Neural Schrödinger Bridge for Minimum Effort Self-assembly

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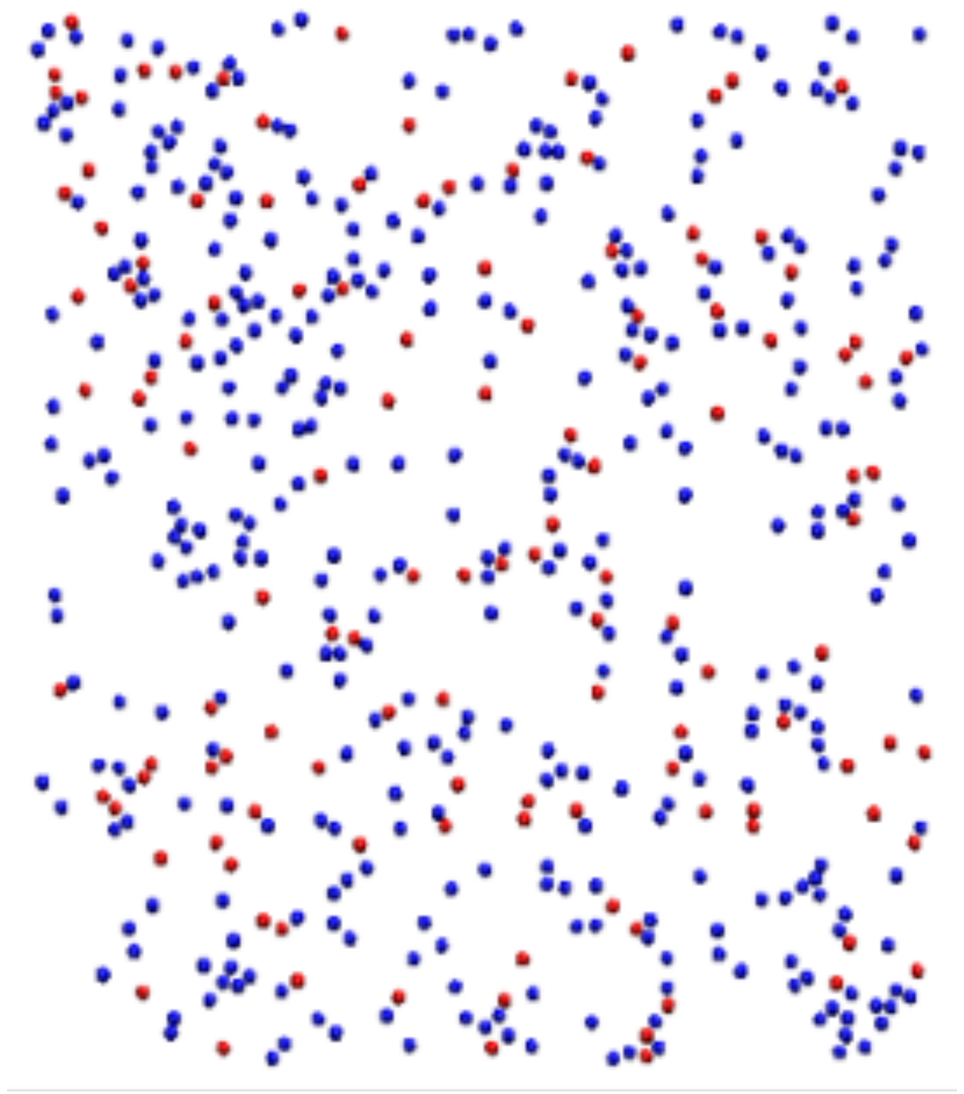
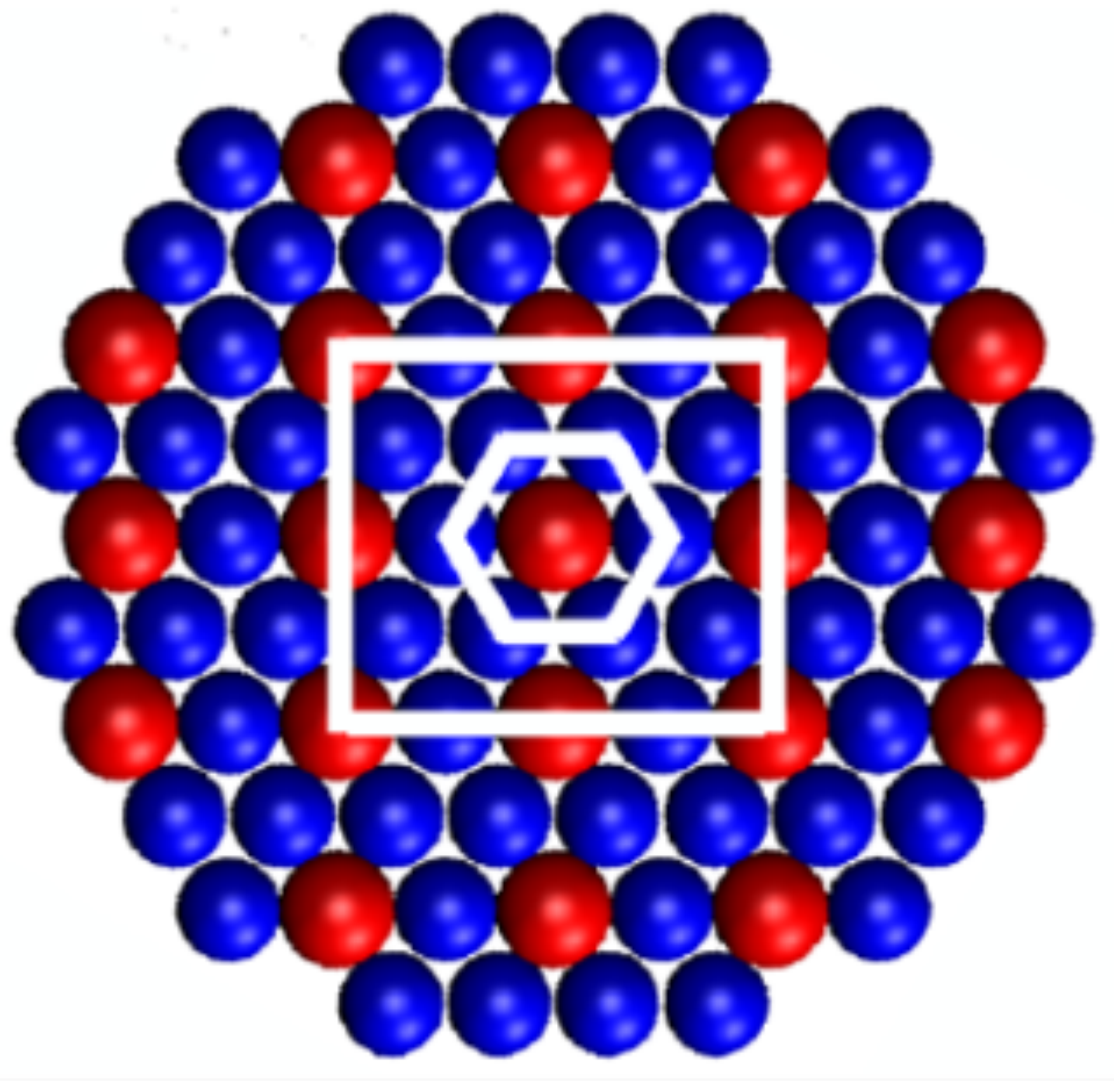
Controlled Self-assembly



