A Physics-informed Deep Learning Approach for Minimum Effort Stochastic Control of Colloidal Self-Assembly

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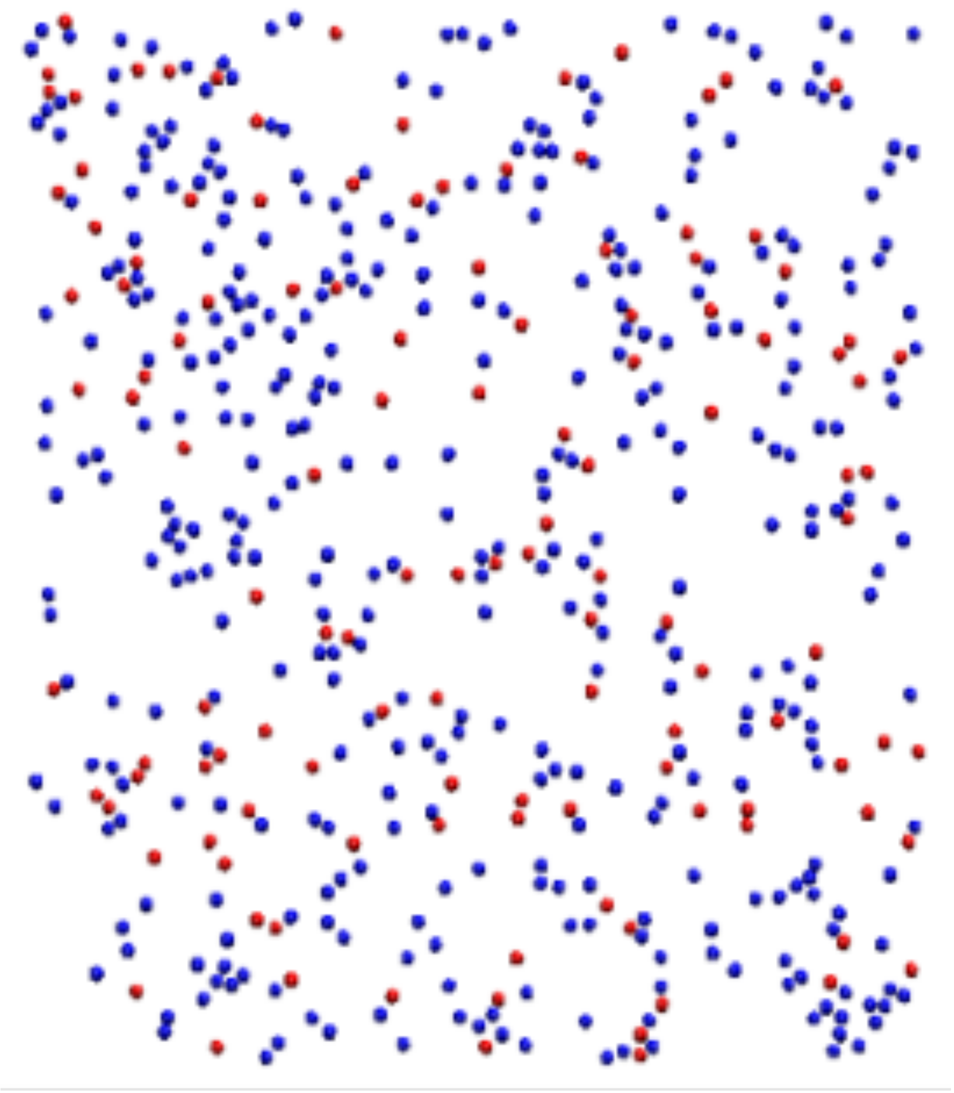
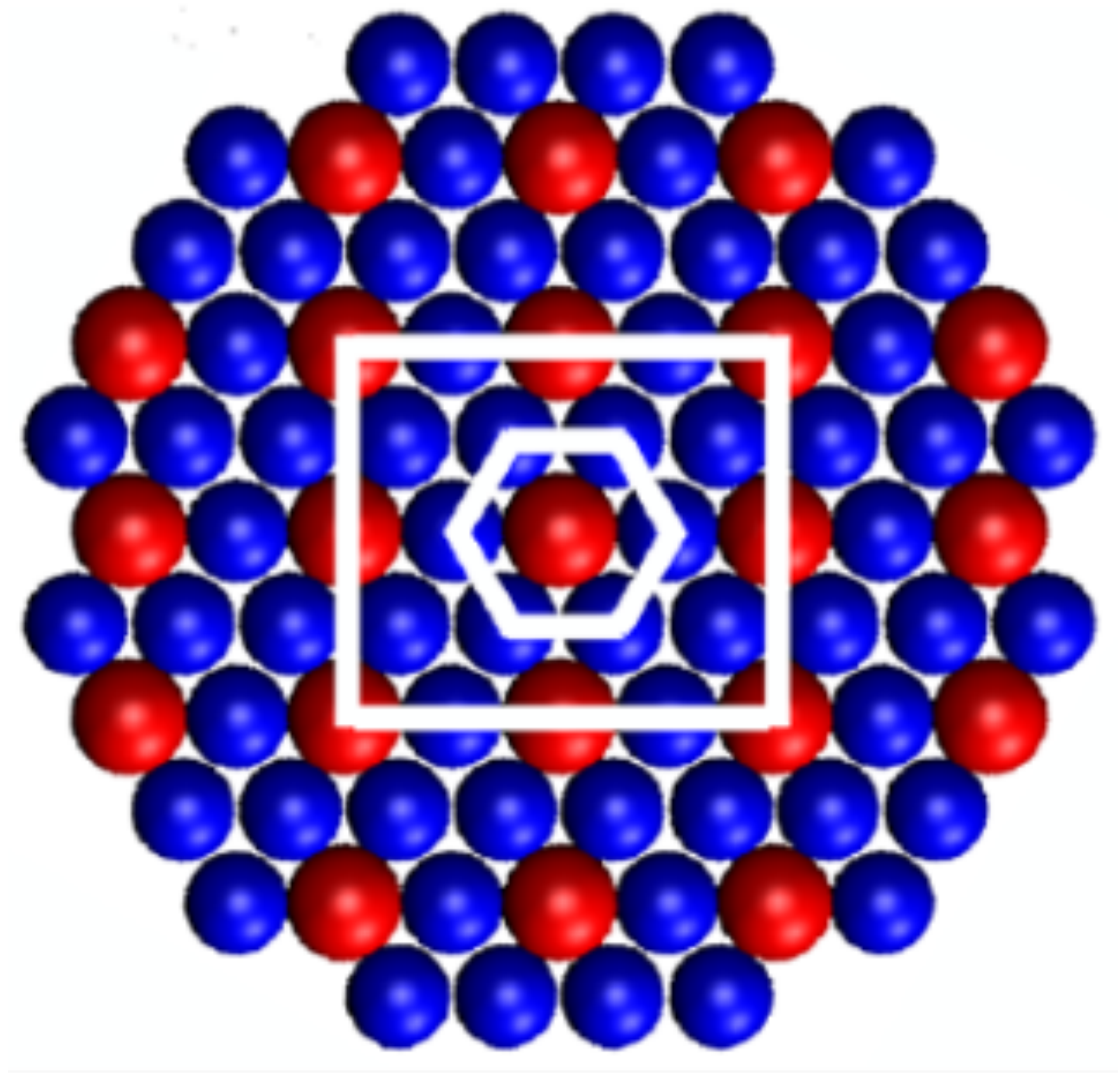
Controlled Self-assembly



