

Neural Schrödinger Bridge for Minimum Effort Self-assembly

Iman Nodoozi

inodozi@ucsc.edu

Department of Electrical and Computer Engineering
University of California, Santa Cruz

Joint work with



Jared O'Leary (UC Berkeley)



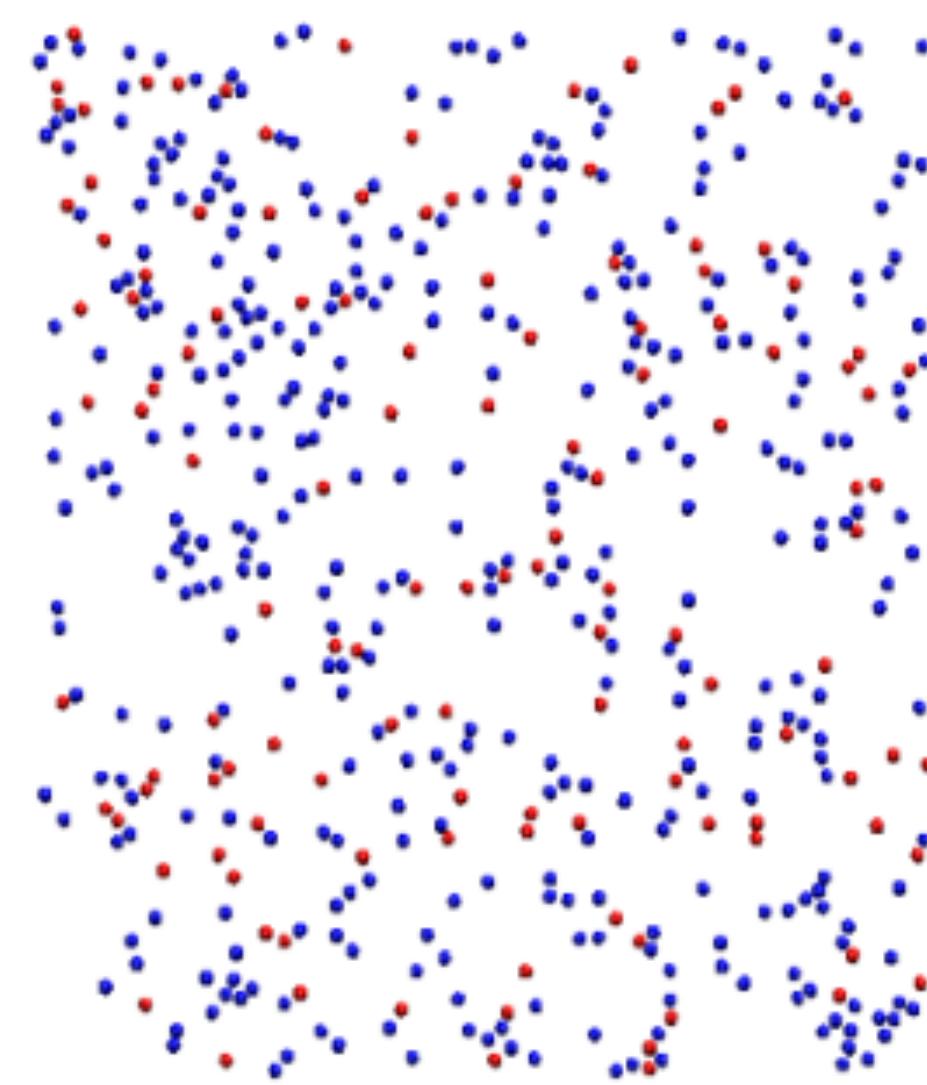
Abhishek Halder (UC Santa Cruz)



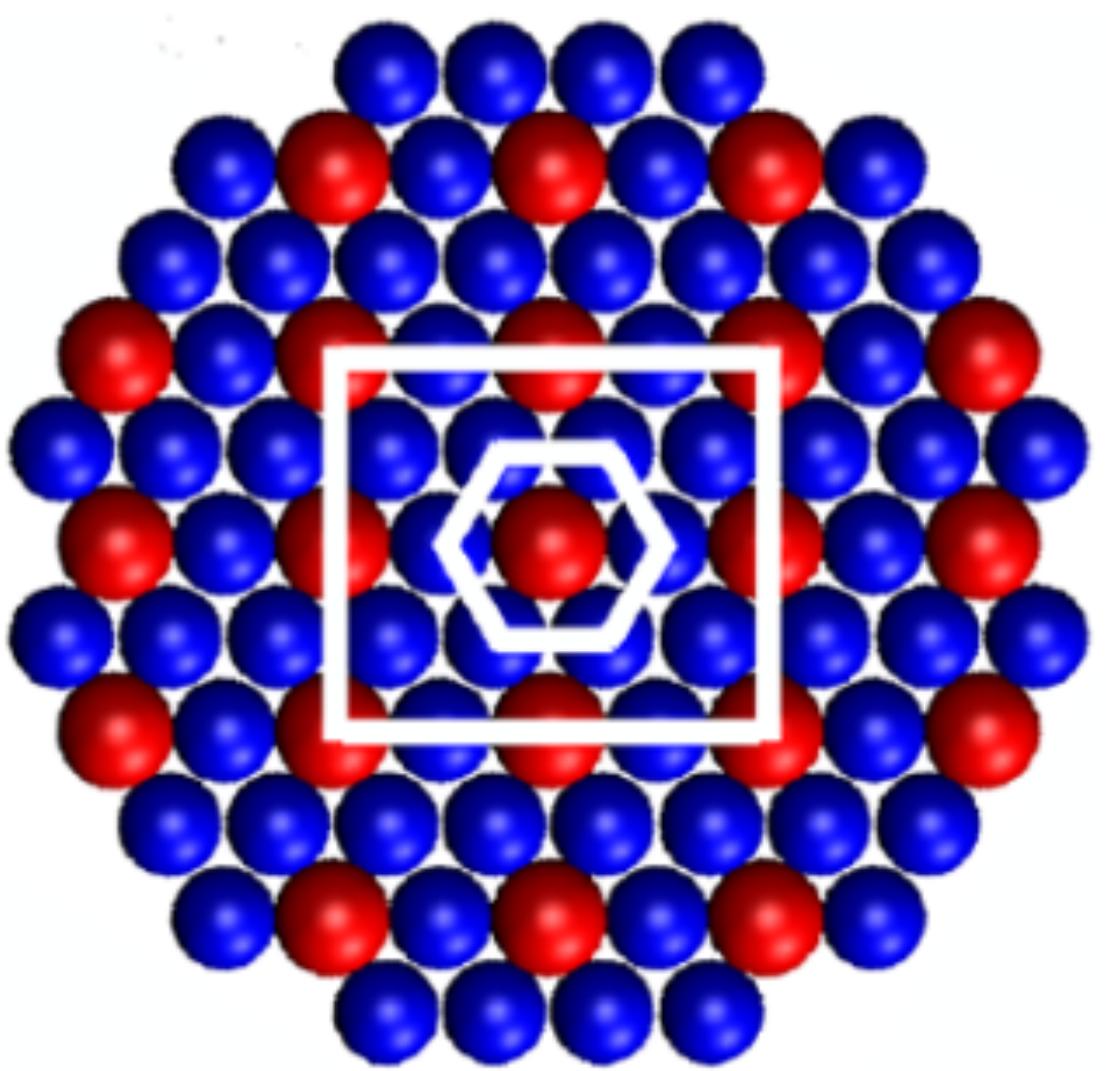
Ali Mesbah (UC Berkeley)