Dispersed particles

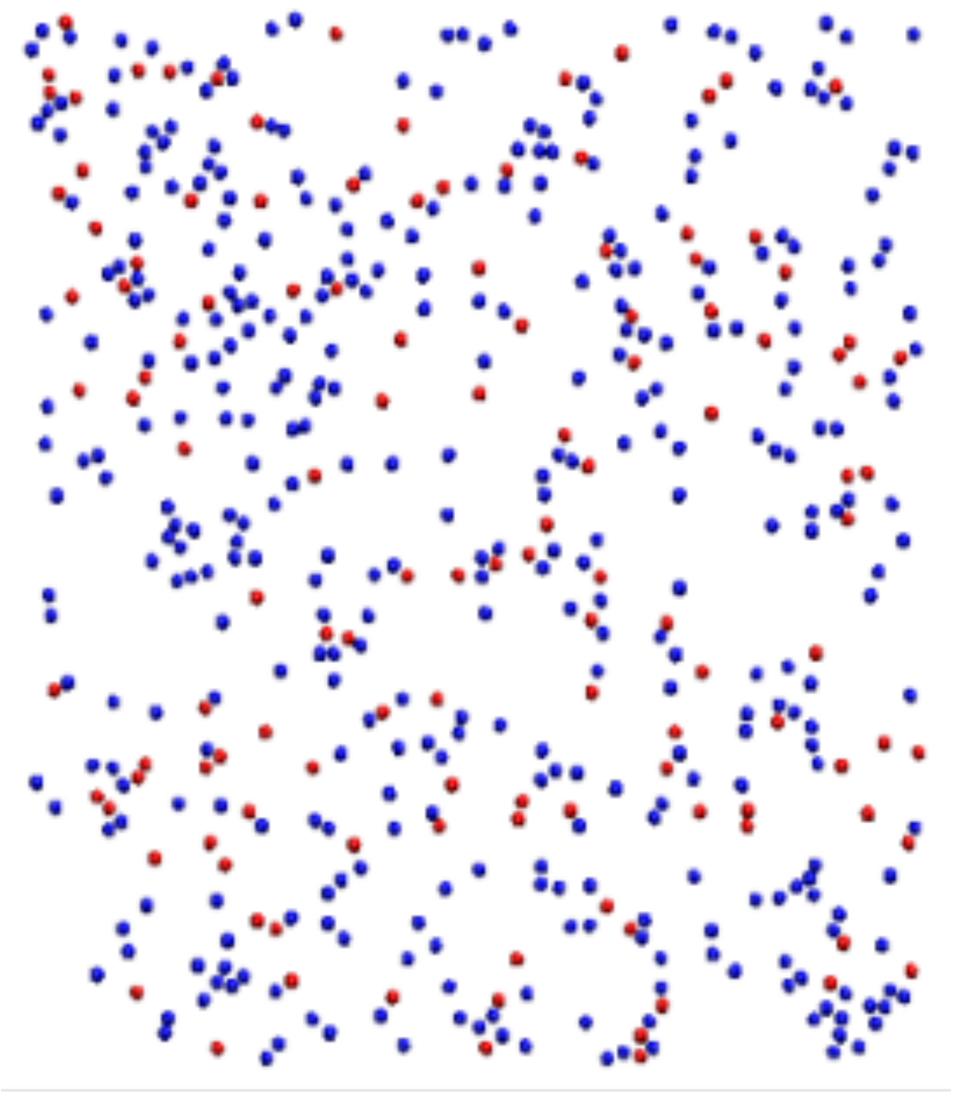


Ordered structure

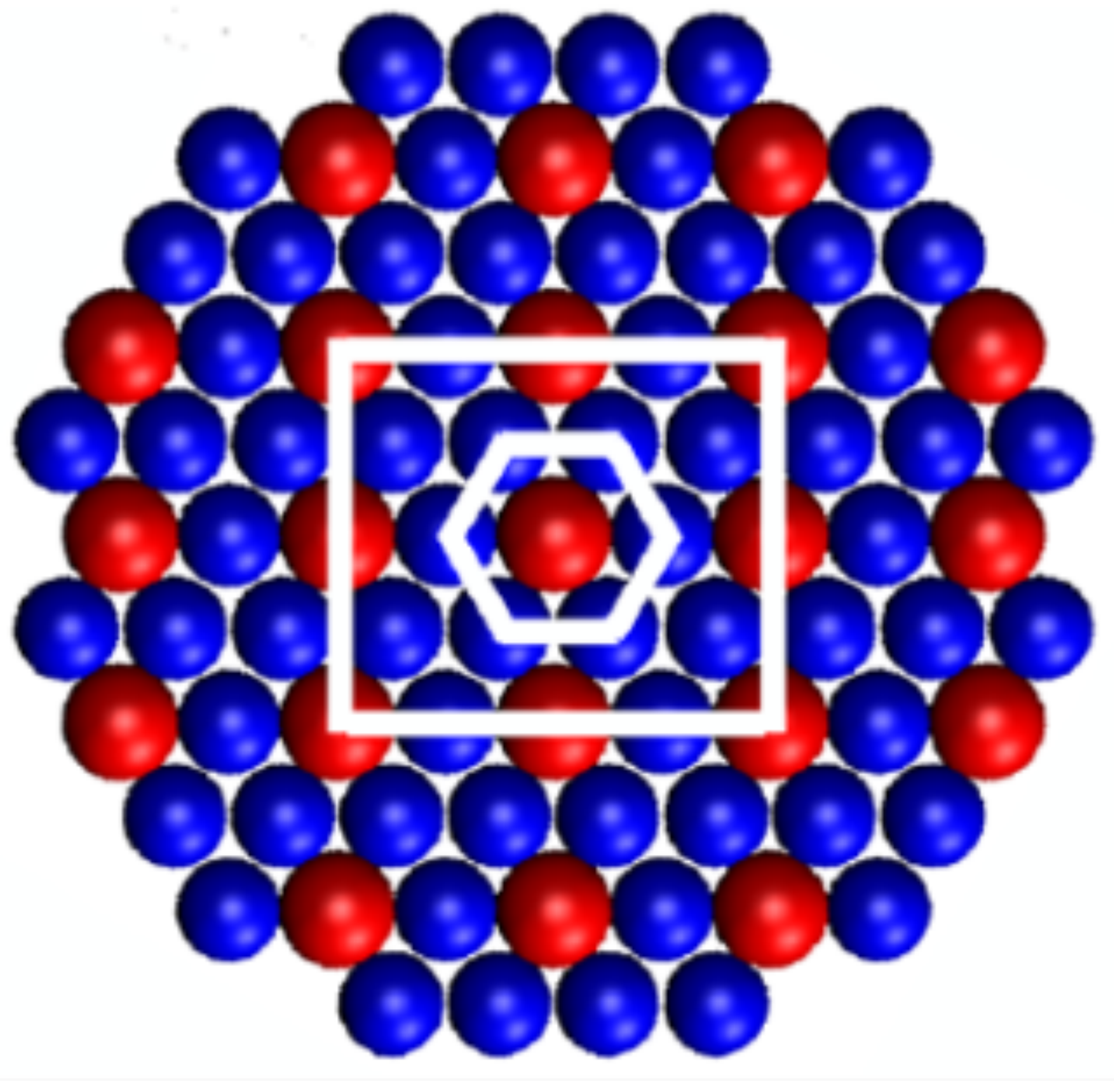
Applications:

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 $\rightsquigarrow$ measure of crystallinity order