Dispersed particles

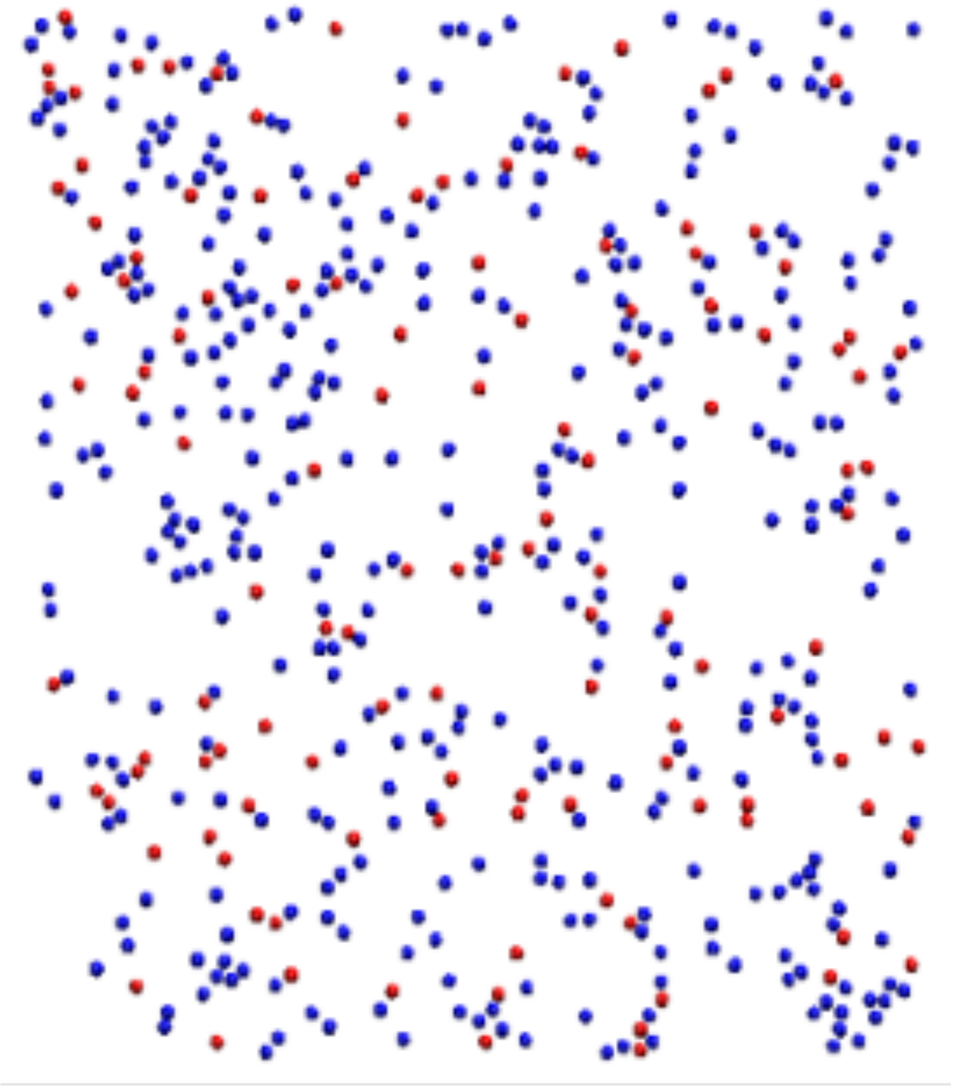


Ordered structure

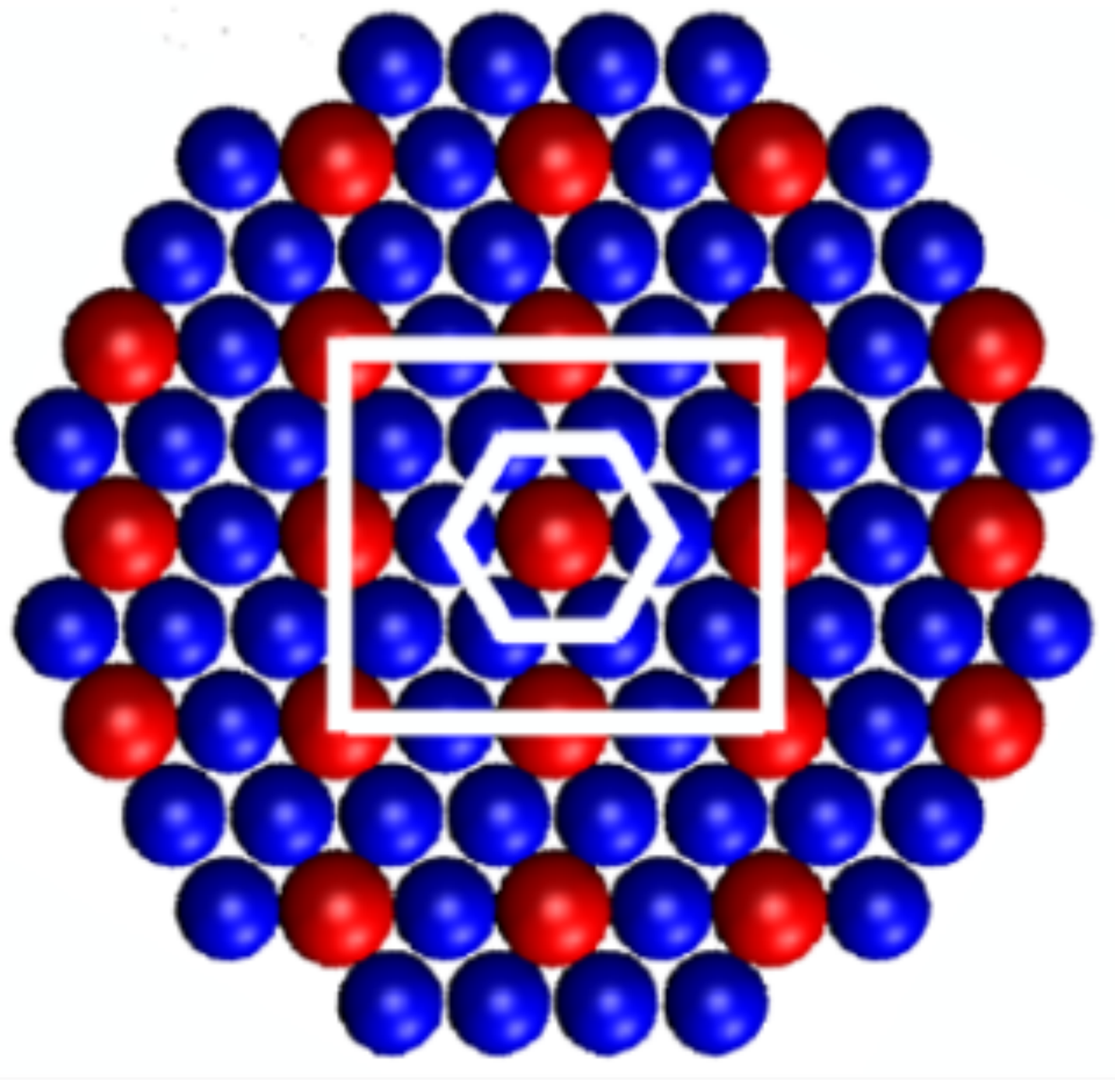
Applications:

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

Controlled Self-assembly



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 ⇝ measure of crystallinity order

Typical control variable: u

Electric field voltage

Technical challenge:

Nonlinear + noisy molecular dynamics

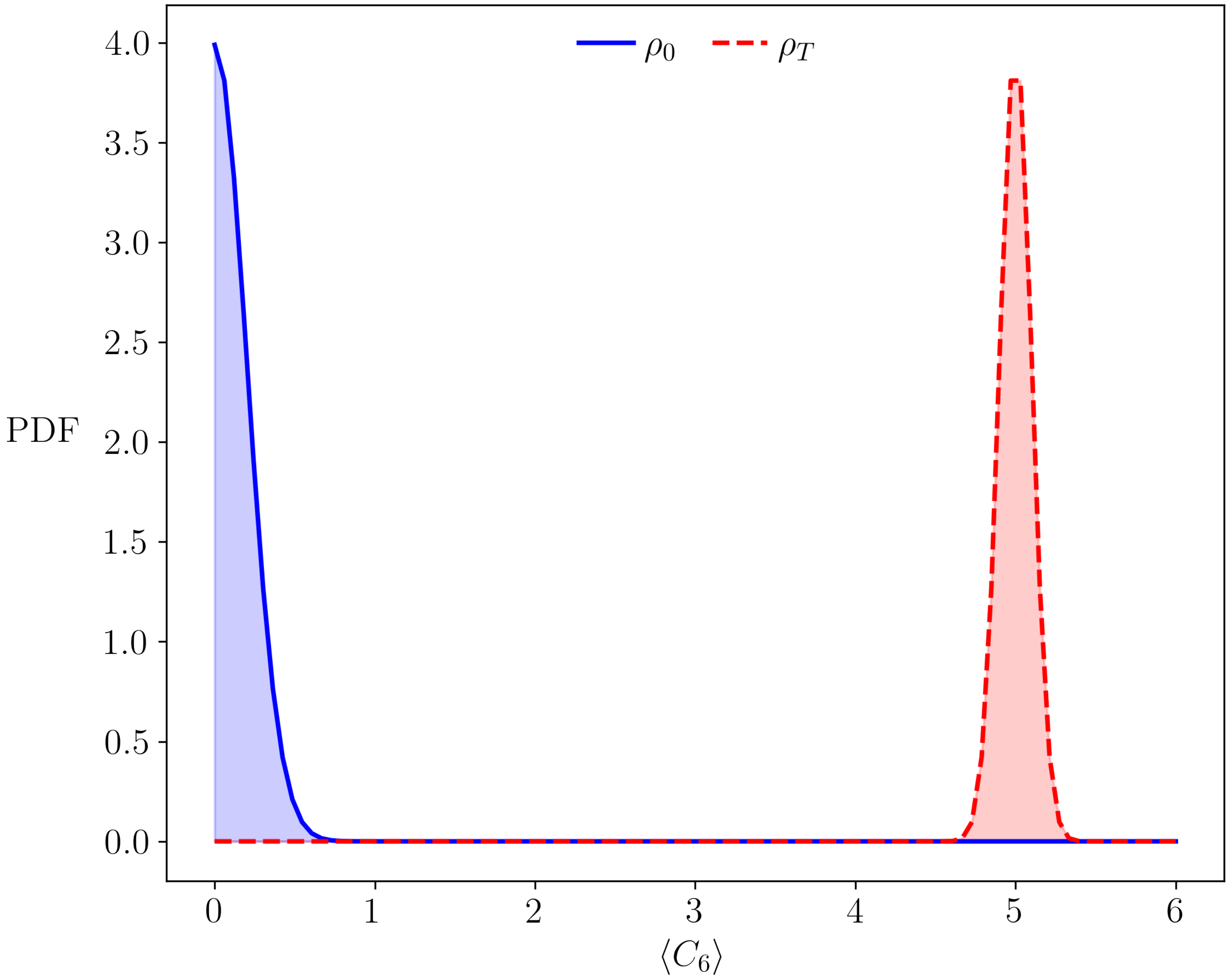
$\langle C_6 \rangle$ is a controlled stochastic process

