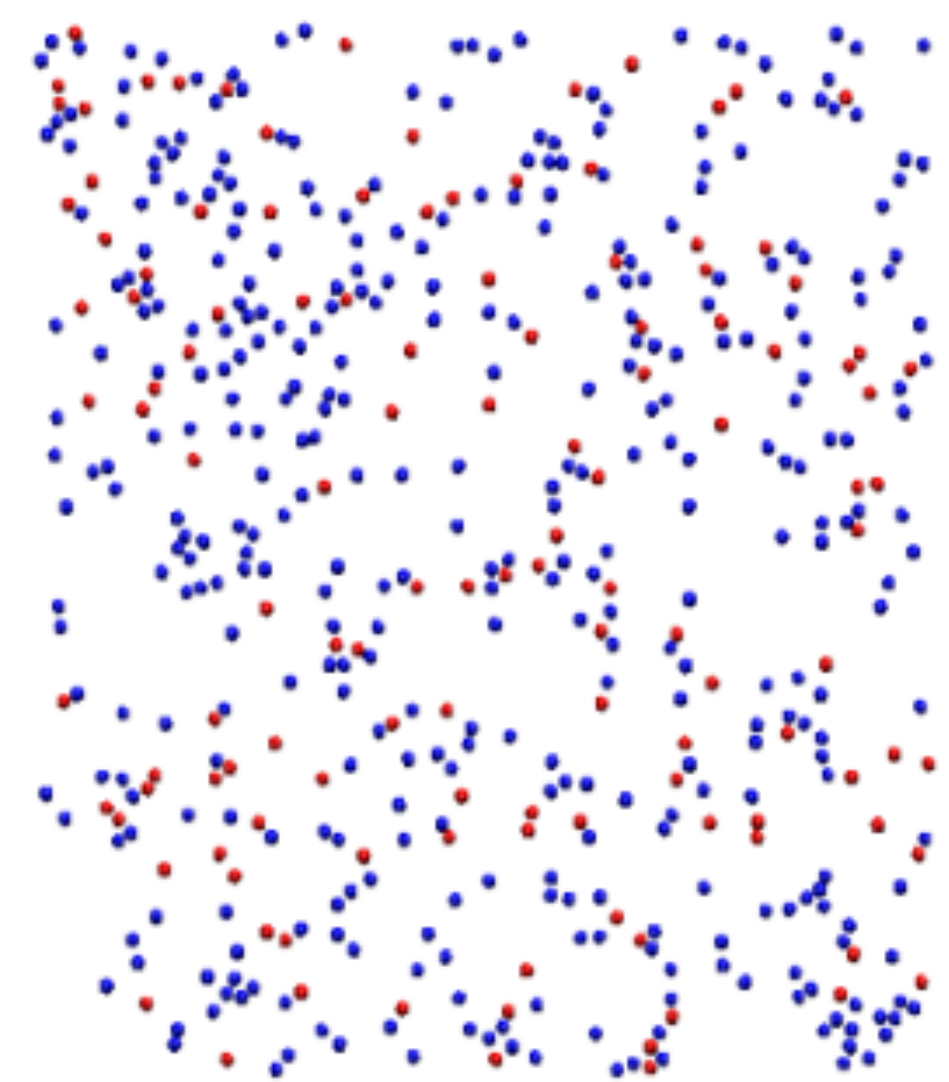
Applications:

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

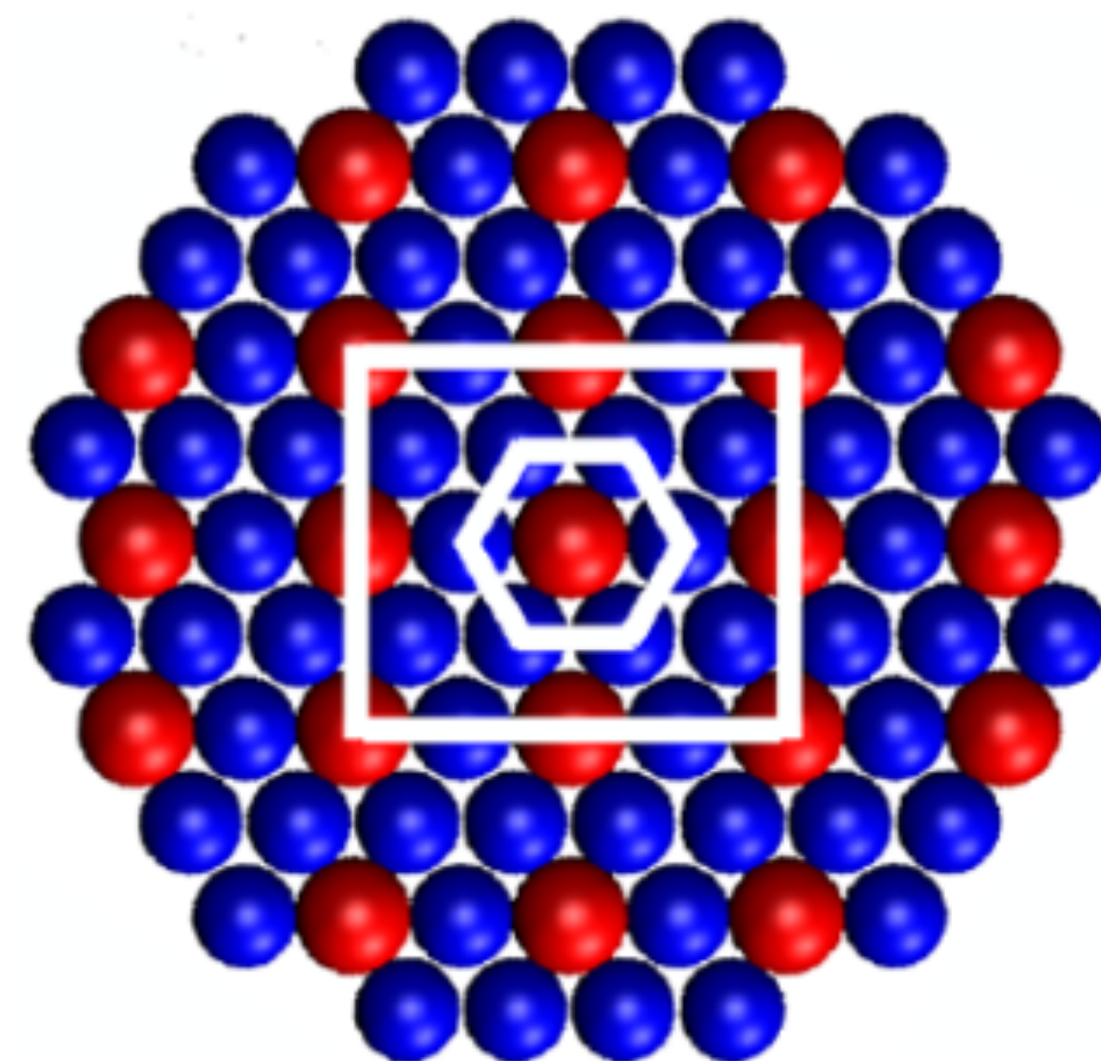
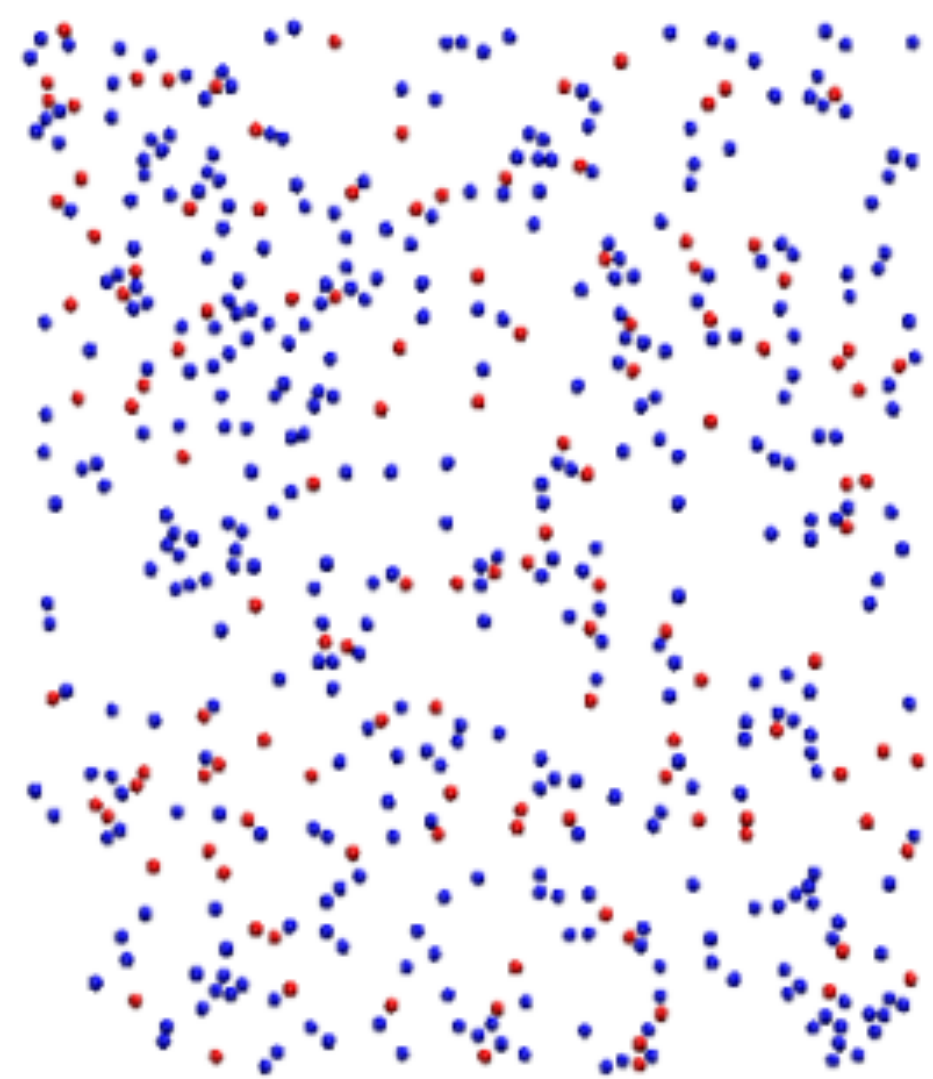
Electric field voltage

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

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

Stochastic Control / Control Non-affine

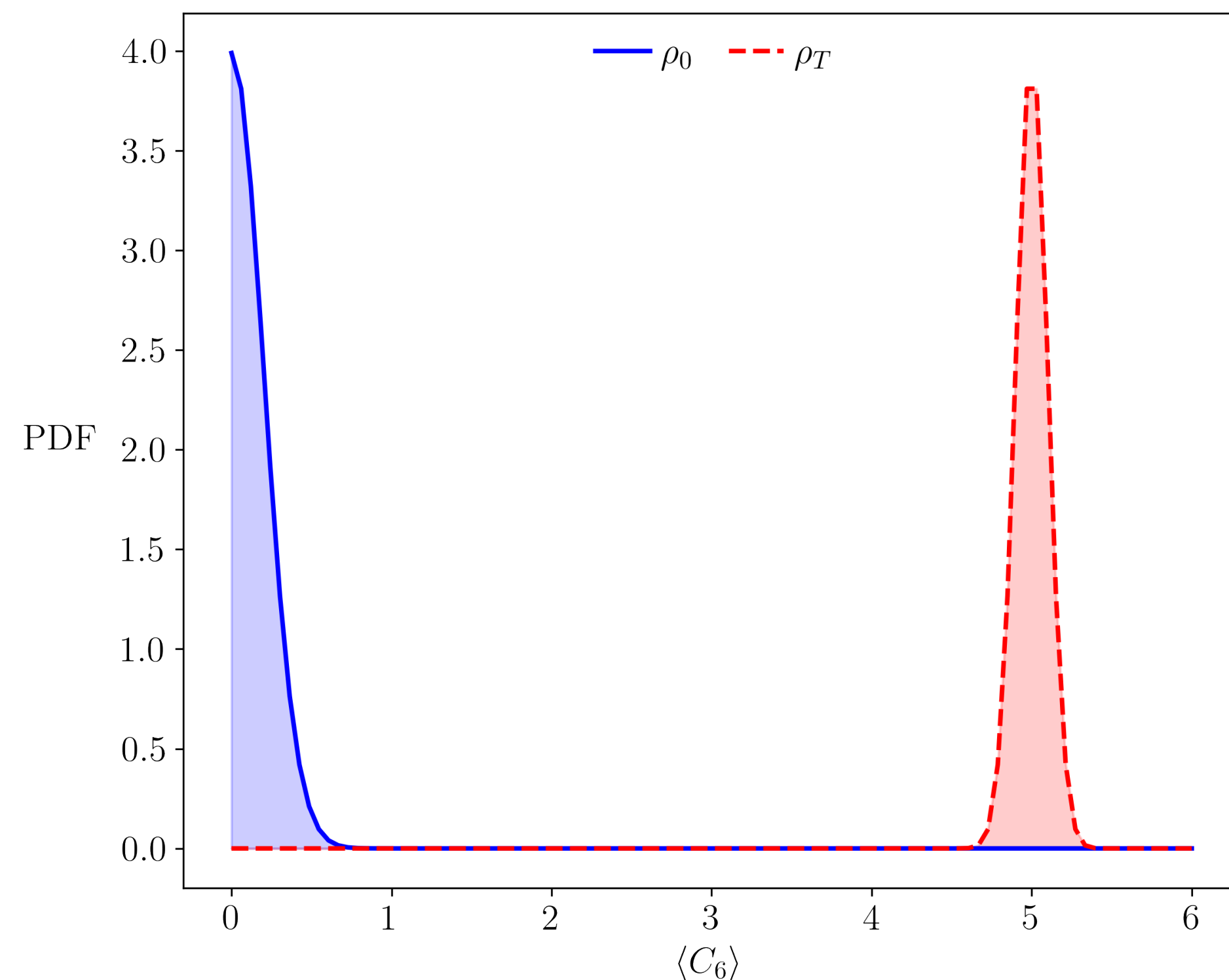
Intuition for Case Study 1:

$\langle C_6 \rangle \approx 0 \Leftrightarrow$ 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:

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

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

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

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

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

Stochastic Control / Control Non-affine

Case 1: Minimum Effort Self-assembly

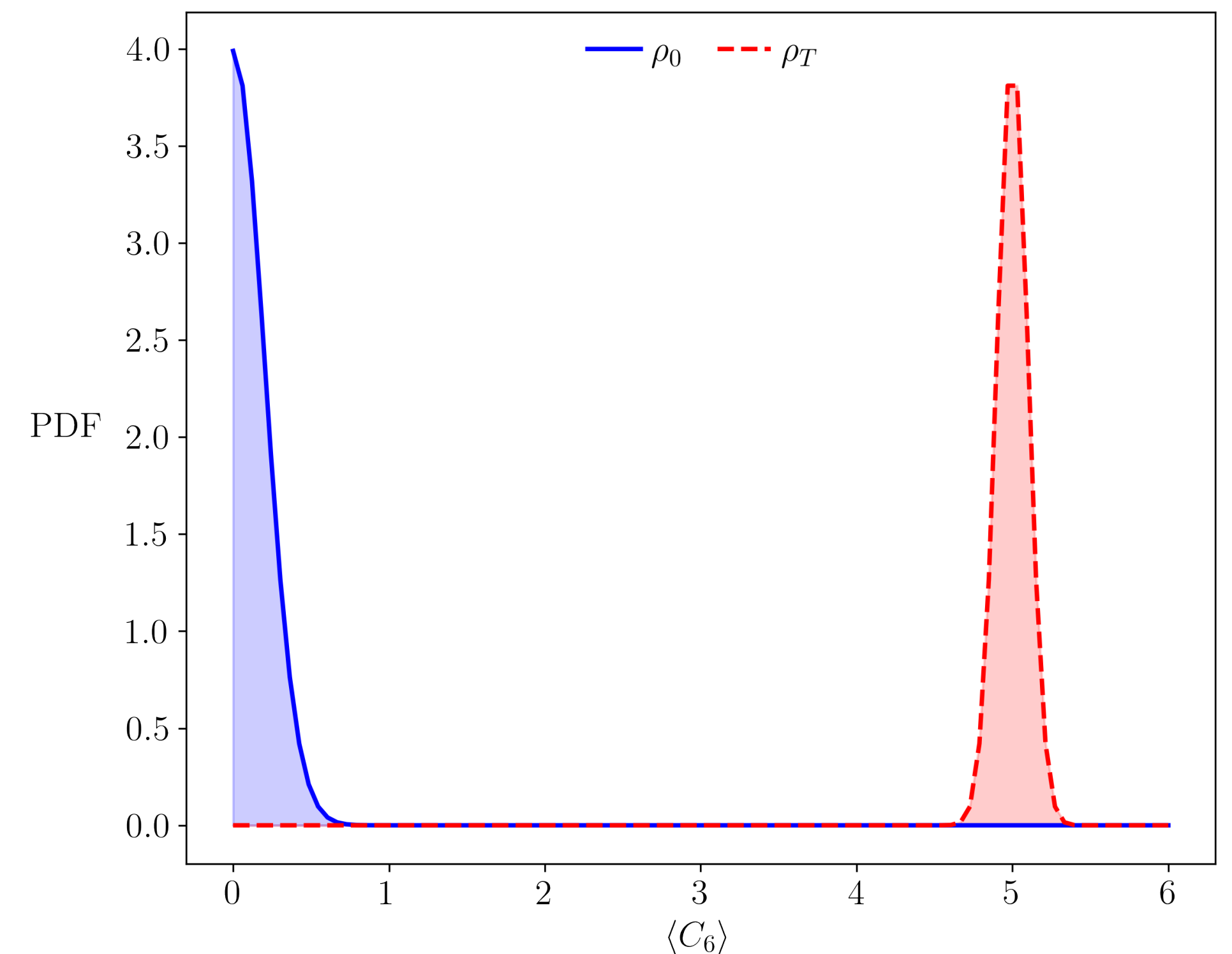
Equivalent formulation:

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

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

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

Guaranteed existence-uniqueness
for compactly supported ρ_0, ρ_T



Stochastic Control / Control Non-affine

Case 1: Conditions for Optimality

$$\frac{\partial \psi}{\partial t} = \frac{1}{2} (\pi^{\text{opt}})^2 - \frac{\partial \psi}{\partial x} D_1 - \frac{\partial^2 \psi}{\partial x^{u2}} D_2$$

HJB PDE

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

Controlled FPK PDE

$$\pi^{\text{opt}}(x^u, t) = \frac{\partial \psi}{\partial x^u} \frac{\partial D_1}{\partial u} + \frac{\partial^2 \psi}{\partial x^{u2}} \frac{\partial D_2}{\partial u}$$

Optimal policy

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

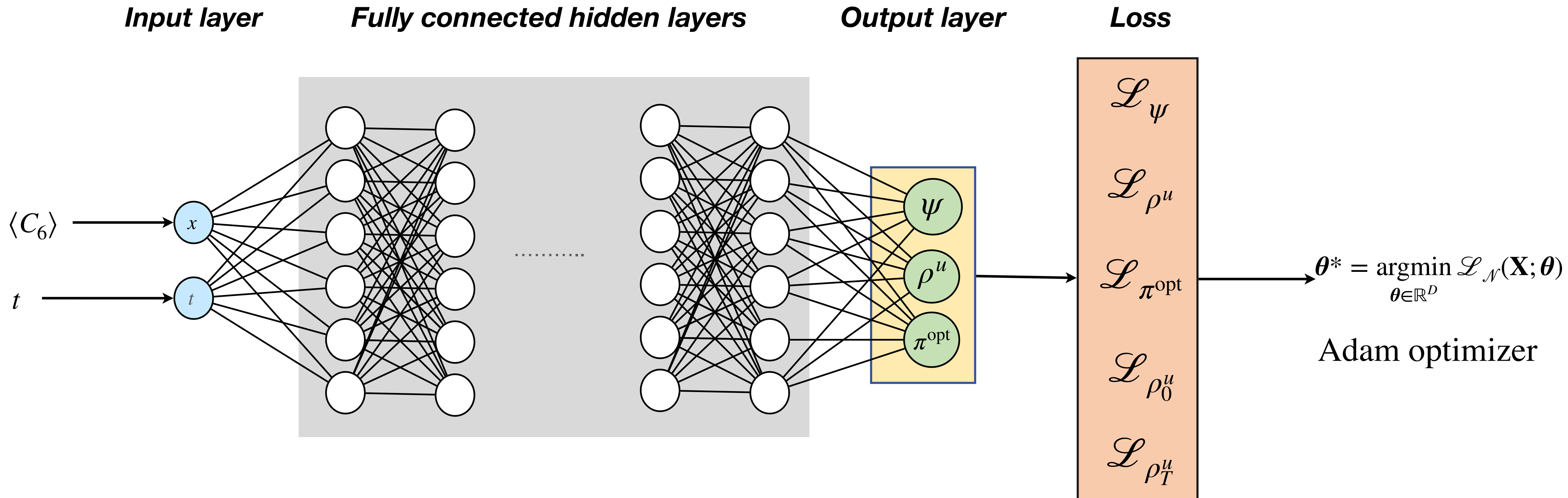
Boundary conditions

value optimally optimal
function controlled PDF policy

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



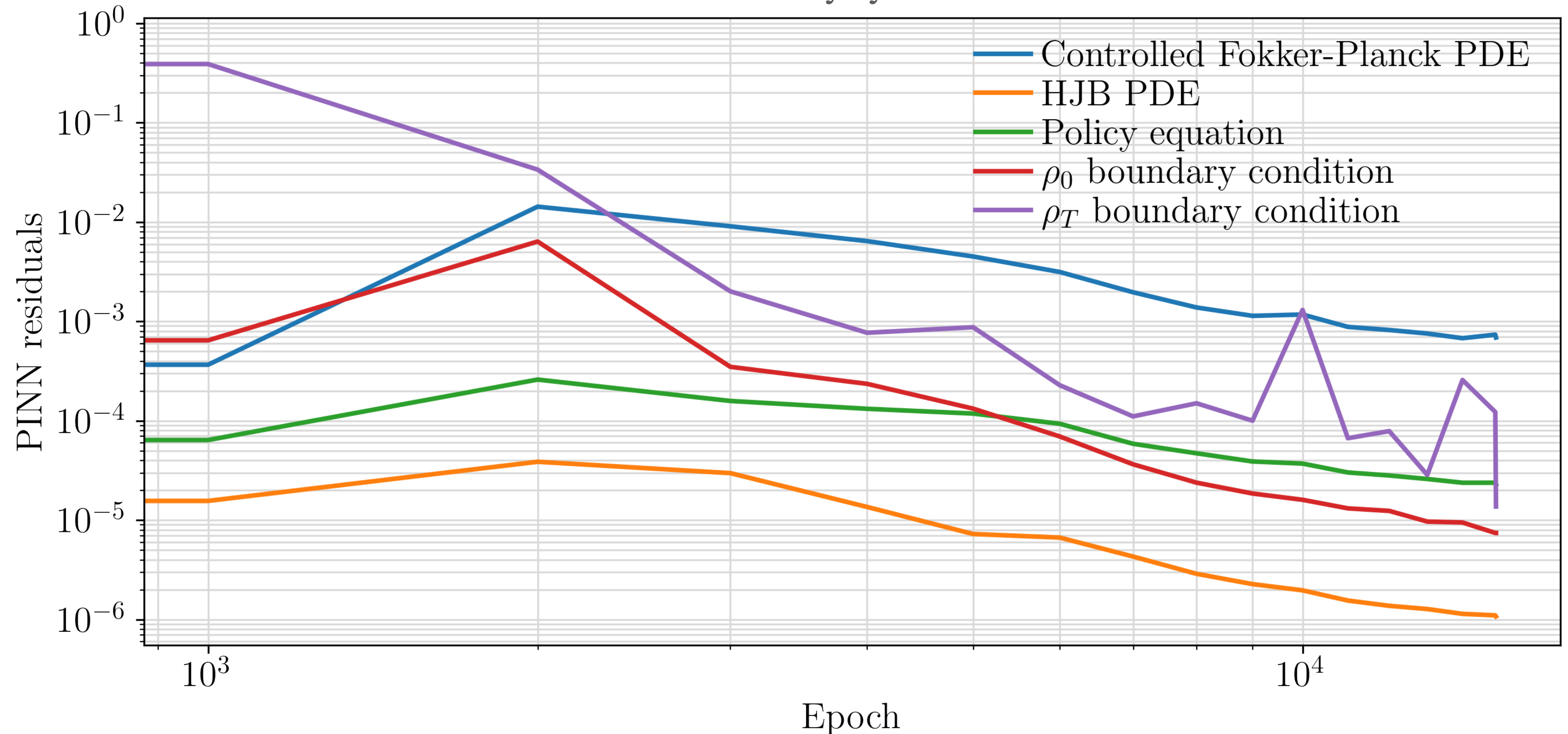
$$\mathcal{L}_{\mathcal{N}} = \mathcal{L}_\psi + \mathcal{L}_{\rho^u} + \mathcal{L}_{\pi^{\text{opt}}} + \mathcal{L}_{\rho_0^u} + \mathcal{L}_{\rho_T^u}$$

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

Stochastic Control / Control Non-affine

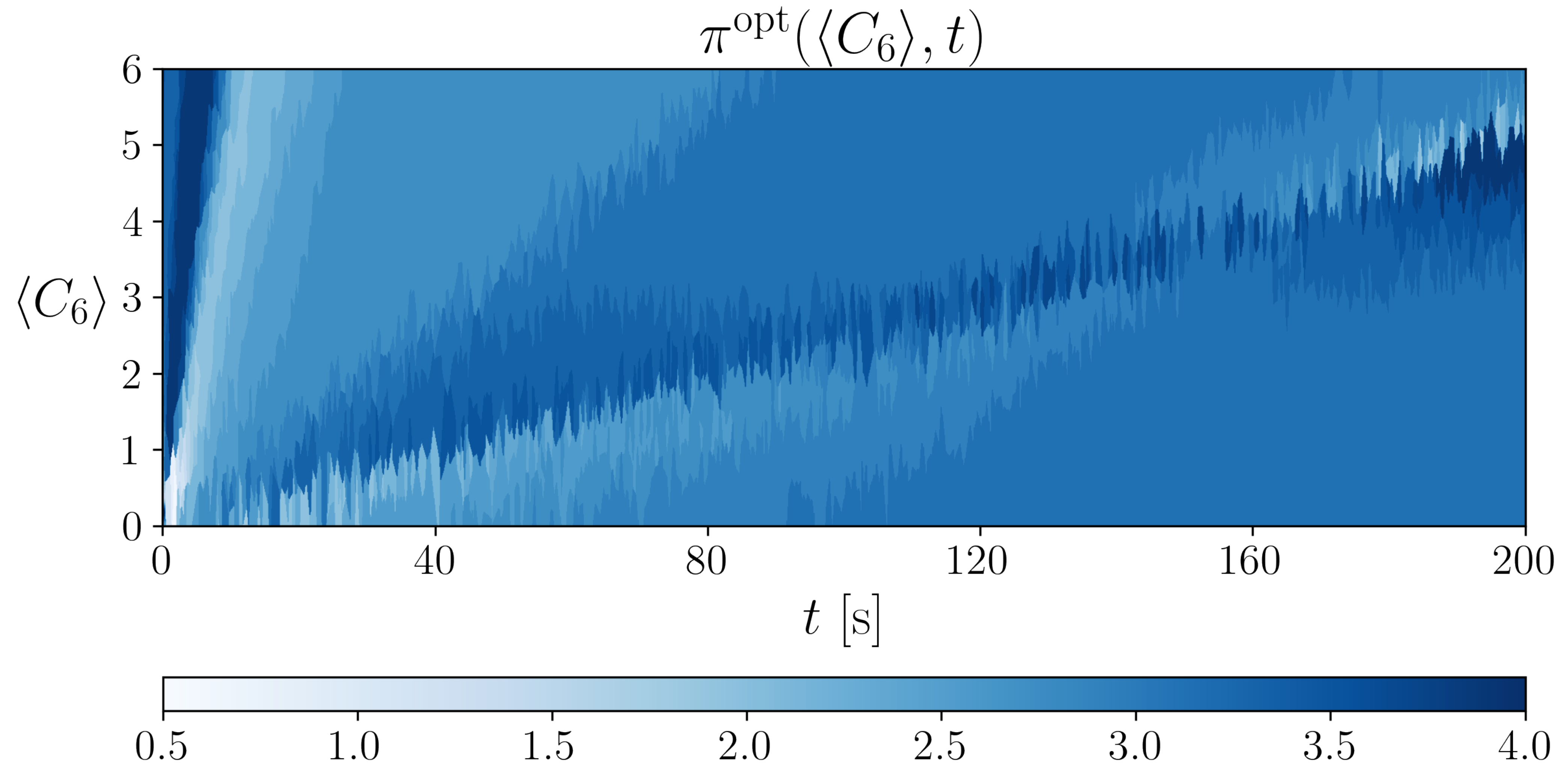
Case 1: Residual for PINN Training

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



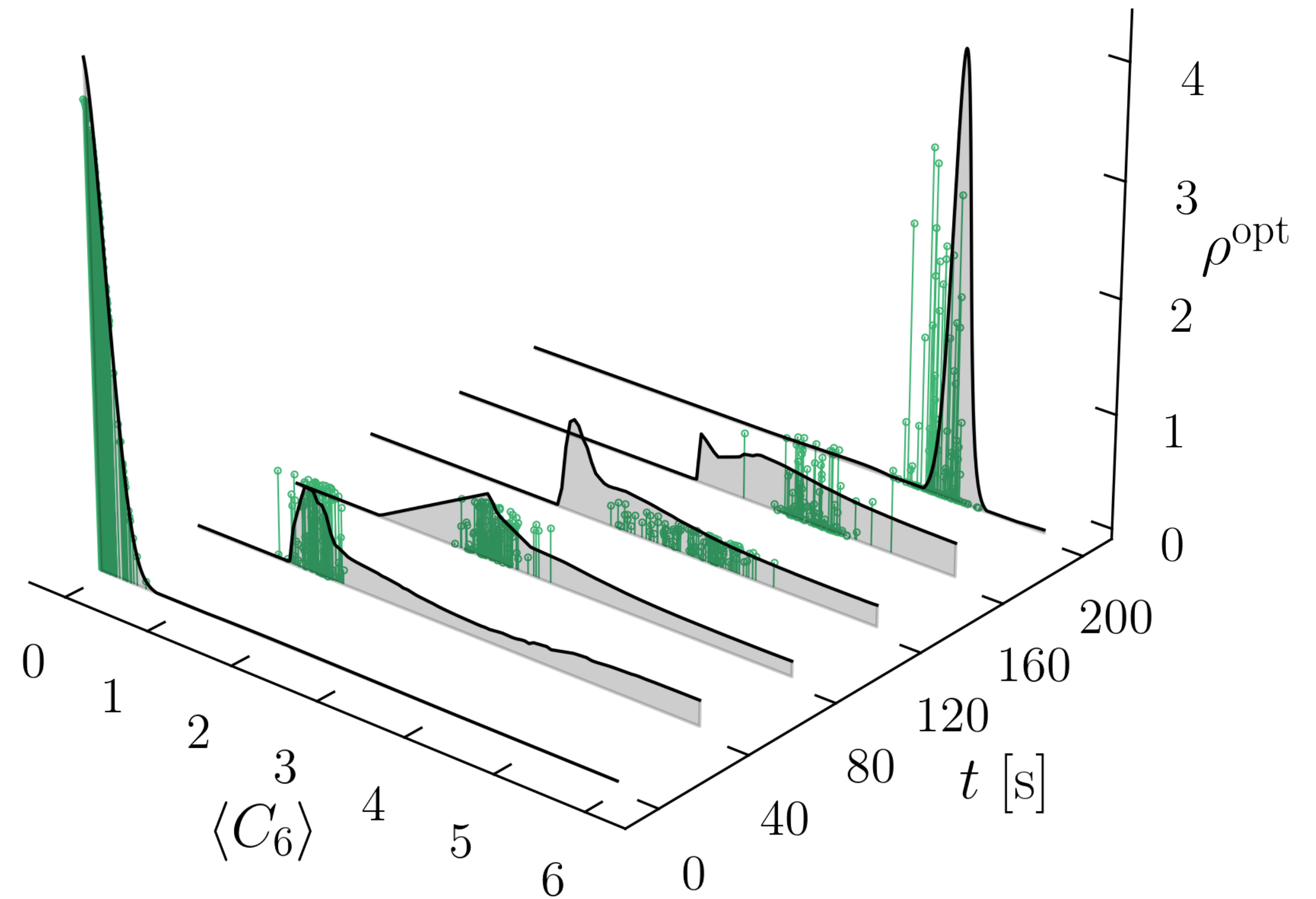
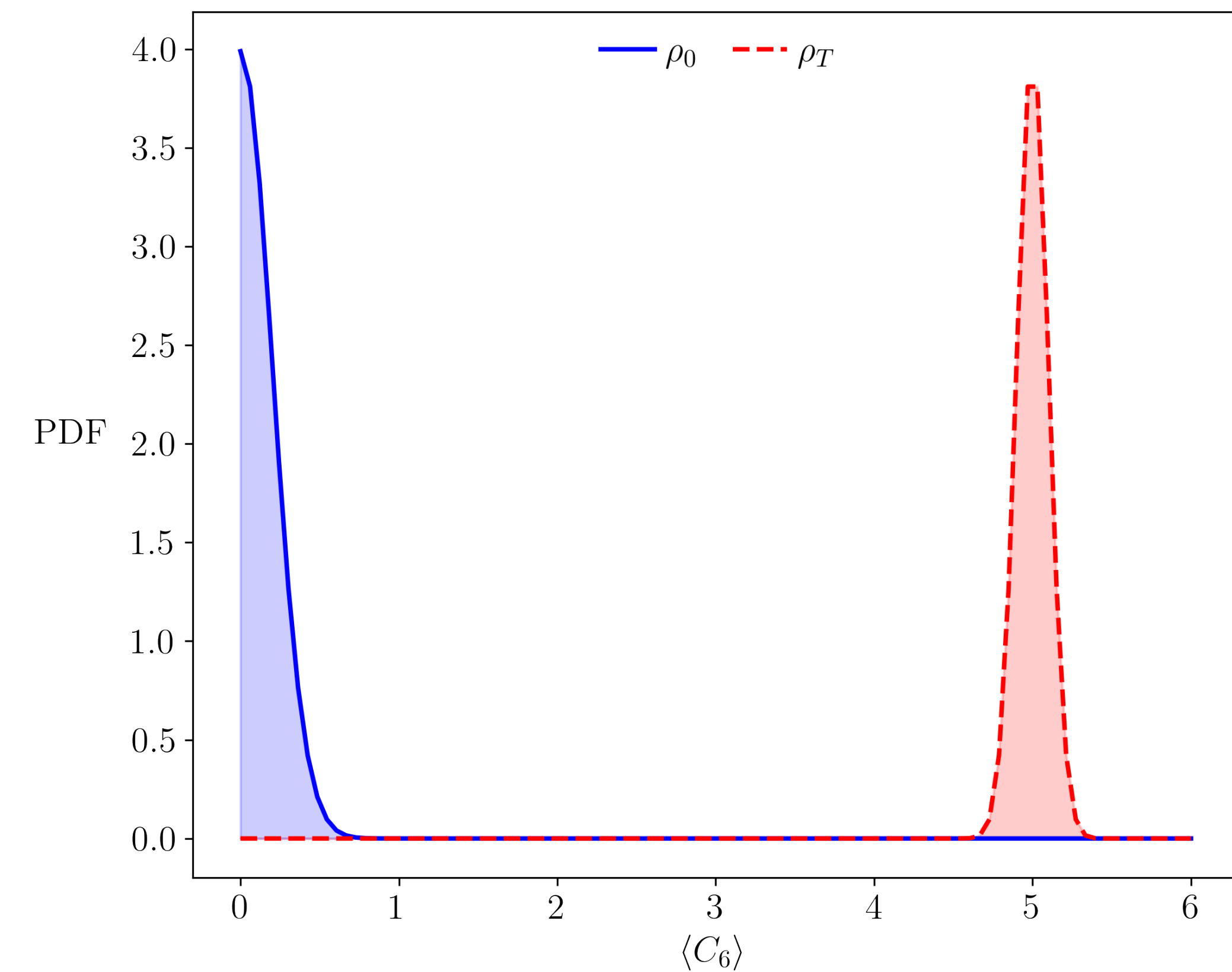
Stochastic Control / Control Non-affine