Typical control variable: u

Electric field voltage

Technical challenge:

Nonlinear + noisy molecular dynamics

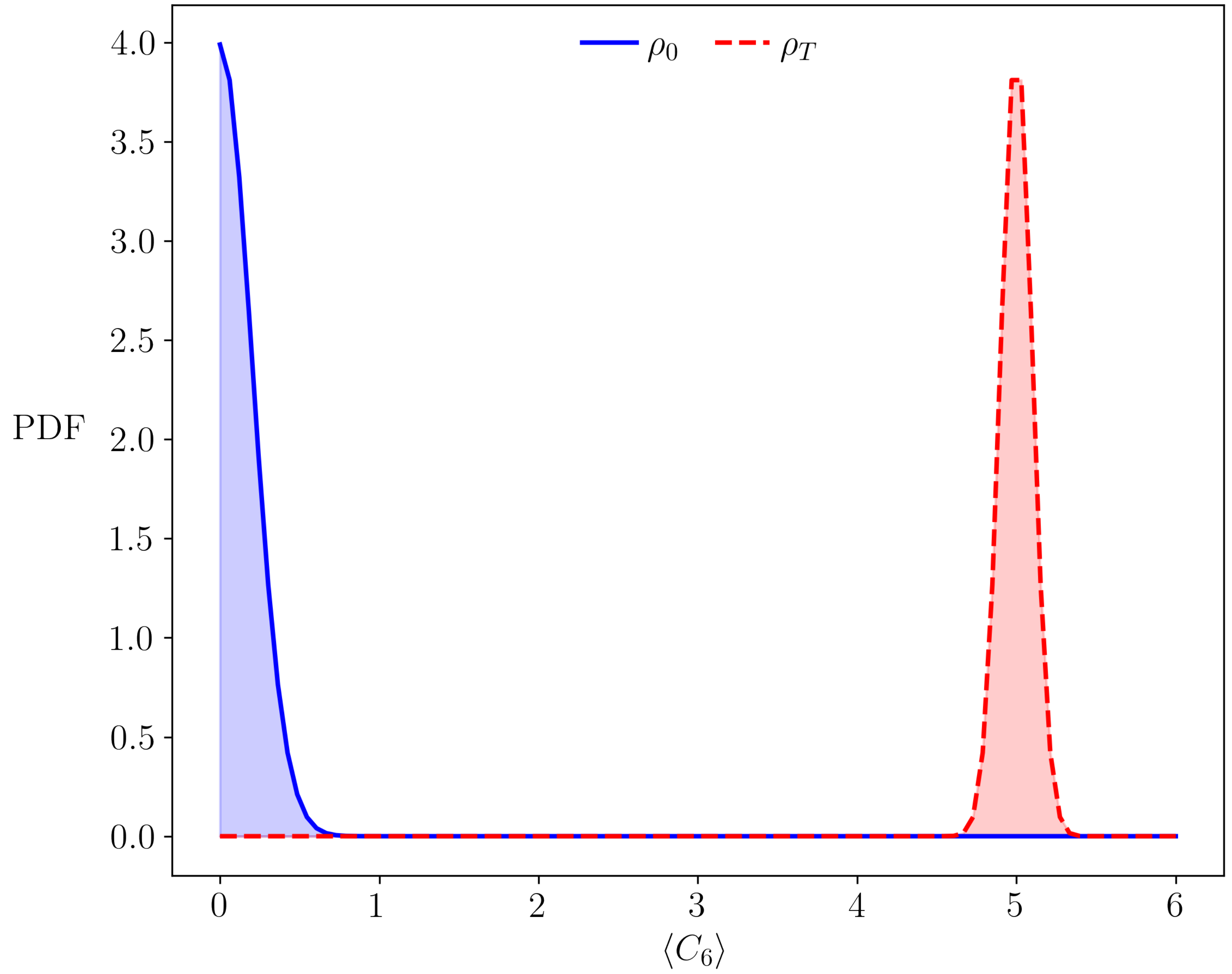
$\langle C_6 \rangle$ is a controlled stochastic process