Controlled Self-assembly as PDF Steering

Intuition: $\langle C_6 \rangle \approx 0 \;\Leftrightarrow\;$ 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 $t = T \equiv 200\,\mathrm{s}$



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

Underdetermined

Minimum Effort Self-assembly

drift landscape

diffusion landscape

free energy landscape

$$D_1(x^u, u) := \frac{\partial}{\partial x} D_2(x^u, u) - \frac{\partial}{\partial x} F(x^u, u) \frac{D_2(x^u, u)}{k_{\mathrm{B}}\theta}$$

either from model or learnt from MD simulation data

Proposed formulation:

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

subject to $\mathrm{d}x^u = D_1(x^u, u)\,\mathrm{d}t + \sqrt{2D_2(x^u, u)}\,\mathrm{d}w,$

$\langle C_6 \rangle$

standard Wiener process

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

Minimum Effort Self-assembly

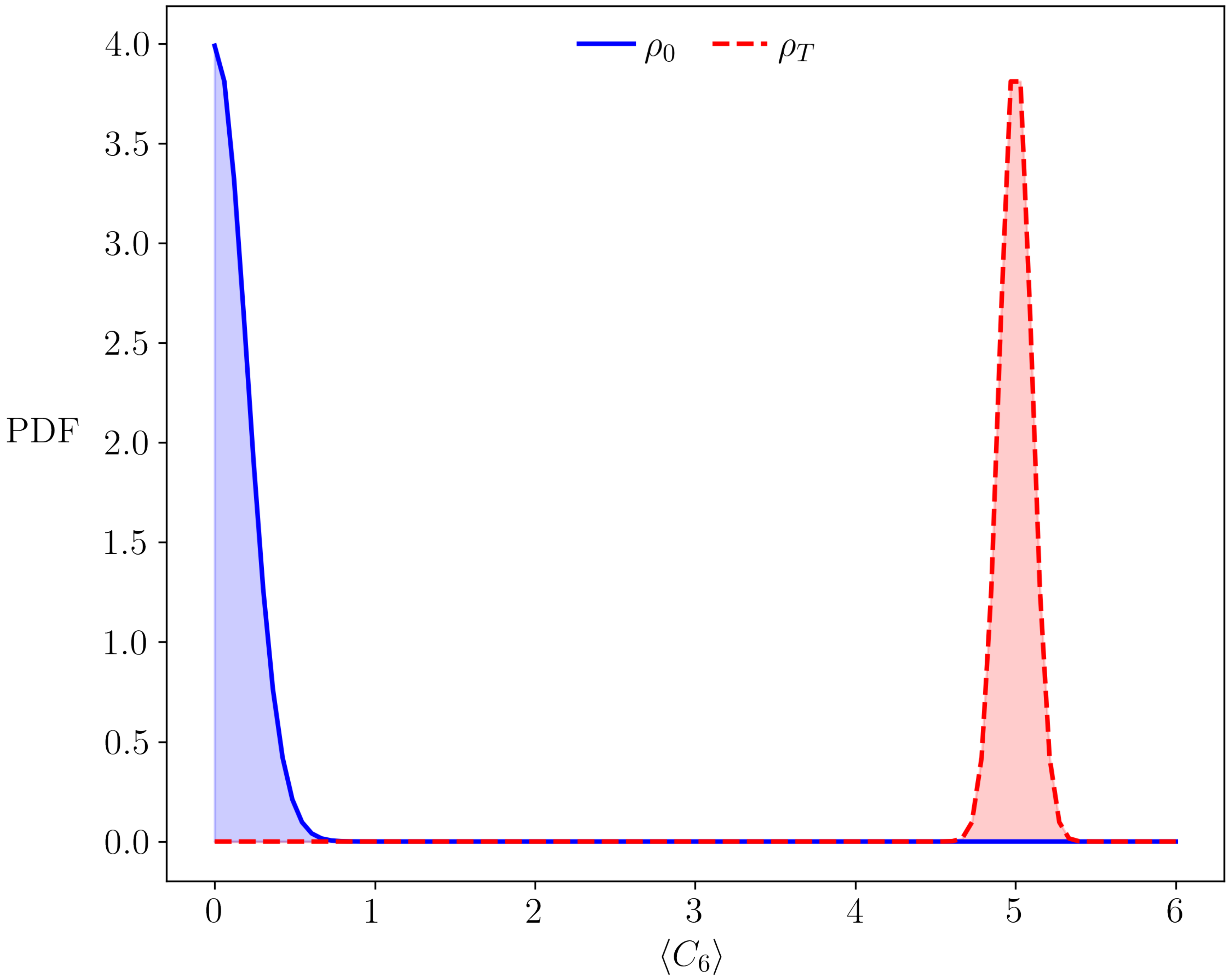
Equivalent formulation:

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

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

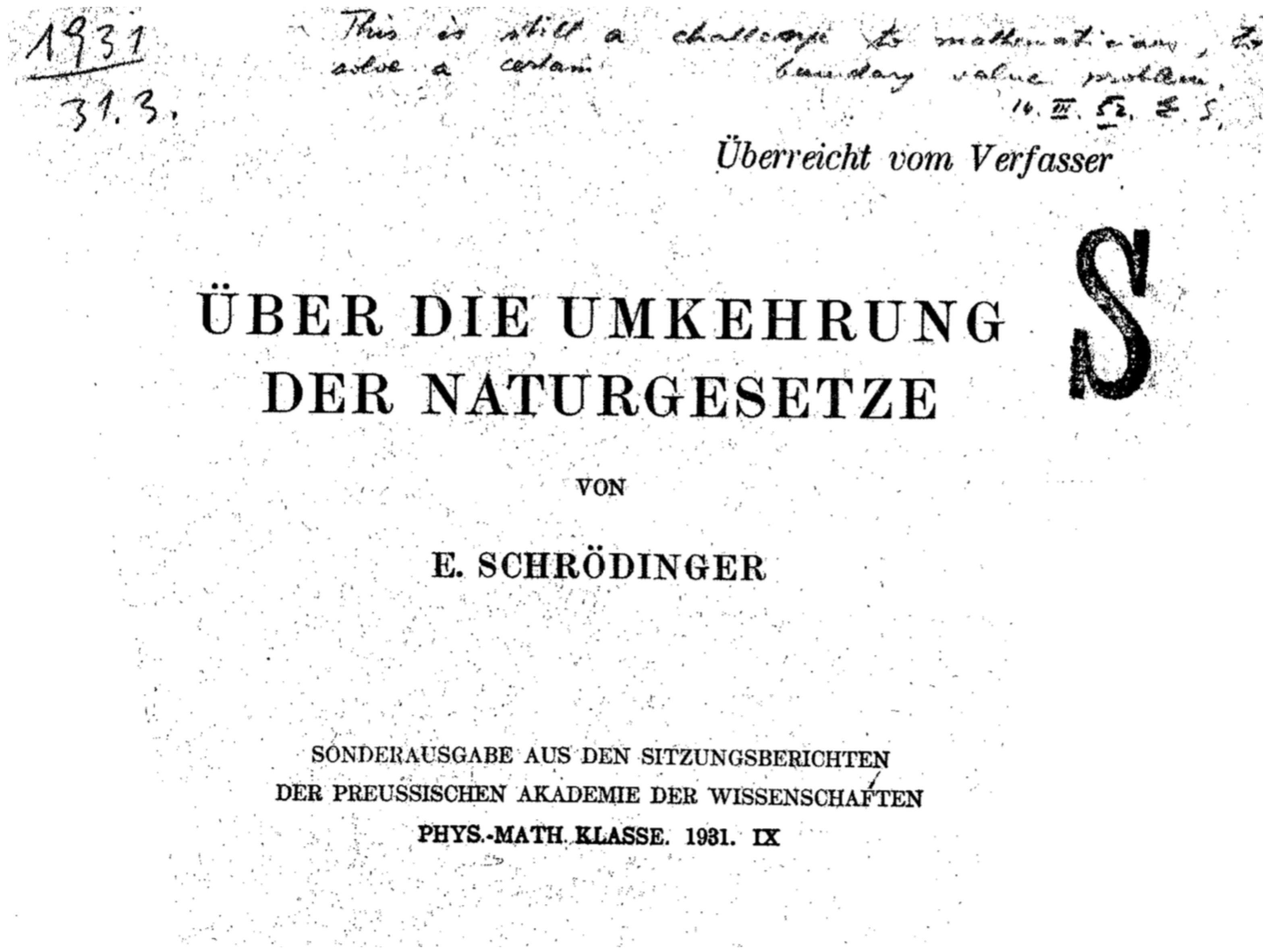
$$\rho^u(x^u, t=0) = \rho_0, \quad \rho^u(x^u, t=T) = \rho_T$$

Guaranteed existence-uniqueness for compactly supported ρ_0, ρ_T



Generalized Schrödinger Bridge

Schrödinger bridge problem: $D_1 \equiv u$ and $D_2 \equiv \text{Identity}$



1931
31.3.

