New Developments in Schrödinger Bridge, Stochastic Control and Stochastic Learning

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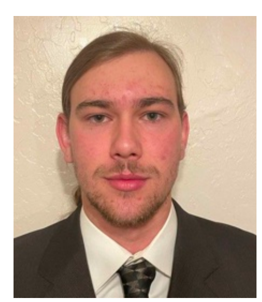
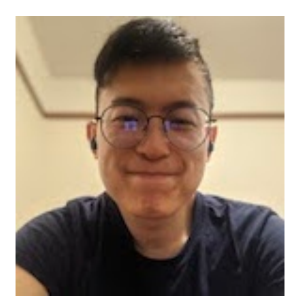
Iowa State University

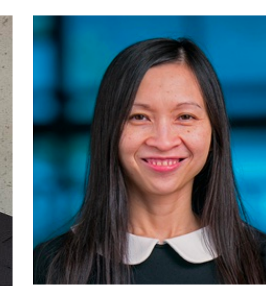
Joint work with students and collaborators







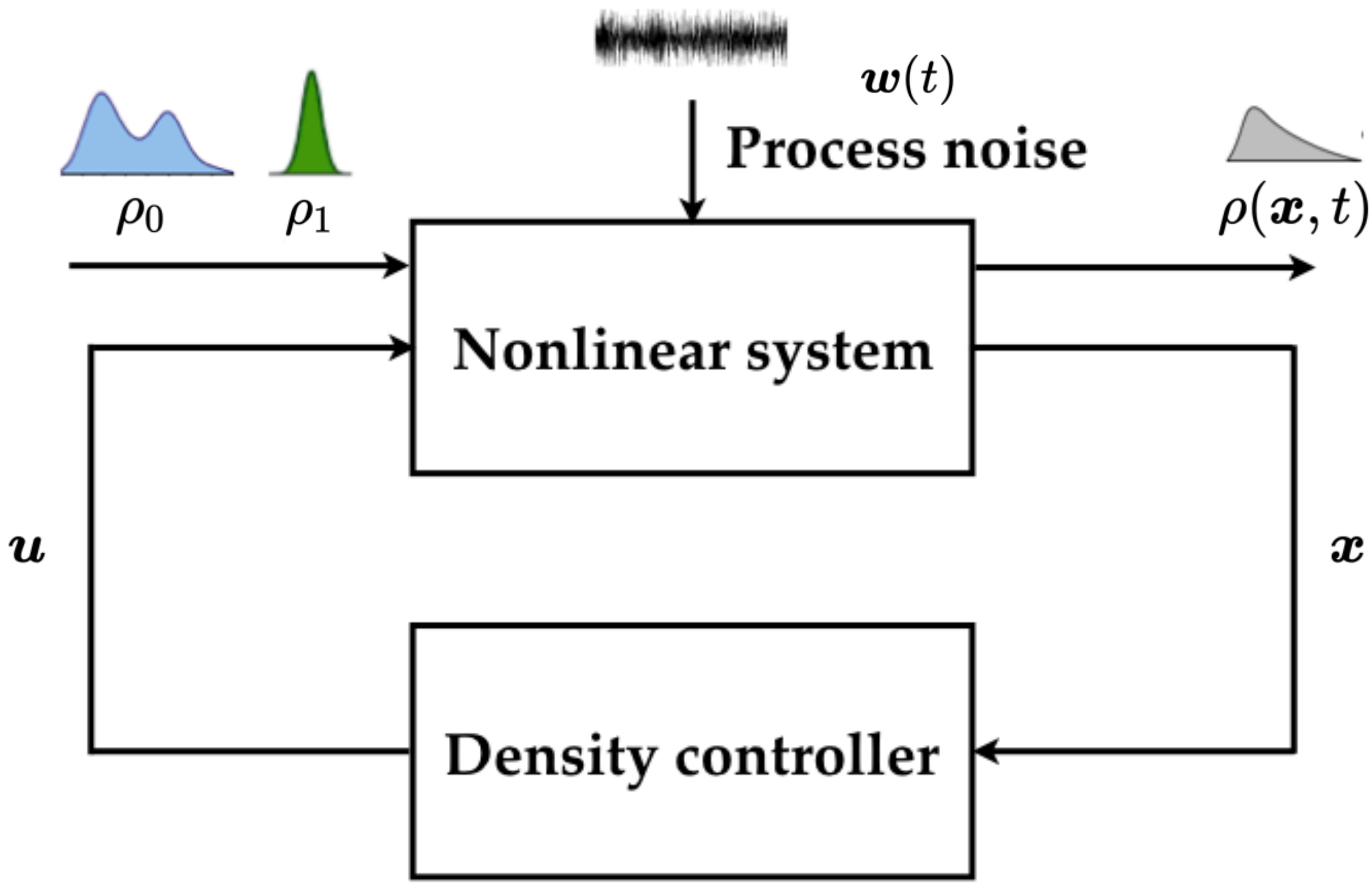


GNC Group Meeting, Department of Aerospace Engineering, Iowa State University
April 02, 2024

Theme of this talk

Control and learning of measures/densities

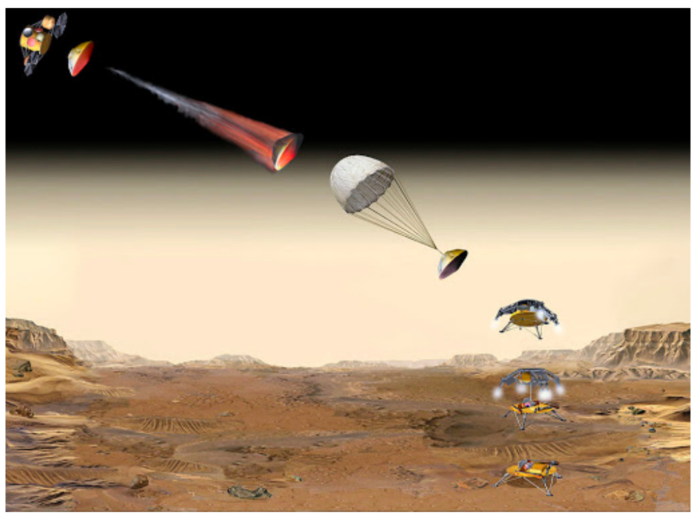
Density Control: Generalized Schrödinger Bridge

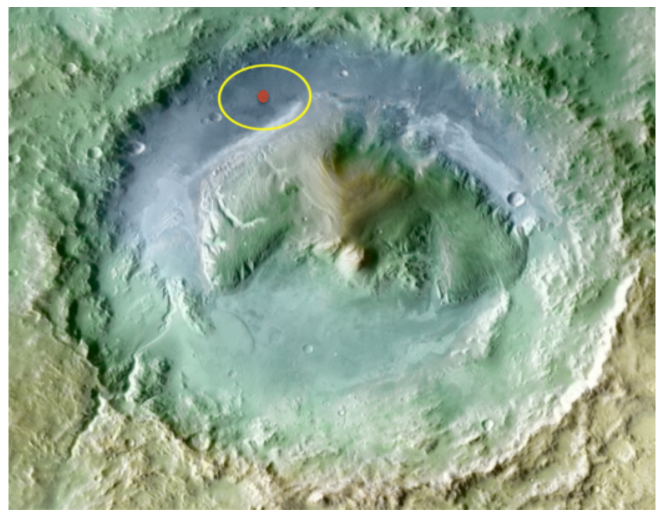


Motivating Applications

Distribution ~ Probability

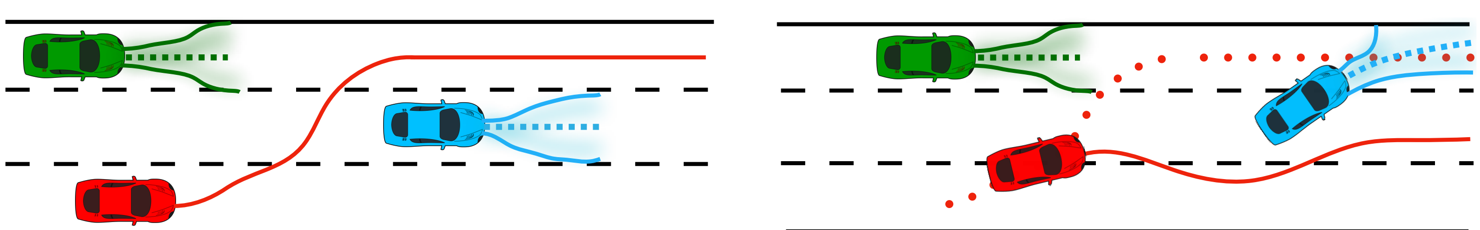
Spacecraft landing with desired statistical accuracy





Gale Crater (4.49S, 137.42E)

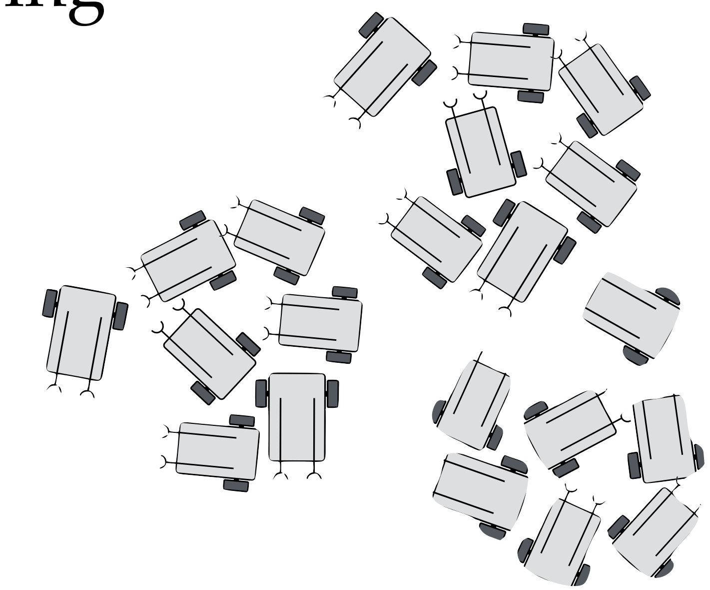
Risk management for automated driving in multi-lane highways