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 $t_0 = 0$ to ordered at $T = 200\,\mathrm{s}$



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

Underdetermined

Minimum Effort Self-assembly

Proposed formulation:

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

drift landscape — diffusion landscape — free energy landscape

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

either from model or learnt from MD simulation data

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

$\langle C_6 \rangle$ — 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

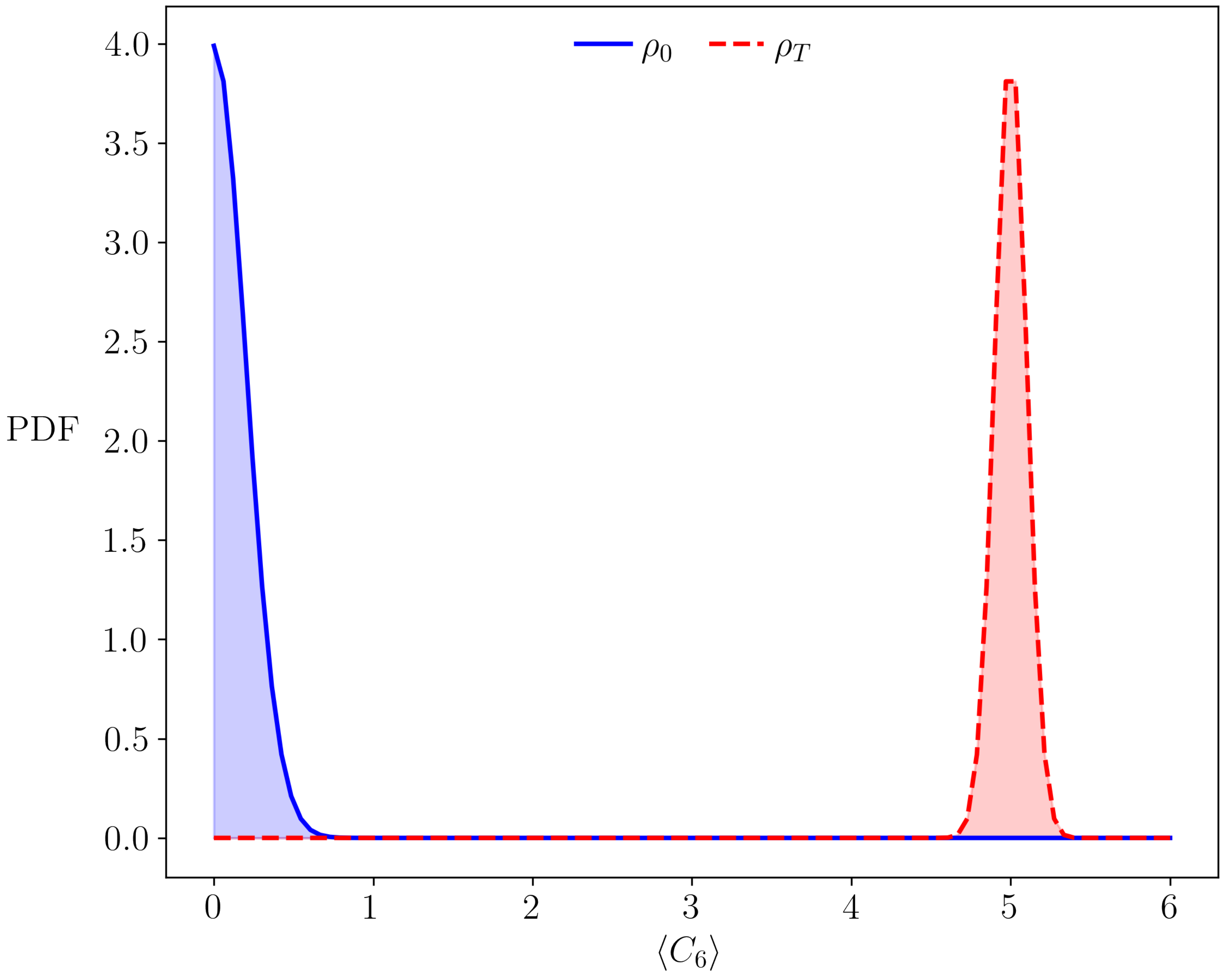
Equivalent formulation:

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

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

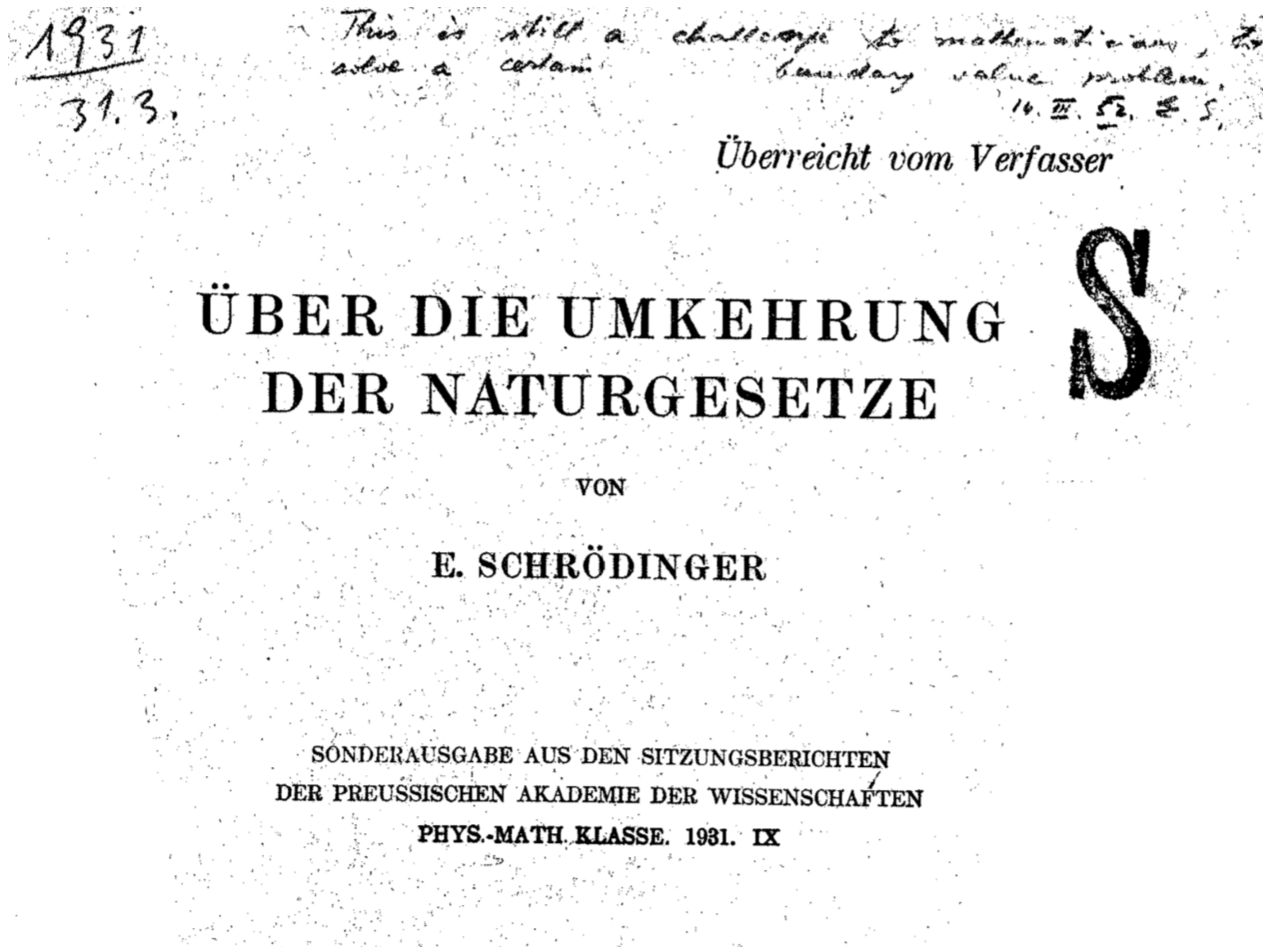
$$\rho(x^u, t=0) = \rho_0, \quad \rho(x^u, t=T) = \rho_T$$

Guaranteed existence-uniqueness for compactly supported ρ_0, ρ_T



Generalized Schrödinger Bridge

Schrödinger bridge problem: $D_1 \equiv 0$ and $D_2 \equiv$ Identity



1931
31.3.