This is still a challenge to mathematicians, to solve a certain boundary value problem.
14.III.52. E.S.

Überreicht vom Verfasser

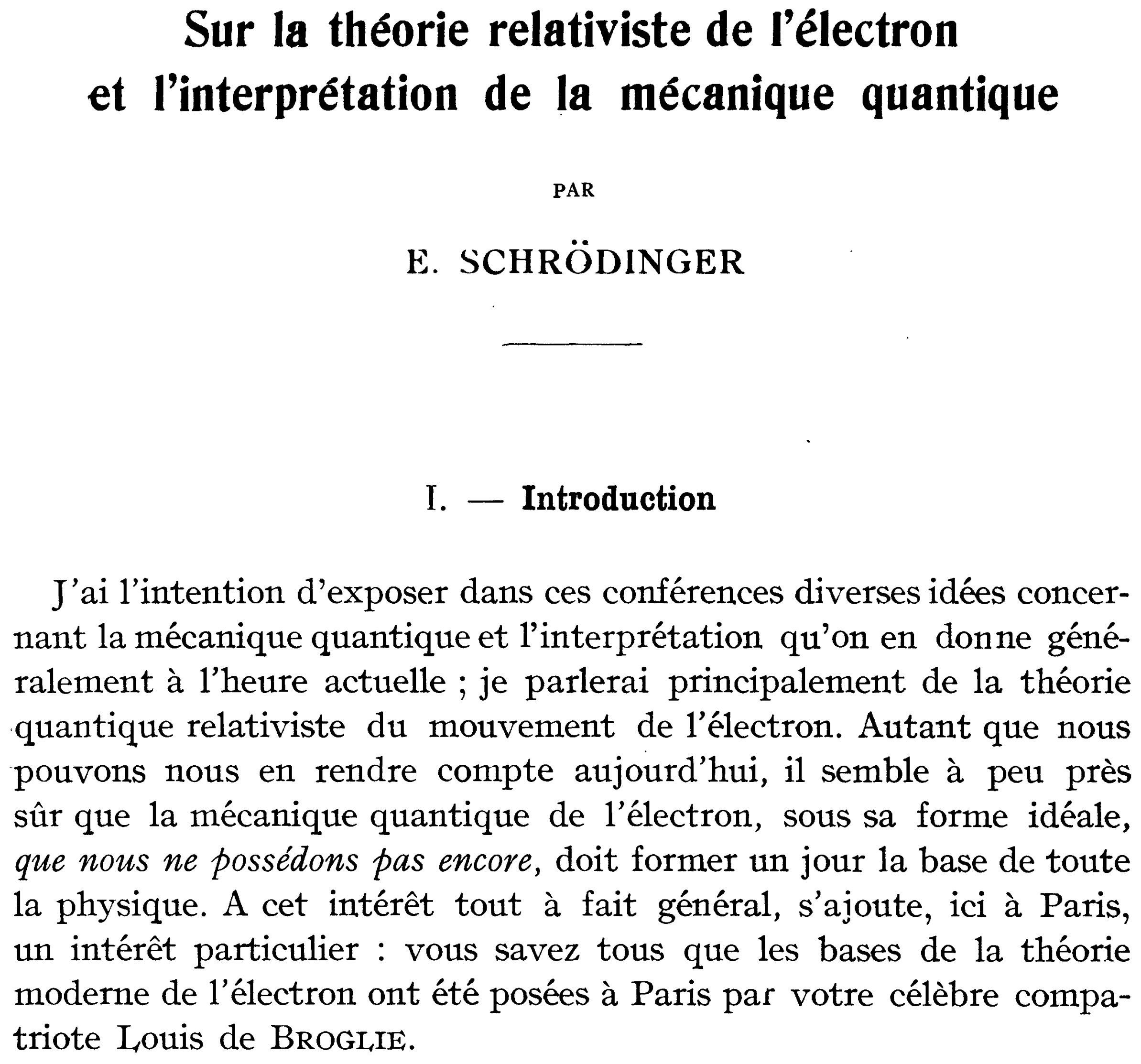
S

ÜBER DIE UMKEHRUNG
DER NATURGESETZE

VON

E. SCHRÖDINGER

SONDERAUSGABE AUS DEN SITZUNGSBERICHTEN
DER PREUSSISCHEN AKADEMIE DER WISSENSCHAFTEN
PHYS.-MATH. KLASSE. 1931. IX



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.

In our setting: both D_1 and D_2 are nonlinear in state + non-affine in control

Conditions for Optimality

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

HJB PDE

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

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 function

optimally controlled PDF

optimal policy

to be solved for the triple: $\psi\left(x^u, t\right), \rho^u\left(x^u, t\right), \pi^{\text{opt}}\left(x^u, t\right)$

Solve via PINN

Loss term for HJB PDE

$$\mathscr{L}_{\psi} = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{\partial \psi}{\partial t}\bigg|_{\boldsymbol{x}_i} - \frac{1}{2}(\pi^{\mathrm{opt}})^2\bigg|_{\boldsymbol{x^u}_i} - + \frac{\partial \psi}{\partial x^u}D_1\bigg|_{\boldsymbol{x}_i^u} - + \frac{\partial^2 \psi}{\partial x^{u2}}D_2\bigg|_{\boldsymbol{x}_i^u}\right)^2$$

Loss term for FPK PDE

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

Loss term for policy equation

$$\mathscr{L}_{\pi^{\mathrm{opt}}} = \frac{1}{n}\sum_{i=1}^{n}\left(\pi^{\mathrm{opt}}\bigg|_{\boldsymbol{x}_i^u} - \frac{\partial \psi}{\partial x^u}\frac{\partial D_1}{\partial u}\bigg|_{\boldsymbol{x}_i^u} - \frac{\partial^2 \psi}{\partial x^{u2}}\frac{\partial D_2}{\partial u}\bigg|_{\boldsymbol{x}_i^u}\right)^2$$