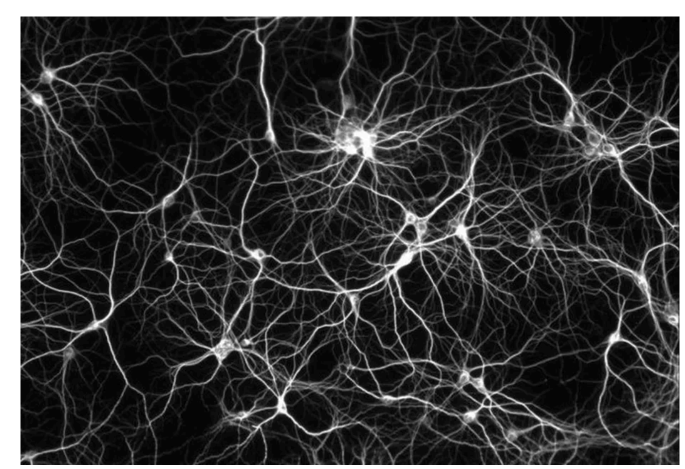
Control of uncertainties

Distribution ~ Population

Dynamic shaping of swarms



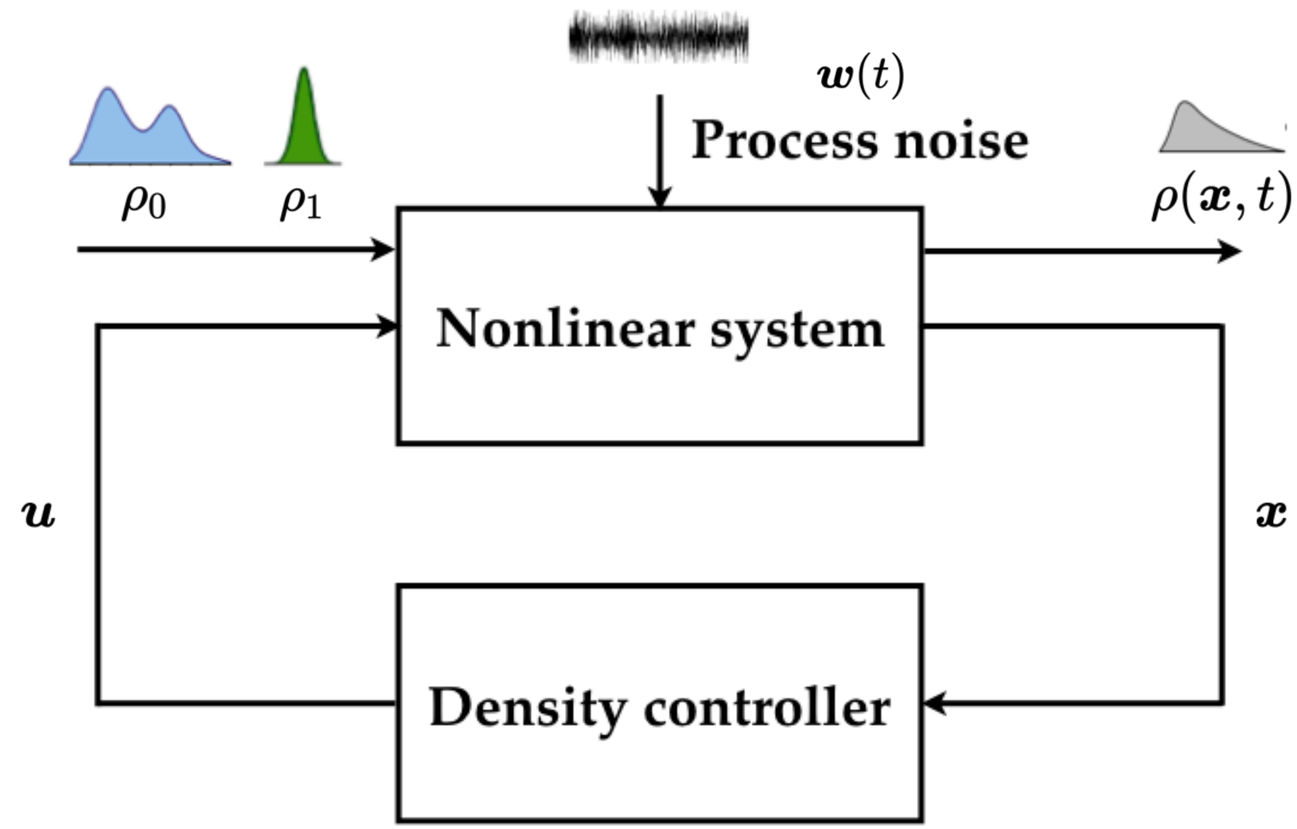
Feedback sync. and desync. of neuronal population



Control of ensemble

State Feedback Density Steering

Steer joint state PDF via feedback control over finite time horizon



Common scenario: $G \equiv B$

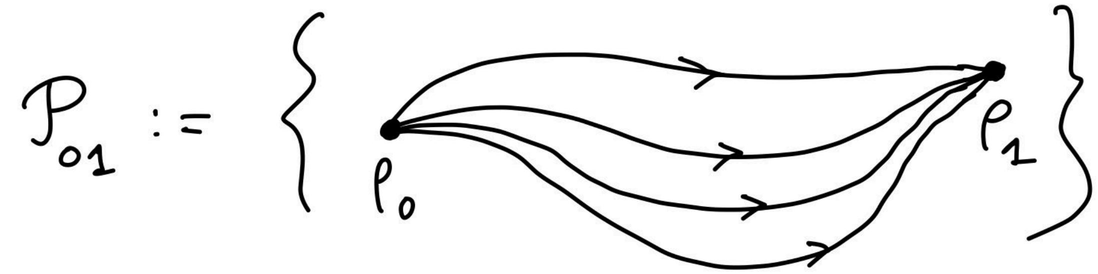
$$\underset{u \in \mathcal{U}}{\text{minimize}} \quad \mathbb{E}\left[\int_0^1 \left(\frac{1}{2}\|u(t, x_t^u)\|_2^2 + q(t, x_t^u)\right) \mathrm{d}t\right]$$

subject to

$$\mathrm{d}x_t^u = \{f(t, x_t^u) + B(t, x_t^u)u\}\mathrm{d}t + \sqrt{2}G(t, x_t^u)\mathrm{d}w_t$$

$$x_0^u := x_t^u(t = 0) \sim \rho_0, \quad x_1^u := x_t^u(t = 1) \sim \rho_1$$

Optimal Control Problem over PDFs



Diffusion tensor: $\boldsymbol{D} := \boldsymbol{G}\boldsymbol{G}^\top$

Hessian operator w.r.t. state: Hess

$$\inf_{(\rho,\boldsymbol{u})\in\mathcal{P}_{01}\times\mathcal{U}} \quad \int_{\mathbb{R}^n}\int_0^1 \left(\frac{1}{2}\|\boldsymbol{u}(t,\boldsymbol{x}_t^{\boldsymbol{u}})\|_2^2 + q(t,\boldsymbol{x}_t^{\boldsymbol{u}})\right)\rho(t,\boldsymbol{x}_t^{\boldsymbol{u}})\,\mathrm{d}t\,\mathrm{d}\boldsymbol{x}_t^{\boldsymbol{u}}$$

subject to

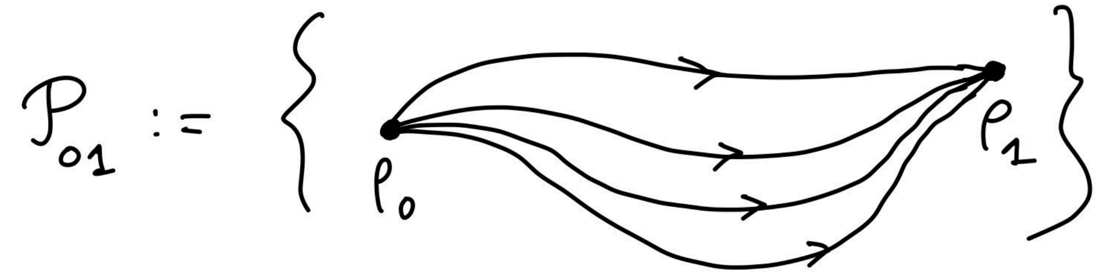
$$\frac{\partial\rho}{\partial t} + \nabla\cdot\left((\boldsymbol{f}+\boldsymbol{B}\boldsymbol{u})\,\rho\right) = \langle \mathrm{Hess}, \boldsymbol{D}\rho\rangle$$

$$\rho(t=0,\boldsymbol{x}_0^{u}) = \rho_0, \quad \rho(t=1,\boldsymbol{x}_1^{u}) = \rho_1$$

Controlled Fokker-Planck or Kolmogorov's forward PDE

Zero Process Noise ⇝ Optimal Mass Transport

Dynamic optimal mass transport
with prior dynamics $\boldsymbol{f}$



$$\inf_{(\rho,\boldsymbol{u})\in\mathcal{P}_{01}\times\mathcal{U}} \quad \int_{\mathbb{R}^n}\int_0^1 \left(\frac{1}{2}\|\boldsymbol{u}(t,\boldsymbol{x}_t^{\boldsymbol{u}})\|_2^2 + q(t,\boldsymbol{x}_t^{\boldsymbol{u}})\right)\rho(t,\boldsymbol{x}_t^{\boldsymbol{u}})\,\mathrm{d}t\,\mathrm{d}\boldsymbol{x}_t^{\boldsymbol{u}}$$

subject to

0

$$\frac{\partial\rho}{\partial t} + \nabla\cdot((\boldsymbol{f}+\boldsymbol{B}\boldsymbol{u})\,\rho) = \langle \mathrm{Hess}, \boldsymbol{D}\rho\rangle$$

$$\rho(t=0,\boldsymbol{x}_0^{u}) = \rho_0, \quad \rho(t=1,\boldsymbol{x}_1^{u}) = \rho_1$$