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

Überreicht vom Verfasser

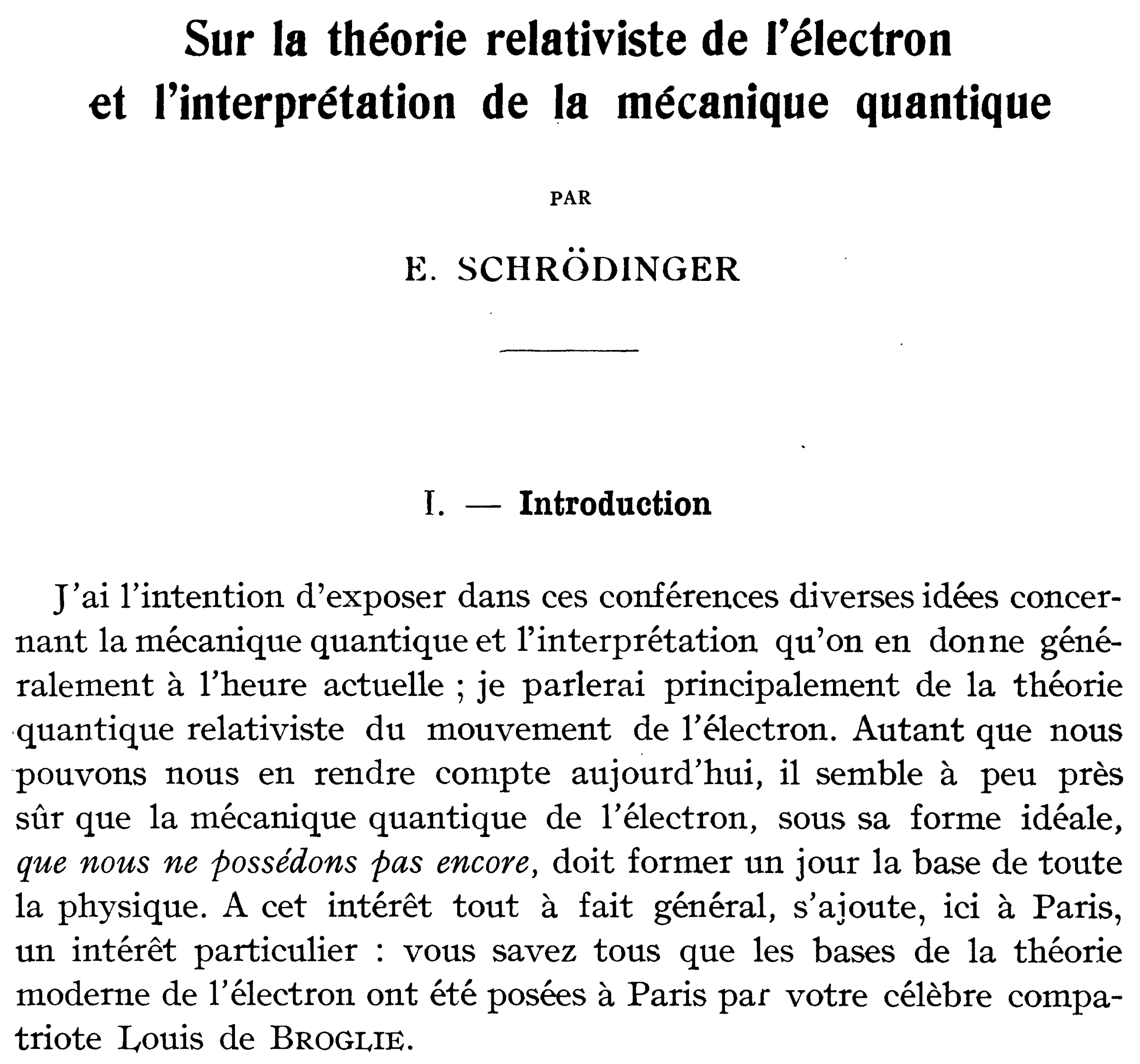
S

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 + control non-affine

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

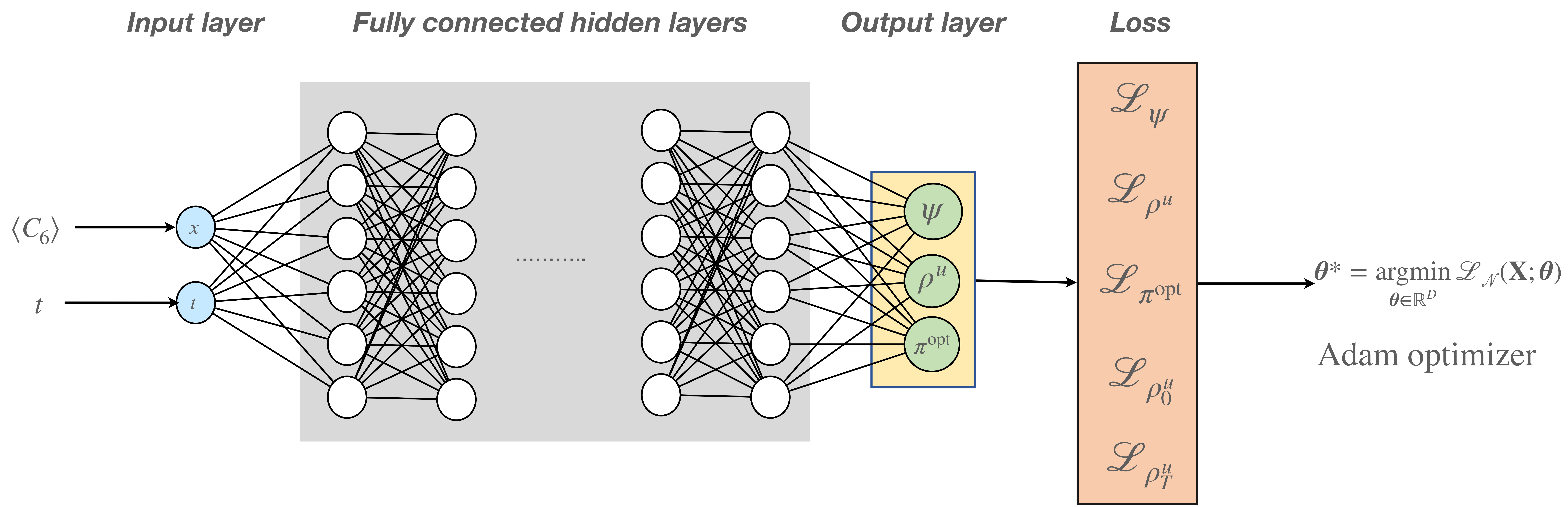
$$\rho(x^u, t = 0) = \rho_0, \quad \rho(x^u, t = T) = \rho_T$$

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



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

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

Losses for Training

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

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

Loss term for initial condition

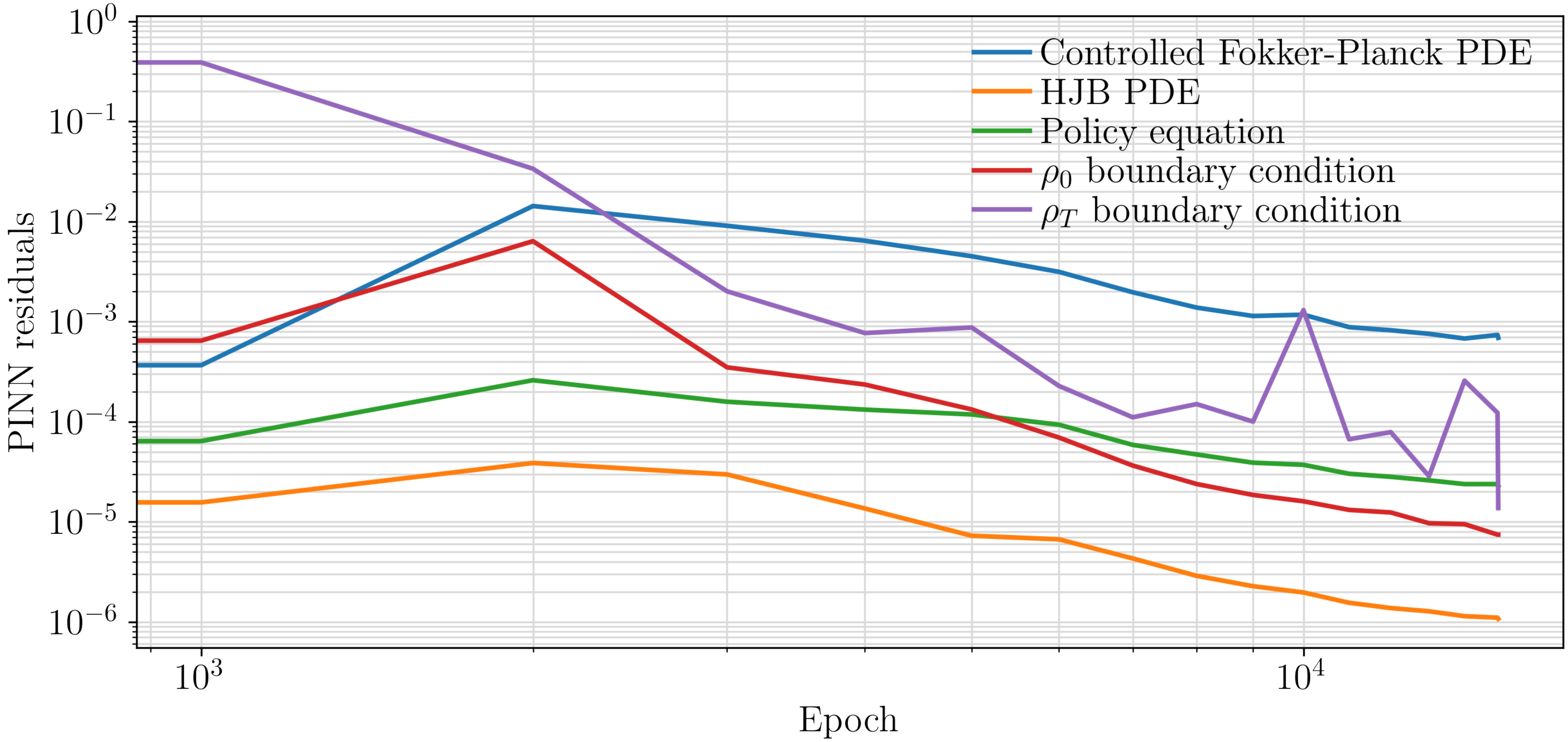
$$\mathscr{L}_{\rho_0^u} = \frac{1}{n}\sum_{i=1}^{n}\left(\rho^u\Big|_{t=0} - \rho_0^u(x)\right)^2$$