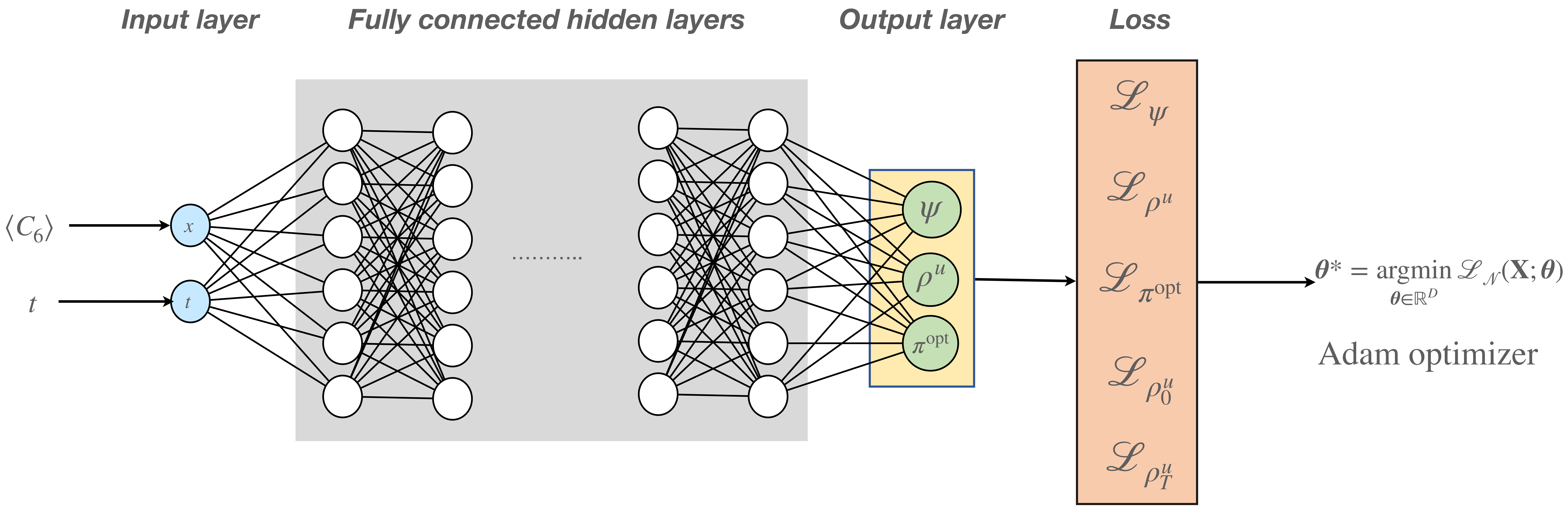
Loss term for initial condition

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

Loss term for terminal condition

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

PINN Architecture



Input layer

Fully connected hidden layers

Output layer

Loss

$\langle C_6 \rangle$

t

$\mathscr{L}_{\psi}$

$\mathscr{L}_{\rho^u}$

$\mathscr{L}_{\pi^{\text{opt}}}$

$\mathscr{L}_{\rho^u_0}$

$\mathscr{L}_{\rho^u_T}$

$$\boldsymbol{\theta}^* = \underset{\boldsymbol{\theta} \in \mathbb{R}^D}{\operatorname{argmin}} \mathscr{L}_{\mathscr{N}}(\mathbf{X}; \boldsymbol{\theta})$$

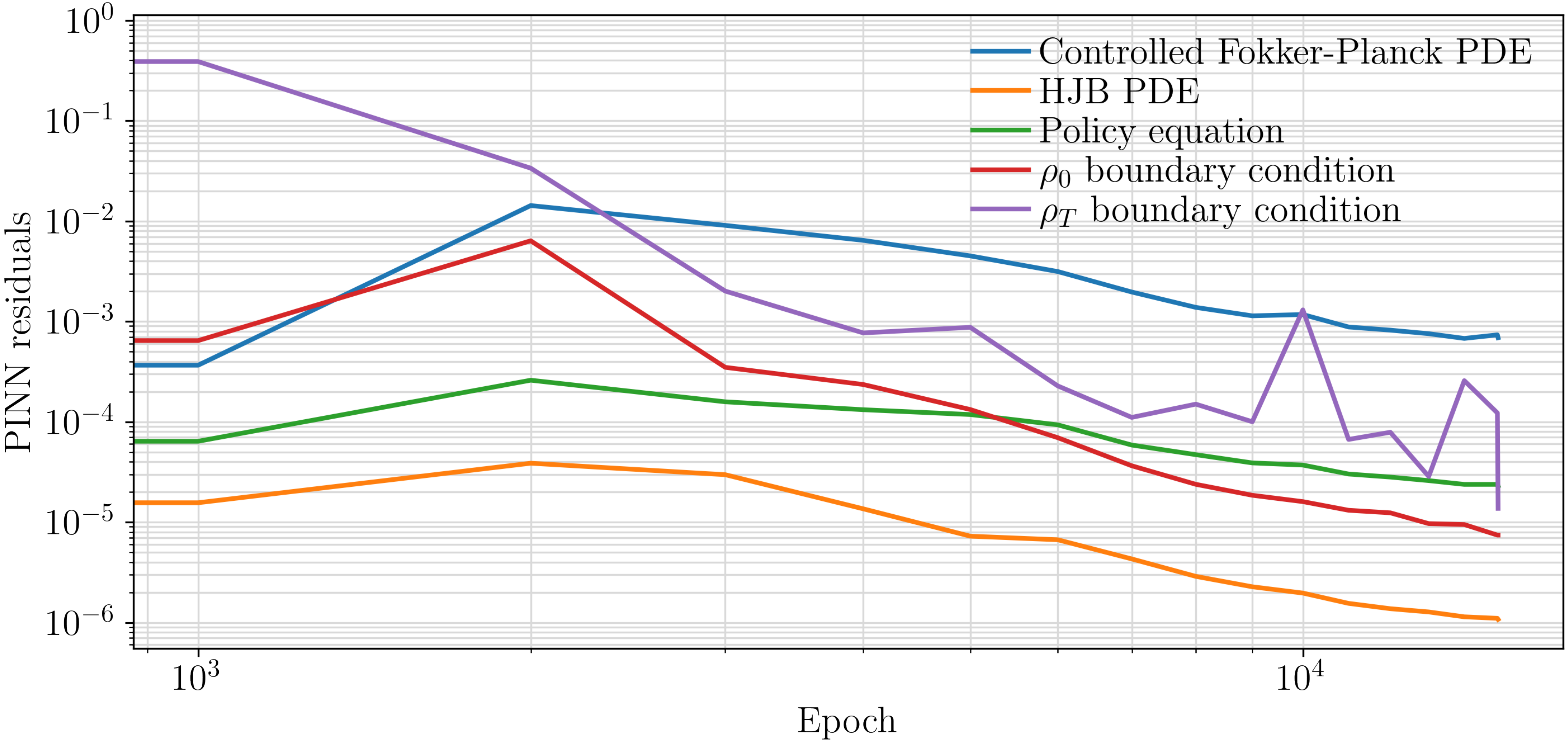
Adam optimizer

$$\mathscr{L}_{\mathscr{N}} = \mathscr{L}_{\psi} + \mathscr{L}_{\rho^u} + \mathscr{L}_{\pi^{\text{opt}}} + \mathscr{L}_{\rho^u_0} + \mathscr{L}_{\rho^u_T}$$

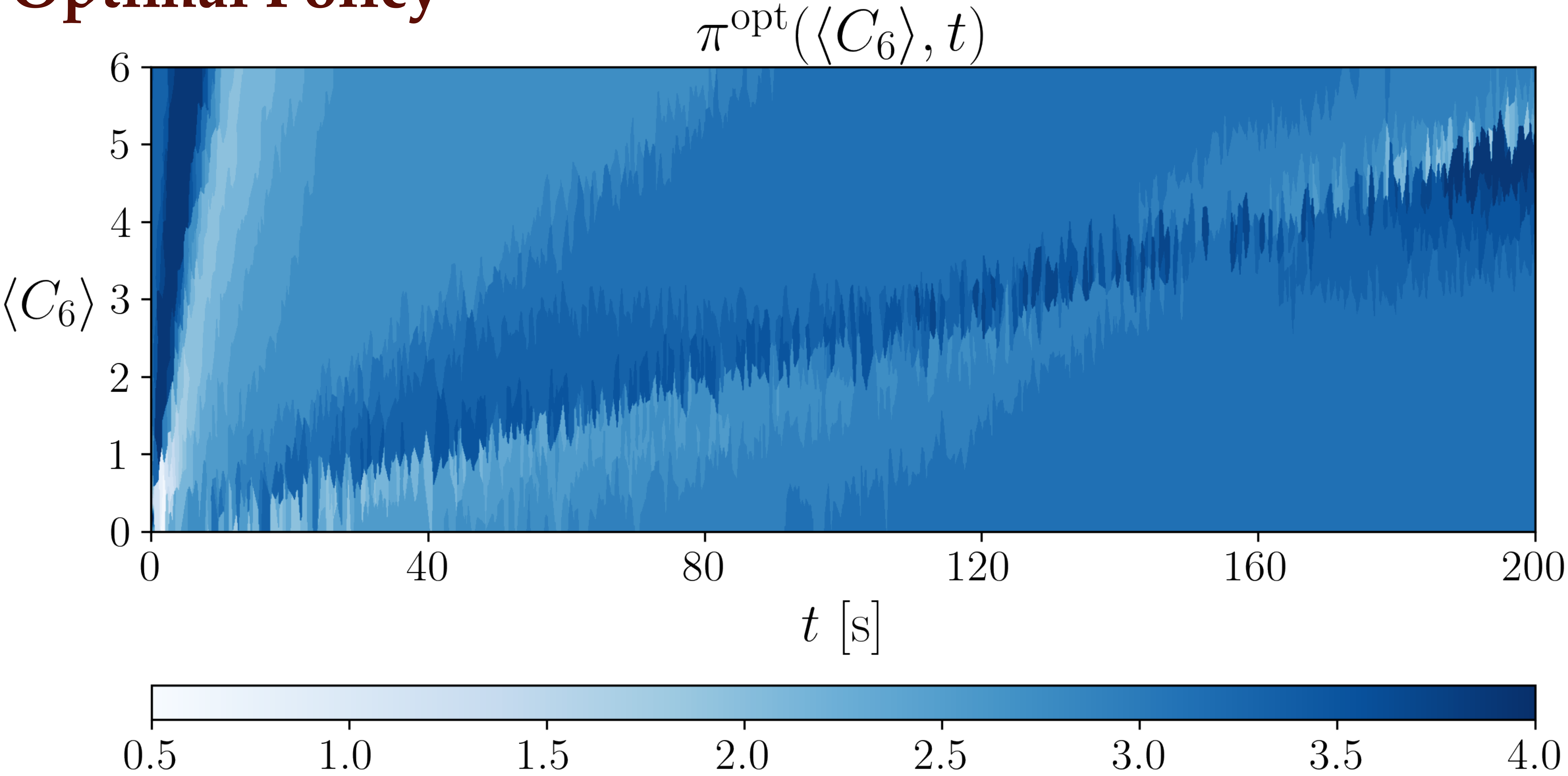
[Lu Lu.et al, 2021] [Niaki.et al, 2021]