Controlled Liouville PDE

Necessary Conditions of Optimality (Assuming $G \equiv B$)

Coupled nonlinear PDEs + linear boundary conditions

Controlled Fokker-Planck or Kolmogorov's forward PDE

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

Hamilton-Jacobi-Bellman-like PDE

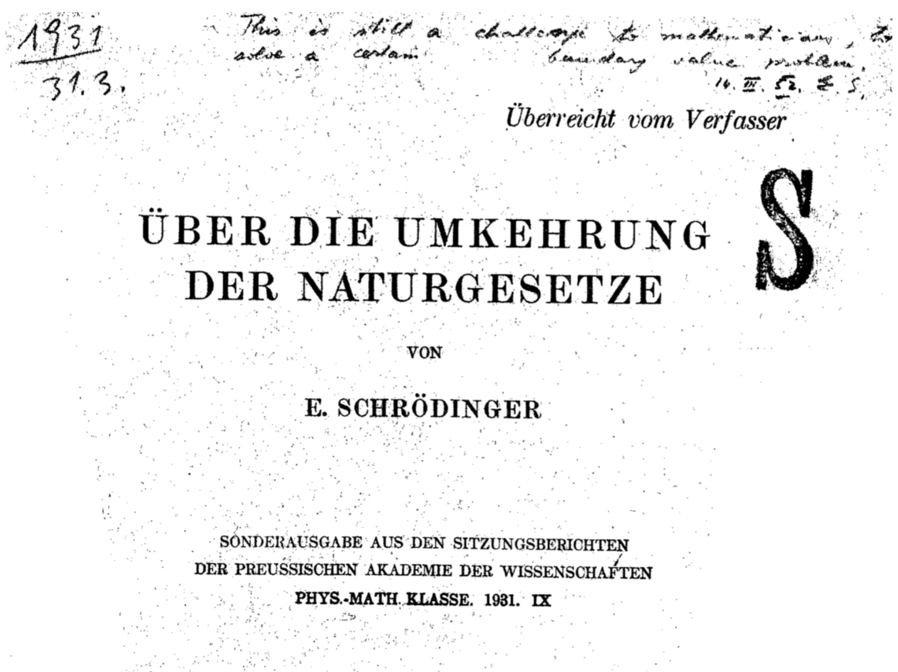
$$\frac{\partial \psi}{\partial t} + \langle \nabla \psi, \boldsymbol{f} \rangle + \langle \boldsymbol{D}, \text{Hess}(\psi) \rangle + \frac{1}{2} \langle \nabla \psi, \boldsymbol{D} \nabla \psi \rangle = q$$

Boundary conditions:

$$\rho^{\text{opt}}(\cdot, t = 0) = \rho_0, \quad \rho^{\text{opt}}(\cdot, t = 1) = \rho_1$$

Optimal control: $\boldsymbol{u}^{\text{opt}} = \boldsymbol{B}^\top \nabla \psi$

Feedback Synthesis via the Schrödinger System



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

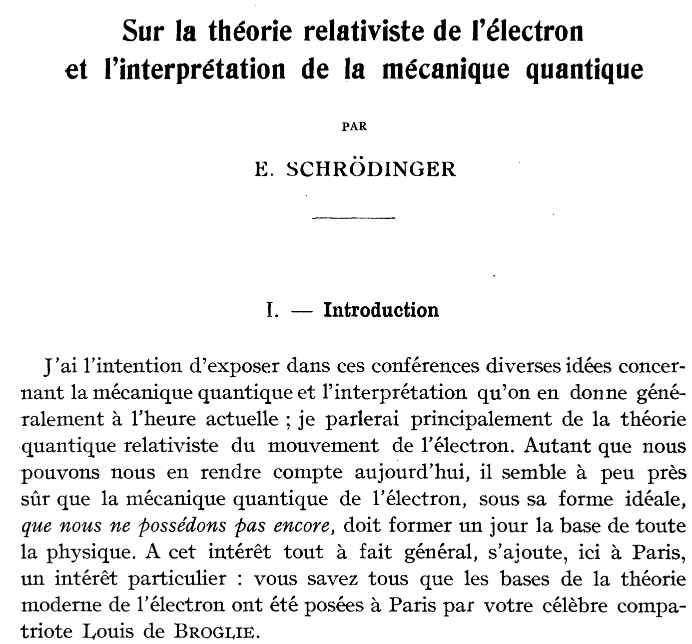
S

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.

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

$$\left(\rho^{\text{opt}}, \psi\right) \mapsto \left(\widehat{\varphi}, \varphi\right)$$ — **Schrödinger factors**

$$\widehat{\varphi}(\boldsymbol{x}, t) = \rho^{\text{opt}}(\boldsymbol{x}, t) \exp\left(-\psi\left(\boldsymbol{x}, t\right)\right)$$

$$\varphi(\boldsymbol{x}, t) = \exp\left(\psi\left(\boldsymbol{x}, t\right)\right) \qquad \text{for all} \qquad (\boldsymbol{x}, t) \in \mathbb{R}^n \times [0, 1]$$

Feedback Synthesis via the Schrödinger System

2 coupled nonlinear PDEs $\longrightarrow$ boundary-coupled linear PDEs!!

Uncontrolled forward-backward Kolmogorov PDEs:

$$\frac{\partial \widehat{\varphi}}{\partial t} = -\nabla \cdot (\widehat{\varphi}\boldsymbol{f}) + \langle \text{Hess}, \boldsymbol{D}\widehat{\varphi} \rangle - q\widehat{\varphi}, \qquad \widehat{\varphi}_0 \varphi_0 = \rho_0,$$

$$\frac{\partial \varphi}{\partial t} = -\langle \nabla \varphi, \boldsymbol{f} \rangle - \langle \text{Hess}(\varphi), \boldsymbol{D} \rangle + q\varphi, \qquad \widehat{\varphi}_1 \varphi_1 = \rho_1,$$

Optimal controlled joint state PDF: $\rho^{\text{opt}}(\boldsymbol{x}, t) = \widehat{\varphi}(\boldsymbol{x}, t)\varphi(\boldsymbol{x}, t)$

Optimal control: $\boldsymbol{u}^{\text{opt}}(\boldsymbol{x}, t) = 2\boldsymbol{B}^{\top} \nabla_{\boldsymbol{x}} \log \varphi(\boldsymbol{x}, t)$

What Exactly are Schrödinger Factors?

Classical: $$\rho^{\text{opt}}(\boldsymbol{x},t) = \varphi(\boldsymbol{x},t)\widehat{\varphi}(\boldsymbol{x},t)$$

$$\left(\frac{\partial}{\partial t} + \frac{1}{2}\Delta - q\right)\varphi = 0$$ [Backward reaction-diffusion PDE]

$$\left(\frac{\partial}{\partial t} - \frac{1}{2}\Delta + q\right)\widehat{\varphi} = 0$$ [Forward reaction-diffusion PDE]

Quantum: $$\rho^{\text{opt}}(\boldsymbol{x},t) = \Psi(\boldsymbol{x},t)\widehat{\Psi}(\boldsymbol{x},t)$$ [Born's relation]

wave function

$$\left(\sqrt{-1}\frac{\partial}{\partial t} + \frac{1}{2}\Delta - q\right)\Psi = 0$$ [Schrödinger PDE]

$$\left(-\sqrt{-1}\frac{\partial}{\partial t} - \frac{1}{2}\Delta + q\right)\widehat{\Psi} = 0$$ [Adjoint Schrödinger PDE]

Feedback Synthesis via the Schrödinger System

2 coupled nonlinear PDEs $\longrightarrow$ boundary-coupled linear PDEs!!

Uncontrolled forward-backward Kolmogorov PDEs:

$$\frac{\partial \widehat{\varphi}}{\partial t} = \boxed{-\nabla \cdot (\widehat{\varphi}\boldsymbol{f}) + \langle \text{Hess}, \boldsymbol{D}\widehat{\varphi}\rangle - q\widehat{\varphi},} \qquad \widehat{\varphi}_0\varphi_0 = \rho_0,$$