Loss term for terminal condition

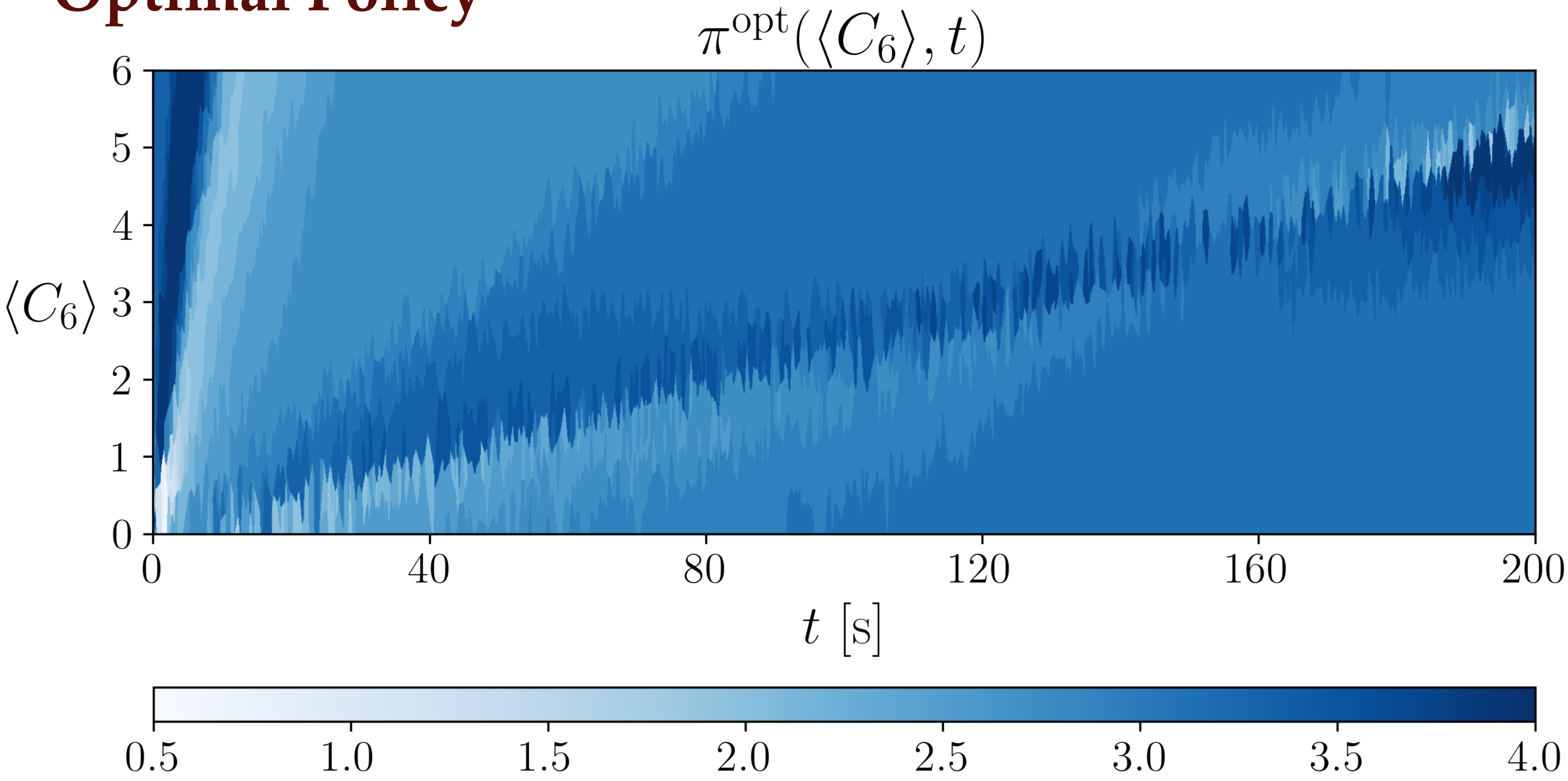
$$\mathscr{L}_{\rho_T^u} = \frac{1}{n}\sum_{i=1}^{n}\left(\rho^u\Big|_{t=T} - \rho_T^u(x)\right)^2$$