Training of the PINN

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

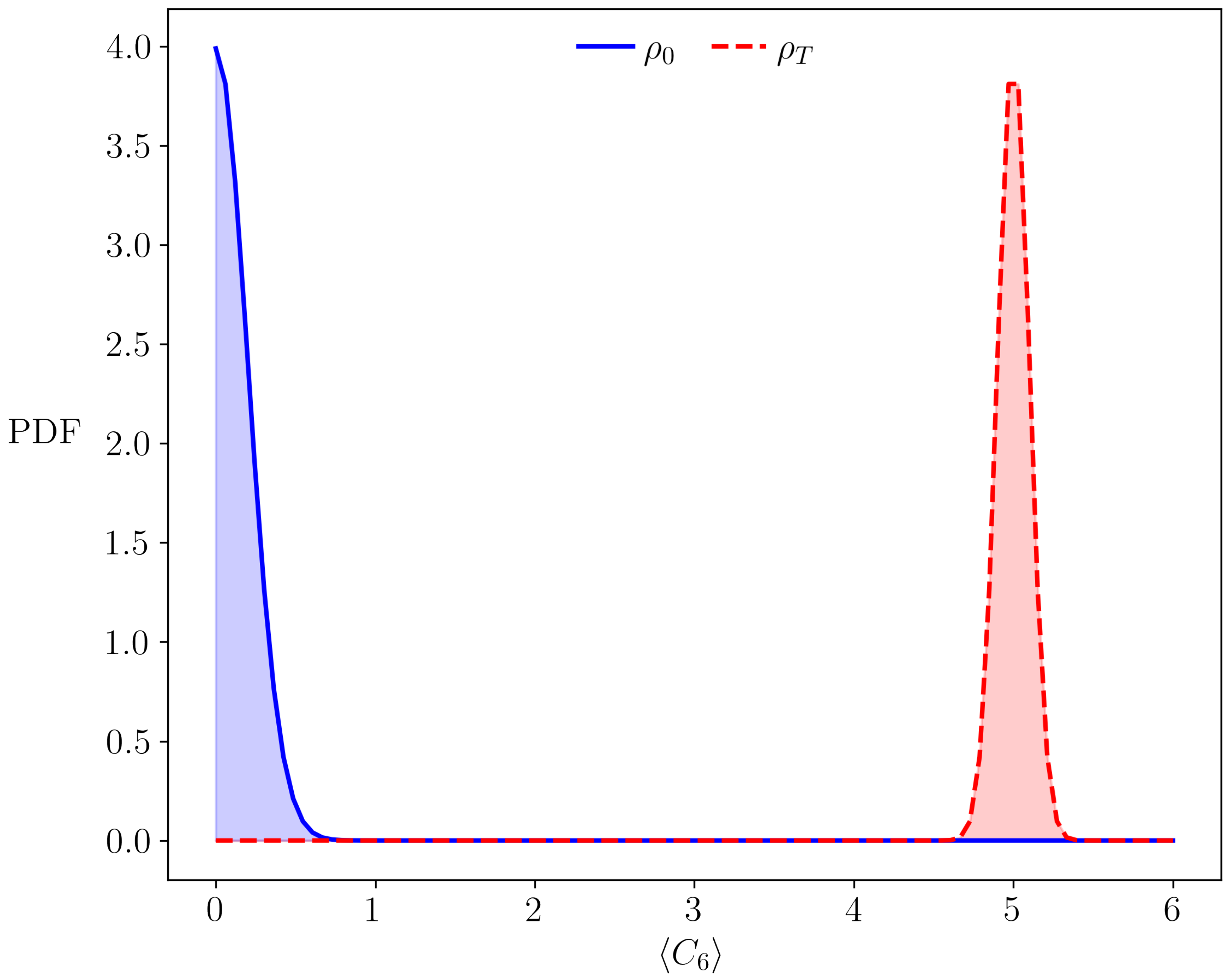


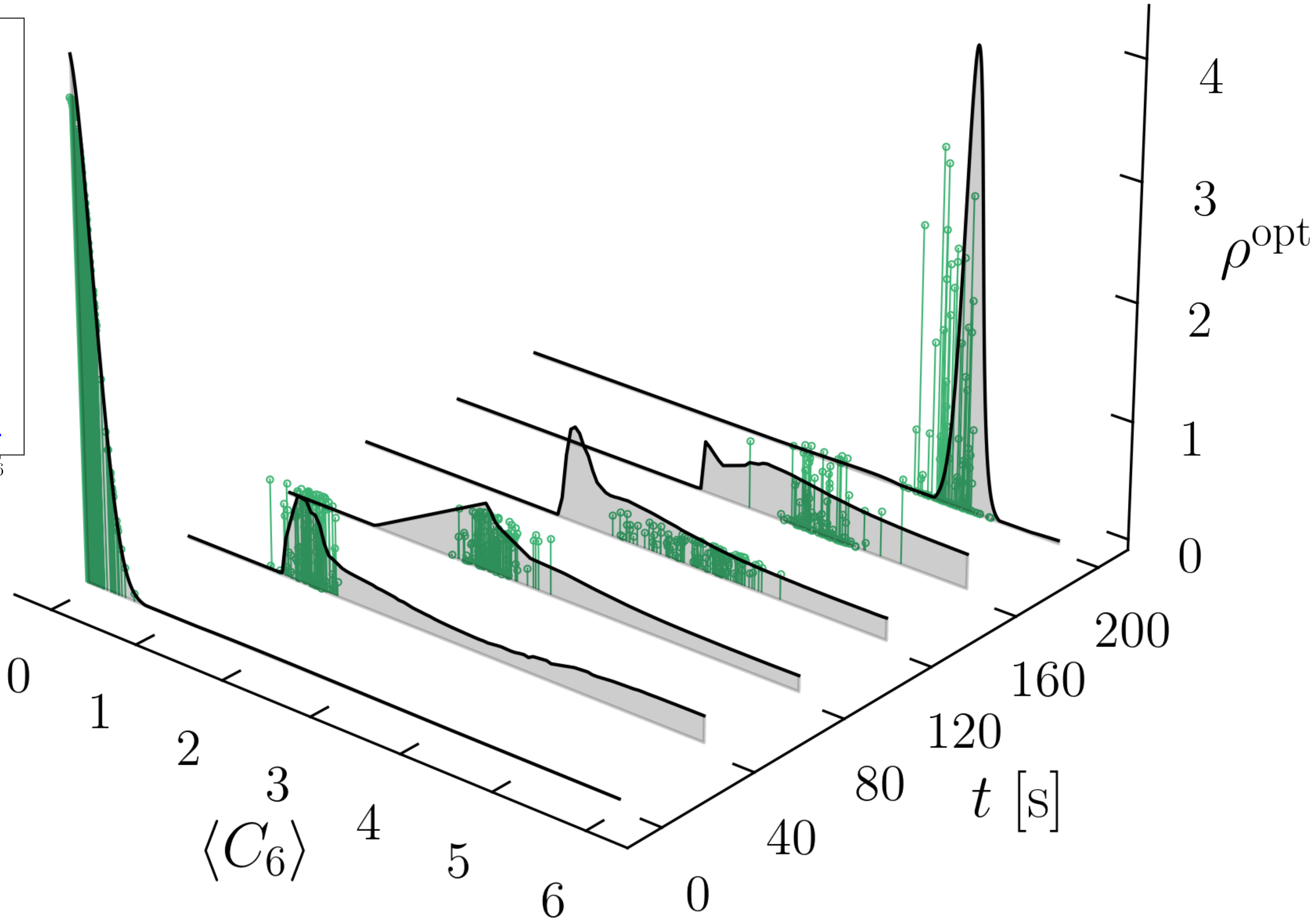
Optimal Policy



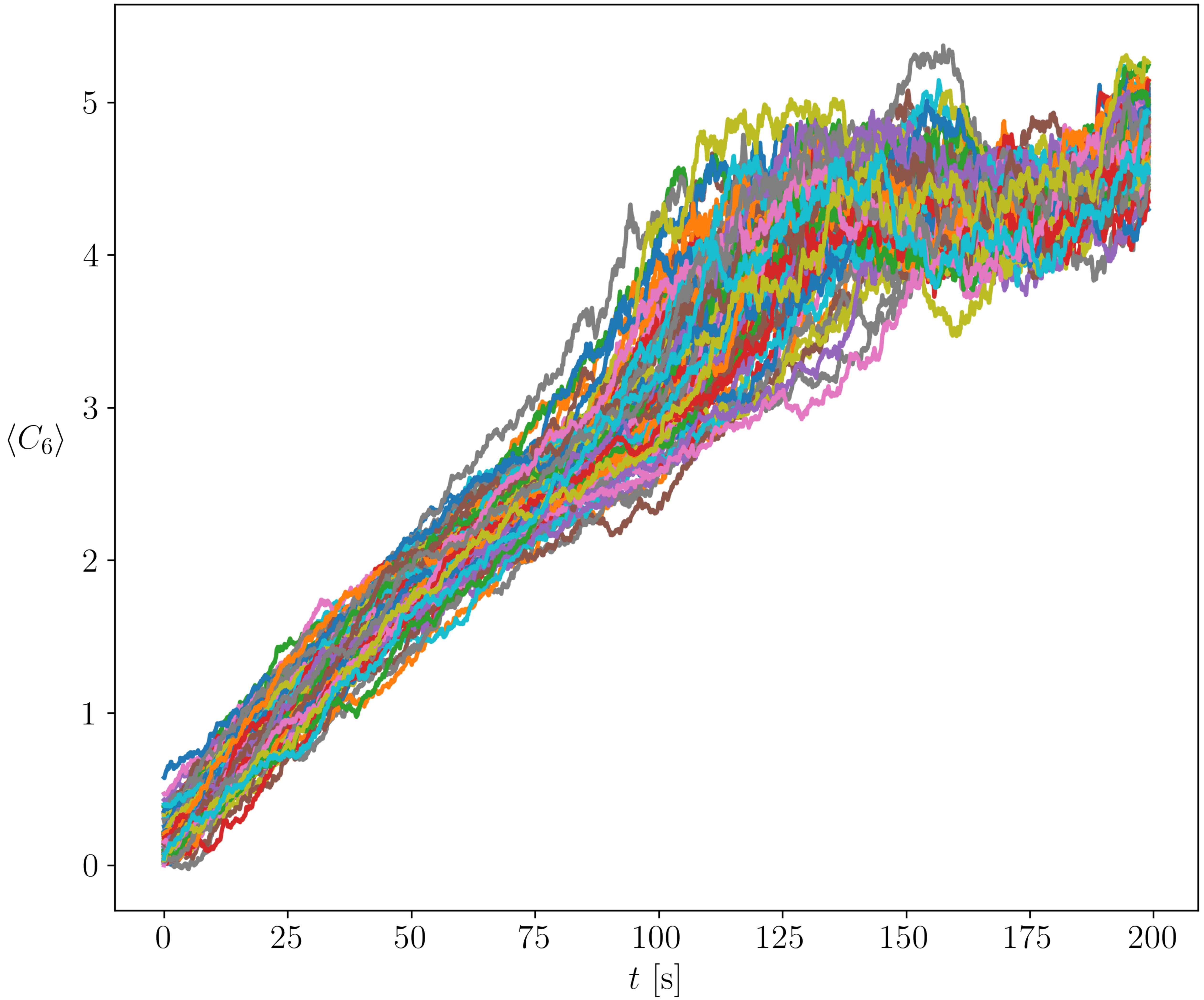
Value Function

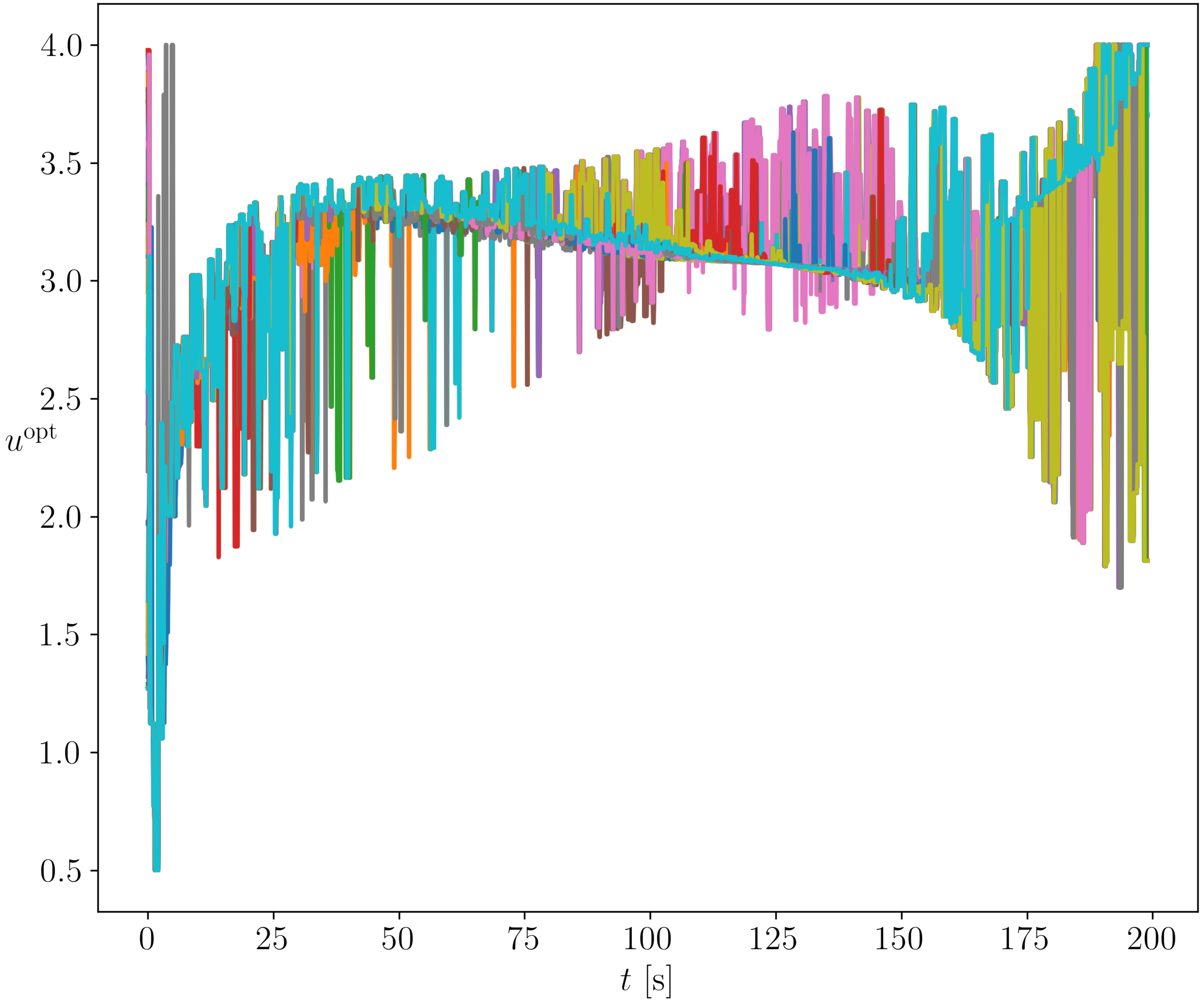
Optimally Controlled State PDFs



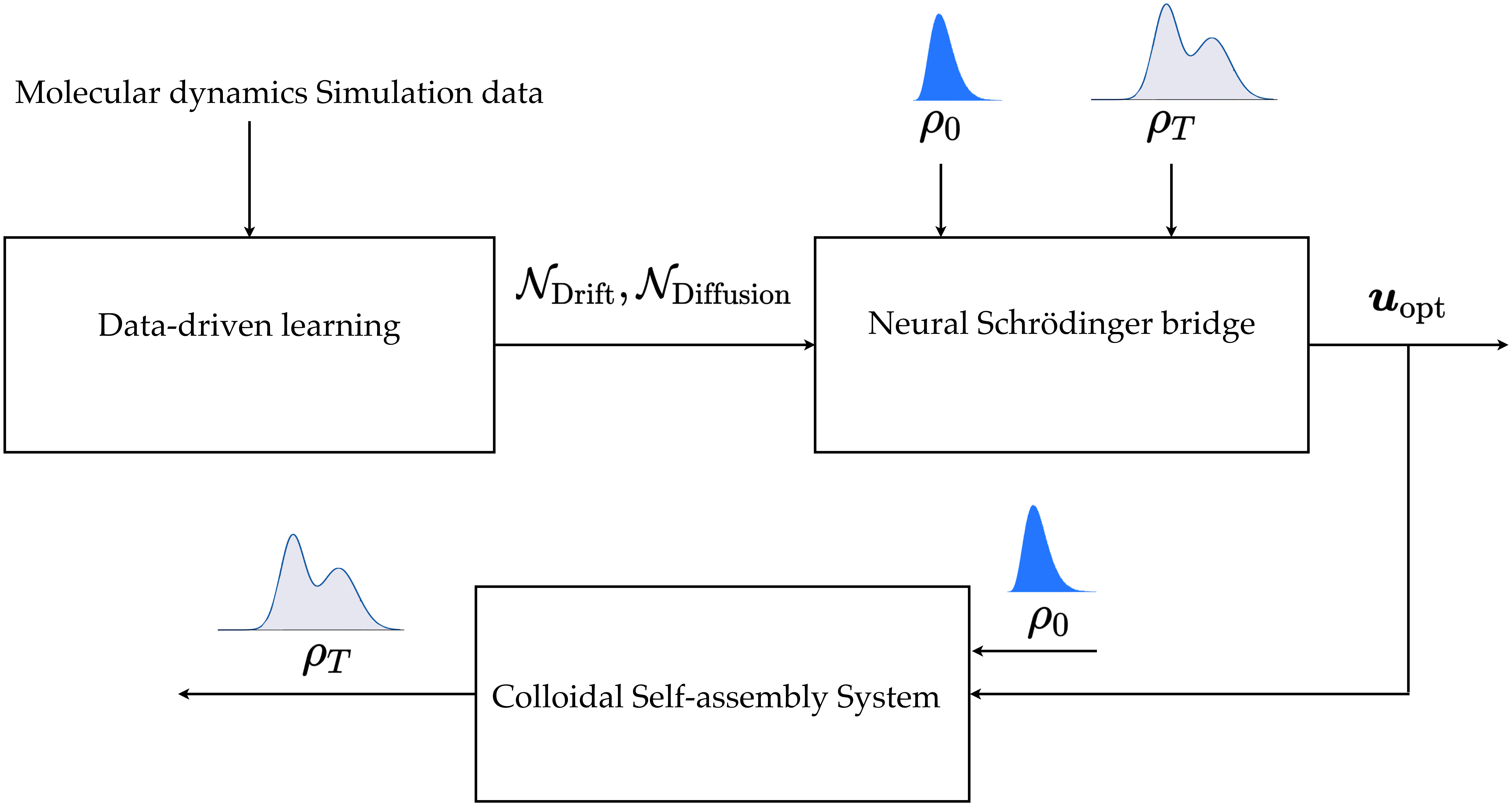