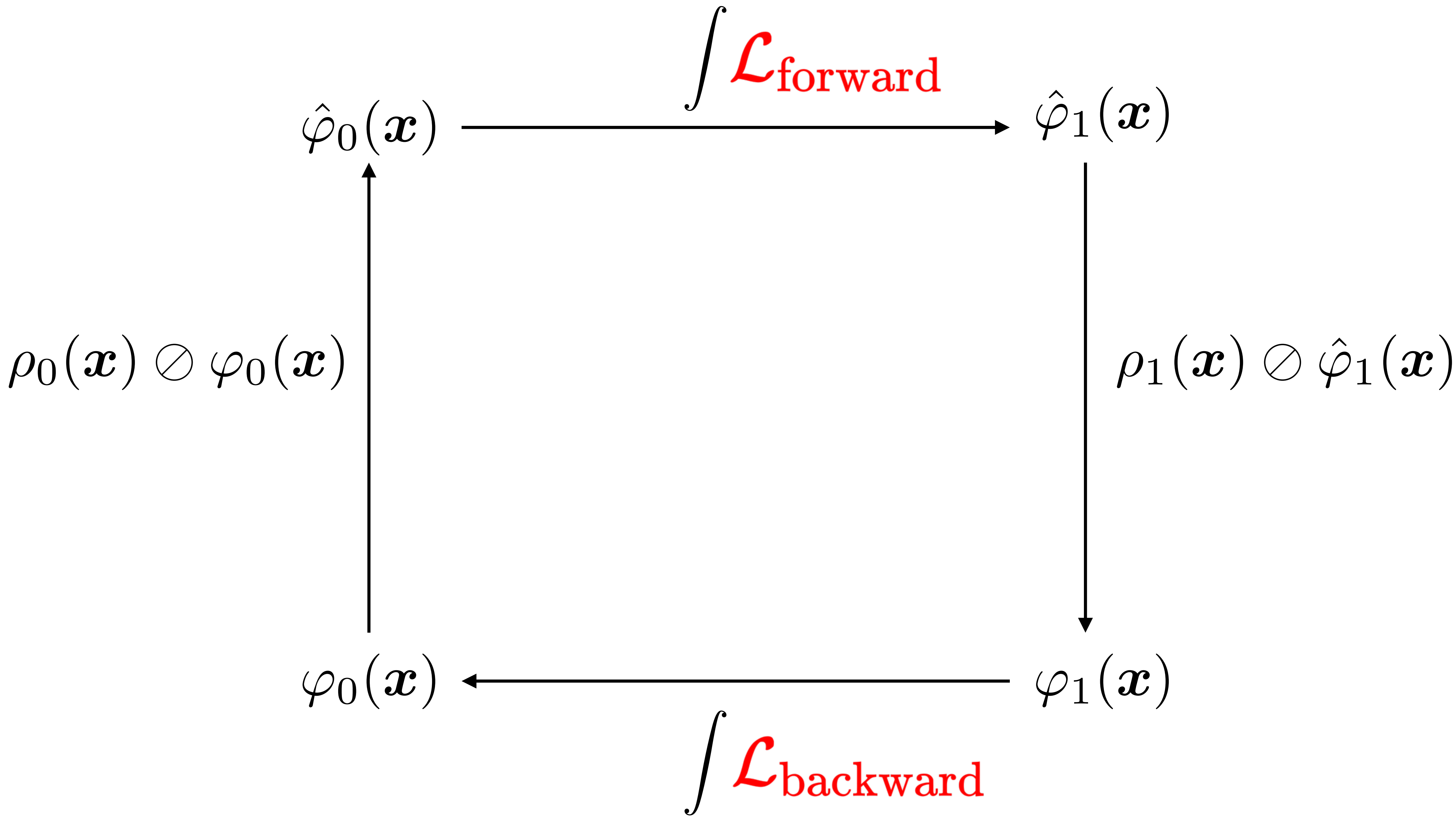
$$\frac{\partial \varphi}{\partial t} = \boxed{-\langle \nabla\varphi, \boldsymbol{f}\rangle - \langle \text{Hess}(\varphi), \boldsymbol{D}\rangle + q\varphi,} \qquad \widehat{\varphi}_1\varphi_1 = \rho_1,$$

$\mathcal{L}_{\text{forward}}\widehat{\varphi}$ $\quad$ $\mathcal{L}_{\text{backward}}\varphi$

Optimal controlled joint state PDF: $\rho^{\text{opt}}(\boldsymbol{x}, t) = \widehat{\varphi}(\boldsymbol{x}, t)\varphi(\boldsymbol{x}, t)$

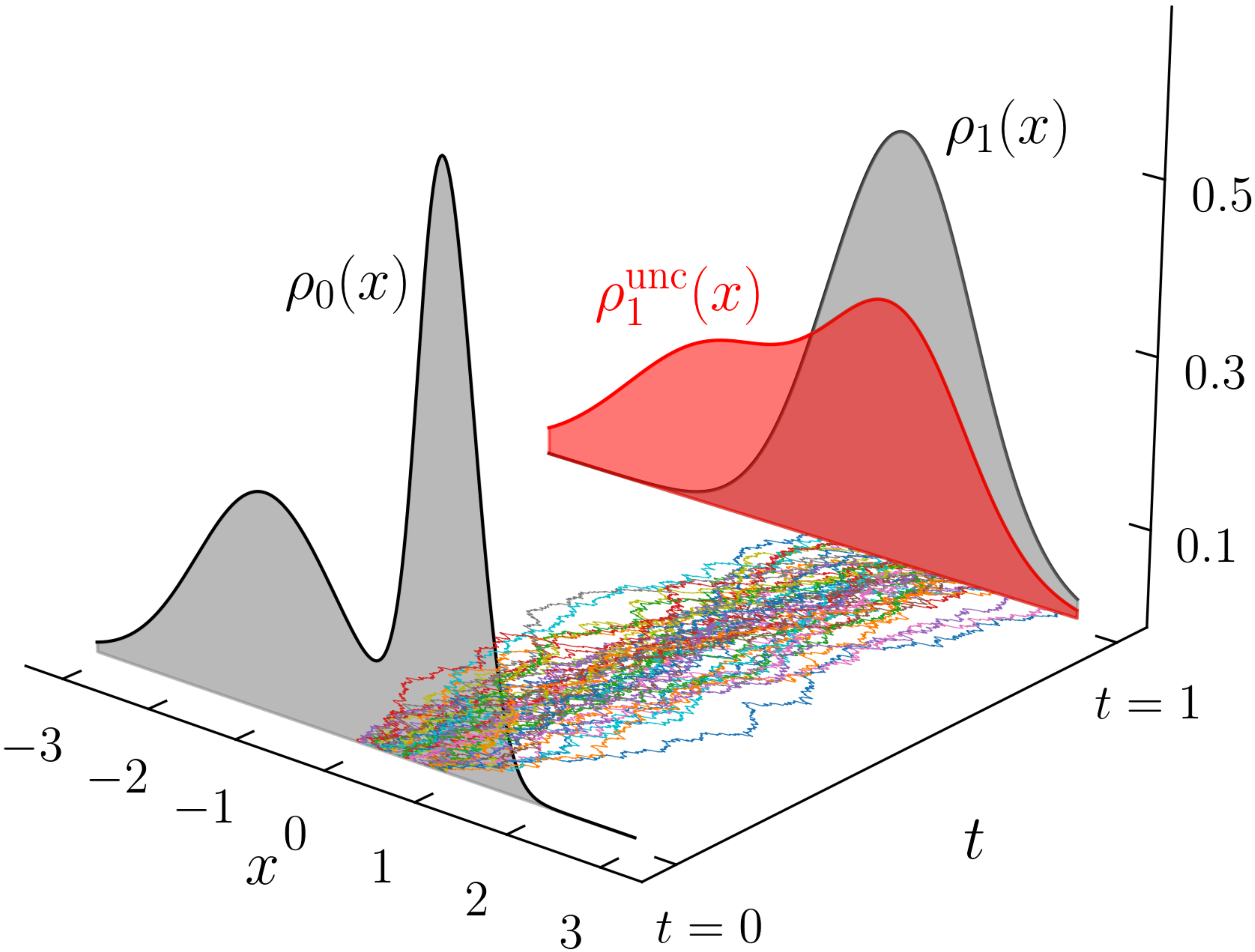
Optimal control: $\boldsymbol{u}^{\text{opt}}(\boldsymbol{x}, t) = 2\boldsymbol{B}^{\top}\nabla_{\boldsymbol{x}} \log \varphi(\boldsymbol{x}, t)$

Fixed Point Recursion Over Pair $(\varphi_1, \hat{\varphi}_0)$



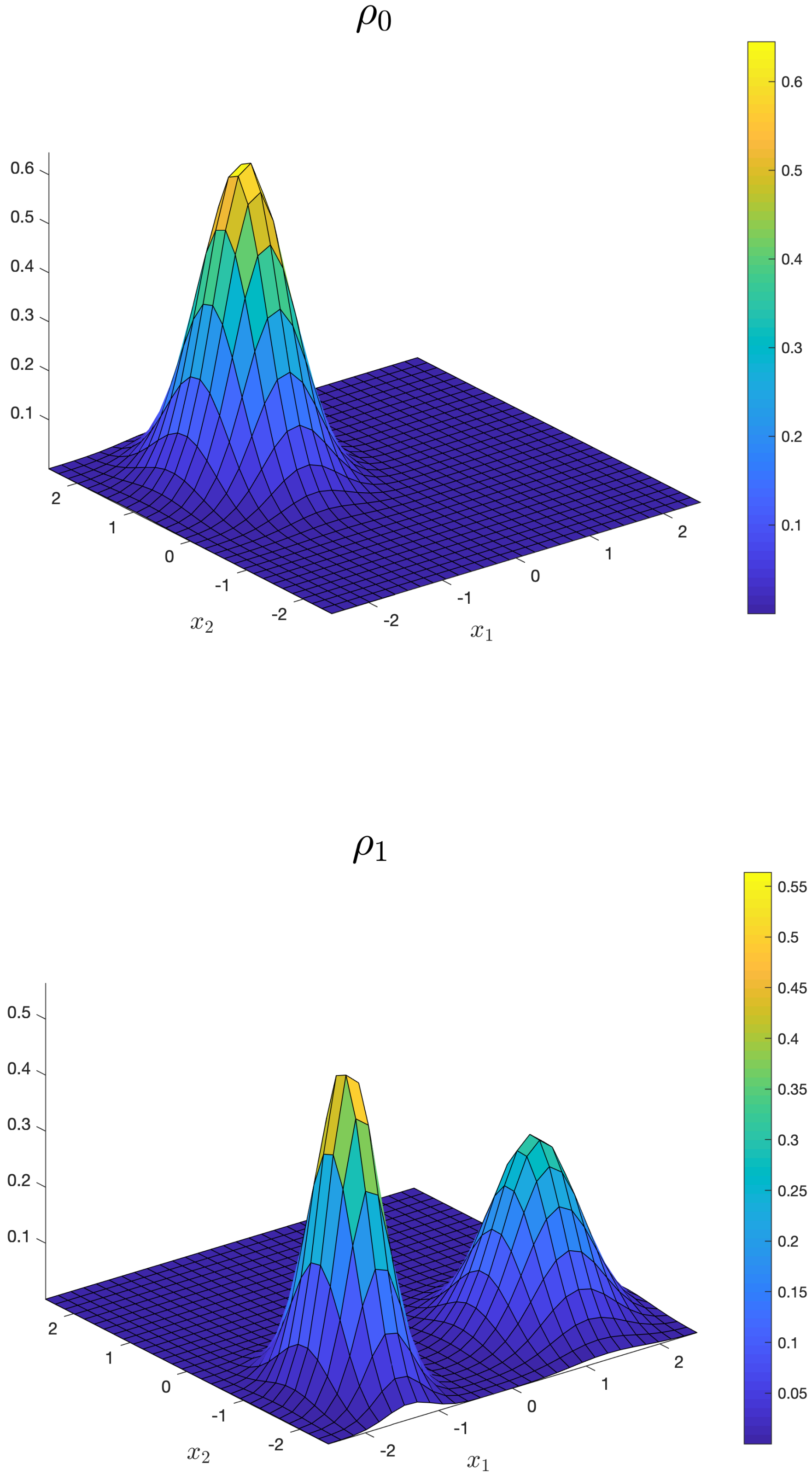
This recursion is contractive in the Hilbert's projective metric!!