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Controlled Self-assembly



Dispersed particles

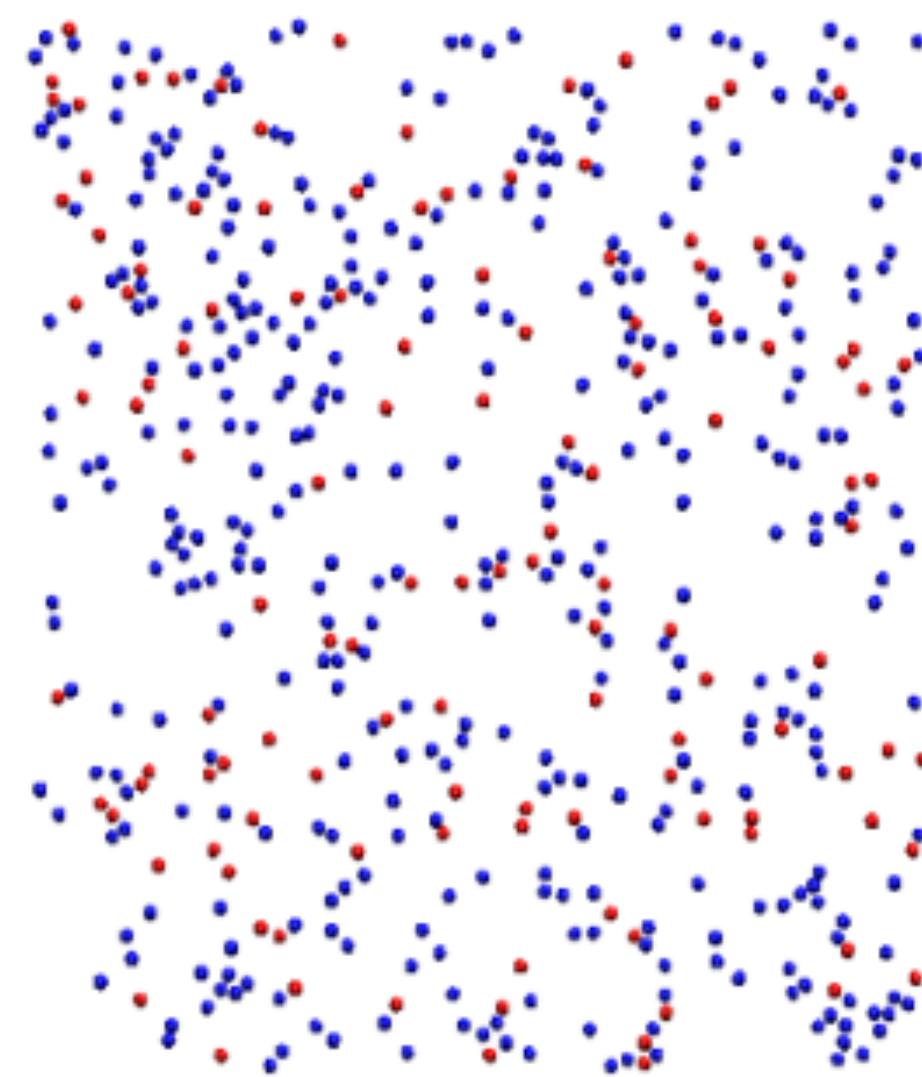


Ordered structure

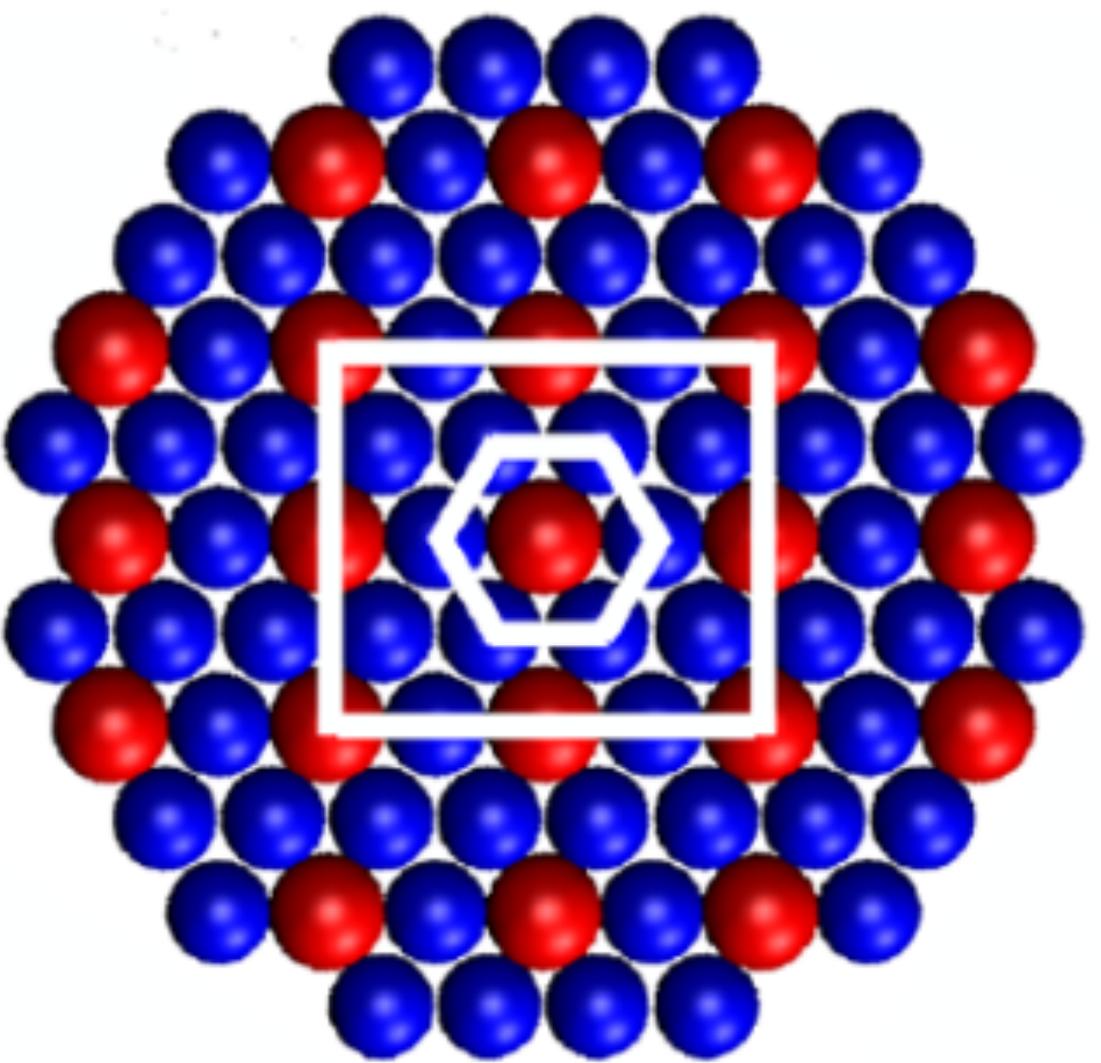
Applications:

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

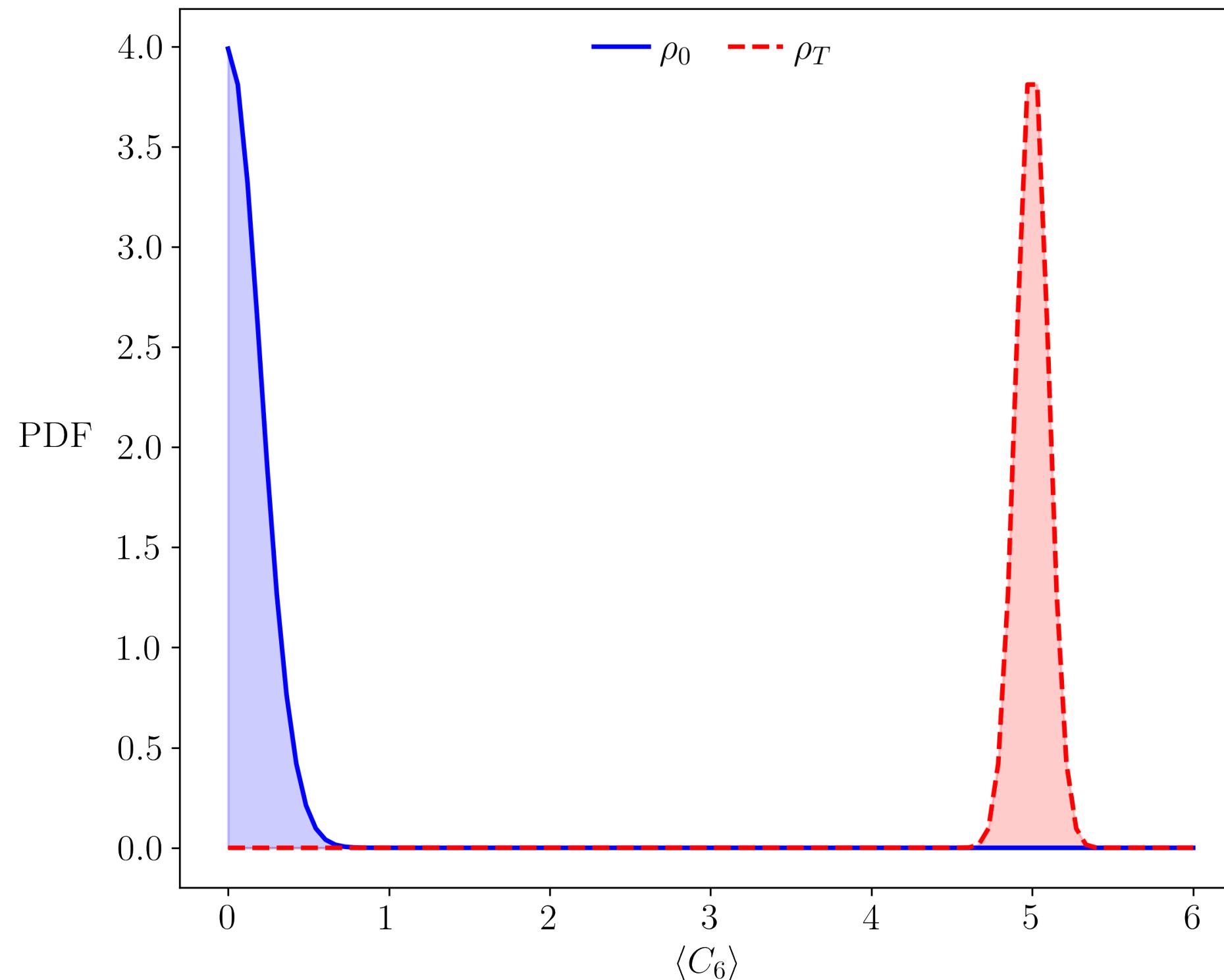
Controlled Self-assembly as PDF Steering

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 $t = T \equiv 200$ 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:**

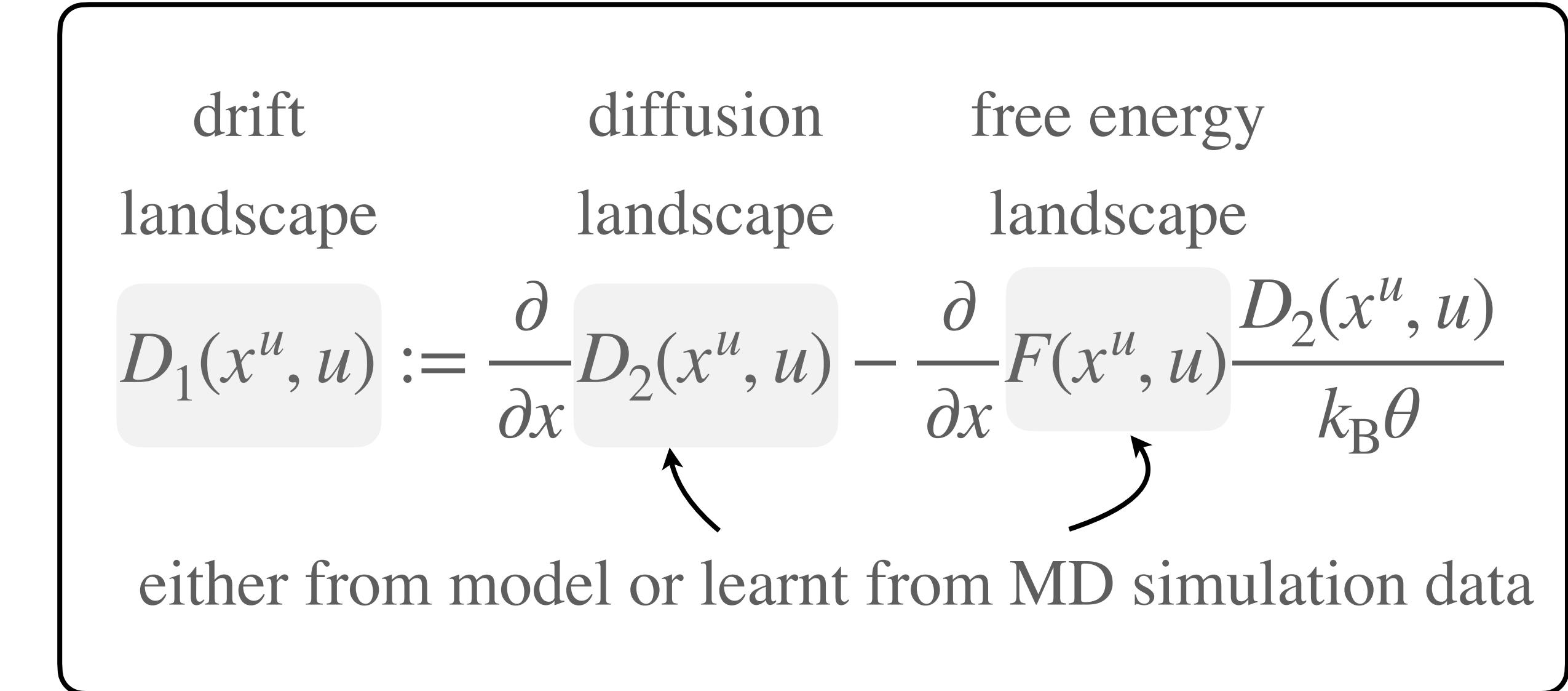
$$u = \pi(\langle C_6 \rangle, t)$$

Underdetermined

Minimum Effort Self-assembly

Proposed formulation:

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



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

$\langle C_6 \rangle$ standard Wiener process

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

Minimum Effort Self-assembly

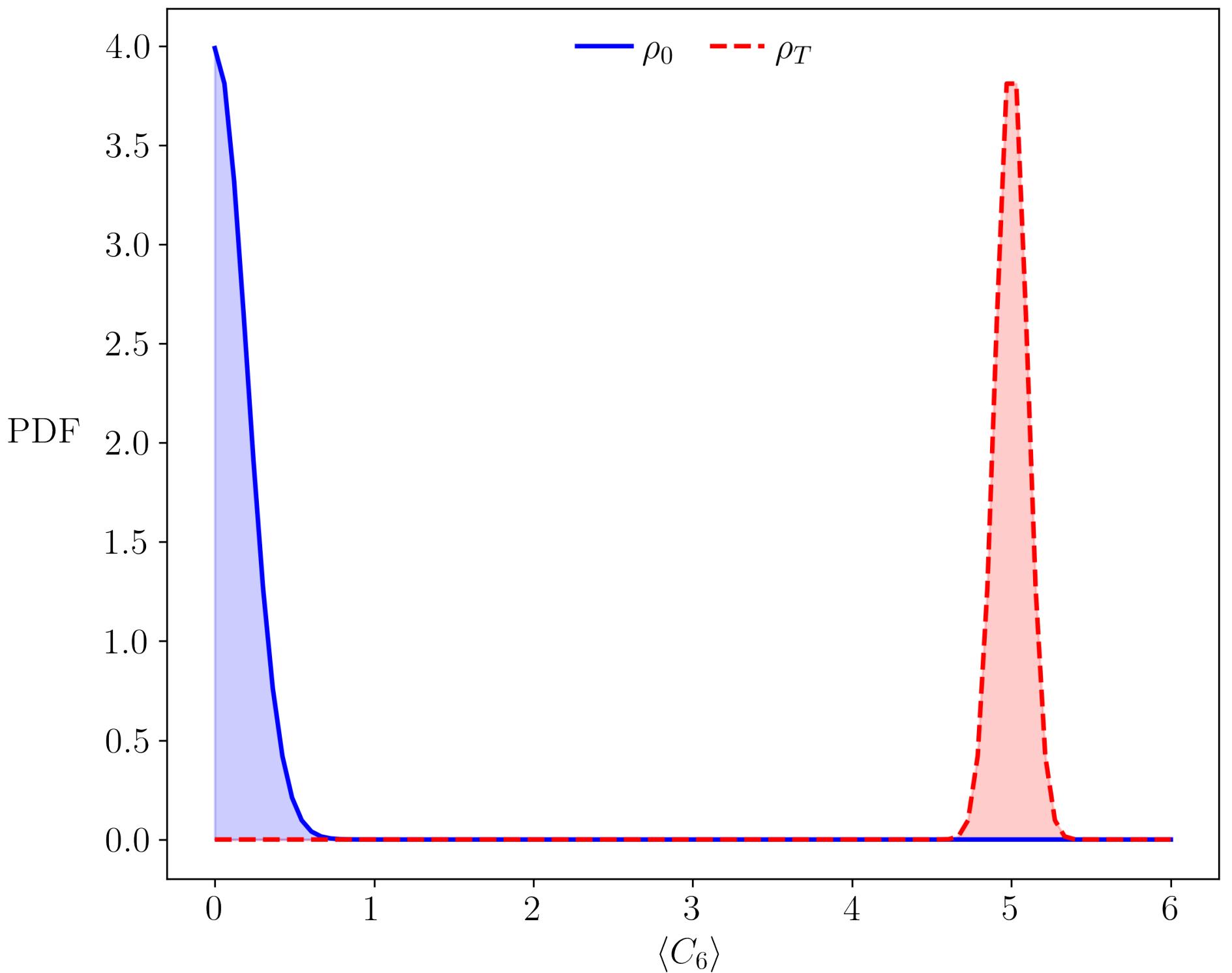
Equivalent formulation:

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

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

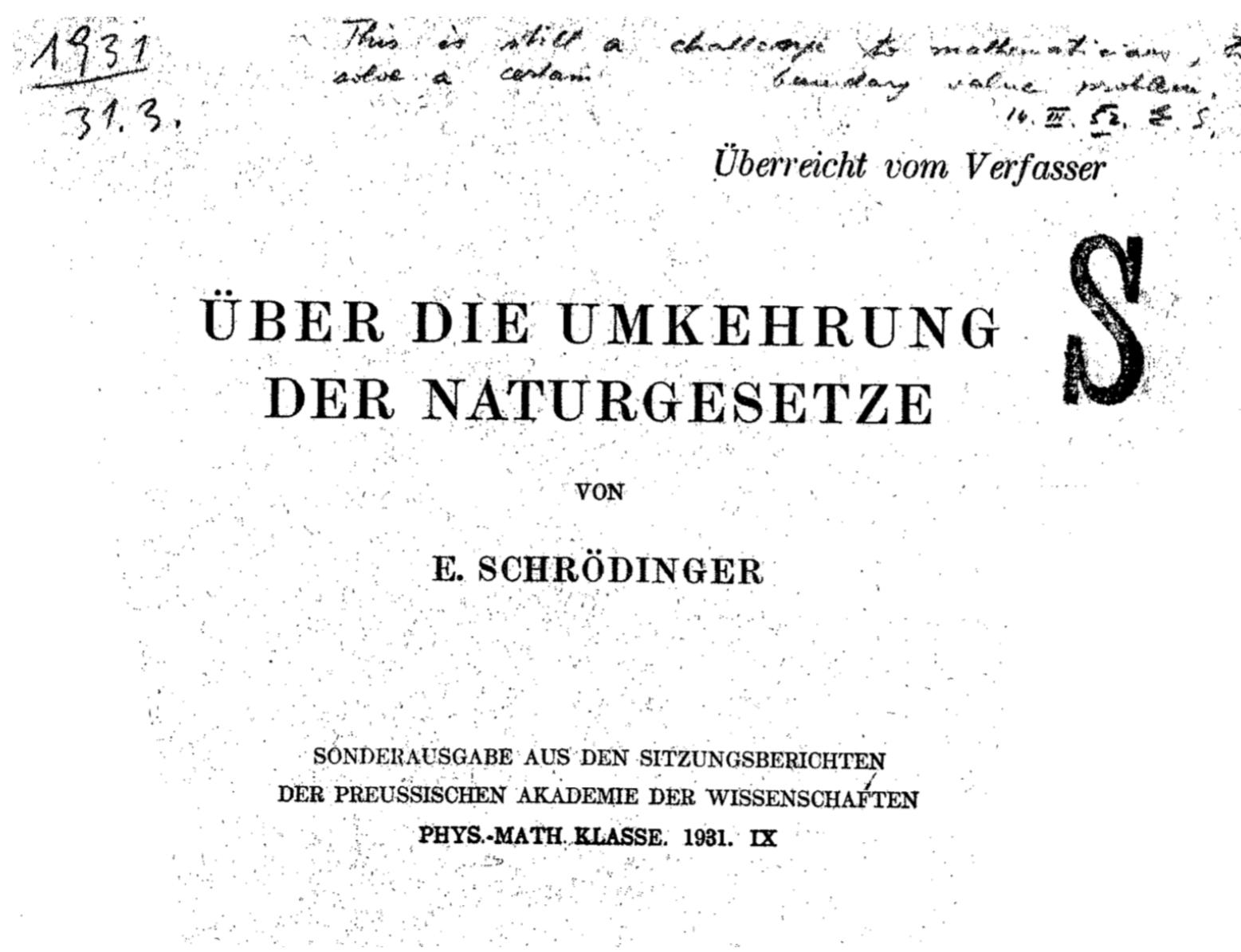
$$\rho^u(x^u, t = 0) = \rho_0, \quad \rho^u(x^u, t = T) = \rho_T$$