Optimal State and Optimal Control Sample Paths

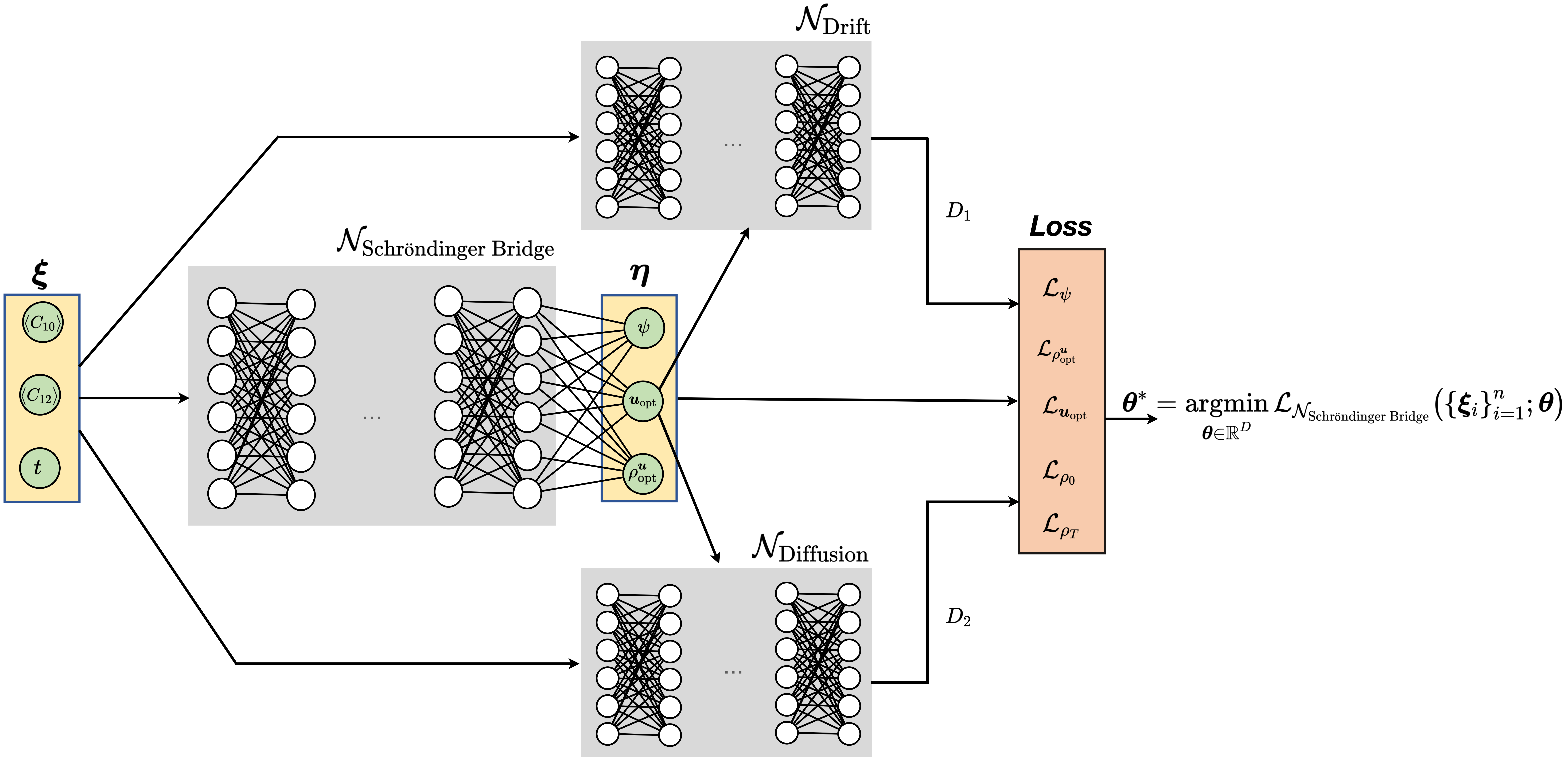




Ongoing Efforts: Learning from Data



Ongoing Efforts: Learning from Data

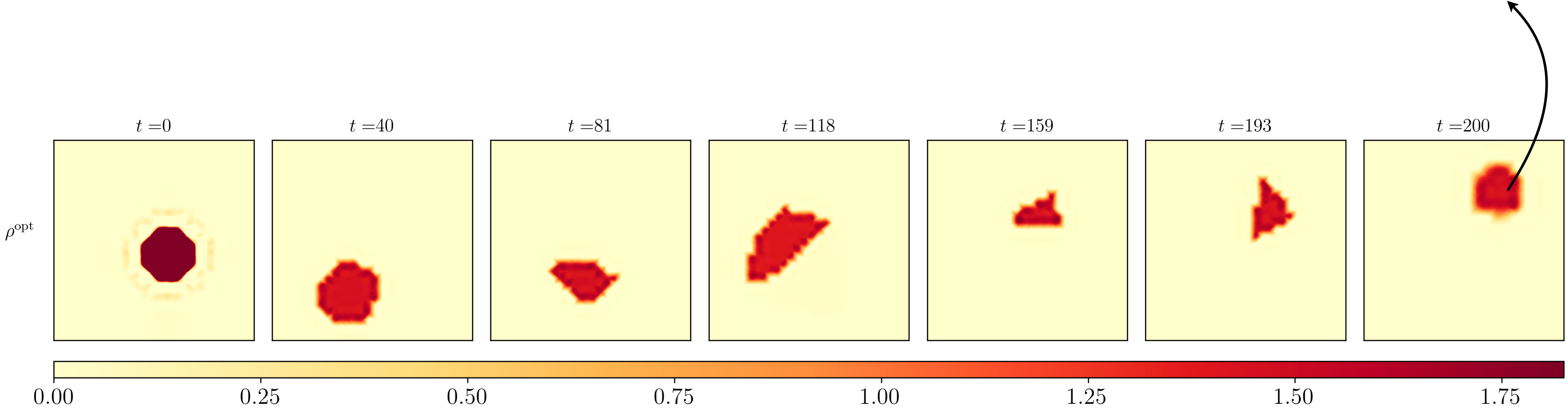


$$\boldsymbol{\theta}^* = \operatorname*{argmin}_{\boldsymbol{\theta}\in\mathbb{R}^D} \mathcal{L}_{\mathcal{N}_{\text{Schröndinger Bridge}}}\left(\{\boldsymbol{\xi}_i\}_{i=1}^{n};\boldsymbol{\theta}\right)$$

Ongoing Efforts: Learning from Data

Ongoing Efforts: Learning from Data

Body-centered cube (BCC) crystal



$\langle C_{10} \rangle \in [-0.1, 0.6]$

$\langle C_{12} \rangle \in [-0.1, 0.6]$

Steinhart bond order parameters

Thank You

Acknowledgment: NSF **CMMI 2112755**