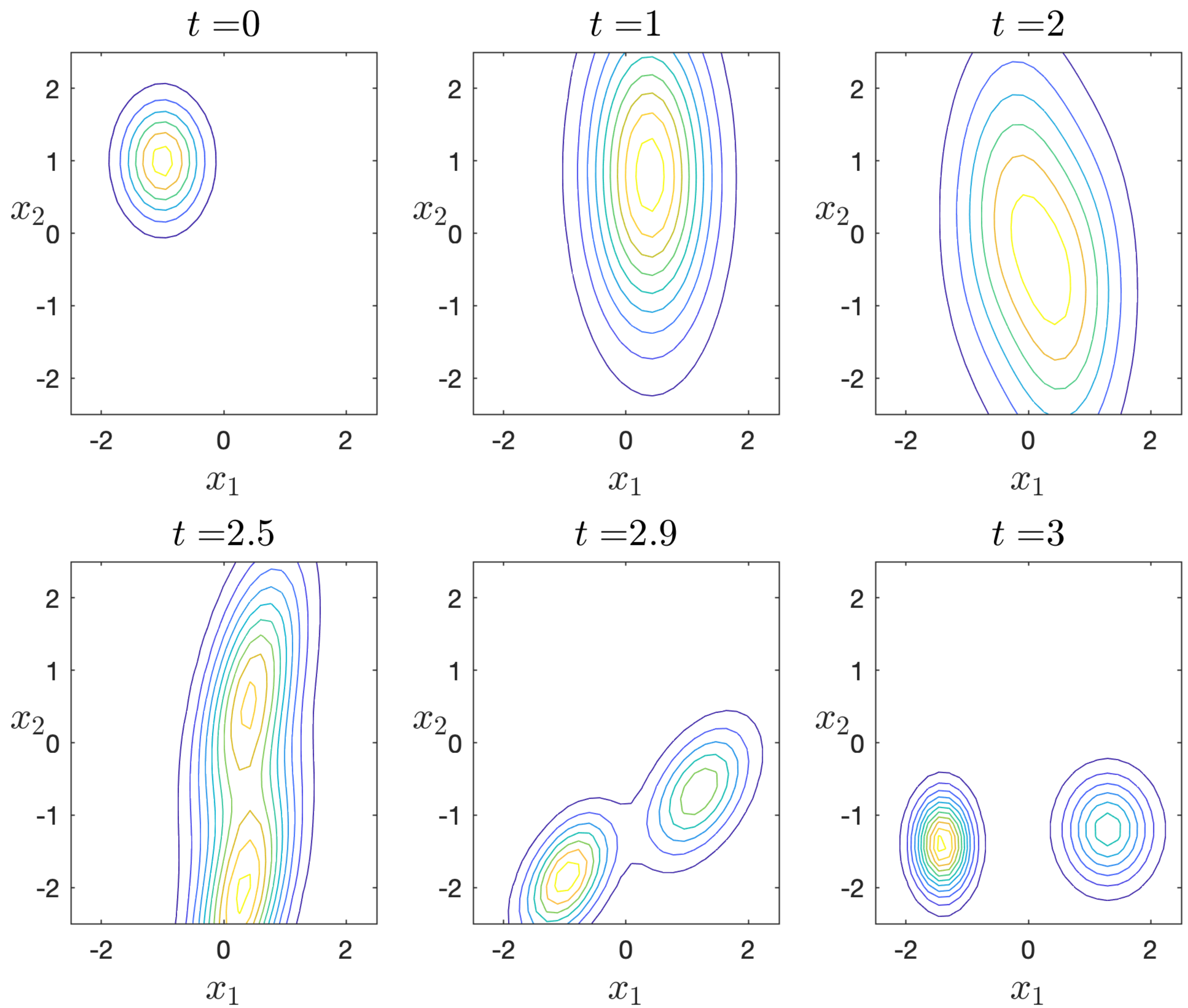
Feedback Density Control: $f \equiv \mathbf{0}, \boldsymbol{B} = \boldsymbol{G} \equiv \boldsymbol{I}, q \equiv 0$