Guaranteed existence-uniqueness
for compactly supported ρ_0, ρ_T



Generalized Schrödinger Bridge

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



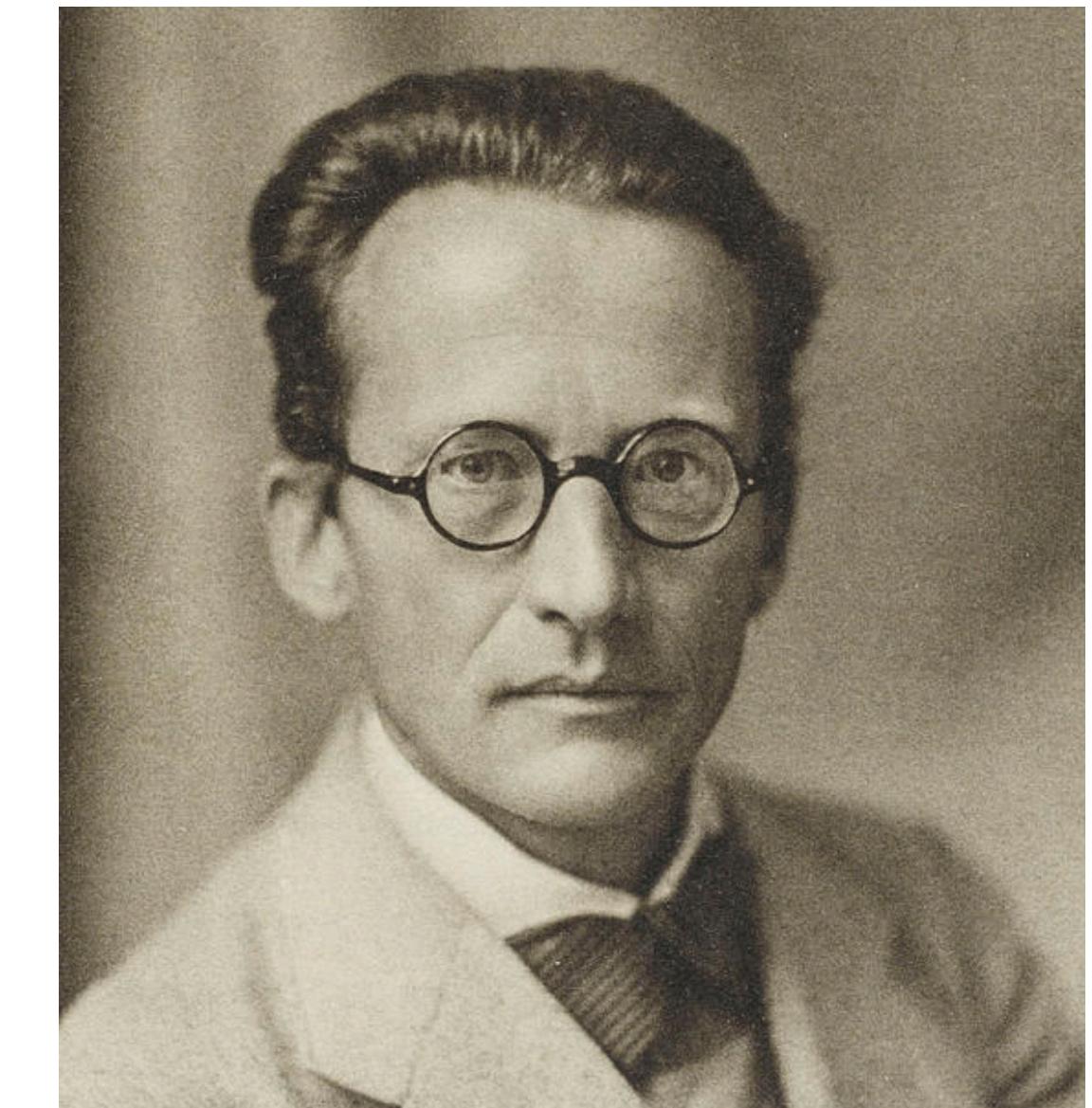
Sur la théorie relativiste de l'électron
et l'interprétation de la mécanique quantique

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

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

HJB PDE

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

Controlled FPK PDE

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

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

Solve via PINN: Losses for Training

Loss term for HJB PDE

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

Loss term for FPK PDE

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

Loss term for policy equation

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

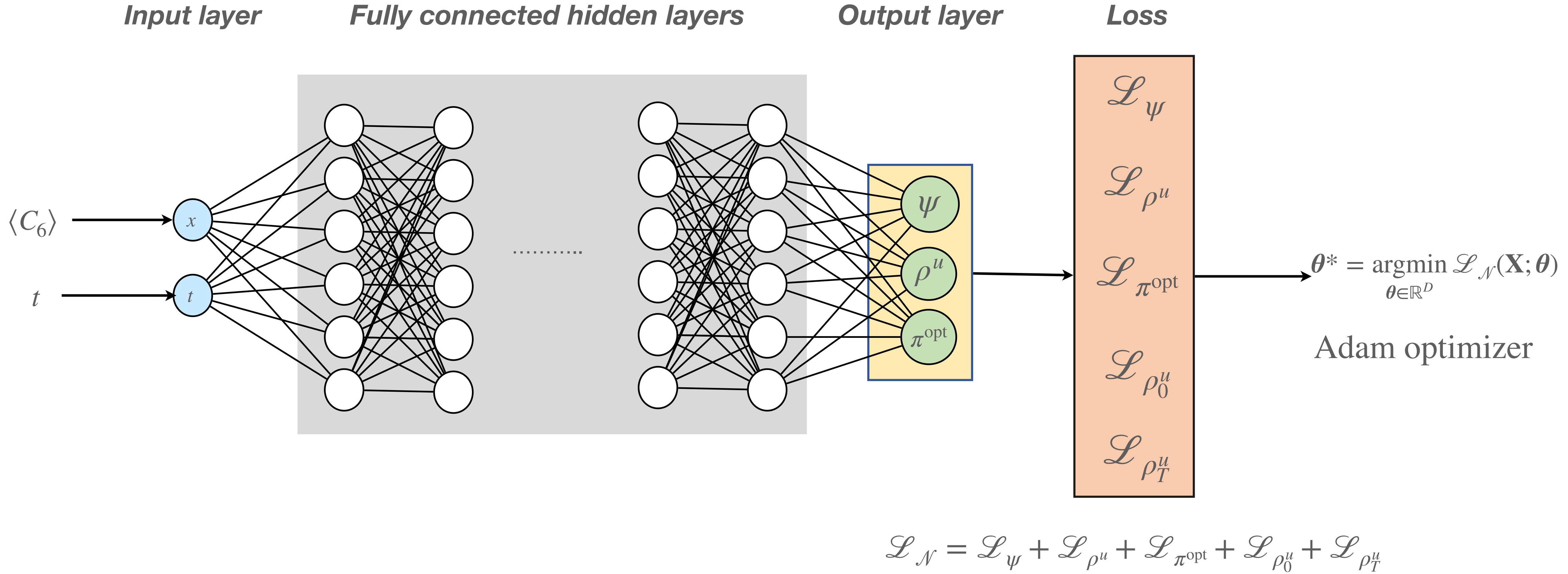
Loss term for initial condition

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

Loss term for terminal condition

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

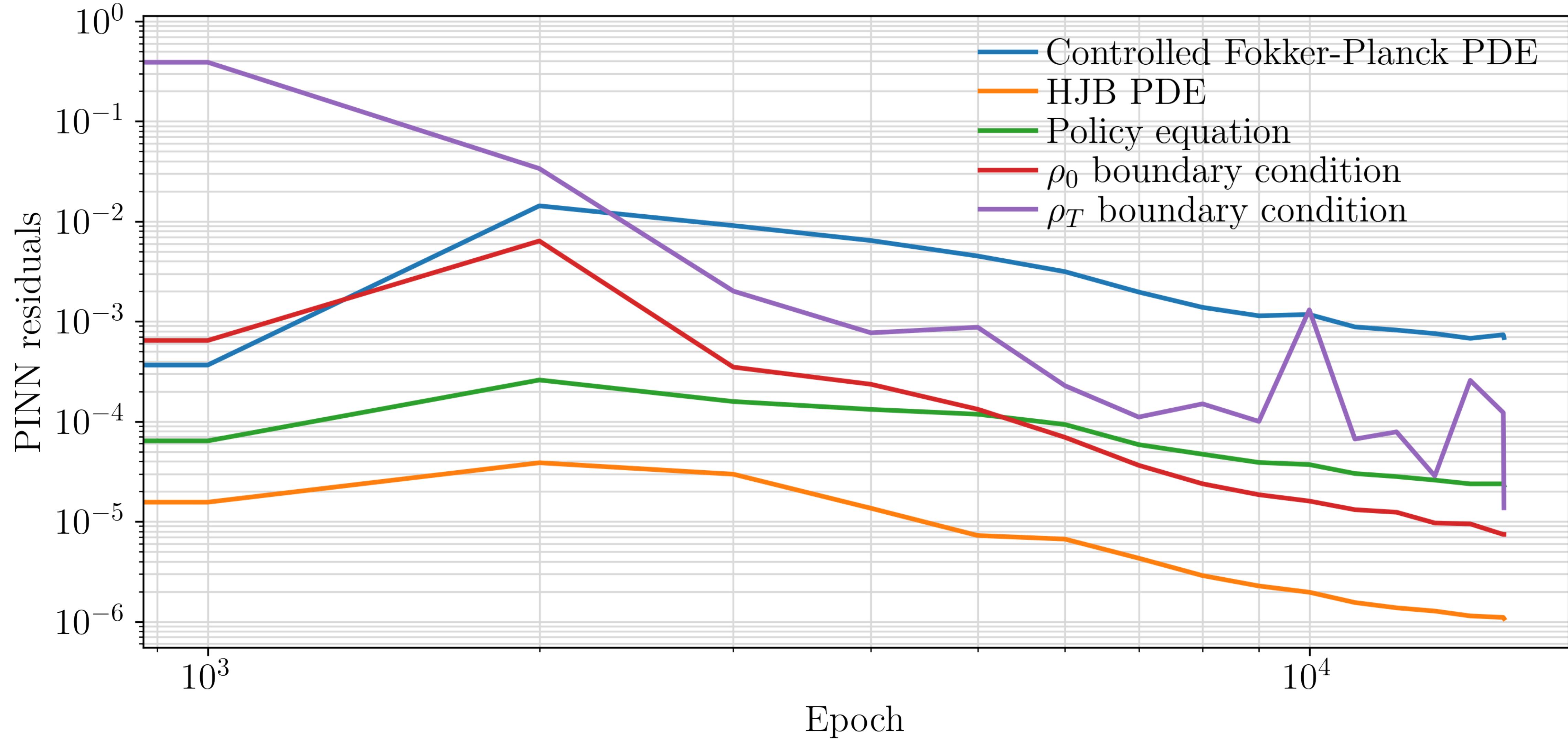
PINN Architecture



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

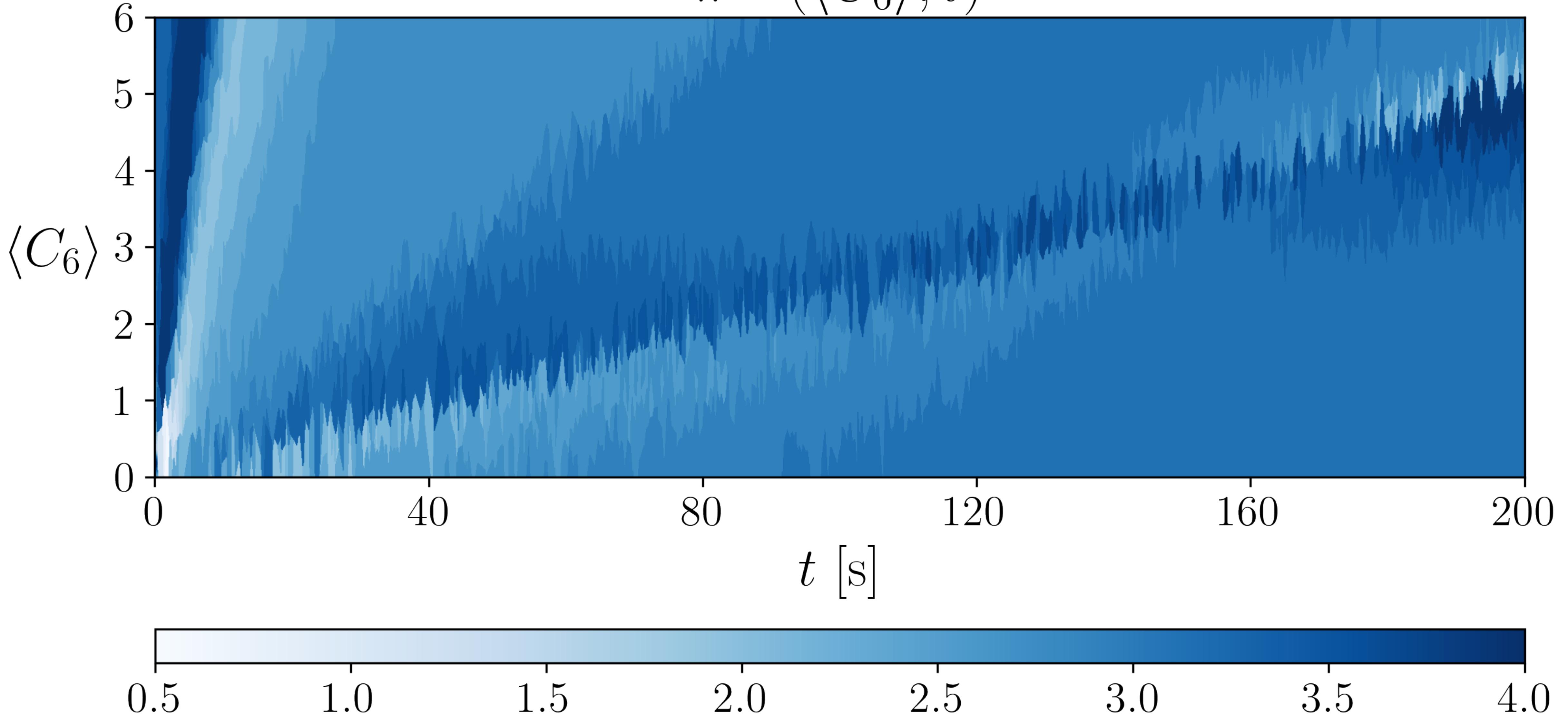