Training of the PINN

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

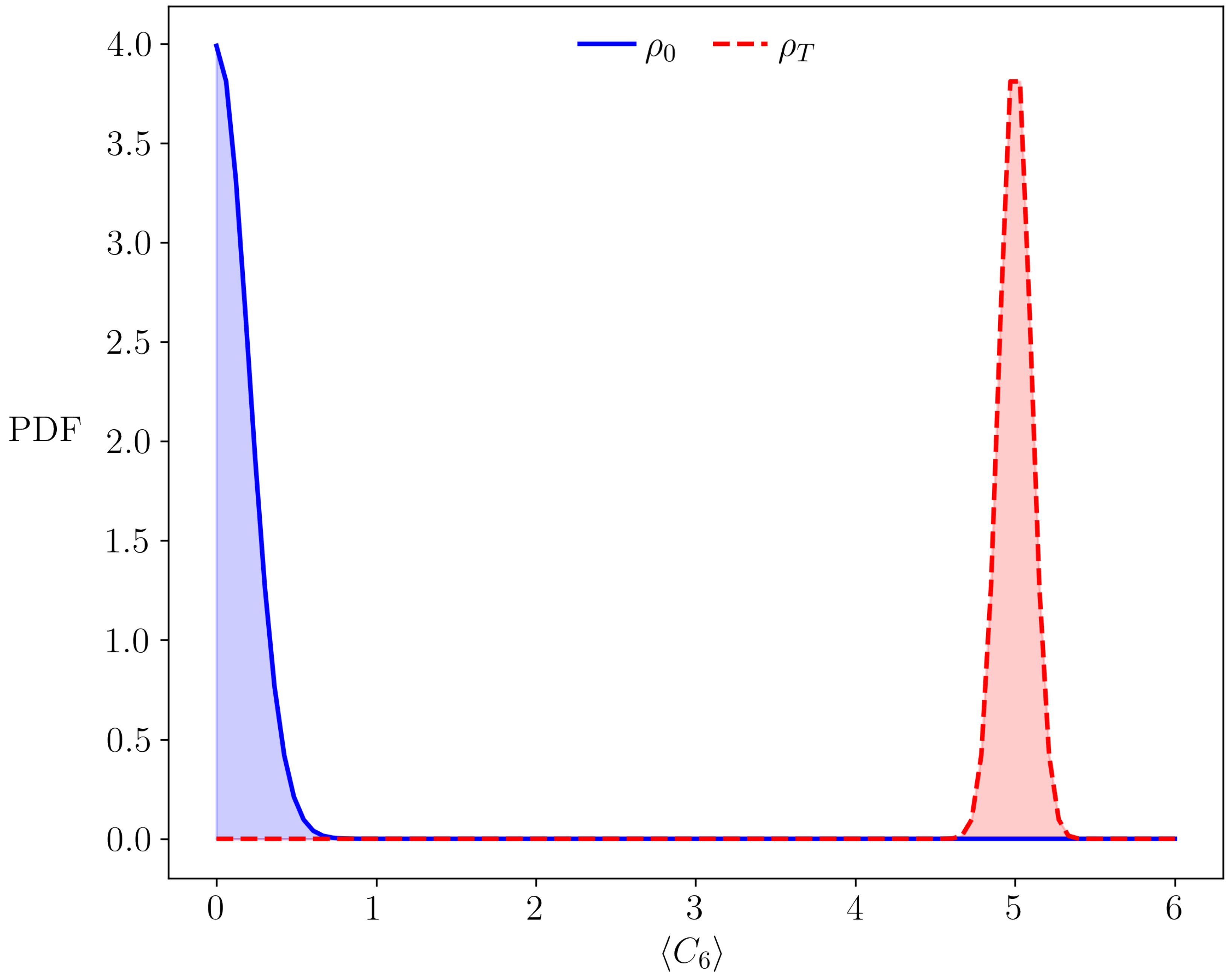


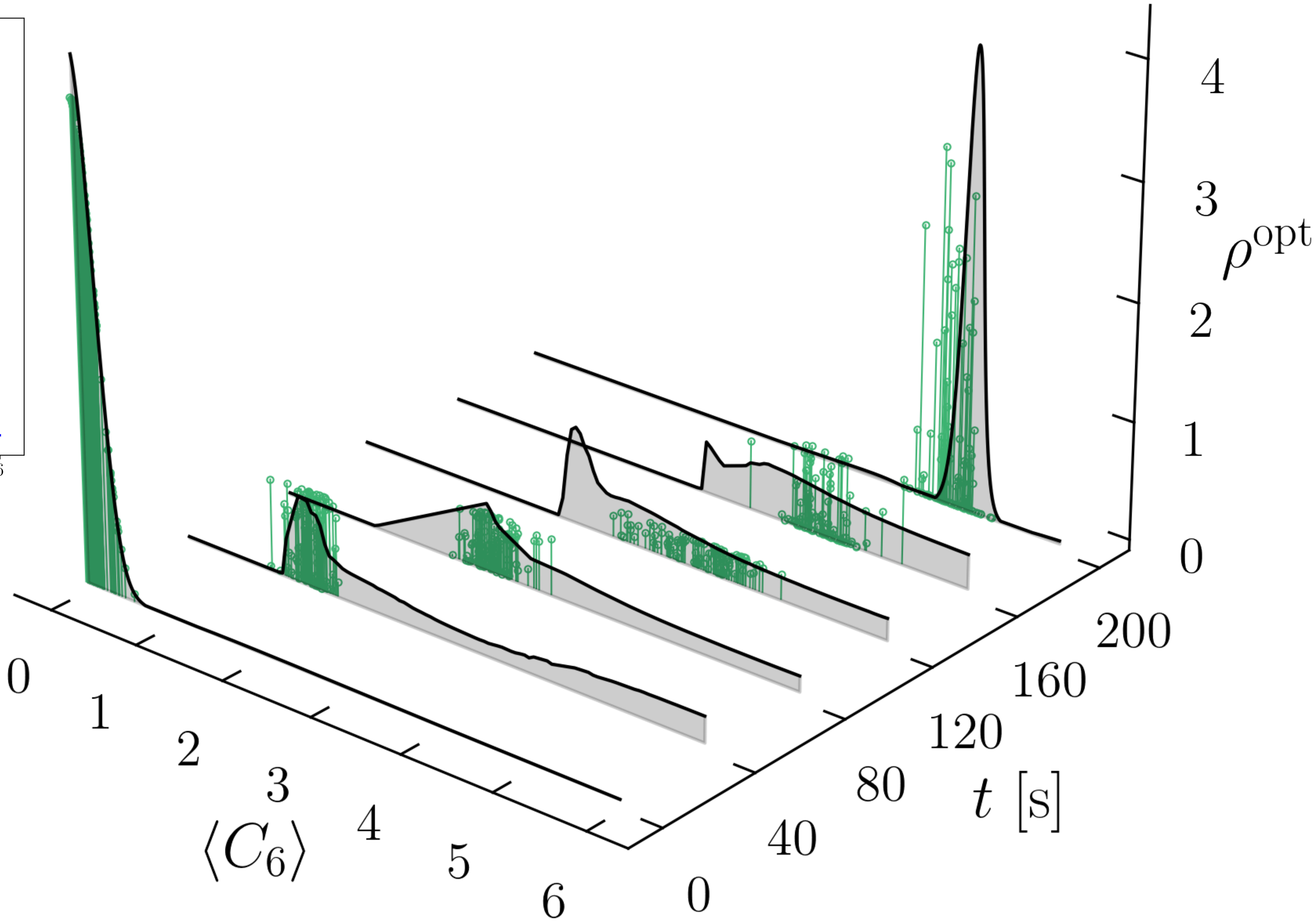
Optimal Policy



Value Function

Optimally Controlled State PDFs





Optimal State and Optimal Control Sample Paths

Ongoing Efforts

Learning from very high fidelity MD simulation data

Online learning and control

Robustness

Thank You

Acknowledgment: NSF