Zero prior dynamics

Feedback Density Control: $f \equiv Ax, B = G, q \equiv 0$

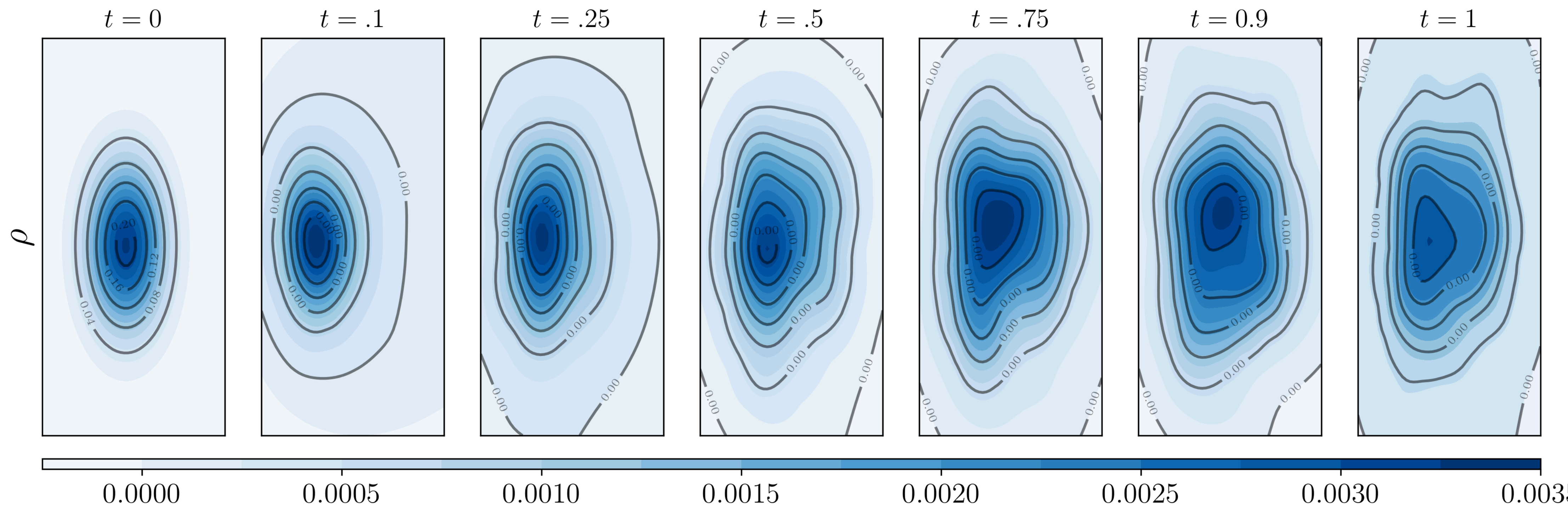




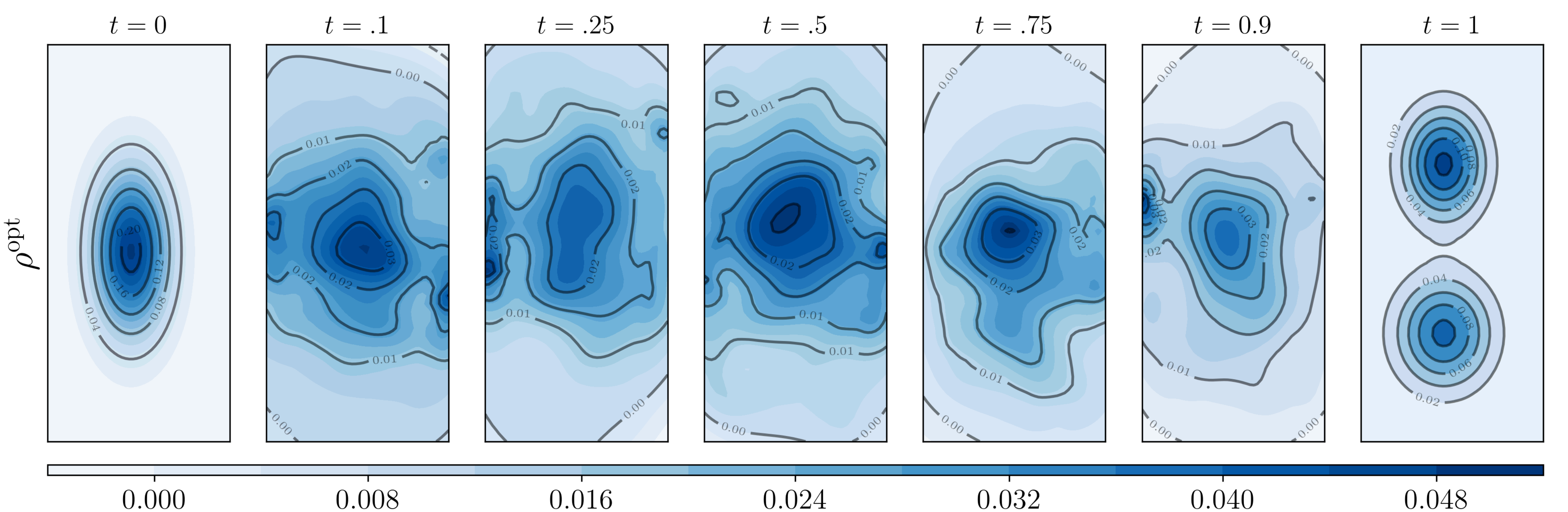
Linear prior dynamics

Feedback Density Control: Nonlinear Grad. Drift

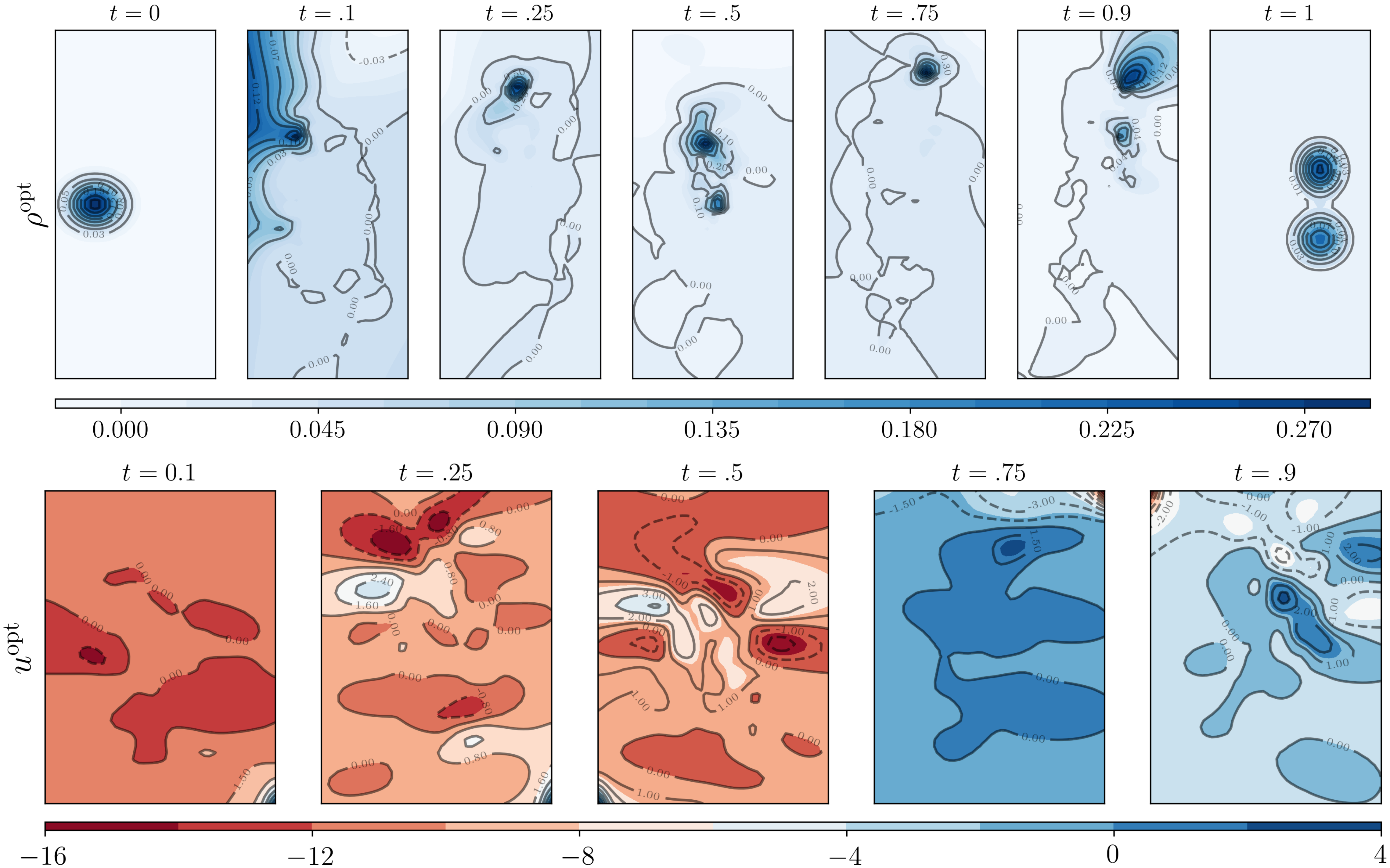
Uncontrolled joint PDF evolution:



Optimal controlled joint PDF evolution:

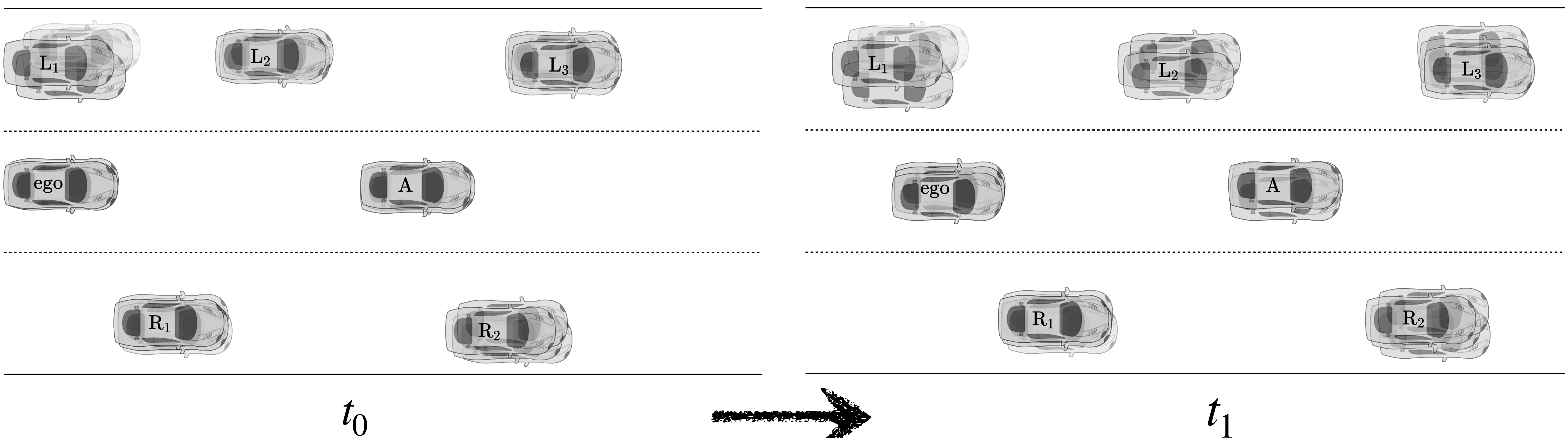


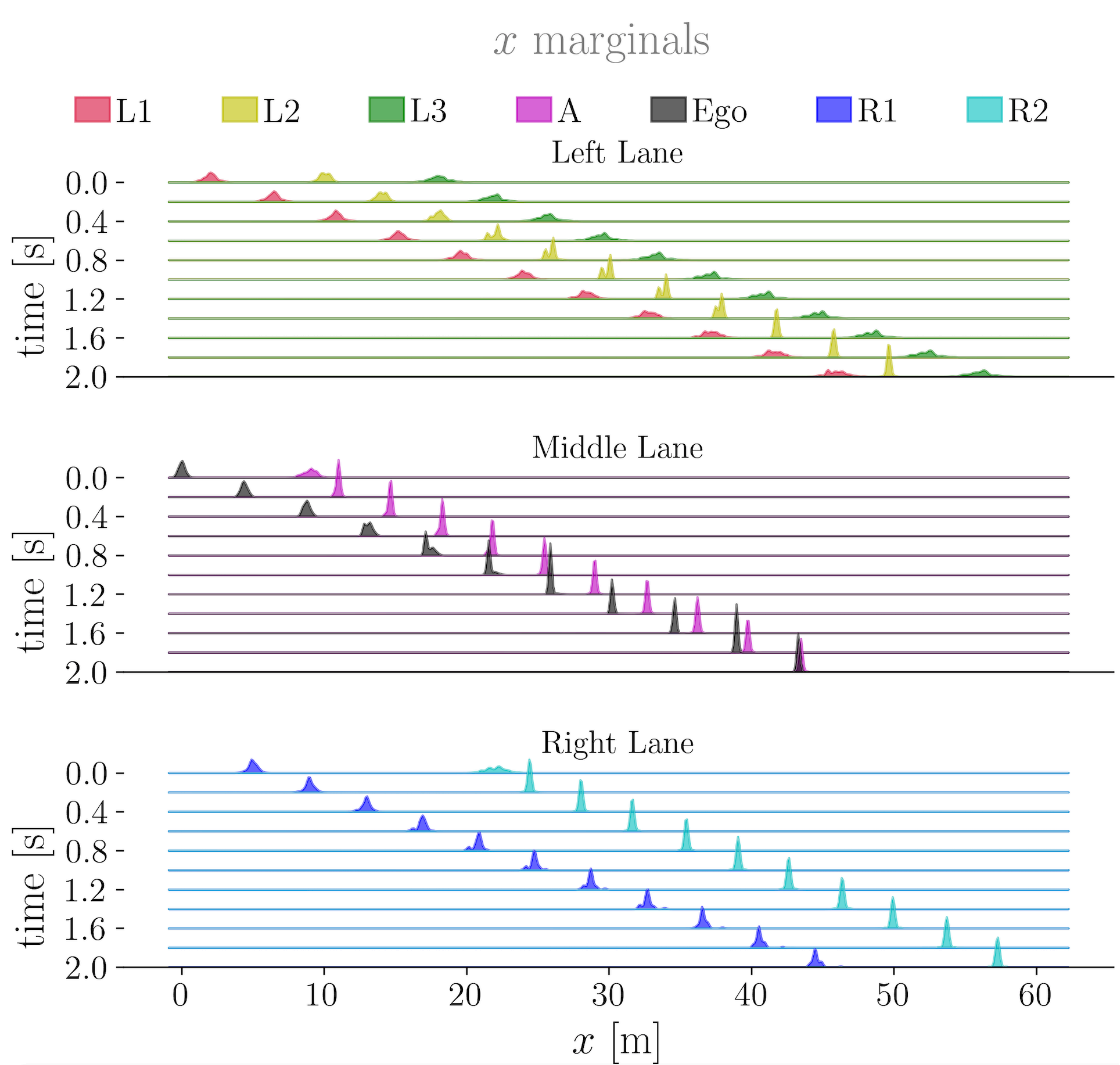
Feedback Density Control: Mixed Conservative-Dissipative Drift