Training of the PINN

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



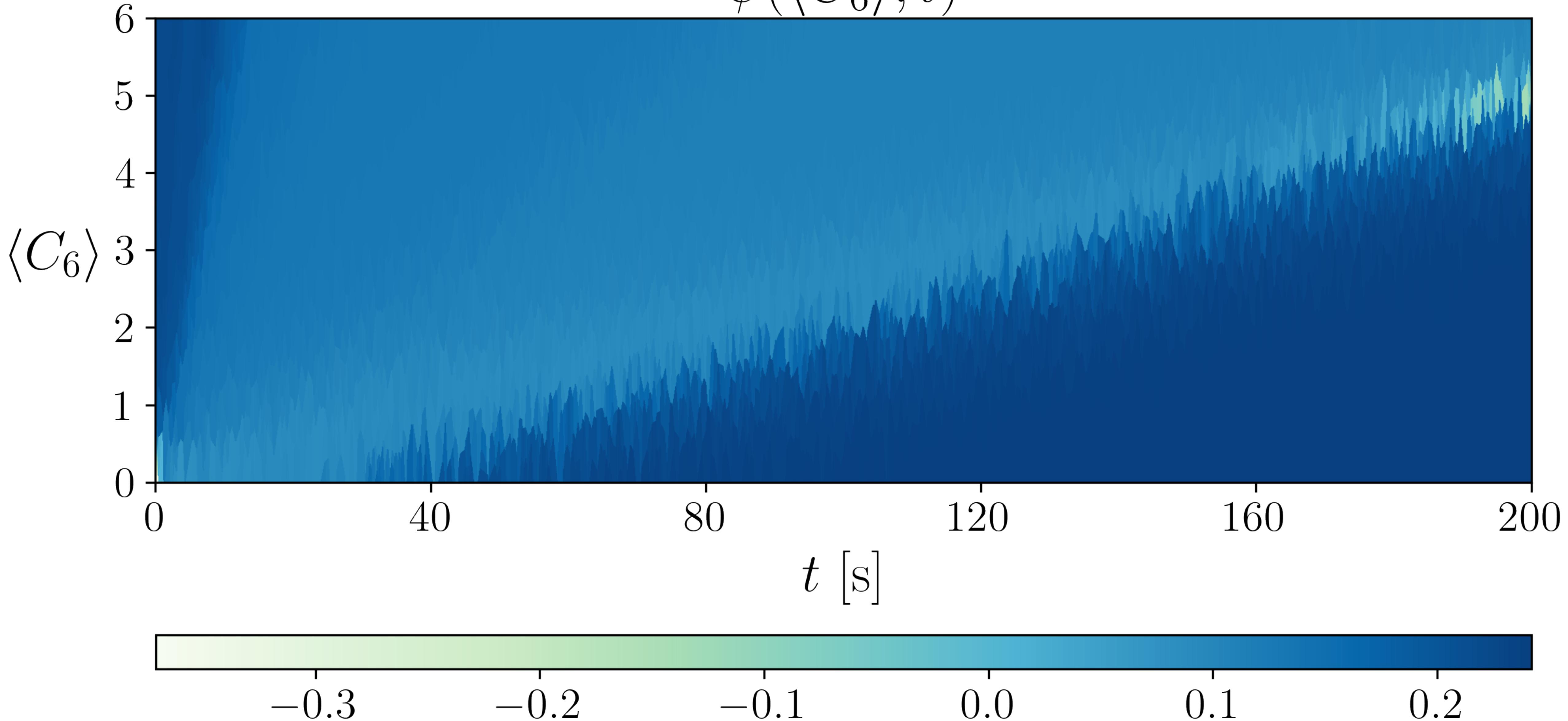
Optimal Policy

$$\pi^{\text{opt}}(\langle C_6 \rangle, t)$$

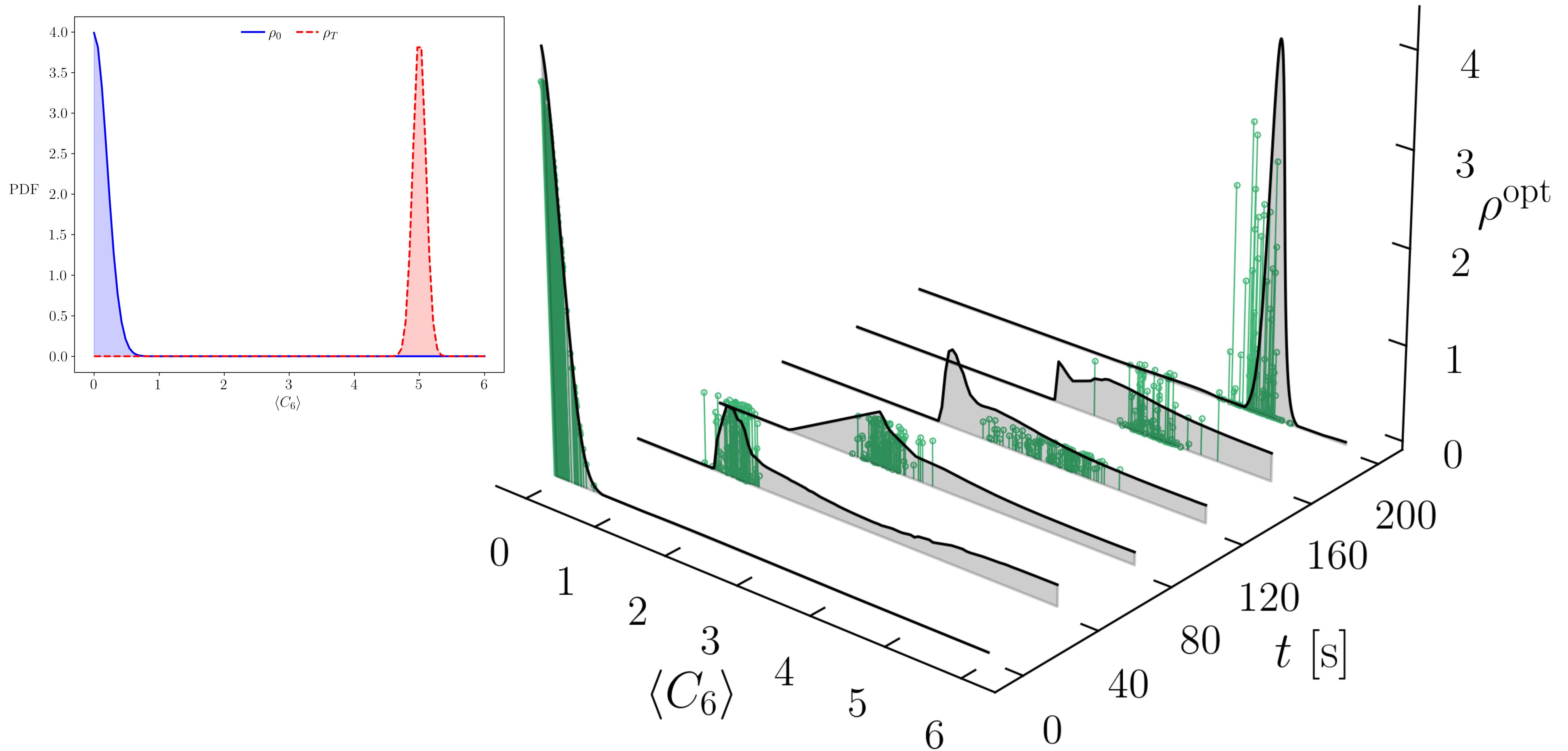


Value Function

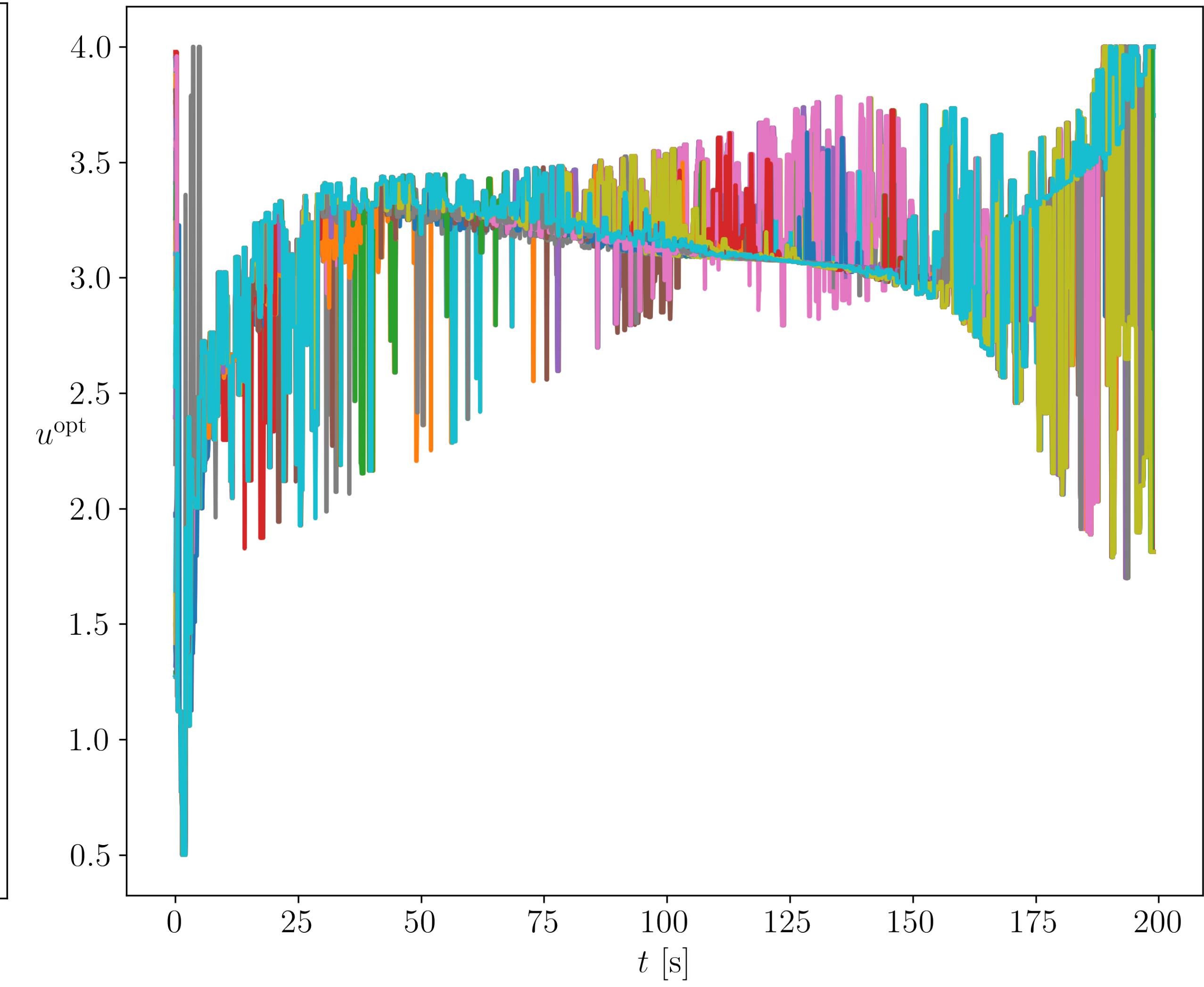
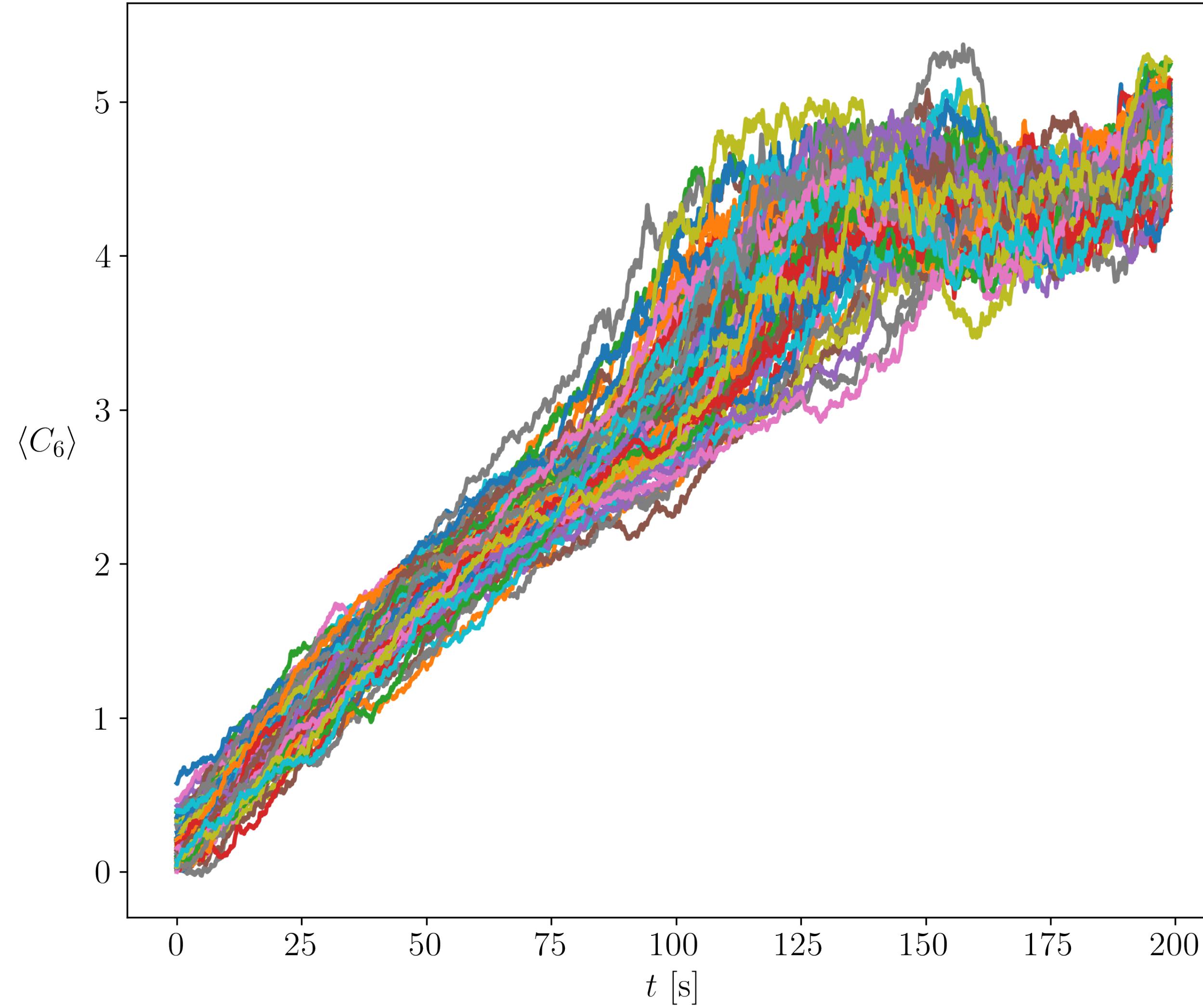
$$\psi(\langle C_6 \rangle, t)$$



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

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