Case 1: Optimal Policy



Stochastic Control / Control Non-affine

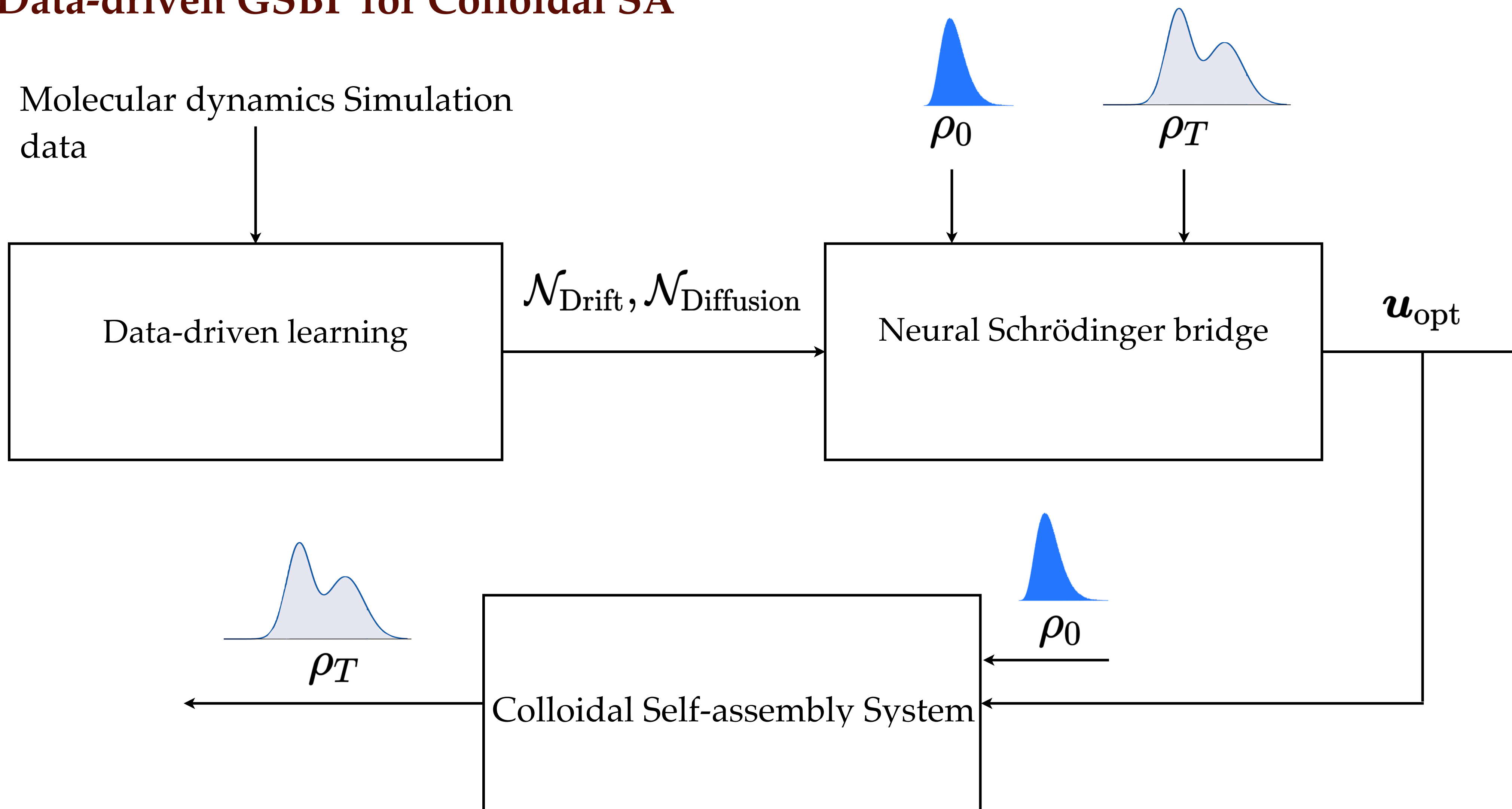
Case 1: Optimally Controlled State PDFs



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

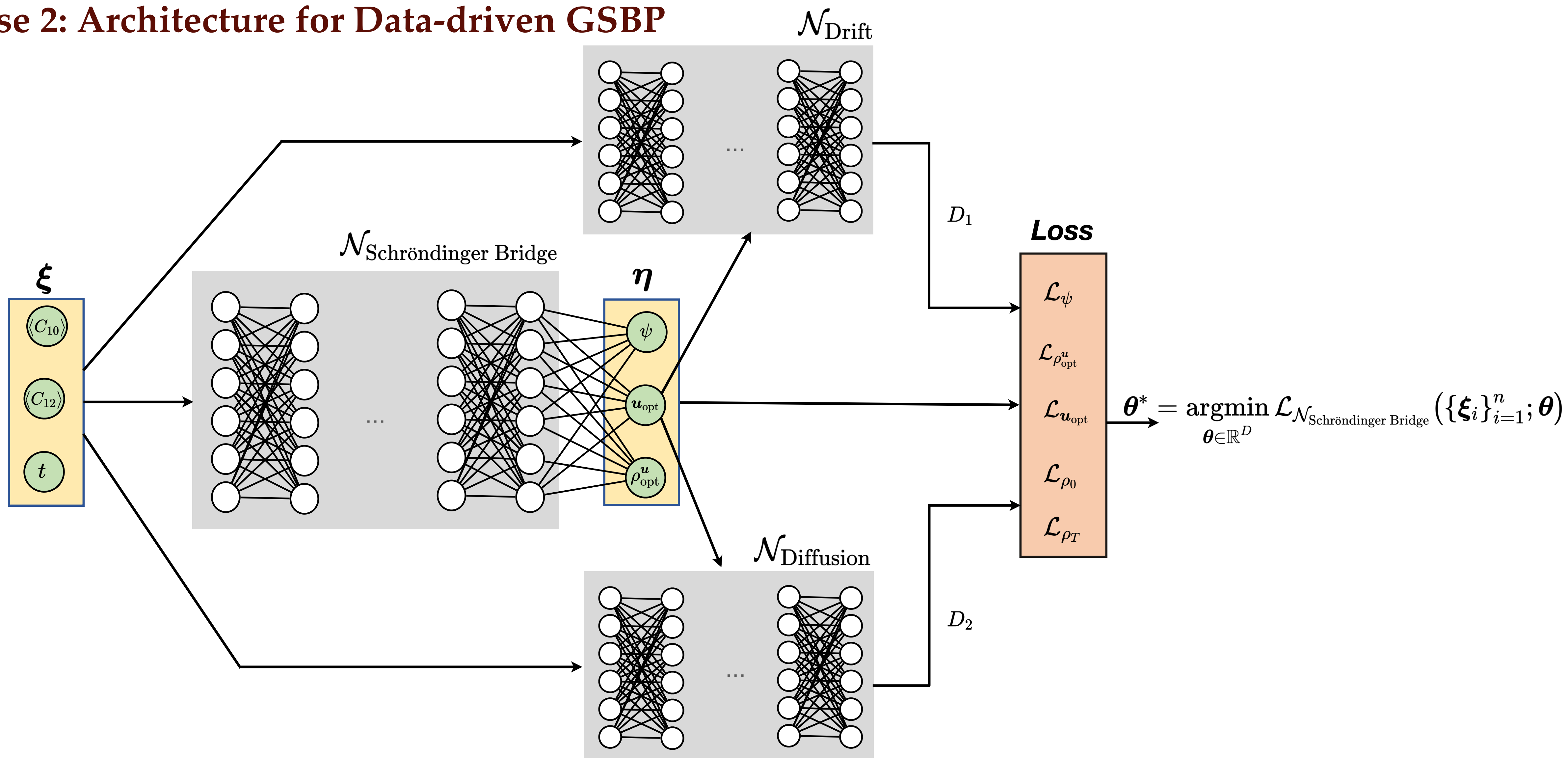
Stochastic Control / Control Non-affine

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

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

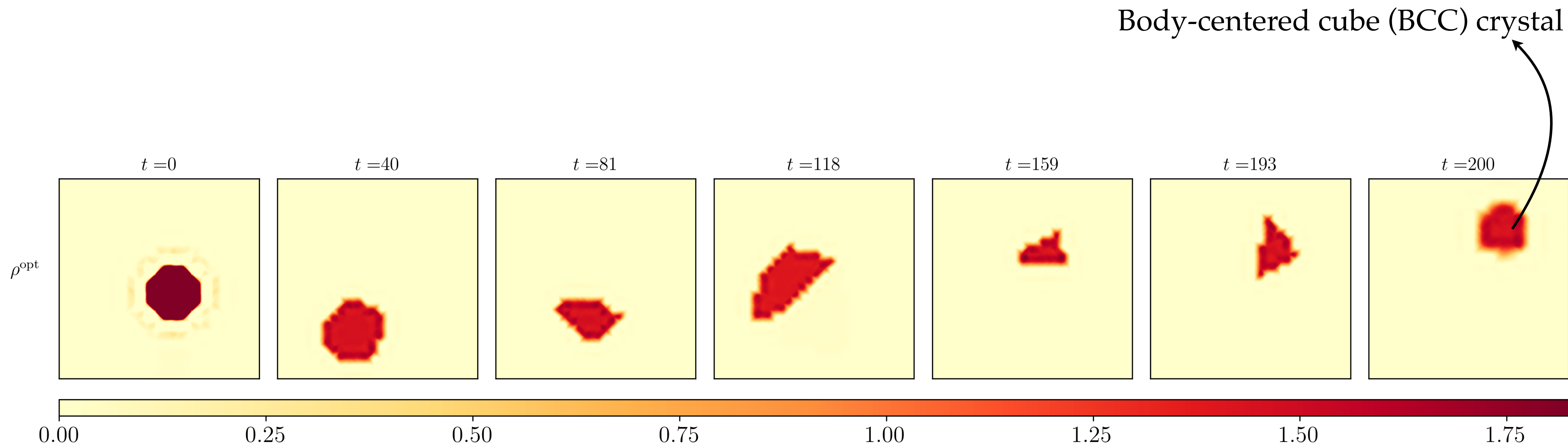
For boundary conditions, use Sinkhorn losses: $\mathcal{L}_{\rho_i} := W_\varepsilon^2 \left(\rho_i, \rho_i^{\text{epoch index}}(\boldsymbol{\theta}) \right)$

Implementation friendly for PINN training:

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

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

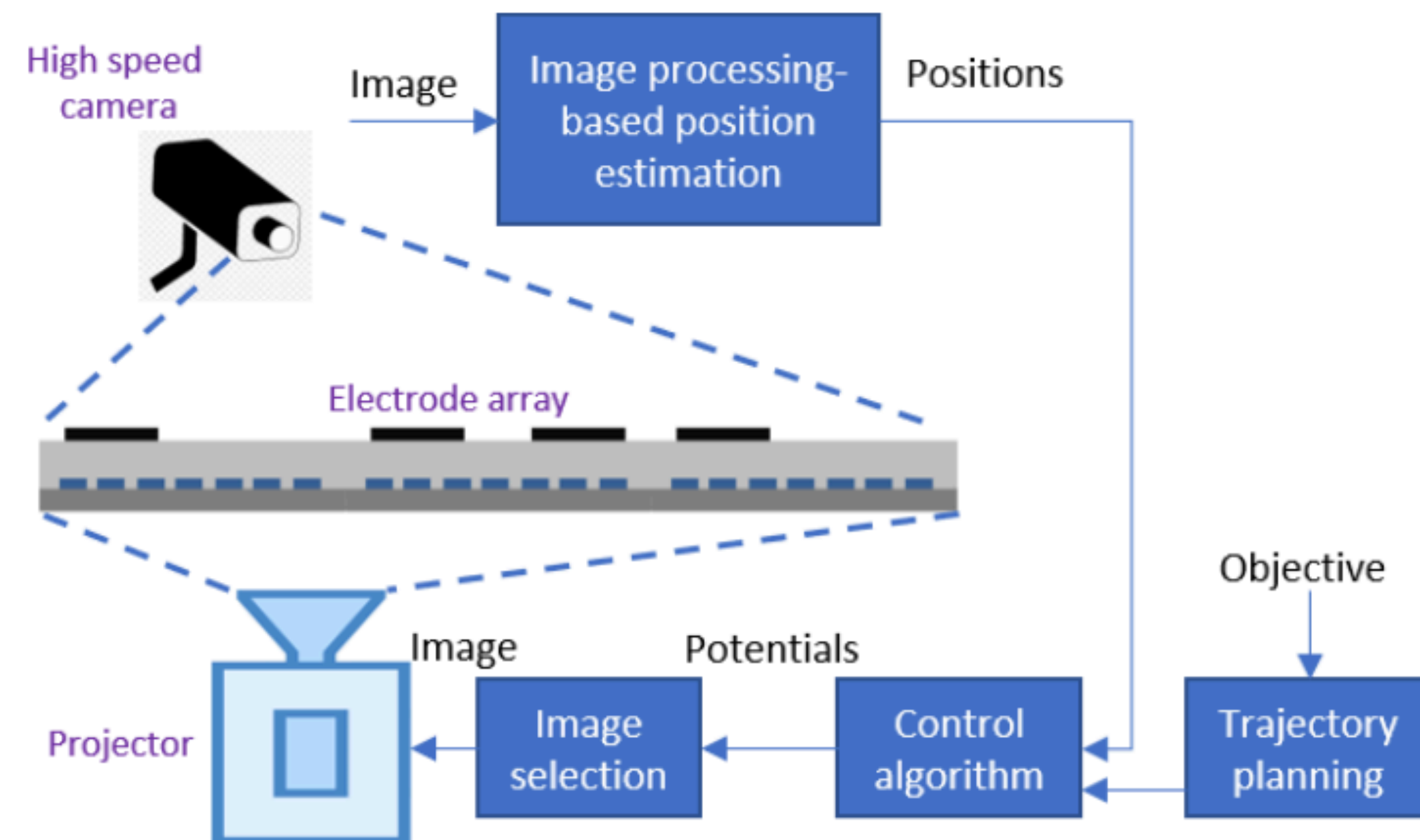


Image credit: PARC

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

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

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

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 ϕ^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 $\rho^n \rightharpoonup \rho$ a.s. in the limit $n \uparrow \infty$

where ρ 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

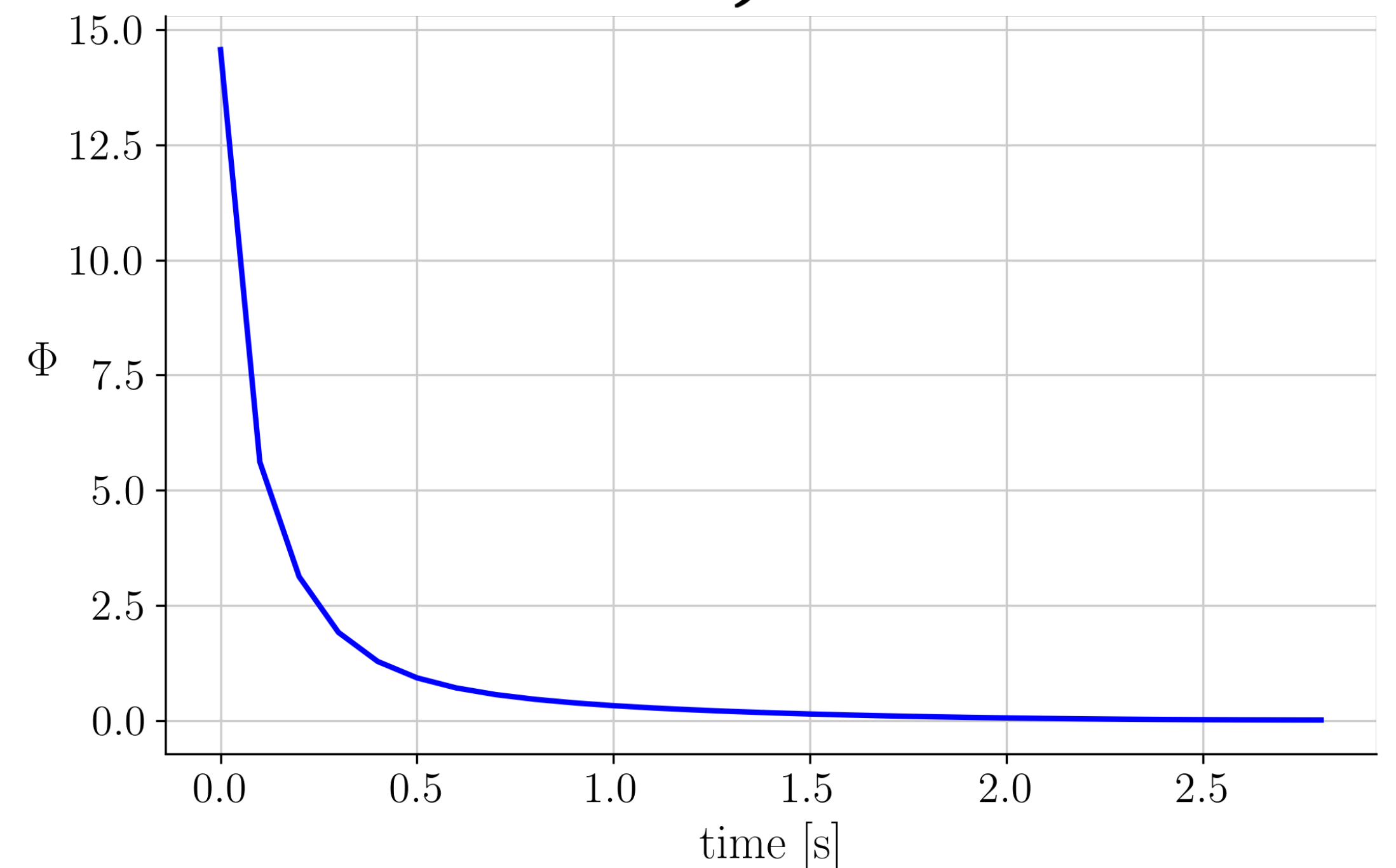
Wasserstein proximal recursion

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

Then the proximal recursion $\varrho_k = \text{prox}_{\tau \hat{\Phi}}^W(\varrho_{k-1})$
 $:= \arg \inf_{\varrho \in \mathcal{P}_2(\mathbb{R}^2)} \left\{ \frac{1}{2} W^2(\varrho, \varrho_{k-1}) + \tau \hat{\Phi}(\varrho, \varrho_{k-1}) \right\}$

approximates the transient solutions of the mean

field nonlinear PDE IVP



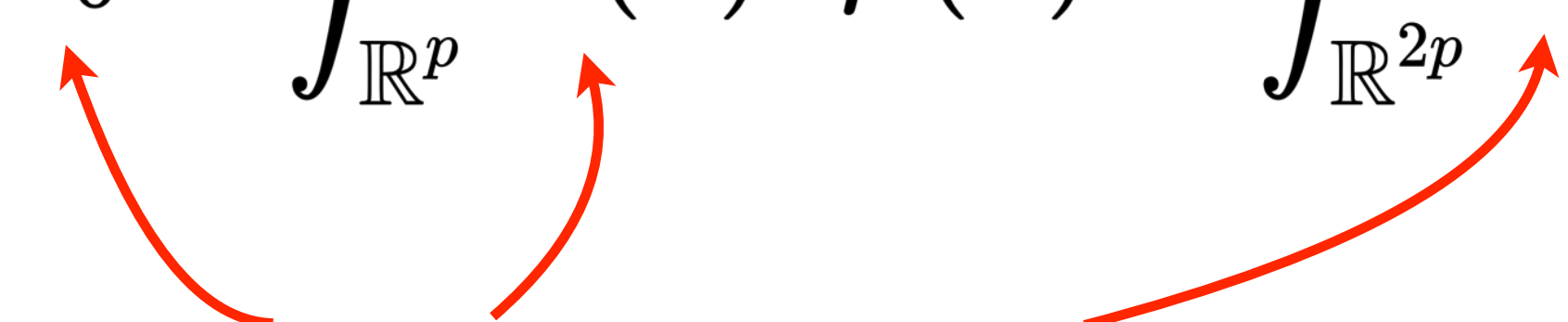
Part III: Stochastic Learning

Stochastic Learning / Centralized Computing

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

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

For quadratic loss:

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


depend on activation functions of the NN

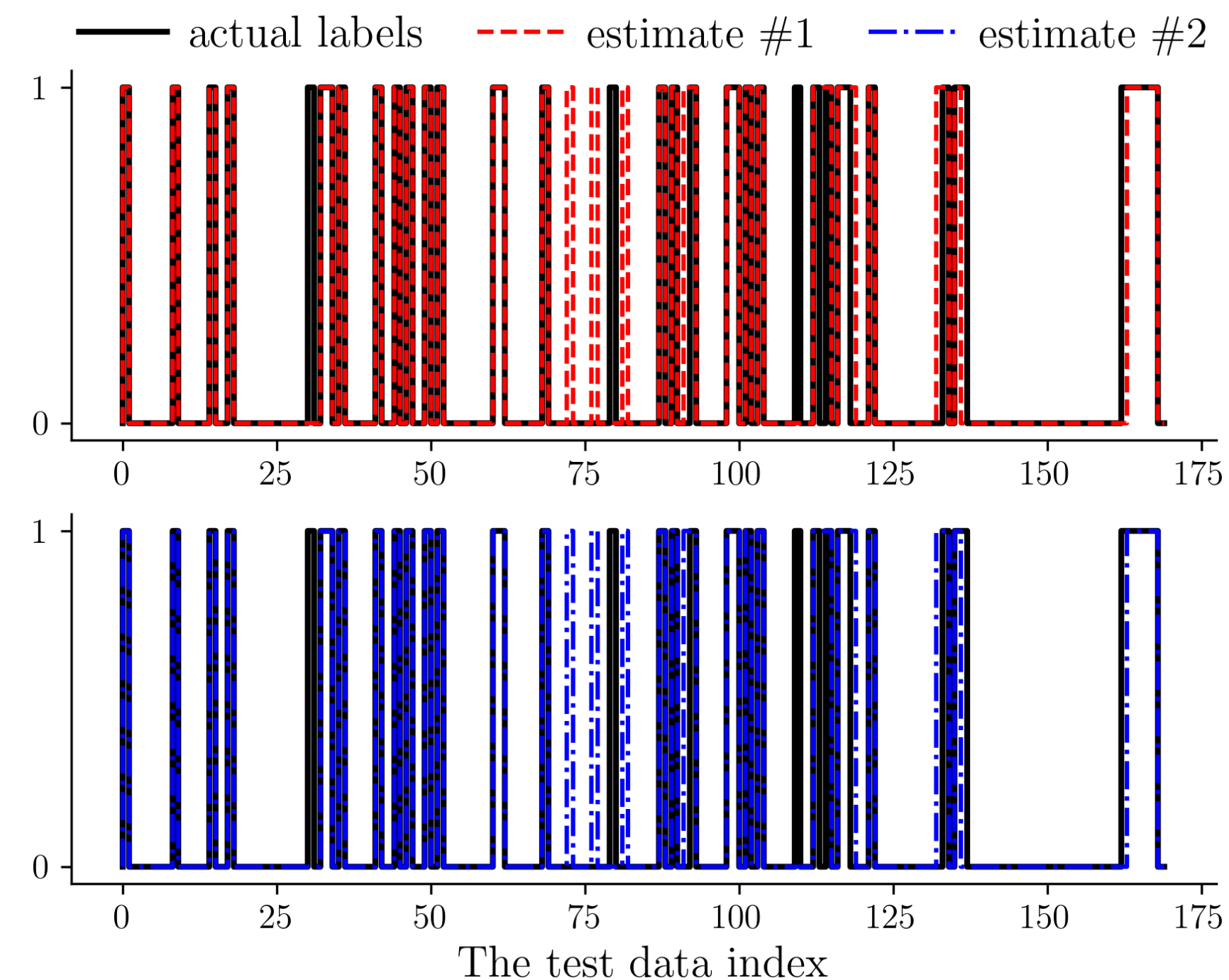
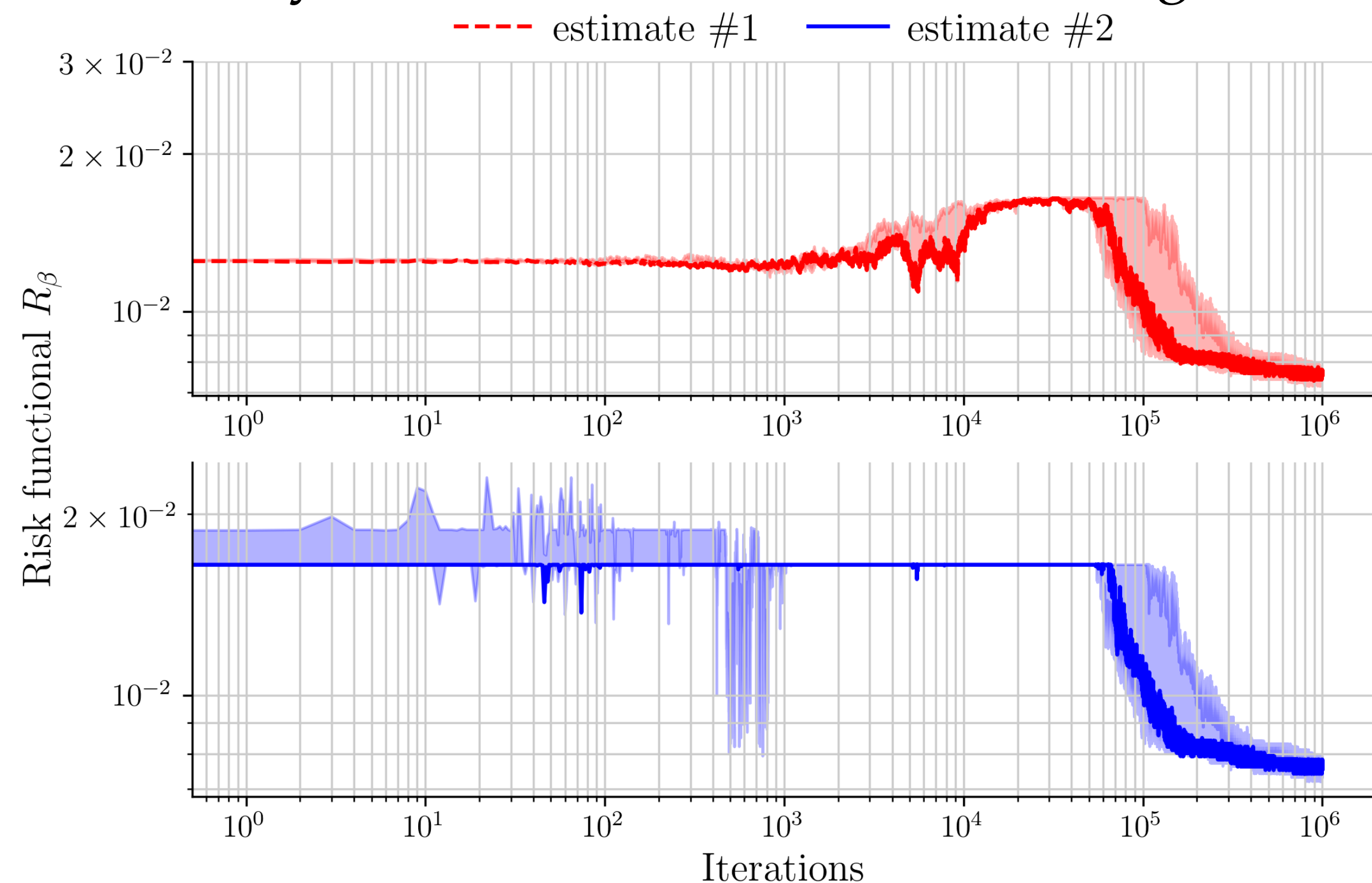
Neuronal population measure dynamics: $\frac{\partial \mu}{\partial t} = \nabla \cdot \left(\mu \nabla \frac{\delta F}{\delta \mu} \right) =: -\nabla^{W_2} F(\mu)$

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



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

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)

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

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

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

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

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

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

Define Wasserstein augmented Lagrangian:

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

regularization > 0

Lagrange multipliers

Stochastic Learning/ Distributed Computing

Proposed Consensus ADMM

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

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

$$\nu_i^{k+1} = \nu_i^k + \alpha(\mu_i^{k+1} - \zeta^{k+1}) \quad \text{where } i \in [n], k \in \mathbb{N}_0$$

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

Euclidean distance matrix

Outer
layer
ADMM

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

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

μ_i update \rightsquigarrow Outer Consensus (Sinkhorn) ADMM

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

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

Stochastic Learning/ Distributed Computing

ζ update \rightsquigarrow Inner (Euclidean) ADMM

Theorem. Consider the convex problem

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

Then

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

Stochastic Learning/ Distributed Computing

ζ update \rightsquigarrow Inner (Euclidean) ADMM

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

Then the following Euclidean ADMM solves

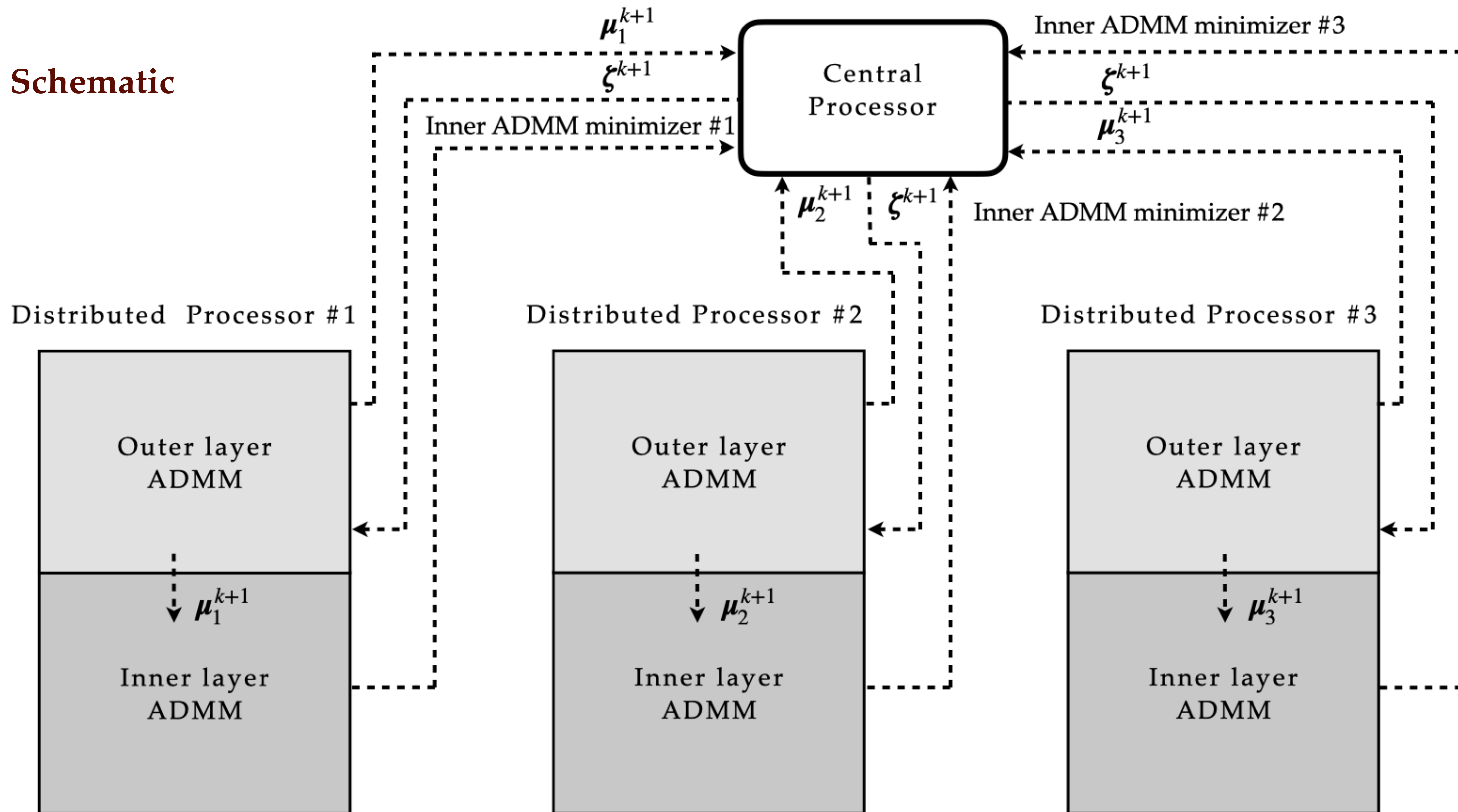
$$\begin{aligned}\mathbf{u}_i^{\ell+1} &= \text{prox}_{\frac{\|\cdot\|_2}{\tau} f_i} \left(\mathbf{z}_i^\ell - \tilde{\mathbf{v}}_i^\ell \right) \\ \mathbf{z}_i^{\ell+1} &= \left(\mathbf{u}_i^{\ell+1} - \frac{1}{n} \sum_{i=1}^n \mathbf{u}_i^{\ell+1} \right) + \left(\tilde{\mathbf{v}}_i^\ell - \frac{1}{n}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

Theorem.

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

Stochastic Learning/ Distributed Computing

Overall Schematic



Stochastic Learning/ Distributed Computing

Experiment #1 Aggregation-drift-diffusion nonlinear PDE

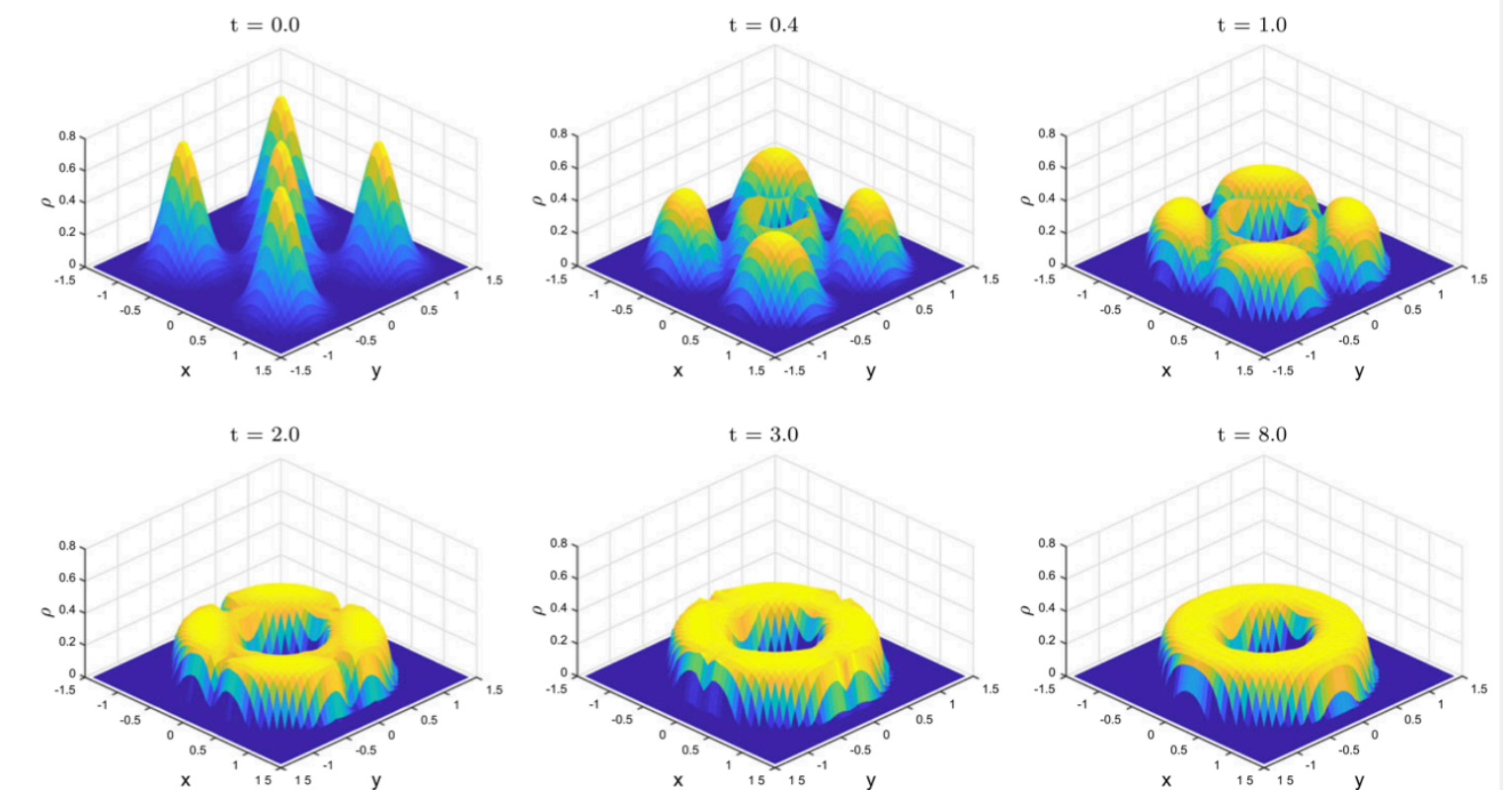
$$\frac{\partial \mu}{\partial t} = \underbrace{\nabla \cdot (\mu \nabla (U * \mu))}_{i=1} + \underbrace{\nabla \cdot (\mu \nabla V)}_{i=2} + \beta^{-1} \Delta \mu^2$$

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

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

Centralized computation:

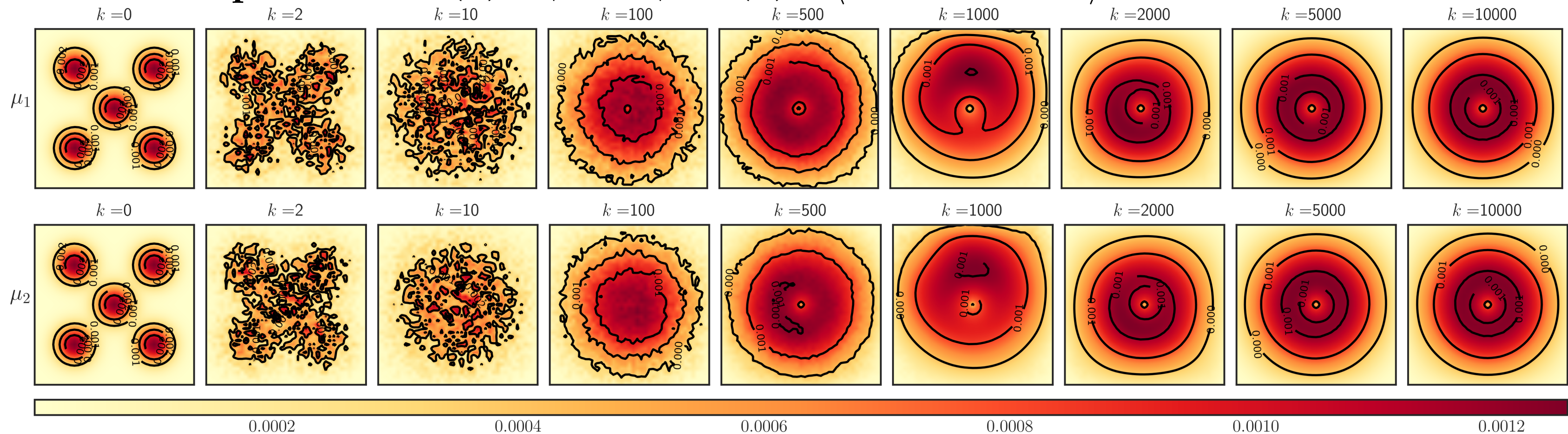
Carrillo, Craig, Wang and Wei, *FOCM*, 2021



$$\lim_{\beta^{-1} \downarrow 0} \mu_\infty = \text{Unif}(\mathcal{A})$$

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

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



Stochastic Learning/ Distributed Computing

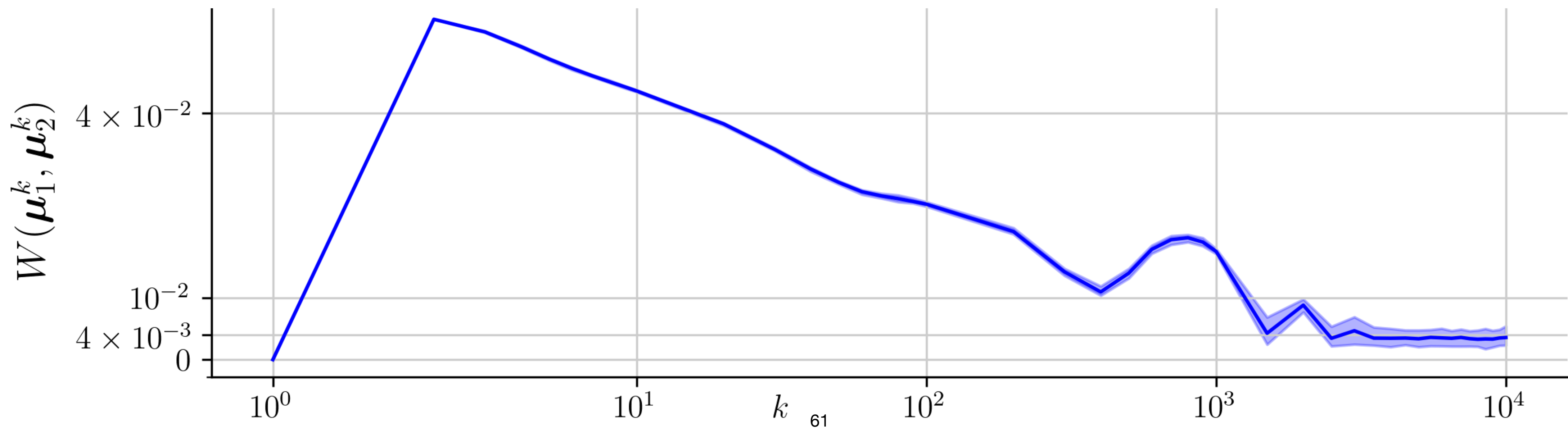
Experiment #1 Aggregation-drift-diffusion nonlinear PDE

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

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

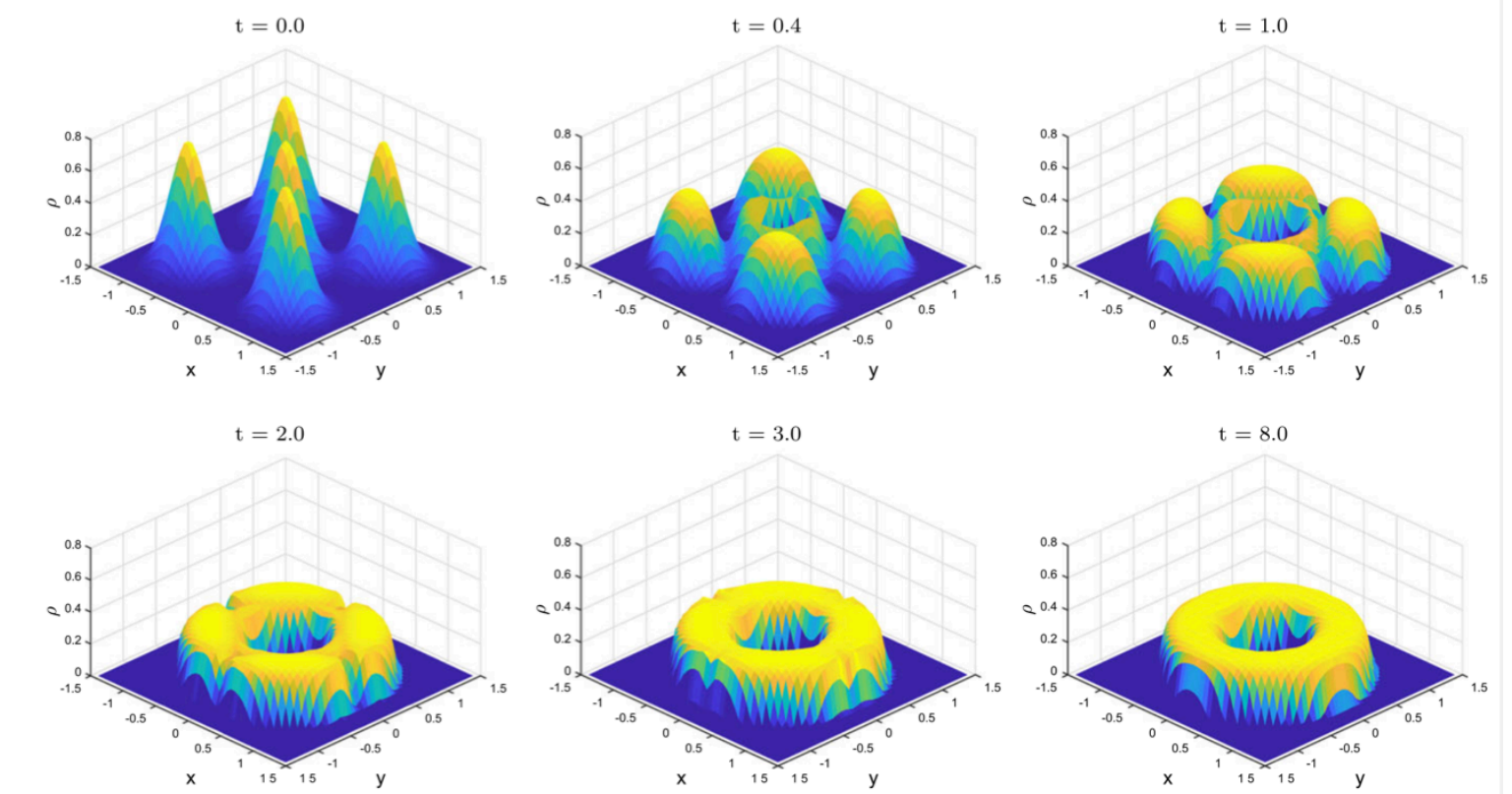
$$V(\mathbf{x}) = -\frac{1}{4} \ln \|\mathbf{x}\|_2$$

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



Centralized computation:

Carrillo, Craig, Wang and Wei, *FOCM*, 2021



$$\lim_{\beta^{-1} \downarrow 0} \mu_\infty = \text{Unif}(\mathcal{A})$$

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

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

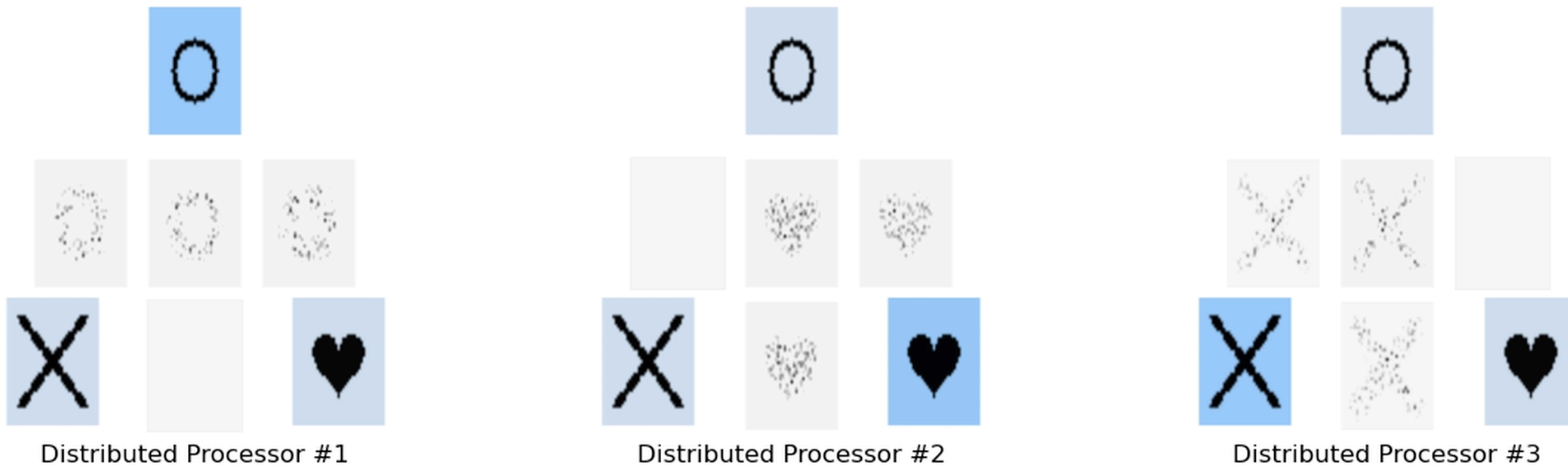
Experiment # 2 Wasserstein barycenter

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



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

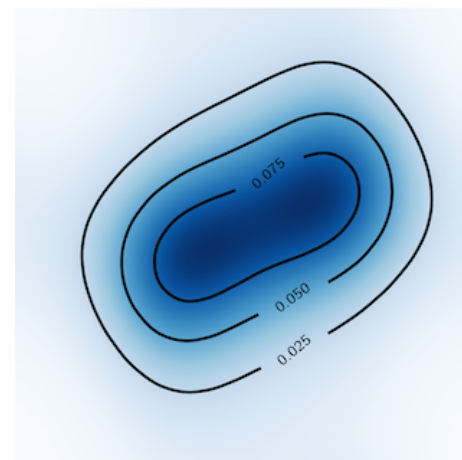
Stochastic Control/ Control-affine: Nonuniform Noisy Kuramoto Oscillators

First order Case Study

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

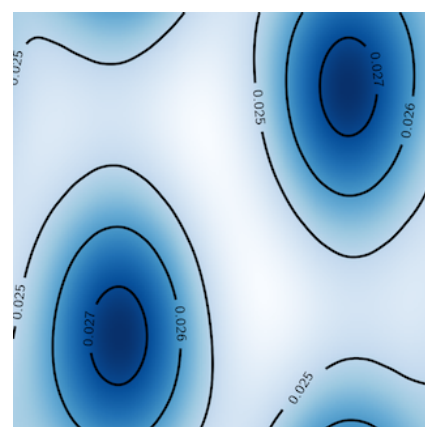
$$\inf_{u \in \mathcal{U}} \mathbb{E}_{\mu^u} \left[\int_0^T \frac{1}{2} u^2 dt \right],$$

$$d\boldsymbol{\theta} = \left(-\nabla_{\boldsymbol{\theta}} V(\boldsymbol{\theta}) + S\mathbf{u} \right) dt + \sqrt{2}S d\mathbf{w} \xrightarrow[\boldsymbol{\theta} \mapsto \boldsymbol{\xi} := S^{-1}\boldsymbol{\theta}]{\text{Change of variables}} d\boldsymbol{\xi} = \left(\mathbf{u} - \Upsilon \nabla_{\boldsymbol{\xi}} \tilde{V}(\boldsymbol{\xi}) \right) dt + \sqrt{2} d\mathbf{w}$$



$\boldsymbol{\theta}(t=0) \sim \mu_0$ (Desynchronized)

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



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

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

Stochastic Control/ Control-affine: Nonuniform Noisy Kuramoto Oscillators

First order
$$d\boldsymbol{\theta} = (-\nabla_{\boldsymbol{\theta}} V(\boldsymbol{\theta}) + \mathbf{S}u) dt + \sqrt{2}\mathbf{S}d\mathbf{w}$$

Second order
$$\begin{pmatrix} d\boldsymbol{\theta} \\ d\boldsymbol{\omega} \end{pmatrix} = \begin{pmatrix} \boldsymbol{\omega} \\ -\mathbf{M}^{-1}\nabla_{\boldsymbol{\theta}} V(\boldsymbol{\theta}) - \mathbf{M}^{-1}\boldsymbol{\Gamma}\boldsymbol{\omega} + \mathbf{M}^{-1}\mathbf{S}u \end{pmatrix} dt + \begin{pmatrix} \mathbf{0}_{n \times 1} \\ \sqrt{2}\mathbf{M}^{-1}\mathbf{S}d\mathbf{w} \end{pmatrix}$$

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

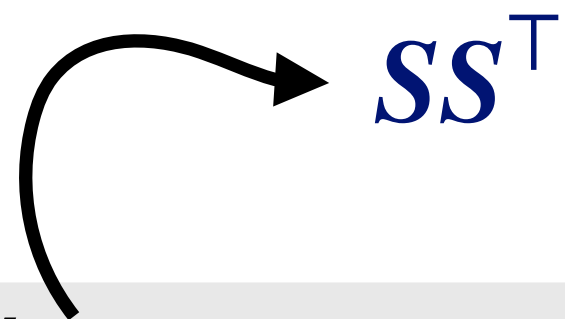
Coupling > 0
Phase difference $\in [0, \pi/2)$
Linear coeff. > 0

Positive diagonal matrices $\mathbf{M}, \boldsymbol{\Gamma}, \mathbf{S}$

Stochastic Control/ Control-affine: Nonuniform Noisy Kuramoto Oscillators

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

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

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


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

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

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

Stochastic Control/ Control-affine: Nonuniform Noisy Kuramoto Oscillators

The Second Order Case

Uncontrolled forward-backward Kolmogorov PDEs

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

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

Initial and Terminal conditions

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

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

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

Stochastic Control/ Control-affine/ Nonuniform Noisy Kuramoto Oscillators

Proximal recursion

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

Distance

Step size

Energy-like functional

First order:

$$d \equiv W_{\Upsilon}$$

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

Second order:

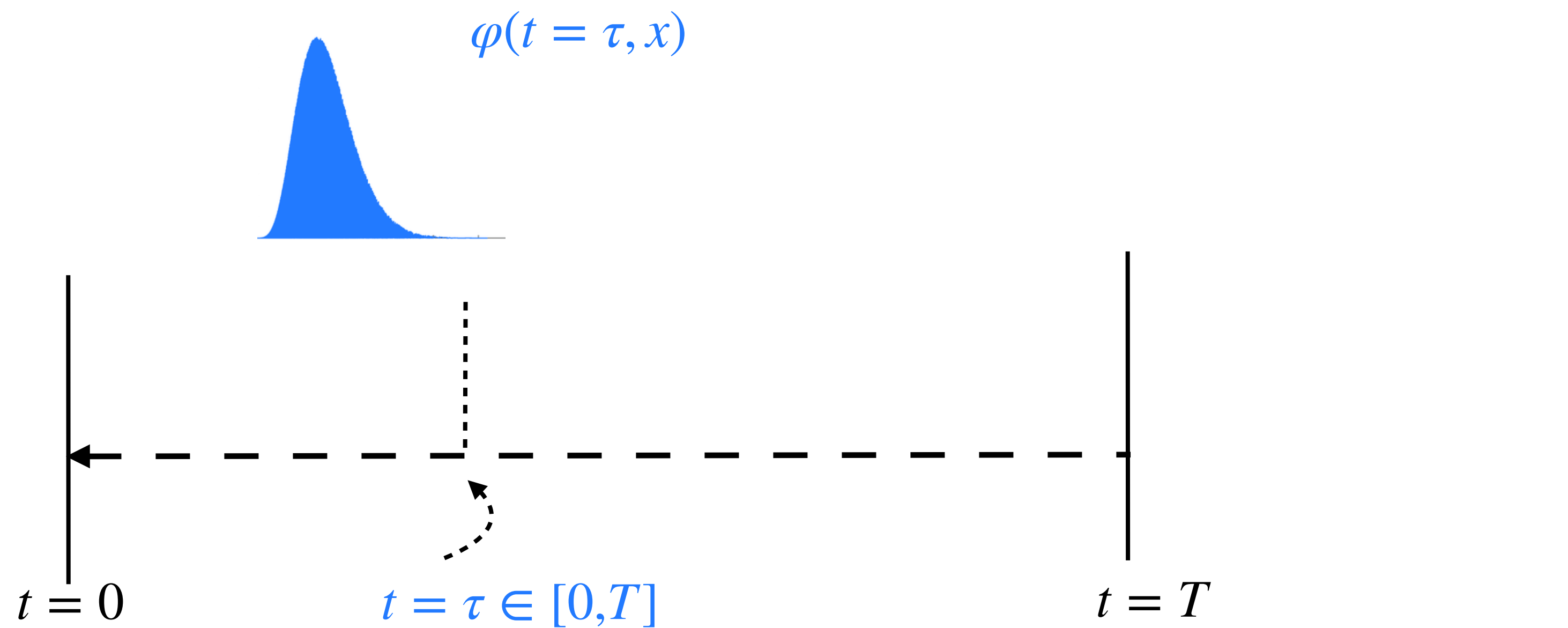
$$d \equiv W_{h, \tilde{\Upsilon}}$$

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

Stochastic Control/ Control-affine/ Nonuniform Noisy Kuramoto Oscillators

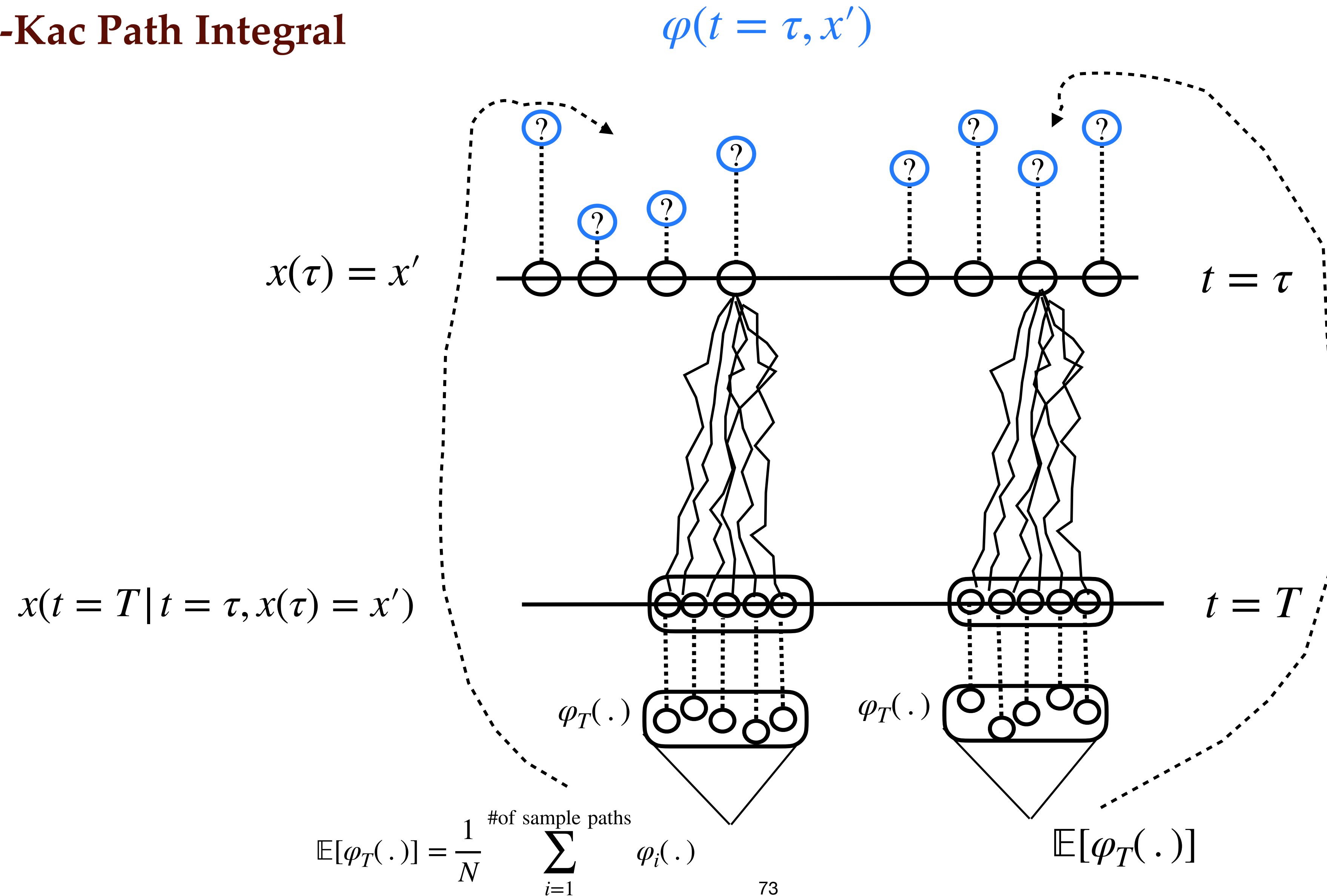
Feynman-Kac Path Integral

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

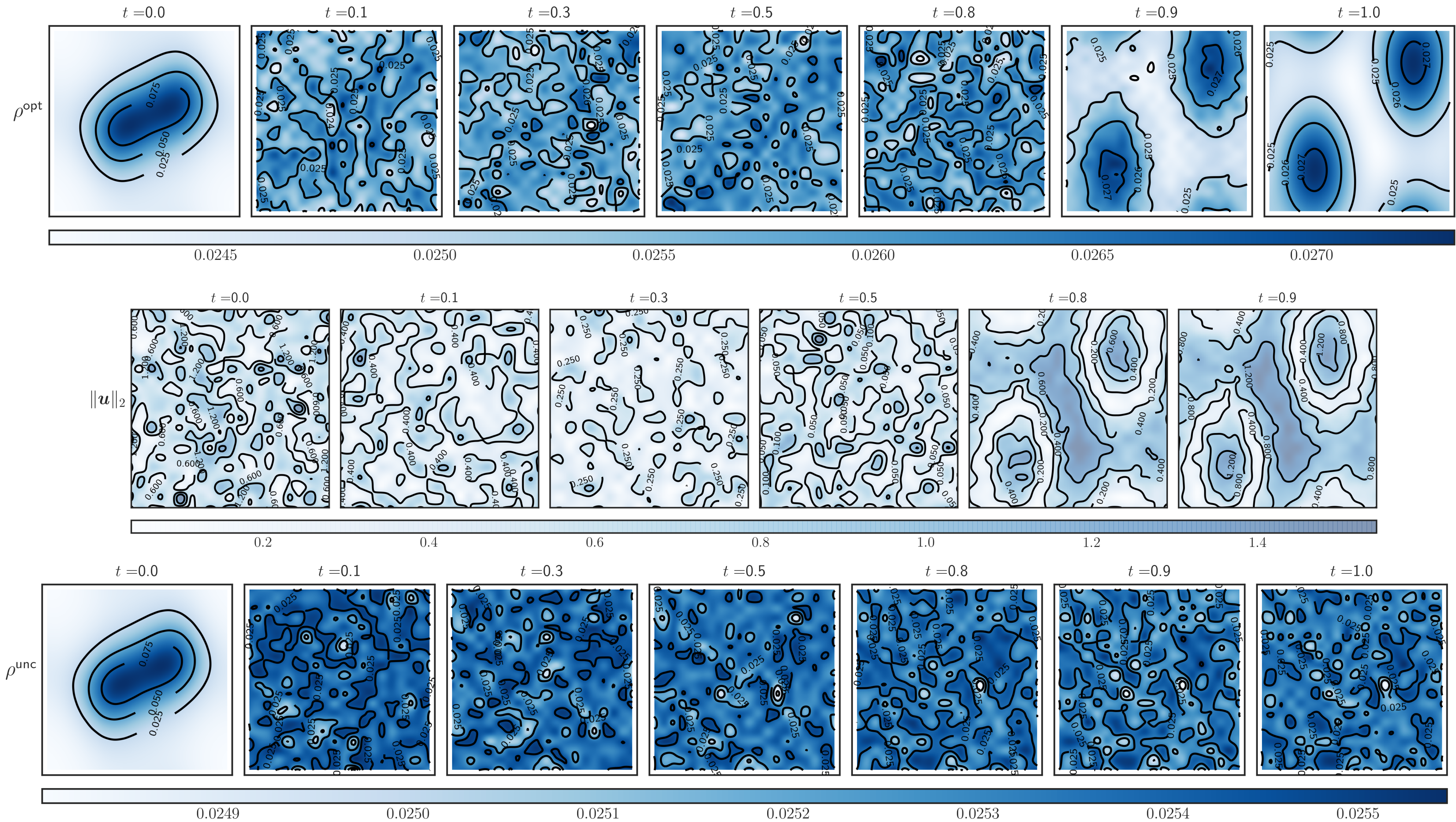


Stochastic Control/ Control-affine/ Nonuniform Noisy Kuramoto Oscillators

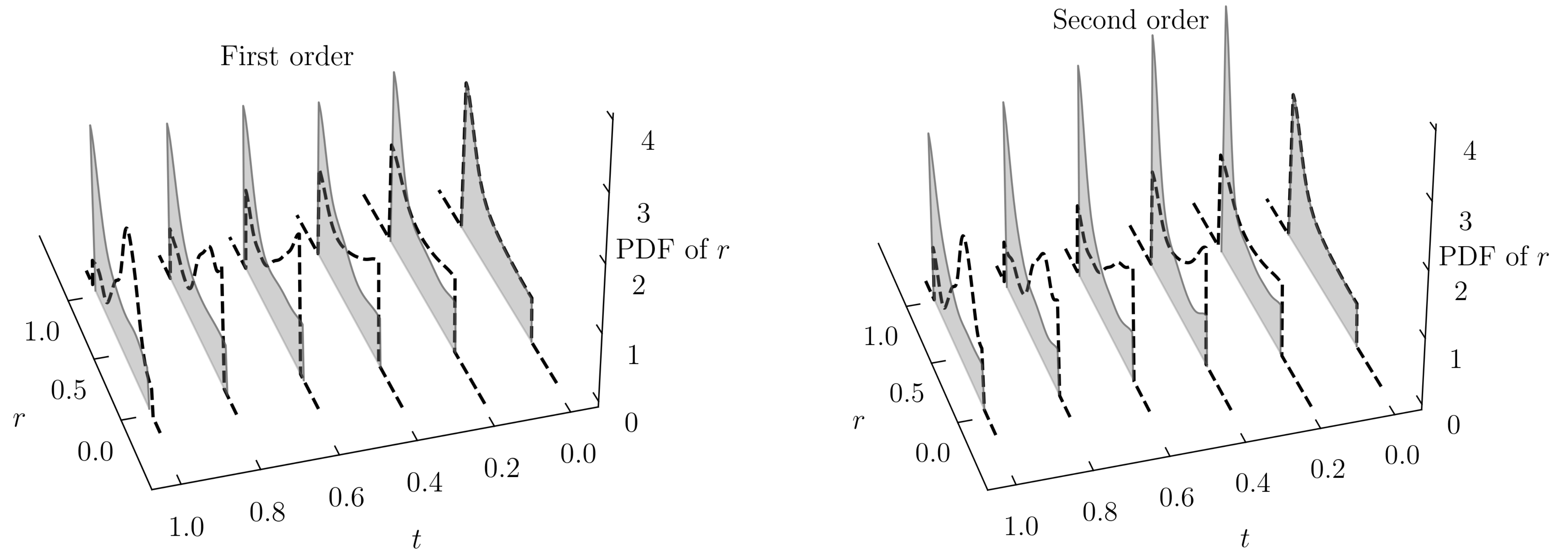
Feynman-Kac Path Integral



Stochastic Control/ Control-affine/ Nonuniform Noisy Kuramoto Oscillators



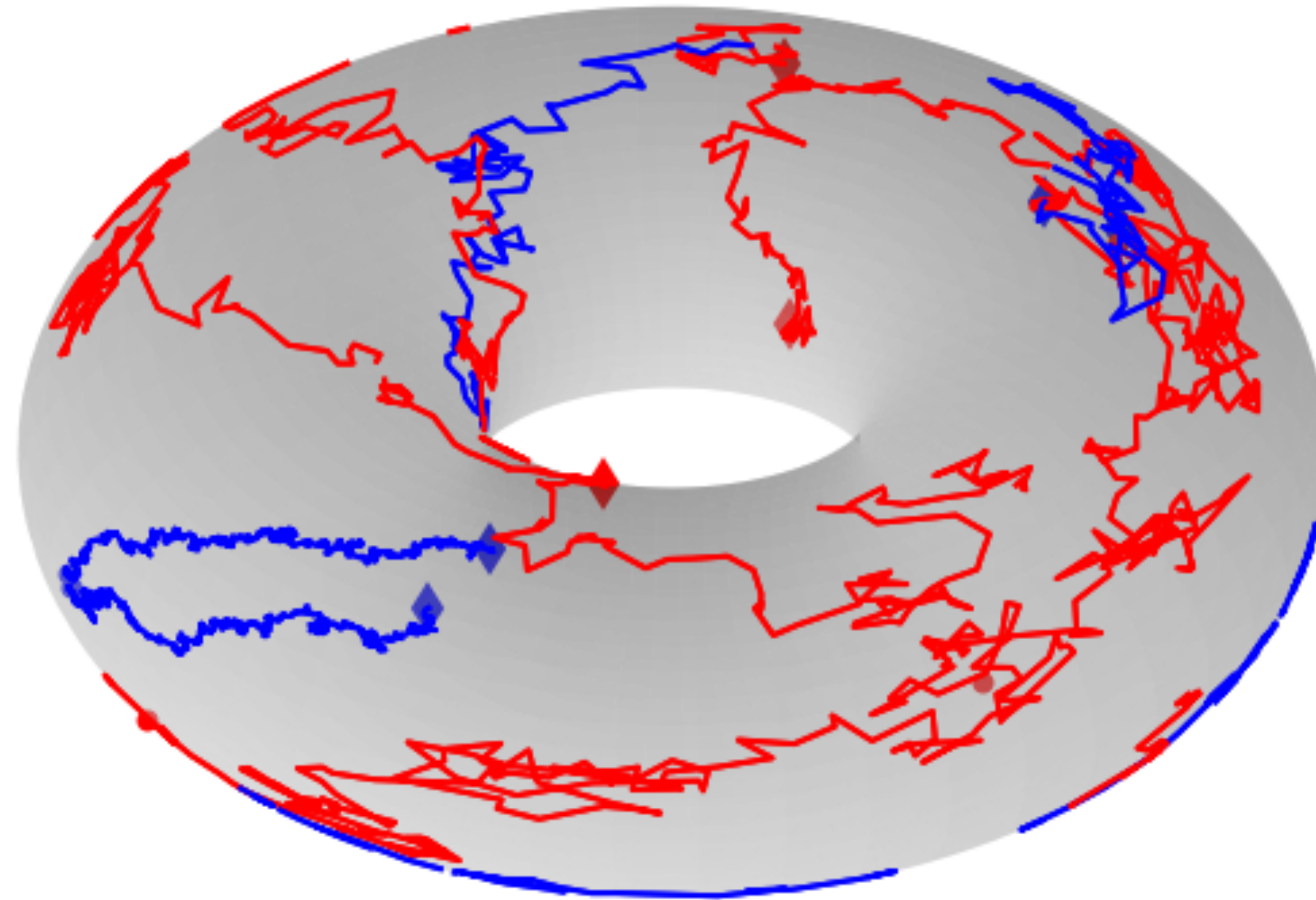
Stochastic Control/ Control-affine/ Nonuniform Noisy Kuramoto Oscillators



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

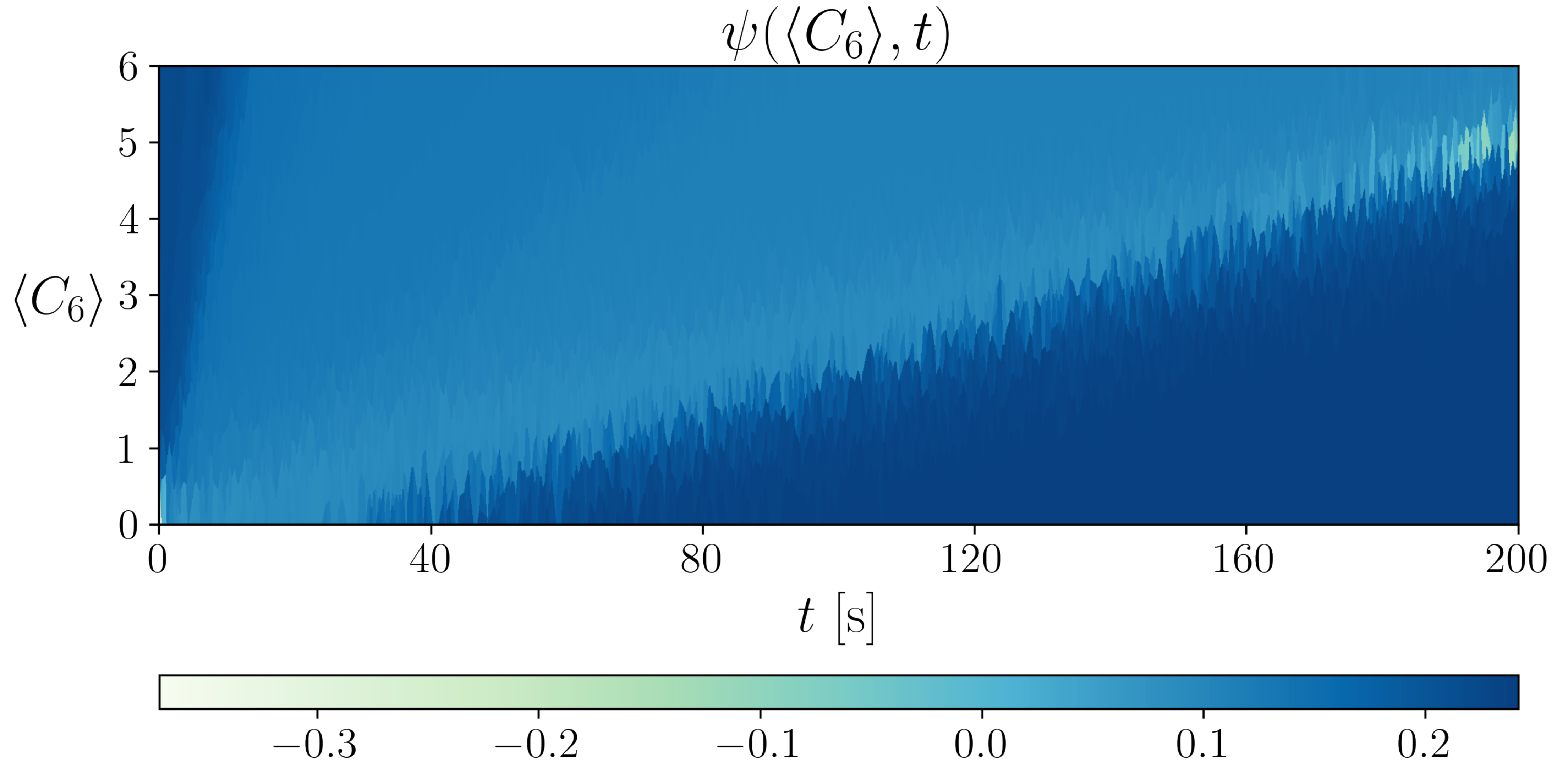
$$\mathcal{L}_{\rho_0^u} = \frac{1}{n} \sum_{i=1}^n \left(\rho^u \Big|_{t=0} - \rho_0^u(x) \right)^2$$

Loss term for terminal condition

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

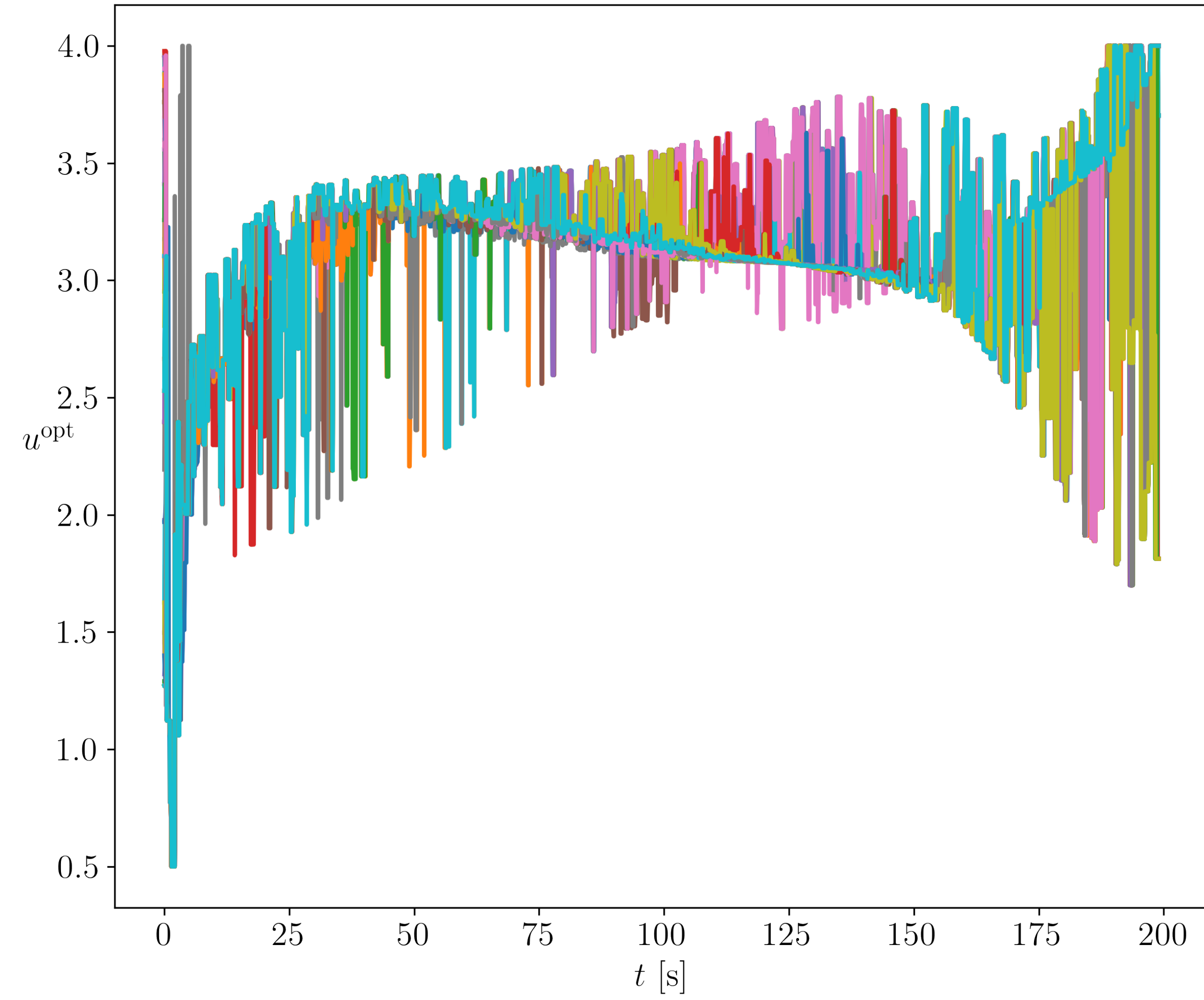
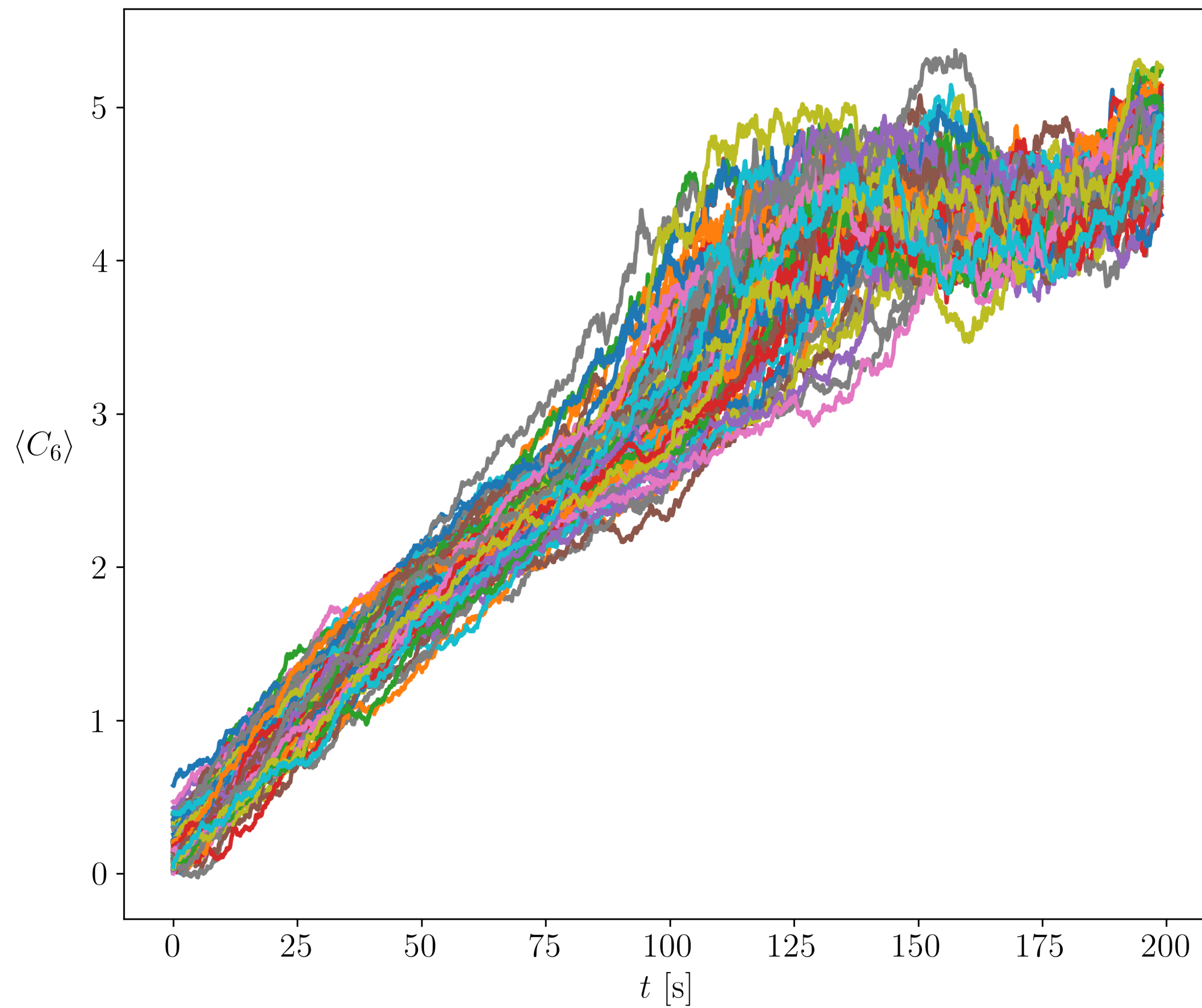
Stochastic Control/ Control Non-affine

Case 1: Value Function



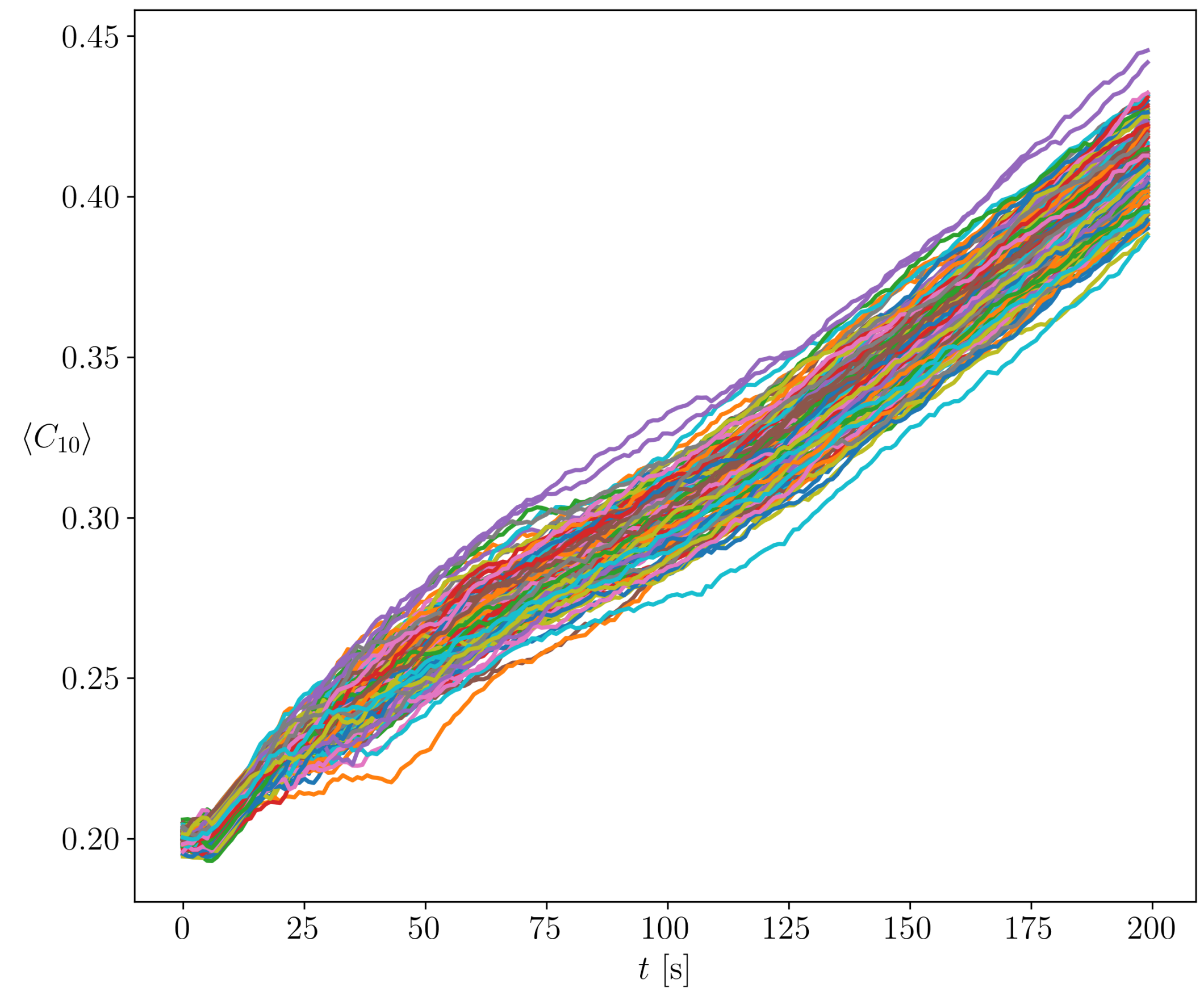
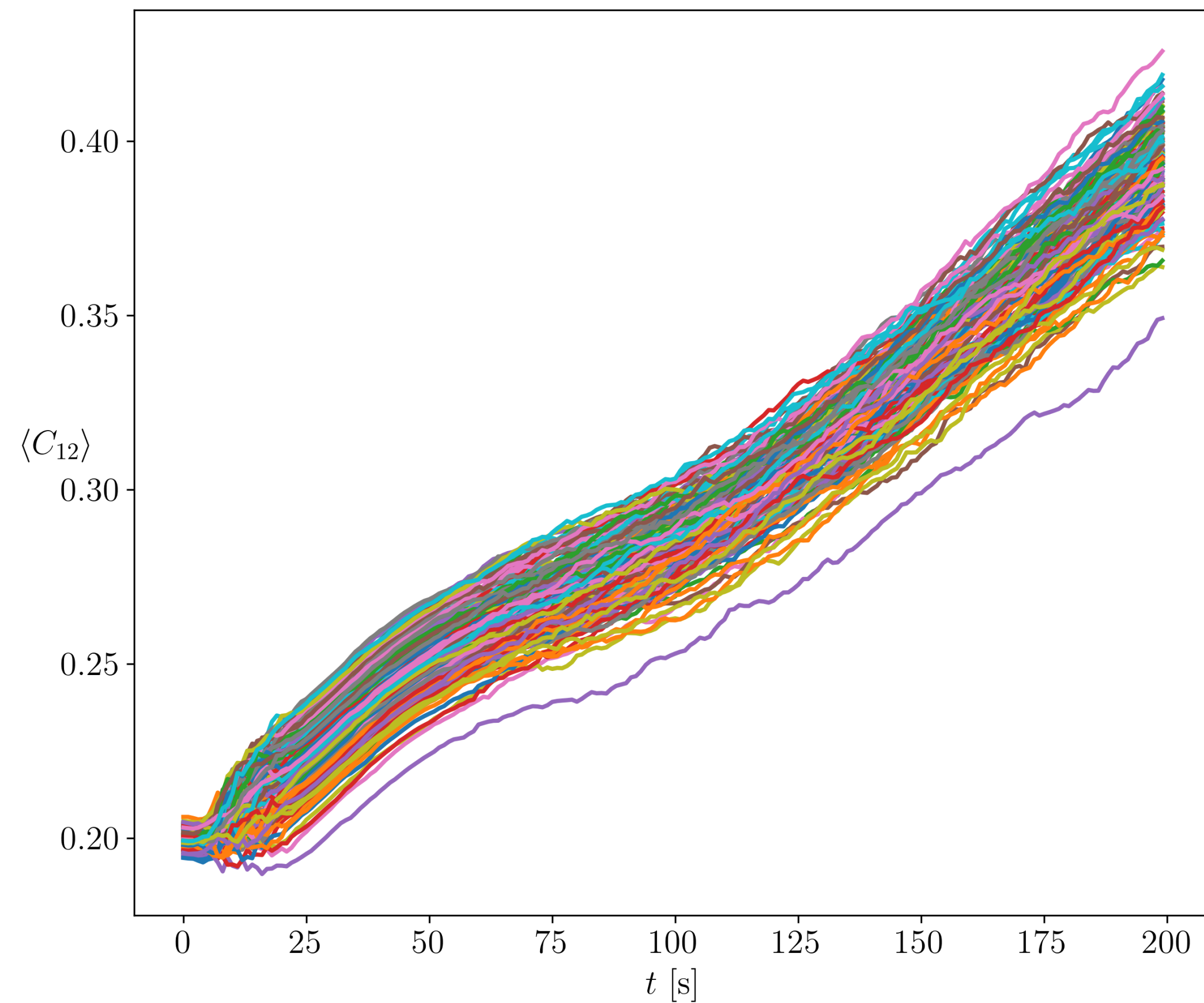
Stochastic Control/ Control Non-affine

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

Outer
layer
ADMM

$$\boldsymbol{\mu}_i^{k+1} = \text{prox}_{\frac{W}{\alpha}}^{F_i(\boldsymbol{\mu}_i) + \langle \boldsymbol{\nu}_i^k, \boldsymbol{\mu}_i \rangle} (\boldsymbol{\zeta}^k)$$

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

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

Inner
layer
ADMM

$$\boldsymbol{\nu}_i^{k+1} = \boldsymbol{\nu}_i^k + \alpha (\boldsymbol{\mu}_i^{k+1} - \boldsymbol{\zeta}^{k+1})$$

where N is the number of samples

With Sinkhorn regularization:

Discrete Sinkhorn divergence

Outer
layer
ADMM

$$\boldsymbol{\mu}_i^{k+1} = \text{prox}_{\frac{W_\varepsilon}{\alpha}}^{F_i(\boldsymbol{\mu}_i) + \langle \boldsymbol{\nu}_i^k, \boldsymbol{\mu}_i \rangle} (\boldsymbol{\zeta}^k)$$

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

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

Inner
layer
ADMM

$$\boldsymbol{\nu}_i^{k+1} = \boldsymbol{\nu}_i^k + \alpha (\boldsymbol{\mu}_i^{k+1} - \boldsymbol{\zeta}^{k+1})$$

Stochastic Learning/ Distributed Computing

μ_i update \rightsquigarrow Outer Consensus (Sinkhorn) ADMM

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

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

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

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

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

Stochastic Learning/ Distributed Computing

ζ update \rightsquigarrow Inner (Euclidean) ADMM

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

Then the following Euclidean ADMM solves

$$\mathbf{u}_i^{\ell+1} = \text{prox}_{\frac{1}{\tau} f_i}^{\|\cdot\|_2} \left(\mathbf{z}_i^\ell - \tilde{\mathbf{v}}_i^\ell \right)$$

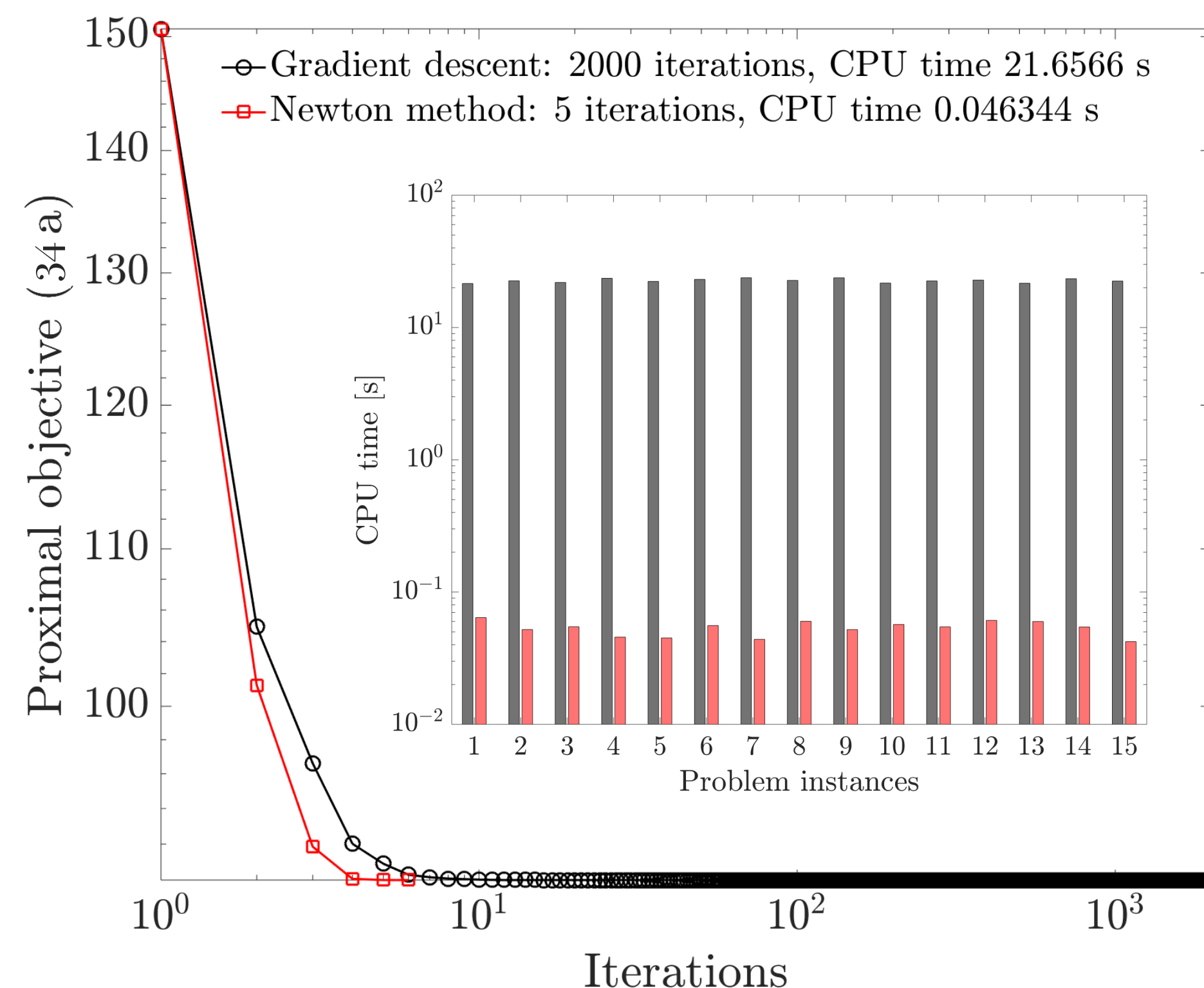
$$\mathbf{z}_i^{\ell+1} = \left(\mathbf{u}_i^{\ell+1} - \frac{1}{n} \sum_{i=1}^n \mathbf{u}_i^{\ell+1} \right) + \left(\tilde{\mathbf{v}}_i^\ell - \frac{1}{n} \sum_{i=1}^n \tilde{\mathbf{v}}_i^\ell \right) + \frac{2}{n\alpha} \boldsymbol{\nu}_{\text{sum}}^k$$

$$\tilde{\mathbf{v}}_i^{\ell+1} = \tilde{\mathbf{v}}_i^\ell + (\mathbf{u}_i^{\ell+1} - \mathbf{z}_i^{\ell+1})$$

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)



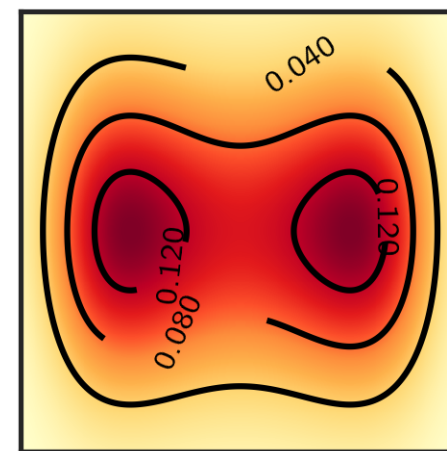
Stochastic Learning/ Distributed Computing

Experiment #3 Linear Fokker-Planck-Kolmogorov PDE

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

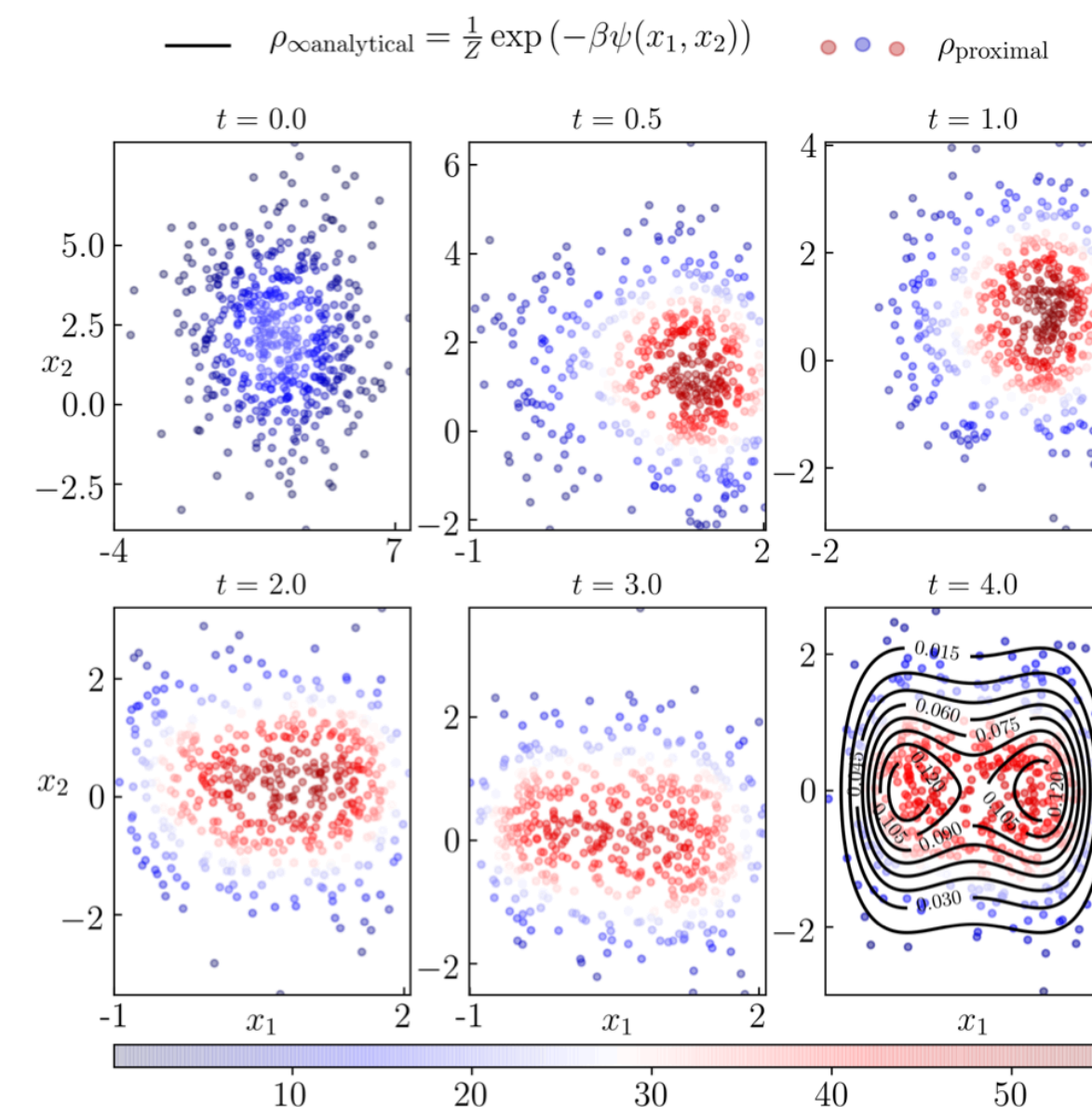
$$V(x_1, x_2) = \frac{1}{4}(1 + x_1^4) + \frac{1}{2}(x_2^2 - x_1^2)$$

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

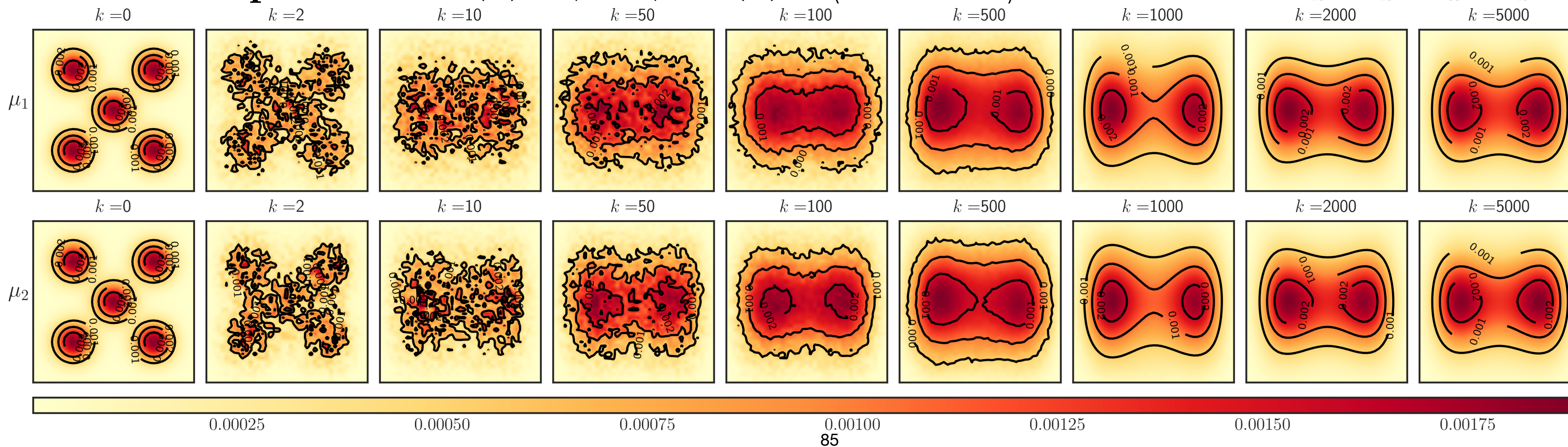


Centralized computation:

Caluya and Halder, *IEEE Trans. Automatic Control*, 2019



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



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

Splitting case	Functionals	Wasserstein distance
#1	$F_1(\boldsymbol{\mu}) = \langle \mathbf{V}_k + \beta^{-1} \boldsymbol{\mu}, \boldsymbol{\mu} \rangle,$ $F_2(\boldsymbol{\mu}) = \langle \mathbf{U}_k \boldsymbol{\mu}^k, \boldsymbol{\mu} \rangle$ <p>av. runtime = 294.06 s</p>	
#2	$F_1(\boldsymbol{\mu}) = \langle \mathbf{U}_k \boldsymbol{\mu}^k + \beta^{-1} \boldsymbol{\mu}, \boldsymbol{\mu} \rangle,$ $F_2(\boldsymbol{\mu}) = \langle \mathbf{V}_k, \boldsymbol{\mu} \rangle$ <p>av. runtime = 285.32 s</p>	
#3	$F_1(\boldsymbol{\mu}) = \langle \mathbf{U}_k \boldsymbol{\mu}^k + \mathbf{V}_k, \boldsymbol{\mu} \rangle,$ $F_2(\boldsymbol{\mu}) = \langle \beta^{-1} \boldsymbol{\mu}, \boldsymbol{\mu} \rangle$ <p>av. runtime = 289.87 s</p>	
#4	$F_1(\boldsymbol{\mu}) = \langle \mathbf{V}_k, \boldsymbol{\mu} \rangle,$ $F_2(\boldsymbol{\mu}) = \langle \mathbf{U}_k \boldsymbol{\mu}^k \rangle,$ $F_3(\boldsymbol{\mu}) = \langle \beta^{-1} \boldsymbol{\mu}, \boldsymbol{\mu} \rangle$ <p>av. runtime = 108.99 s</p>	

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

Case	Functionals	Wasserstein distances
#1	$F_1(\boldsymbol{\mu}) = \langle \mathbf{V}_k + \beta^{-1} \boldsymbol{\mu}, \boldsymbol{\mu} \rangle,$ $F_2(\boldsymbol{\mu}) = \langle \mathbf{U}_k \boldsymbol{\mu}^k, \boldsymbol{\mu} \rangle$	
#2	$F_1(\boldsymbol{\mu}) = \langle \mathbf{U}_k \boldsymbol{\mu}^k + \beta^{-1} \boldsymbol{\mu}, \boldsymbol{\mu} \rangle,$ $F_2(\boldsymbol{\mu}) = \langle \mathbf{V}_k, \boldsymbol{\mu} \rangle$	
#3	$F_1(\boldsymbol{\mu}) = \langle \mathbf{U}_k \boldsymbol{\mu}^k + \mathbf{V}_k, \boldsymbol{\mu} \rangle,$ $F_2(\boldsymbol{\mu}) = \langle \beta^{-1} \boldsymbol{\mu}, \boldsymbol{\mu} \rangle$	
#4	$F_1(\boldsymbol{\mu}) = \langle \mathbf{V}_k, \boldsymbol{\mu} \rangle,$ $F_2(\boldsymbol{\mu}) = \langle \mathbf{U}_k \boldsymbol{\mu}^k, \boldsymbol{\mu} \rangle,$ $F_3(\boldsymbol{\mu}) = \langle \beta^{-1} \boldsymbol{\mu}, \boldsymbol{\mu} \rangle$	

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."