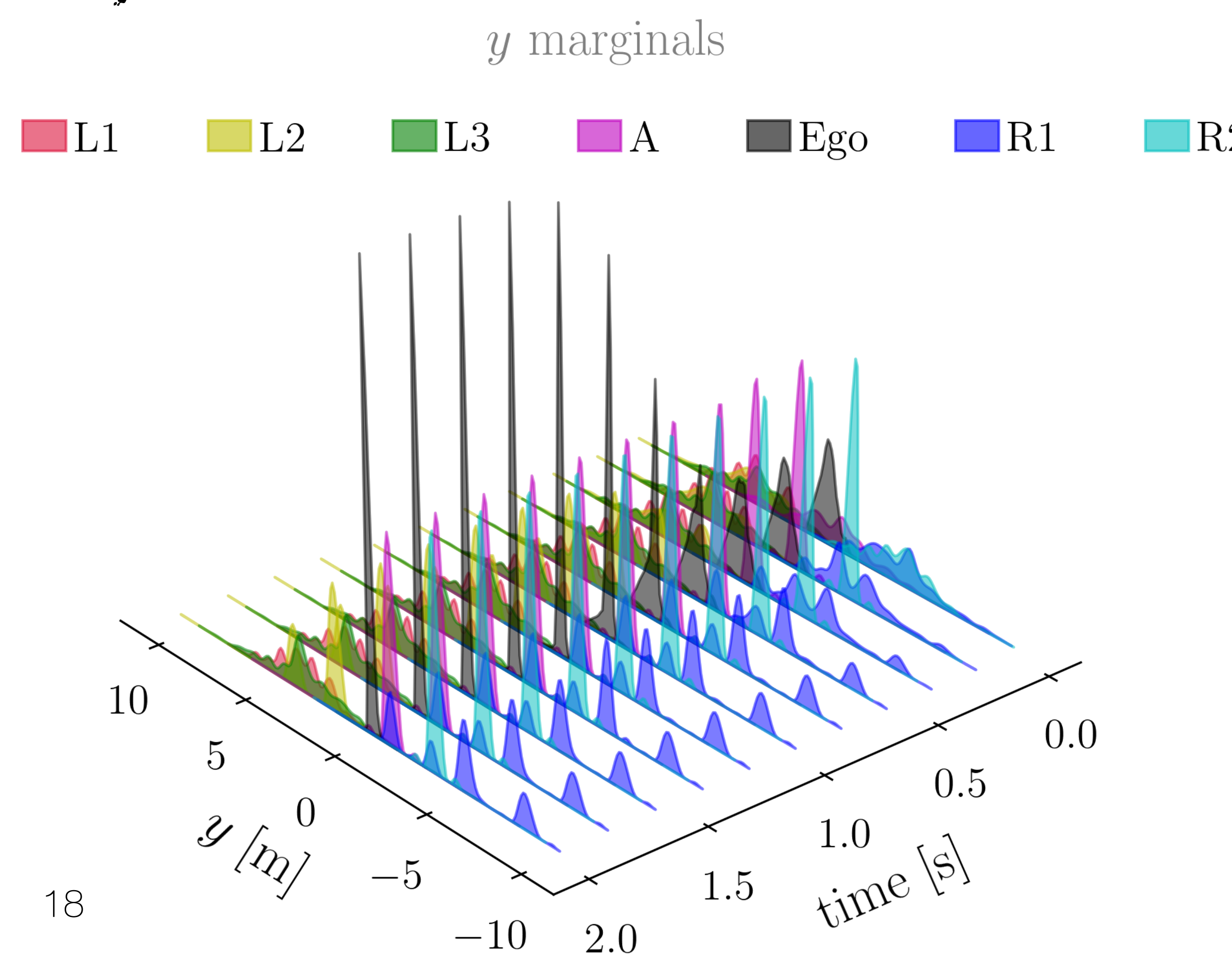


K.F. Caluya and A.H., Wasserstein proximal algorithms for the Schrödinger bridge problem: density control with nonlinear drift, *IEEE TAC* 2021.

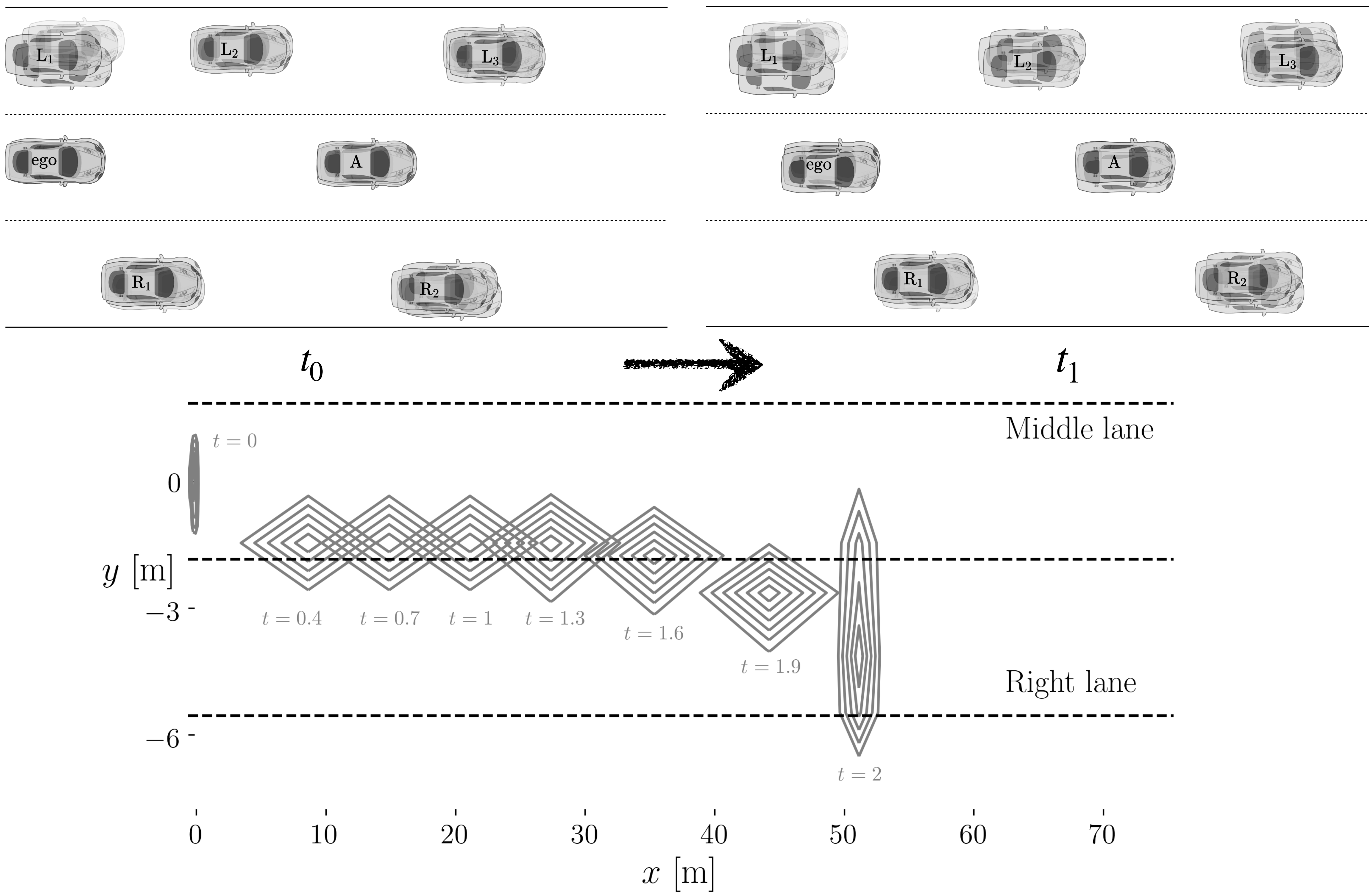
Application: Multi-lane Automated Driving







Application: Multi-lane Automated Driving



Hard Path Constraints: Reflected SBP

Main idea: path constraints $\sim$ reflected Itô SDEs
modify the controlled sample path dynamics to

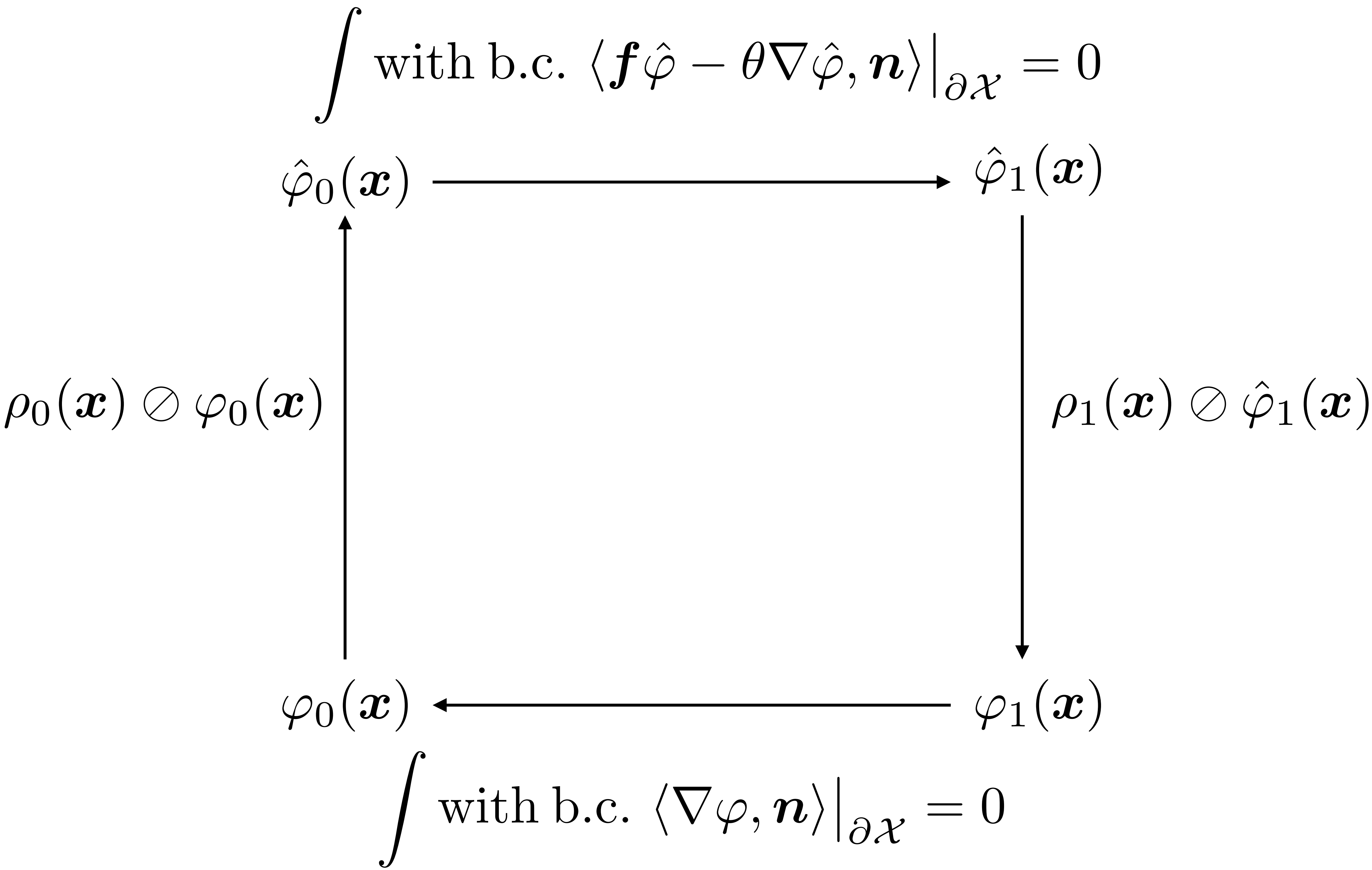
$$\mathrm{d}\boldsymbol{x}_t^{\boldsymbol{u}} = \{\boldsymbol{f}(t, \boldsymbol{x}_t^{\boldsymbol{u}}) + \boldsymbol{B}(t)\boldsymbol{u}(t, \boldsymbol{x}_t^{\boldsymbol{u}})\}\mathrm{d}t + \sqrt{2\theta}\boldsymbol{G}(t)\mathrm{d}\boldsymbol{w}_t + \boldsymbol{n}(\boldsymbol{x}_t^{\boldsymbol{u}})\mathrm{d}\gamma_t$$

$\boldsymbol{x}_t^{\boldsymbol{u}} \in \overline{\mathcal{X}} := \mathcal{X} \cup \partial\mathcal{X}$, closure of connected smooth $\mathcal{X}$

$\boldsymbol{n}$ is inward unit normal to the boundary $\partial\mathcal{X}$

γ_t is minimal local time stochastic process

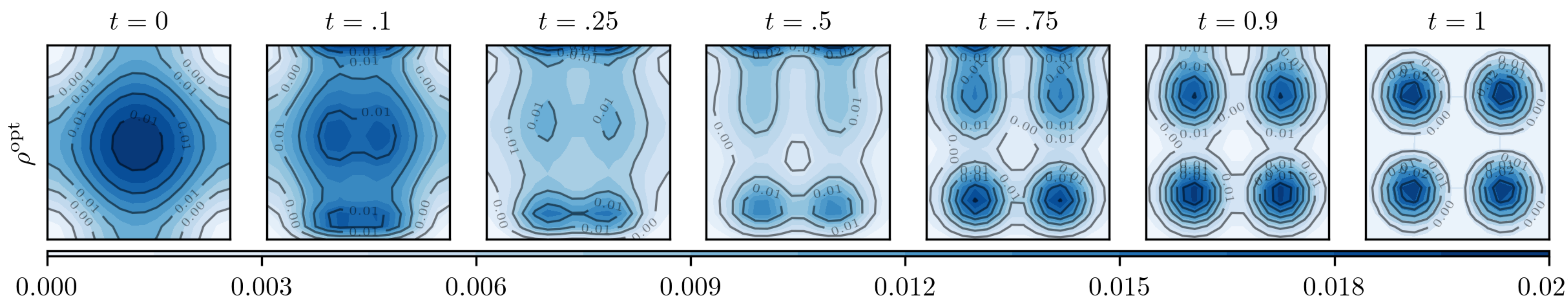
Reflected SBP: Schrödinger Factor Recursion



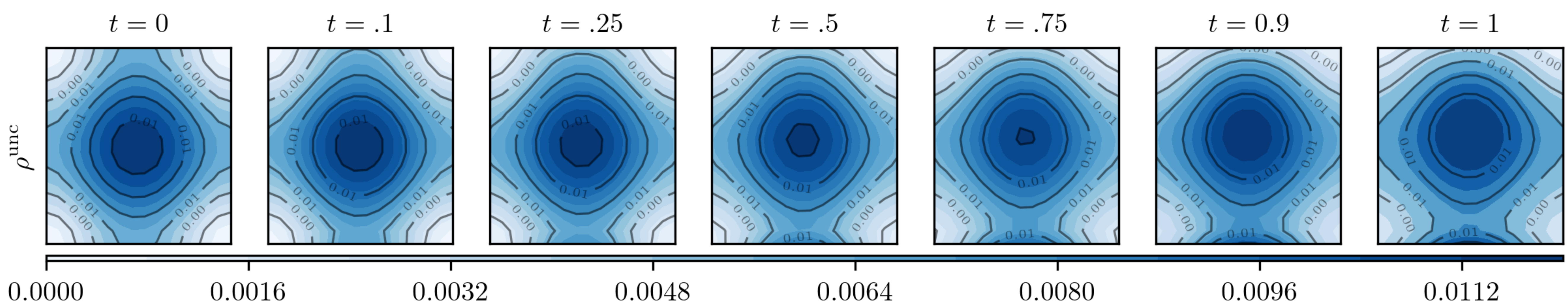
Reflected SBP: Numerics with Gradient Drift

$$V(x_1, x_2) = (x_1^2 + x_2^3)/5, \quad \overline{\mathcal{X}} = [-4, 4]^2$$

Optimal controlled state PDFs:



Uncontrolled state PDFs:



Control Non-affine SBP: Optimality Conditions

$m+2$ coupled PDEs with endpoint boundary conditions:

Drift coefficient   Diffusion tensor

$$\frac{\partial \psi}{\partial t} = \frac{1}{2}\|\boldsymbol{u}_{\text{opt}}\|_2^2 - \langle \nabla_{\boldsymbol{x}}\psi, \boldsymbol{f}\rangle - \langle \boldsymbol{G}, \textbf{Hess}(\psi)\rangle,$$

$$\frac{\partial \rho_{\text{opt}}^{\boldsymbol{u}}}{\partial t} = -\nabla.(\rho_{\text{opt}}^{\boldsymbol{u}}\boldsymbol{f}) + \langle \boldsymbol{G}, \textbf{Hess}(\rho_{\text{opt}}^{\boldsymbol{u}})\rangle,$$

$$\boldsymbol{u}_{\text{opt}} = \nabla_{\boldsymbol{u}_{\text{opt}}}\left(\langle \nabla_{\boldsymbol{x}}\psi, \boldsymbol{f}\rangle + \langle \boldsymbol{G}, \textbf{Hess}(\psi)\rangle\right),$$

$$\rho_{\text{opt}}^{\boldsymbol{u}}(0,\boldsymbol{x}) = \rho_0, \qquad \rho_{\text{opt}}^{\boldsymbol{u}}(T,\boldsymbol{x}) = \rho_T,$$

Cf. classical SBP: two coupled PDEs + optimal policy explicit in value fn ψ

Outlook

- Density control and learning: undergoing rapid developments

- Lots of mathematics, algorithms and applications to be done

- Growing community in systems-control

- Strong intersections with many areas: probability, analysis, geometry, optimization, AI/ML, statistics, information theory, robotics, systems biology

Thank You

Support: