

# Gradient Flows for Prediction and Control of Densities

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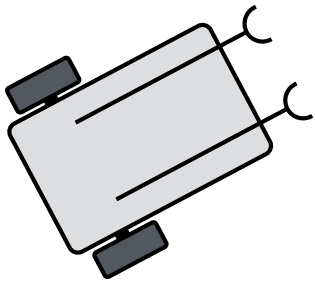
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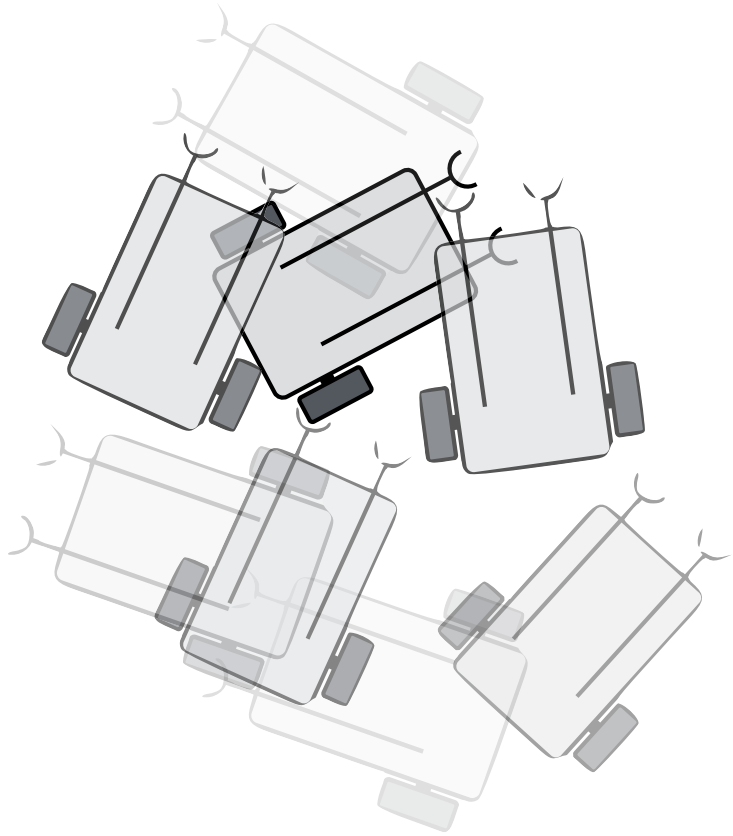
**What is density?**

# Probability Density Fn.



$$x(t) \in \mathcal{X} \equiv \mathbb{R}^2 \times S^1$$

# Probability Density Fn.



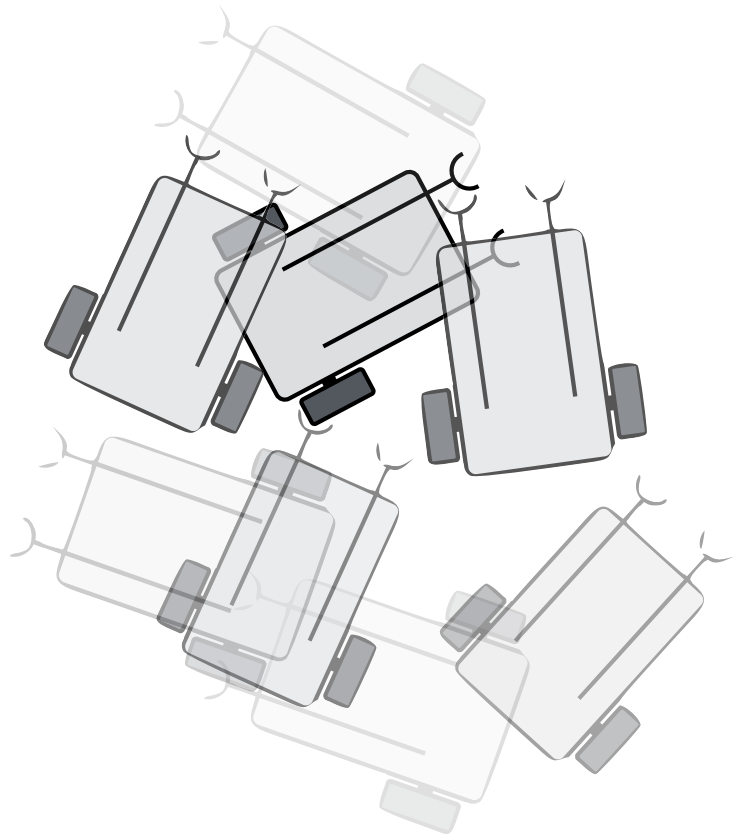
$$x(t) \in \mathcal{X} \equiv \mathbb{R}^2 \times \mathbb{S}^1$$

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

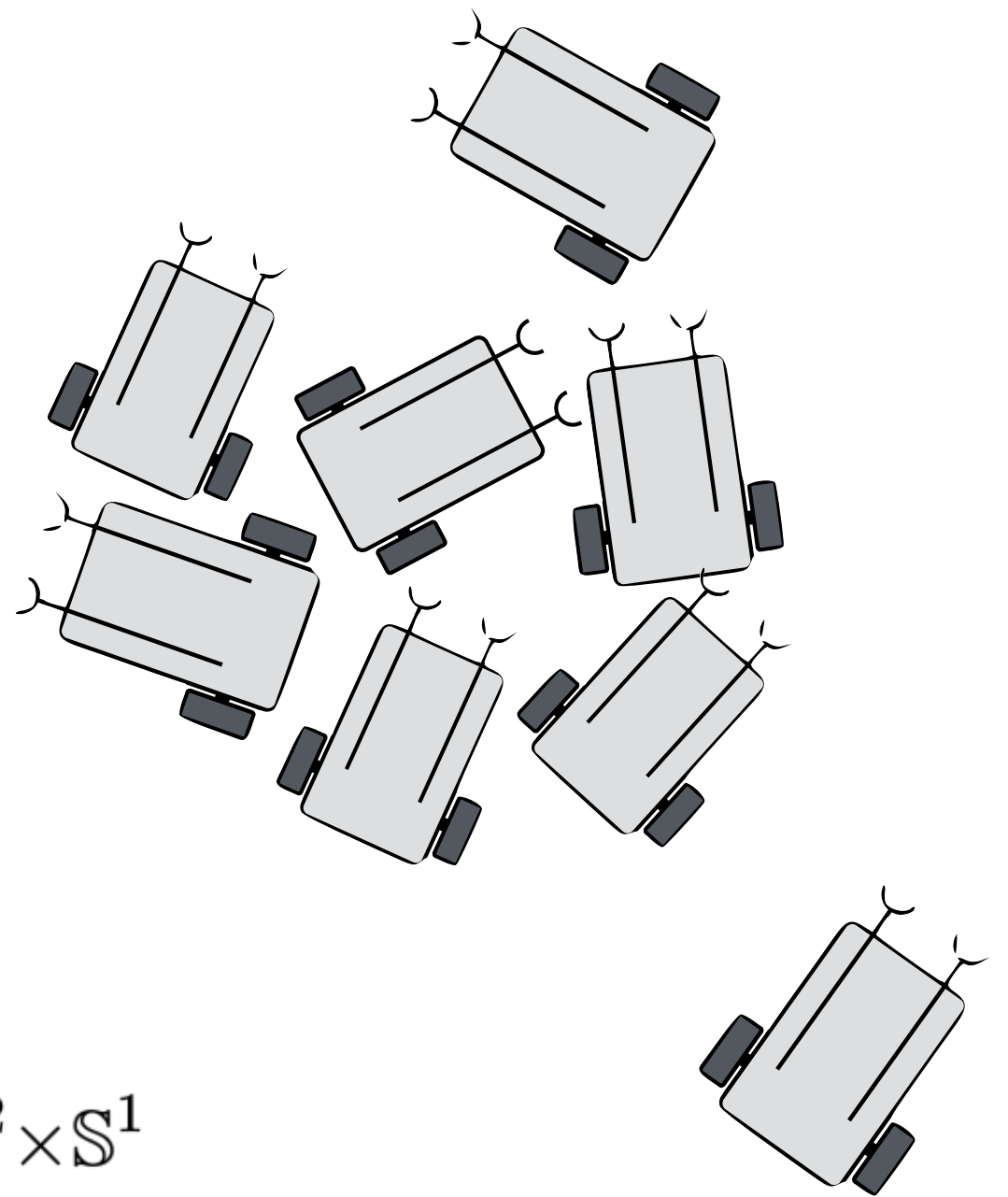
$$\int_{\mathcal{X}} \rho \, dx = 1 \quad \text{for all } t \in [0, \infty)$$



# Probability Density Fn.



# Population Density Fn.



$$x(t) \in \mathcal{X} \equiv \mathbb{R}^2 \times \mathbb{S}^1$$

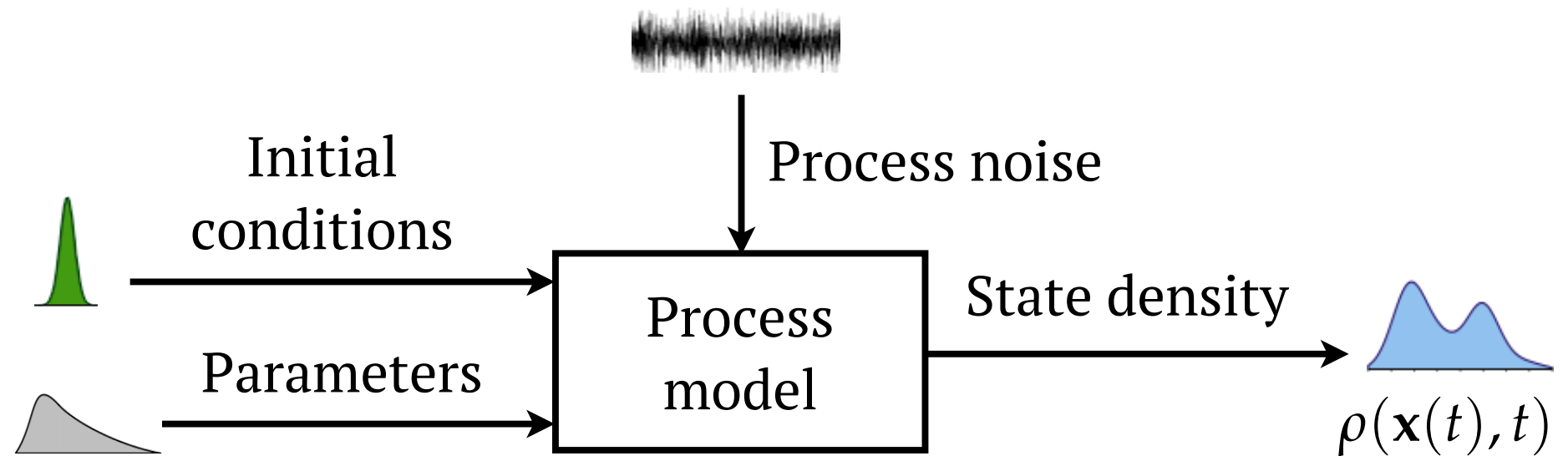
$$\rho(x, t) : \mathcal{X} \times [0, \infty) \mapsto \mathbb{R}_{\geq 0}$$

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

**Why bother about densities?**

# Prediction Problem

Compute  
joint state PDF  
 $\rho(x, t)$



**Trajectory flow:**

$$d\mathbf{x}(t) = \mathbf{f}(\mathbf{x}, t) dt + \mathbf{g}(\mathbf{x}, t) d\mathbf{w}(t), \quad d\mathbf{w}(t) \sim \mathcal{N}(0, \mathbf{Q}dt)$$

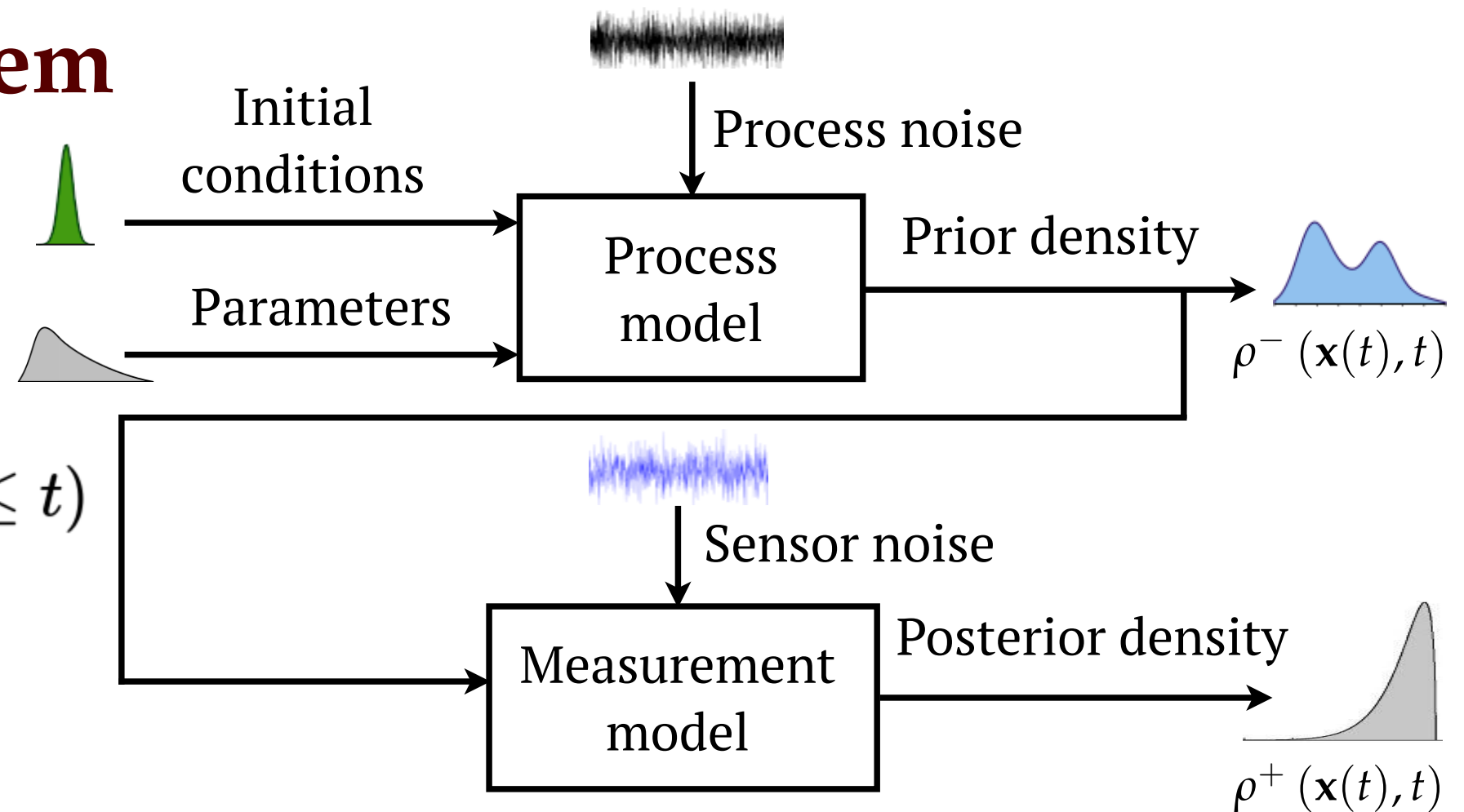
**Density flow:**

$$\frac{\partial \rho}{\partial t} = \mathcal{L}_{\text{FP}}(\rho) := -\nabla \cdot (\rho \mathbf{f}) + \frac{1}{2} \sum_{i,j=1}^n \frac{\partial^2}{\partial x_i \partial x_j} \left( \left( \mathbf{g} \mathbf{Q} \mathbf{g}^\top \right)_{ij} \rho \right)$$

# Filtering Problem

Compute conditional  
joint state PDF

$$\rho^+ \equiv \rho(x, t | z(s), 0 \leq s \leq t)$$



## Trajectory flow:

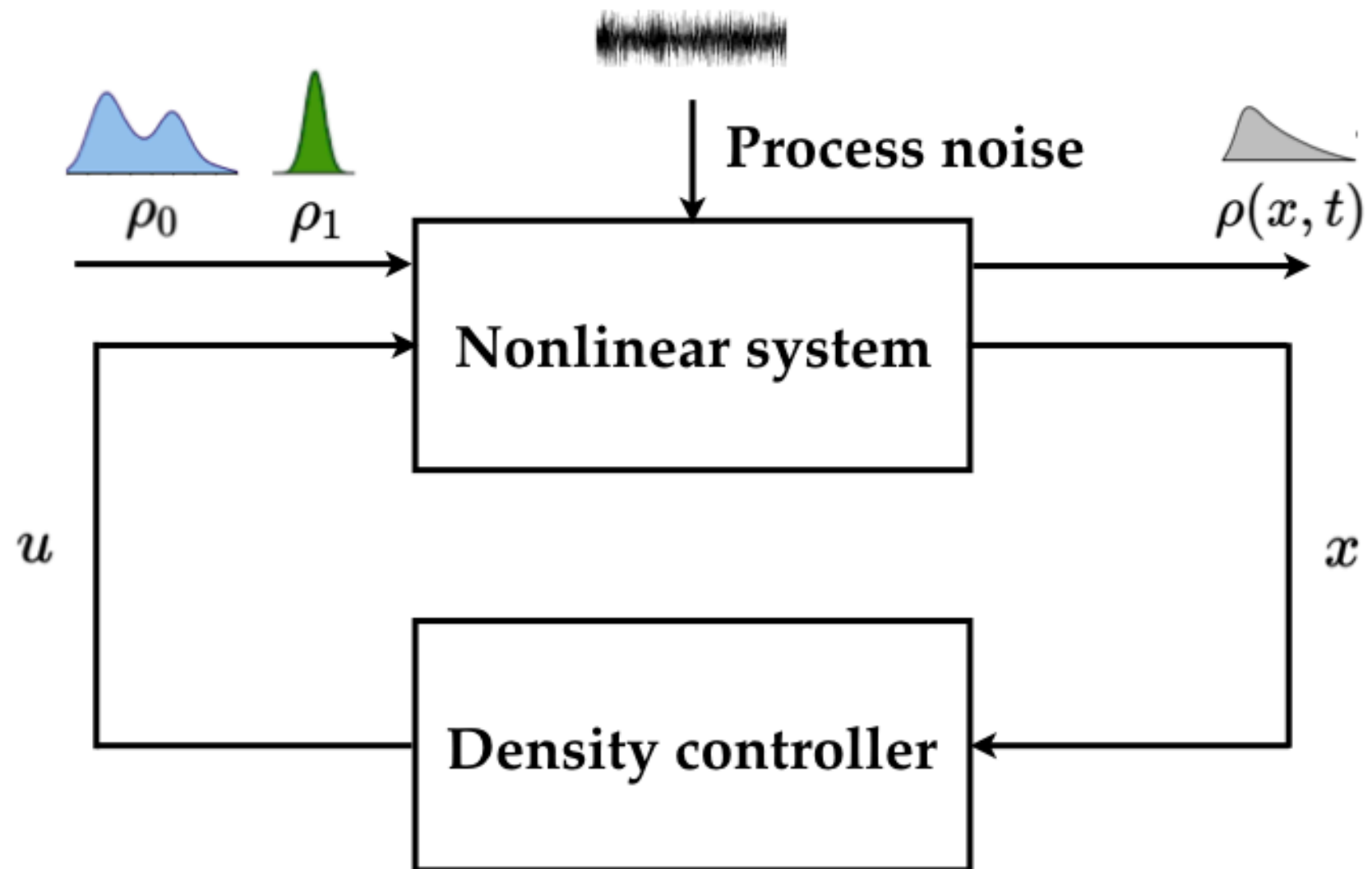
$$\begin{aligned} d\mathbf{X}(t) &= \mathbf{f}(\mathbf{X}, t) dt + \mathbf{g}(\mathbf{X}, t) d\mathbf{w}(t), & d\mathbf{w}(t) &\sim \mathcal{N}(0, \mathbf{Q}dt) \\ d\mathbf{Z}(t) &= \mathbf{h}(\mathbf{X}, t) dt + d\mathbf{v}(t), & d\mathbf{v}(t) &\sim \mathcal{N}(0, \mathbf{R}dt) \end{aligned}$$

## Density flow:

$$d\rho^+ = \left[ \mathcal{L}_{\text{FP}} dt + (\mathbf{h}(\mathbf{x}, t) - \mathbb{E}_{\rho^+}\{\mathbf{h}(\mathbf{x}, t)\})^\top \mathbf{R}^{-1} (d\mathbf{z}(t) - \mathbb{E}_{\rho^+}\{\mathbf{h}(\mathbf{x}, t)\} dt) \right] \rho^+$$

# Control Problem

Steer joint state PDF  
via feedback control



$$\underset{u \in \mathcal{U}}{\text{minimize}} \mathbb{E} \left[ \int_0^1 \|u\|_2^2 dt \right]$$

subject to

$$dx = f(x, u, t) dt + g(x, t) dw,$$

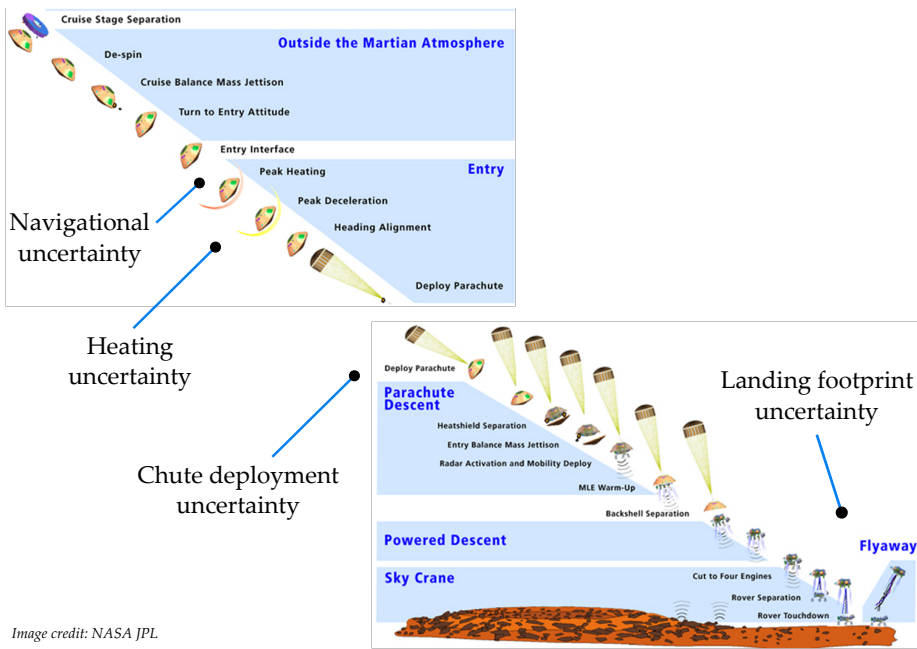
$$x(t=0) \sim \rho_0, \quad x(t=1) \sim \rho_1$$

# PDFs in Mars Entry-Descent-Landing

Prediction Problem

Filtering Problem

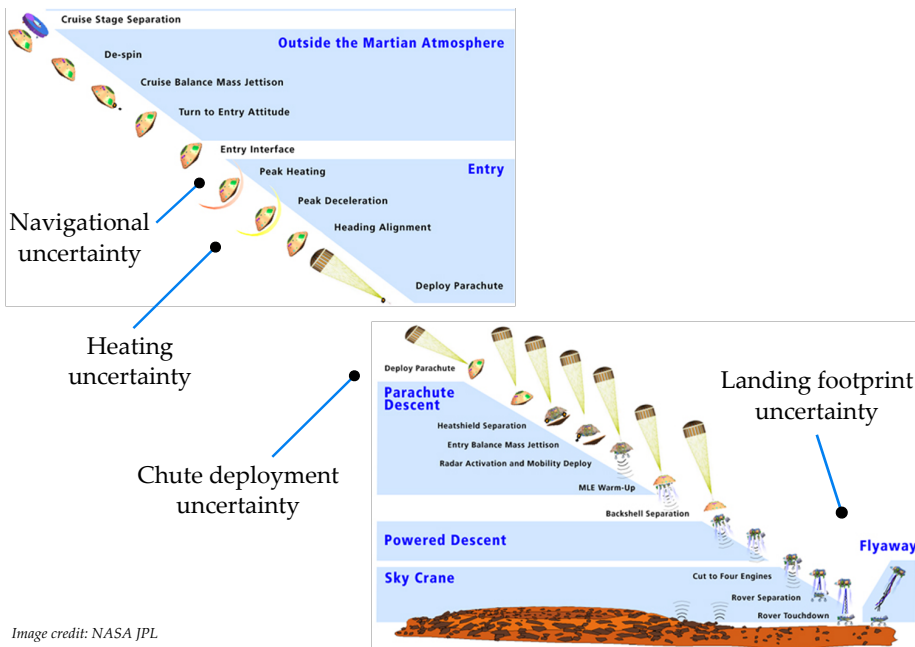
Control Problem



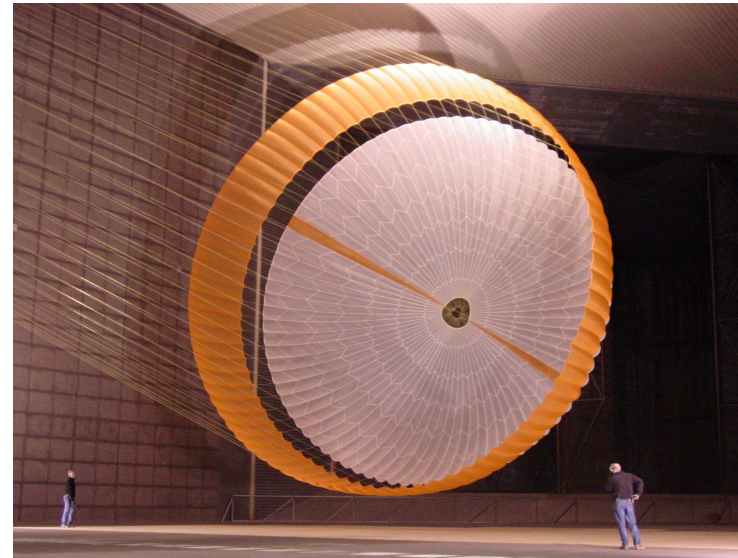
Predict heating rate uncertainty

# PDFs in Mars Entry-Descent-Landing

## Prediction Problem

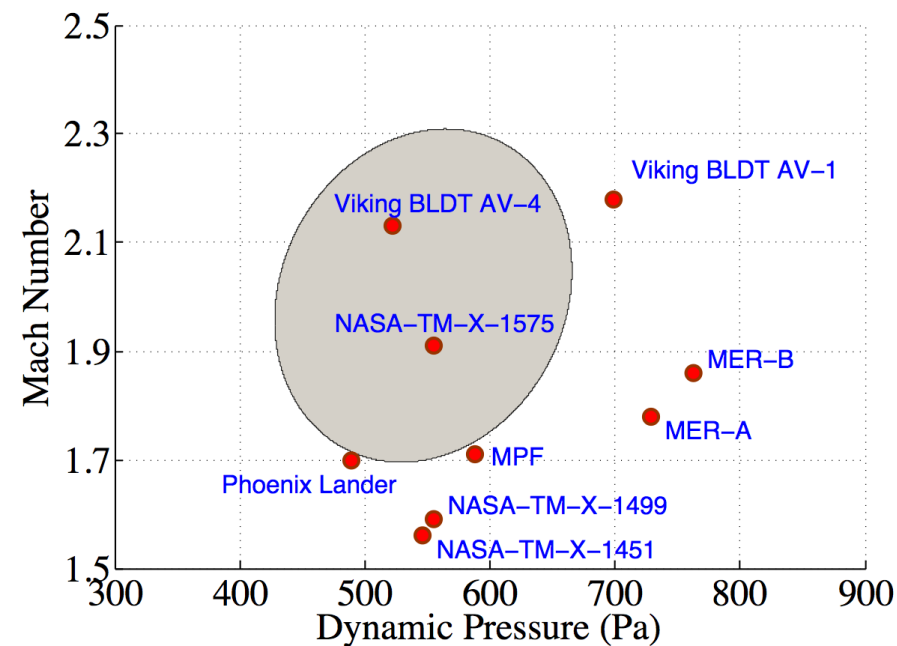


## Filtering Problem



Supersonic parachute

## Control Problem



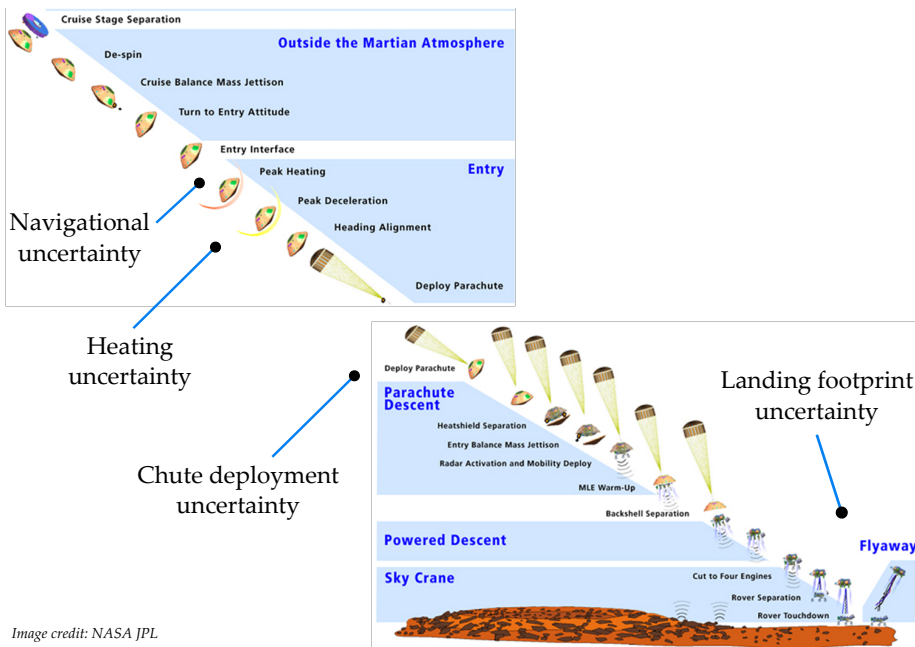
Predict heating rate uncertainty

Estimate state to deploy parachute

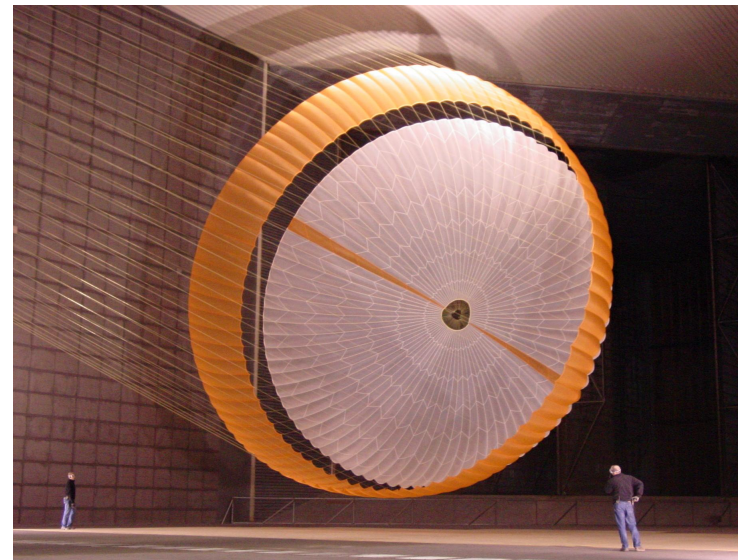


# PDFs in Mars Entry-Descent-Landing

## Prediction Problem

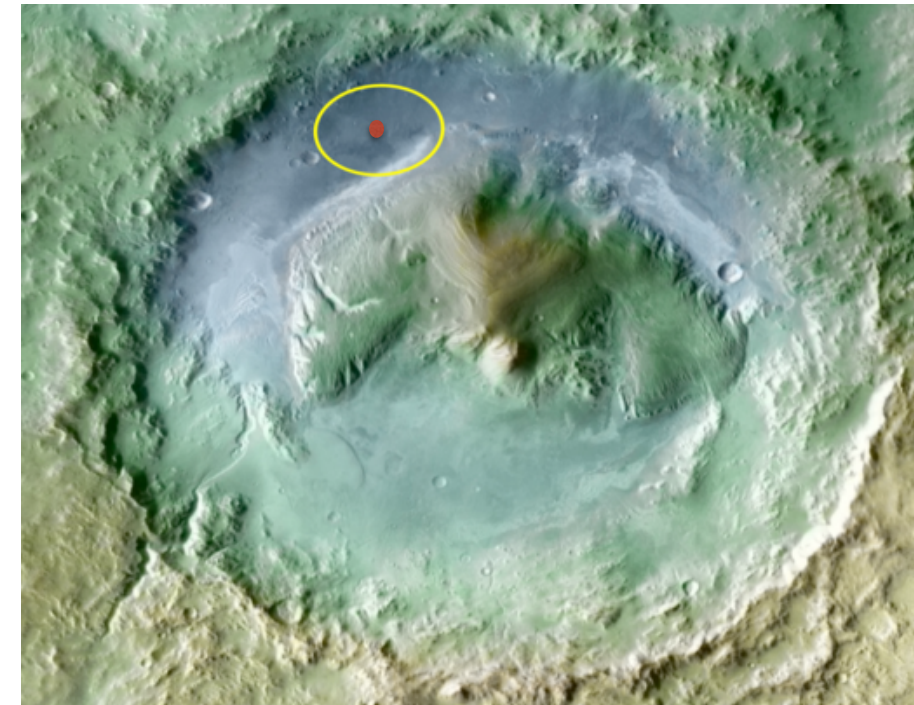


## Filtering Problem

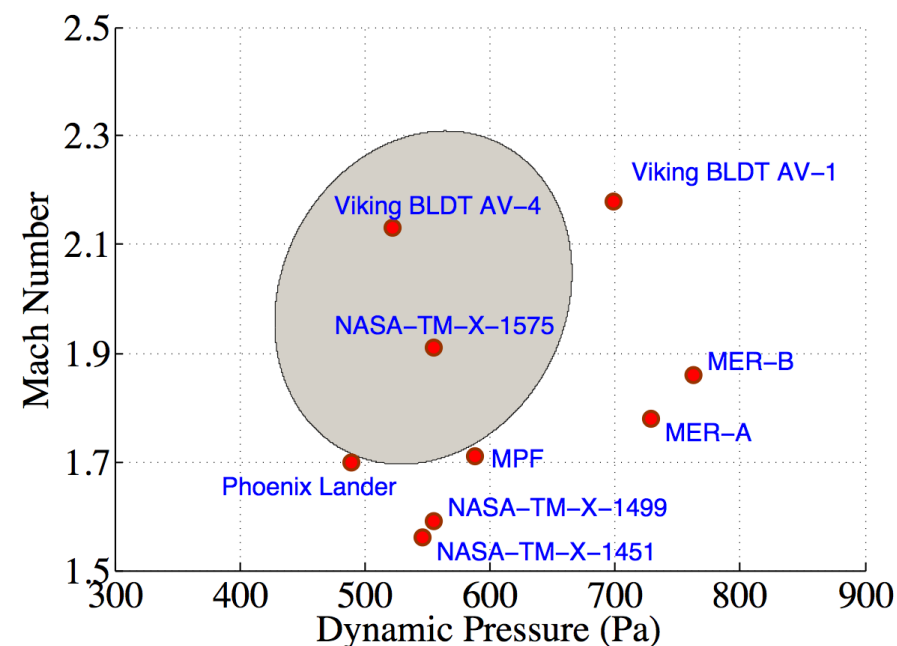


Supersonic parachute

## Control Problem



Gale Crater (4.49S, 137.42E)



Predict heating rate uncertainty

Estimate state to deploy parachute

Steer state PDF to achieve desired landing footprint accuracy

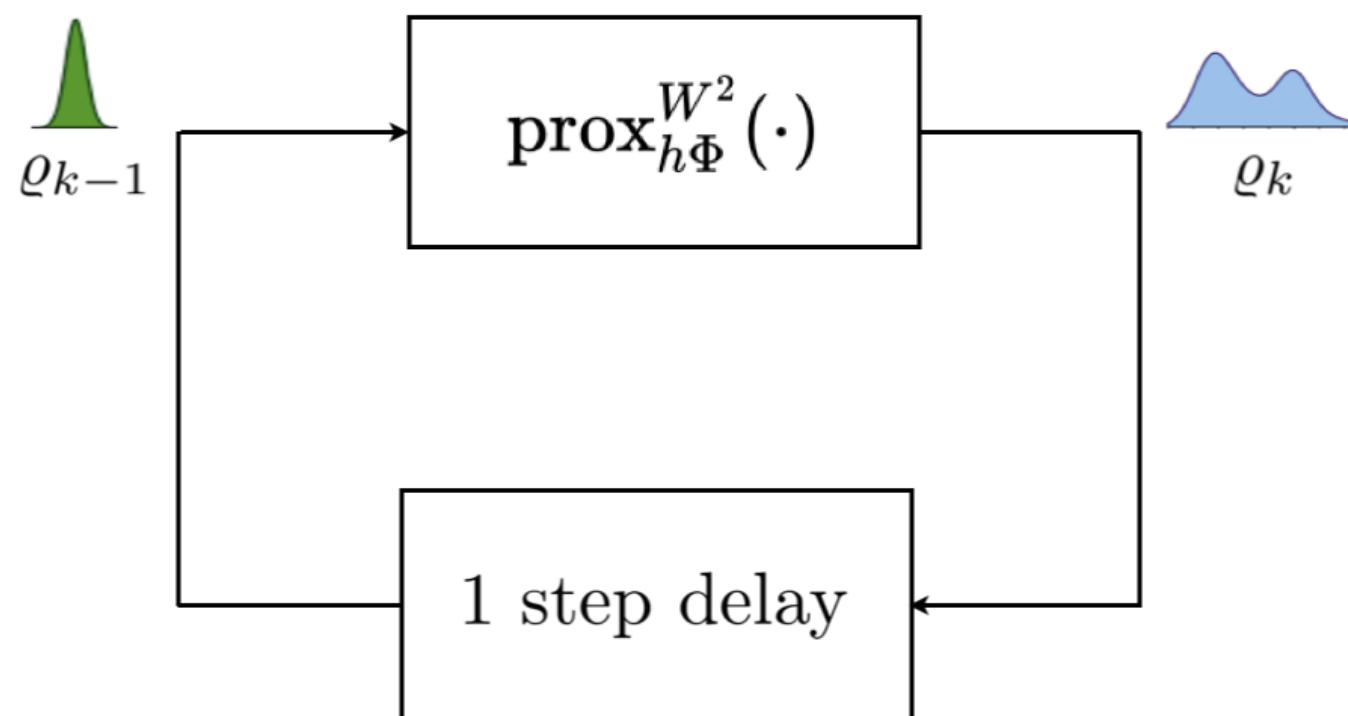


# Solving prediction problem as gradient flow

# What's New?

Main idea: Solve  $\frac{\partial \rho}{\partial t} = \mathcal{L}_{\text{FP}} \rho$ ,  $\rho(x, t = 0) = \rho_0$  as gradient flow in  $\mathcal{P}_2(\mathcal{X})$

Infinite dimensional variational recursion:



Proximal operator:  $\varrho_k = \text{prox}_{h\Phi}^{W^2}(\varrho_{k-1}) := \arg \inf_{\varrho \in \mathcal{P}_2(\mathcal{X})} \left\{ \frac{1}{2} W^2(\varrho, \varrho_{k-1}) + h\Phi(\varrho) \right\}$

Optimal transport cost:  $W^2(\varrho, \varrho_{k-1}) := \inf_{\pi \in \Pi(\varrho, \varrho_{k-1})} \int_{\mathcal{X} \times \mathcal{X}} c(x, y) \, \mathrm{d}\pi(x, y)$

Free energy functional:  $\Phi(\varrho) := \int_{\mathcal{X}} \psi \varrho \, \mathrm{d}x + \beta^{-1} \int_{\mathcal{X}} \varrho \log \varrho \, \mathrm{d}x$

# Gradient Flow

## Gradient Flow in $\mathcal{X}$

---

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

**Recursion:**

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

**Convergence:**

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

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

---

$$\frac{\partial \rho}{\partial t} = -\nabla^W \Phi(\rho), \quad \rho(\mathbf{x}, 0) = \rho_0$$

**Recursion:**

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

**Convergence:**

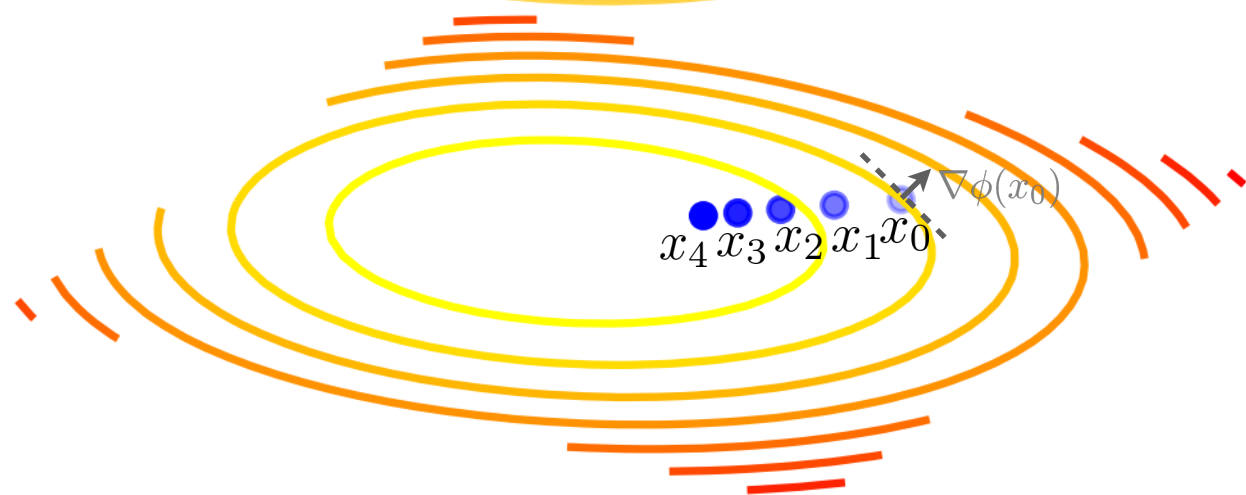
$$\rho_k \rightarrow \rho(\cdot, t = kh) \quad \text{as} \quad h \downarrow 0$$

# Gradient Flow

## Gradient Flow in $\mathcal{X}$

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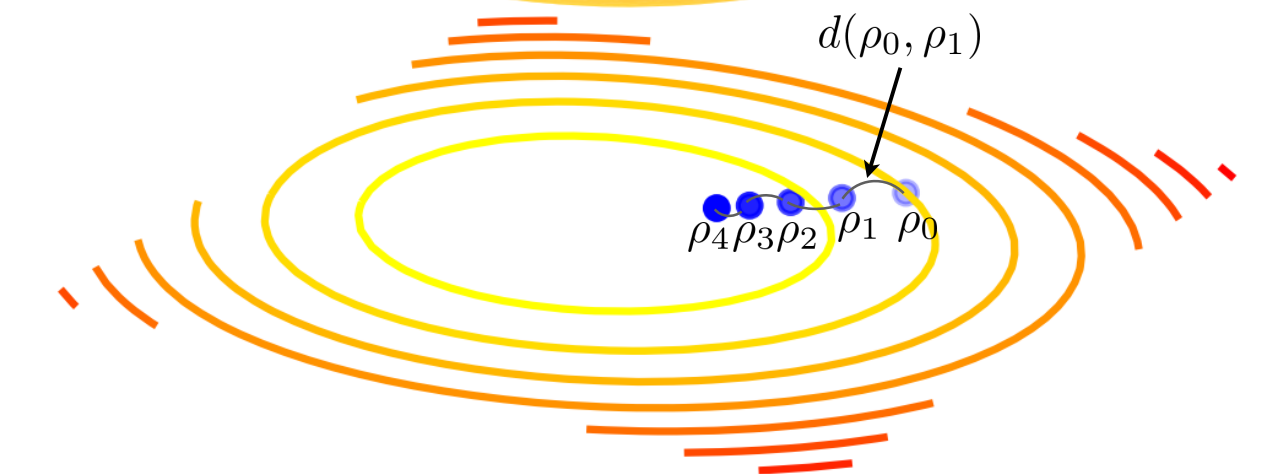
$$z = \phi(x), \quad x \in \mathbb{R}^2$$



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

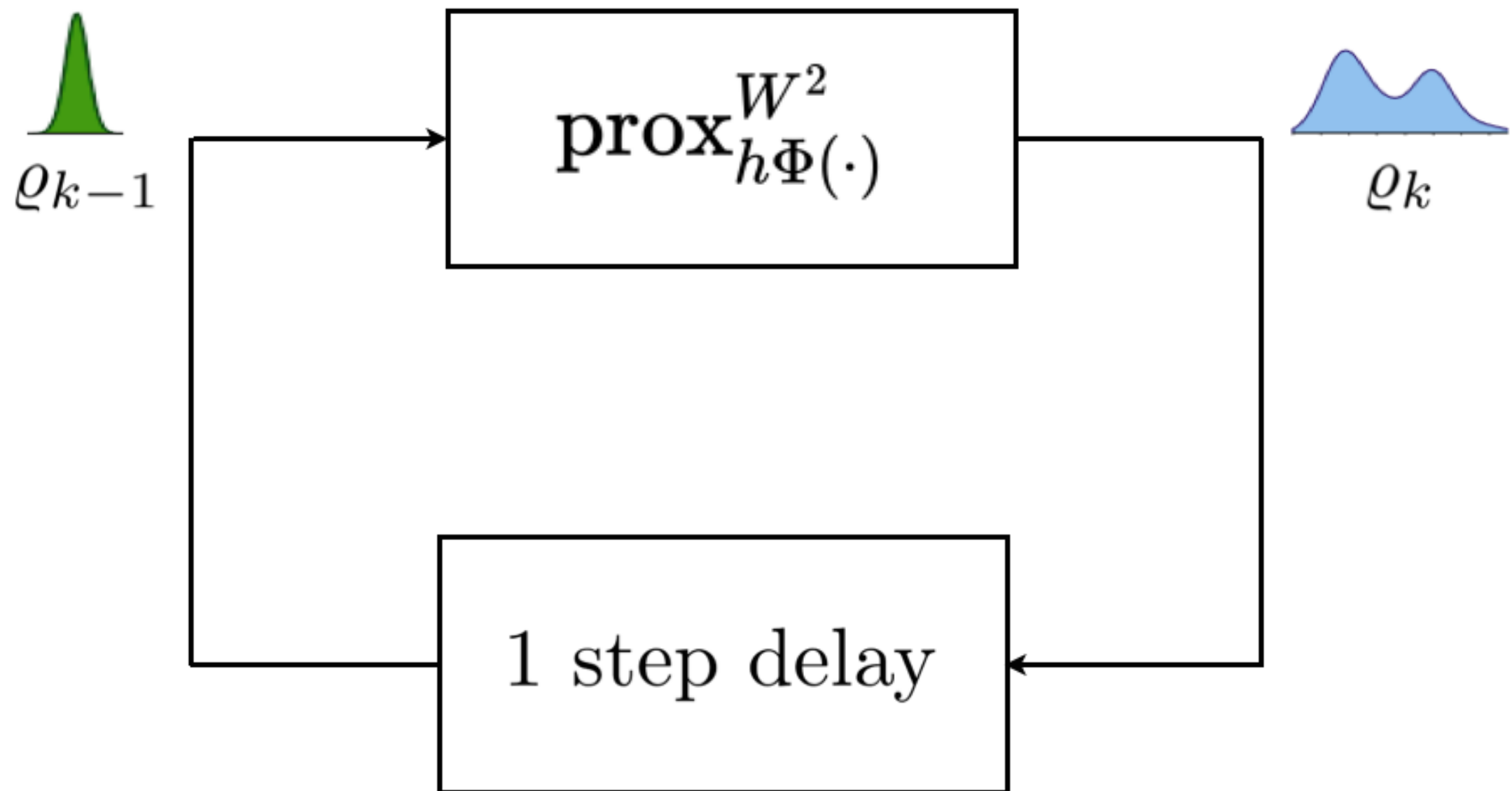
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$$z = \Phi(\rho), \quad \rho \in \mathcal{D}$$



# Algorithm: Gradient Ascent on the Dual Space

Uncertainty propagation via point clouds



No spatial discretization or function approximation

# Algorithm: Gradient Ascent on the Dual Space

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

$\Updownarrow$  **Proximal Recursion**

$$\rho_k = \rho(\mathbf{x}, t = kh) = \arg \inf_{\rho \in \mathcal{P}_2(\mathbb{R}^n)} \left\{ \frac{1}{2} W^2(\rho, \rho_{k-1}) + h \Phi(\rho) \right\}$$

# Algorithm: Gradient Ascent on the Dual Space

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$\Downarrow$  **Discrete Primal Formulation**

$$\varrho_k = \arg \min_{\varrho} \left\{ \min_{\mathbf{M} \in \Pi(\varrho_{k-1}, \varrho)} \frac{1}{2} \langle \mathbf{C}_k, \mathbf{M} \rangle + h \langle \psi_{k-1} + \beta^{-1} \log \varrho, \varrho \rangle \right\}$$

# Algorithm: Gradient Ascent on the Dual Space

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

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$\Downarrow$  **Entropic Regularization**

$$\varrho_k = \arg \min_{\varrho} \left\{ \min_{\mathbf{M} \in \Pi(\varrho_{k-1}, \varrho)} \frac{1}{2} \langle \mathbf{C}_k, \mathbf{M} \rangle + \epsilon H(\mathbf{M}) + h \langle \psi_{k-1} + \beta^{-1} \log \varrho, \varrho \rangle \right\}$$



# Algorithm: Gradient Ascent on the Dual Space

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

$\Updownarrow$  **Proximal Recursion**

$$\rho_k = \rho(\mathbf{x}, t = kh) = \arg \inf_{\rho \in \mathcal{P}_2(\mathbb{R}^n)} \left\{ \frac{1}{2} W^2(\rho, \rho_{k-1}) + h \Phi(\rho) \right\}$$

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$\Updownarrow$  **Dualization**

$$\begin{aligned} \lambda_0^{\text{opt}}, \lambda_1^{\text{opt}} = \arg \max_{\lambda_0, \lambda_1 \geq 0} & \left\{ \langle \lambda_0, \varrho_{k-1} \rangle - F^*(-\lambda_1) \right. \\ & \left. - \frac{\epsilon}{h} \left( \exp(\lambda_0^\top h / \epsilon) \exp(-\mathbf{C}_k / 2\epsilon) \exp(\lambda_1 h / \epsilon) \right) \right\} \end{aligned}$$

# Fixed Point Recursion

$$\mathbf{y} = e^{\frac{\lambda_0^*}{\epsilon} h} \Big| \quad \Big| \quad \mathbf{z} = e^{\frac{\lambda_1^*}{\epsilon} h}$$

Coupled Transcendental Equations in  $\mathbf{y}$  and  $\mathbf{z}$

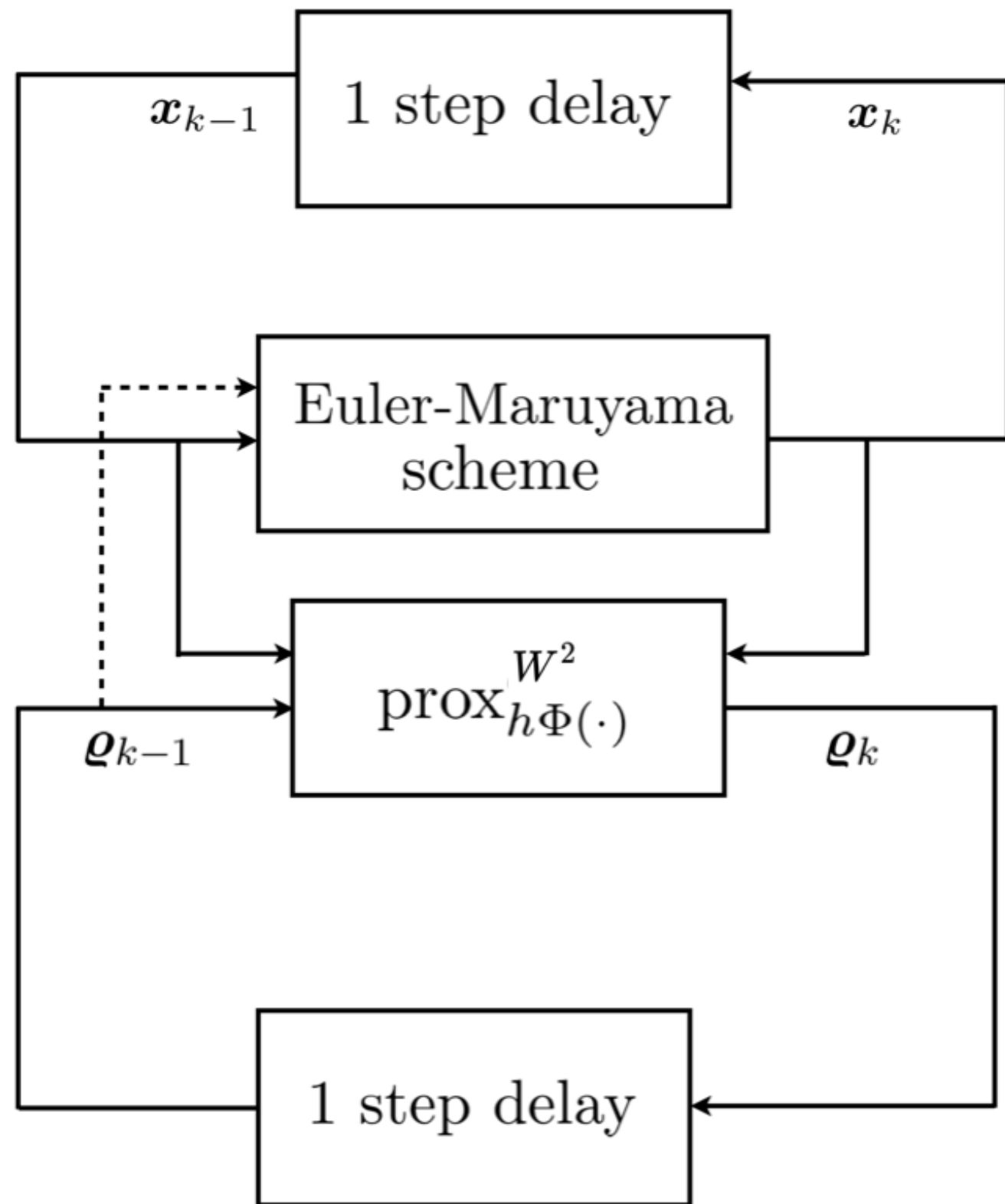
$$\begin{array}{l} \Gamma_k = e^{\frac{-\mathcal{C}_k}{2\epsilon}} \\ \varrho_{k-1} \\ \xi_{k-1} = \frac{e^{-\beta\psi_{k-1}}}{e} \end{array} \begin{array}{l} \longrightarrow \\ \longrightarrow \\ \longrightarrow \end{array} \boxed{\begin{array}{l} \mathbf{y} \odot \Gamma_k \mathbf{z} = \varrho_{k-1} \\ \mathbf{z} \odot \Gamma_k^\top \mathbf{y} = \xi_{k-1} \odot \mathbf{z}^{-\beta\epsilon/2h} \end{array}} \longrightarrow \varrho_k = \mathbf{z} \odot \Gamma_k^\top \mathbf{y}$$

**Theorem:** Consider the recursion on the cone  $\mathbb{R}_{\geq 0}^n \times \mathbb{R}_{\geq 0}^n$

$$\mathbf{y} \odot (\Gamma_k \mathbf{z}) = \varrho_{k-1}, \quad \mathbf{z} \odot (\Gamma_k^\top \mathbf{y}) = \xi_{k-1} \odot \mathbf{z}^{-\frac{\beta\epsilon}{h}},$$

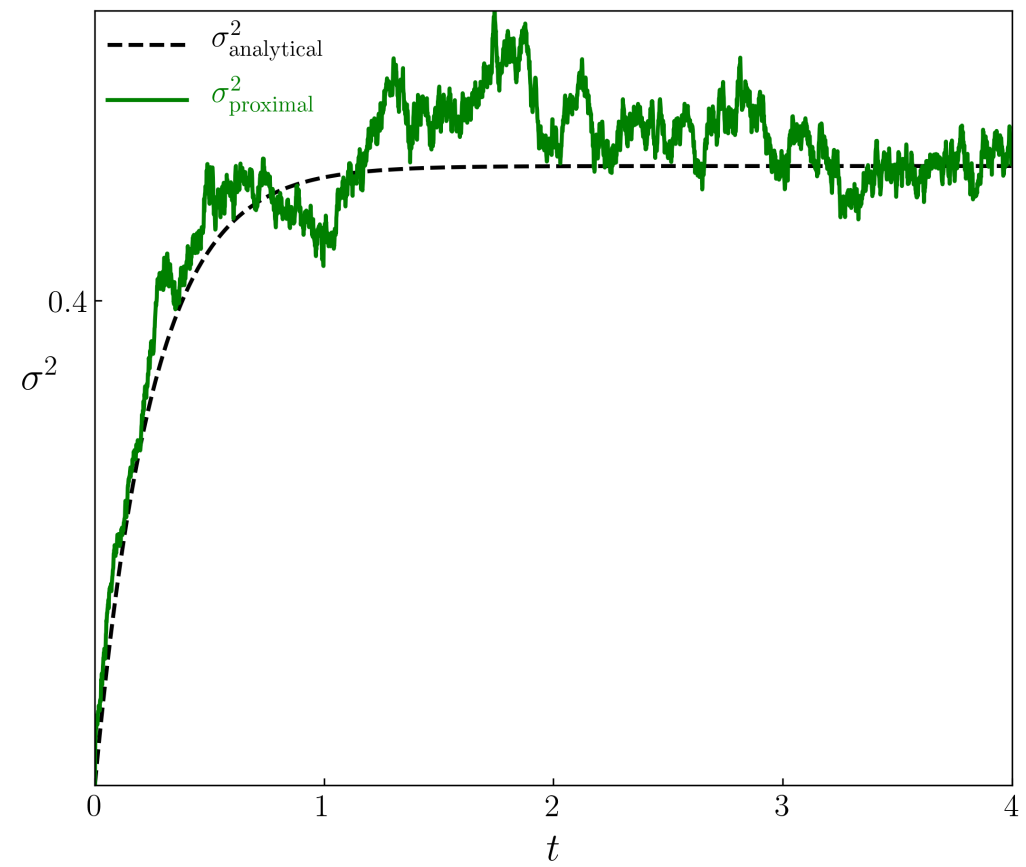
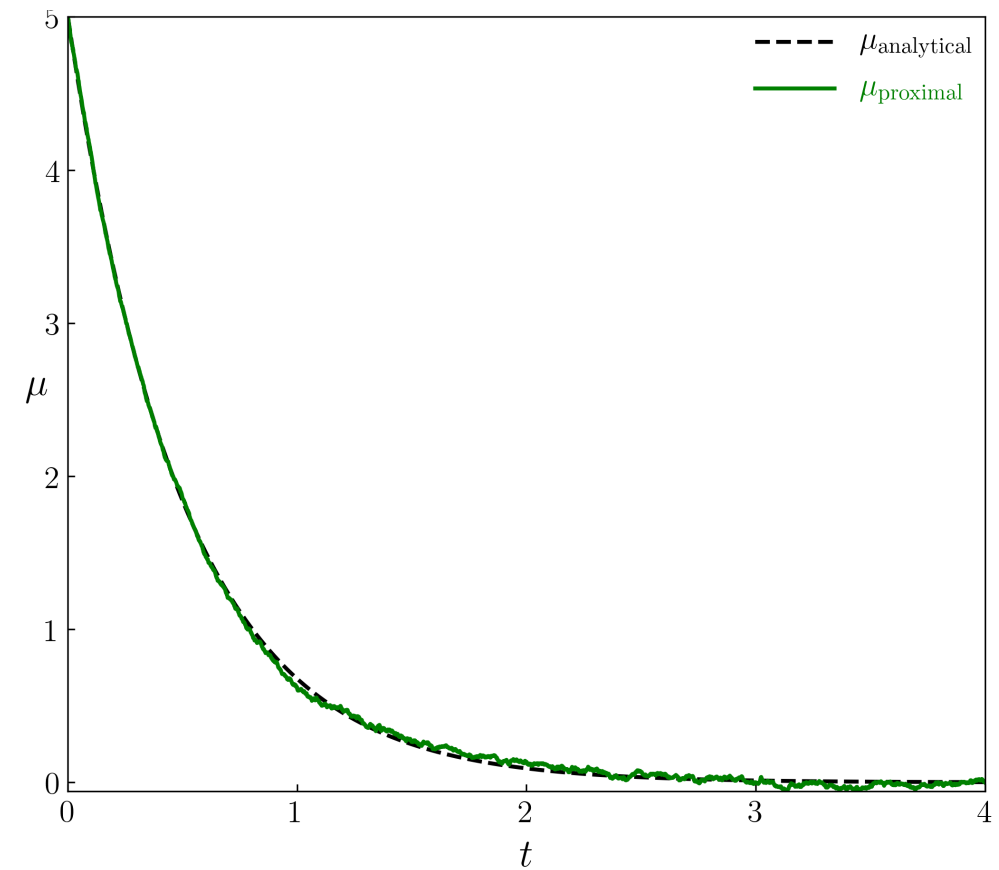
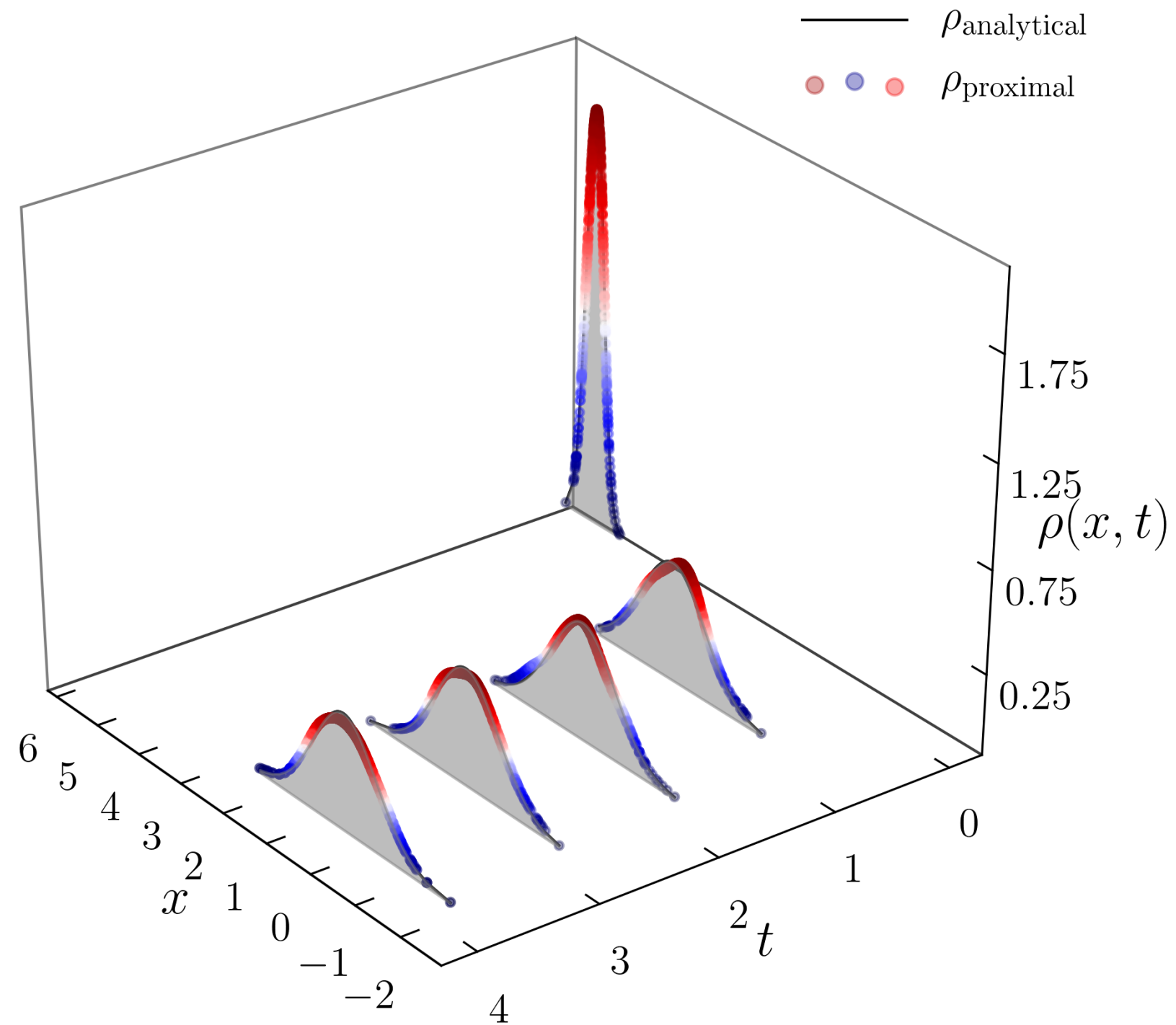
Then the solution  $(\mathbf{y}^*, \mathbf{z}^*)$  gives the proximal update  $\varrho_k = \mathbf{z}^* \odot (\Gamma_k^\top \mathbf{y}^*)$

# Algorithmic Setup

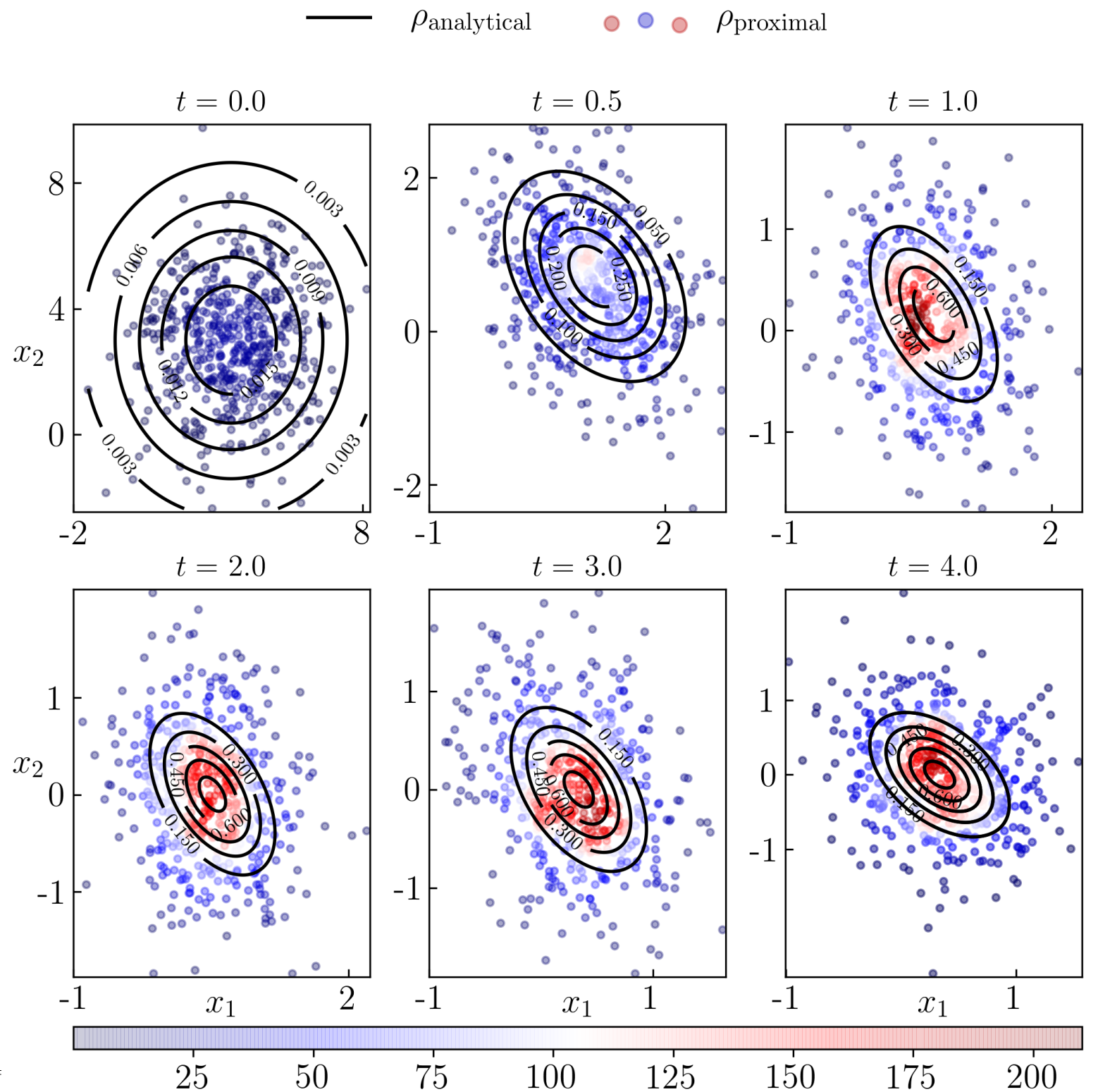
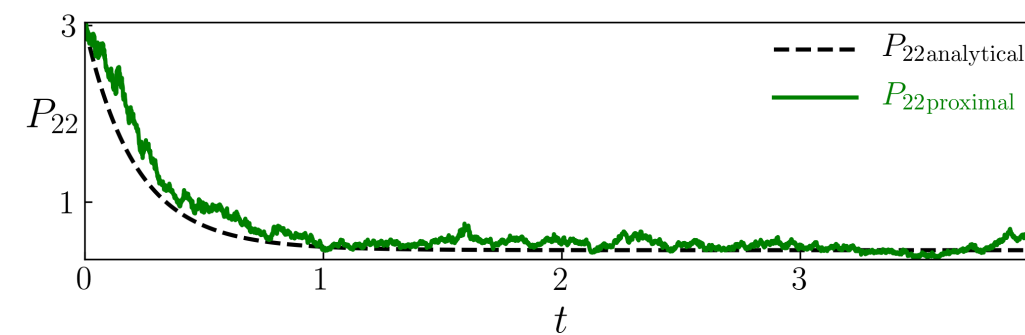
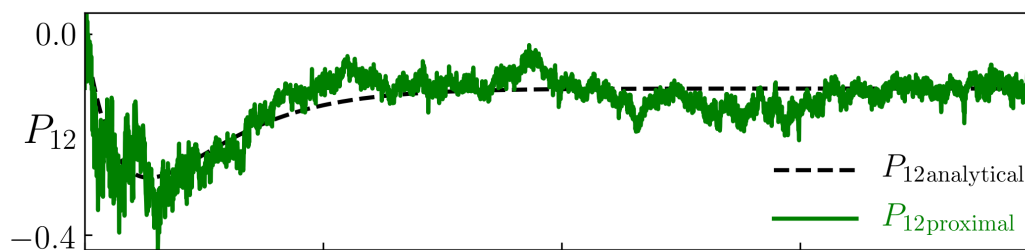
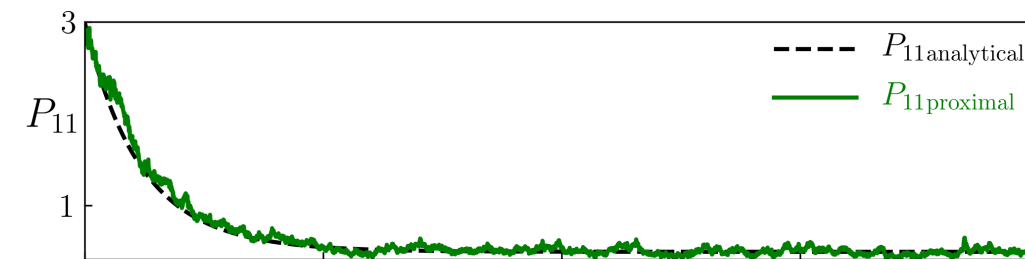
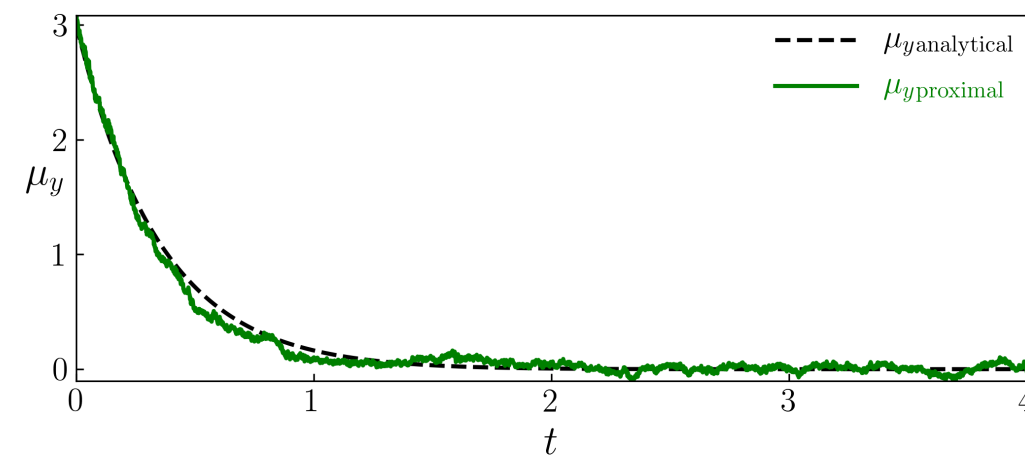
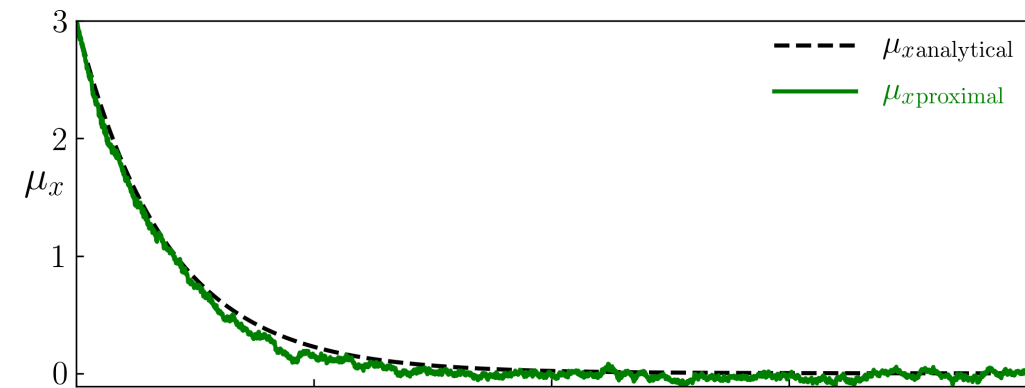


**Theorem:** Block co-ordinate iteration of  $(\mathbf{y}, \mathbf{z})$  recursion is contractive on  $\mathbb{R}_{>0}^n \times \mathbb{R}_{>0}^n$ .

# Proximal Prediction: 1D Linear Gaussian

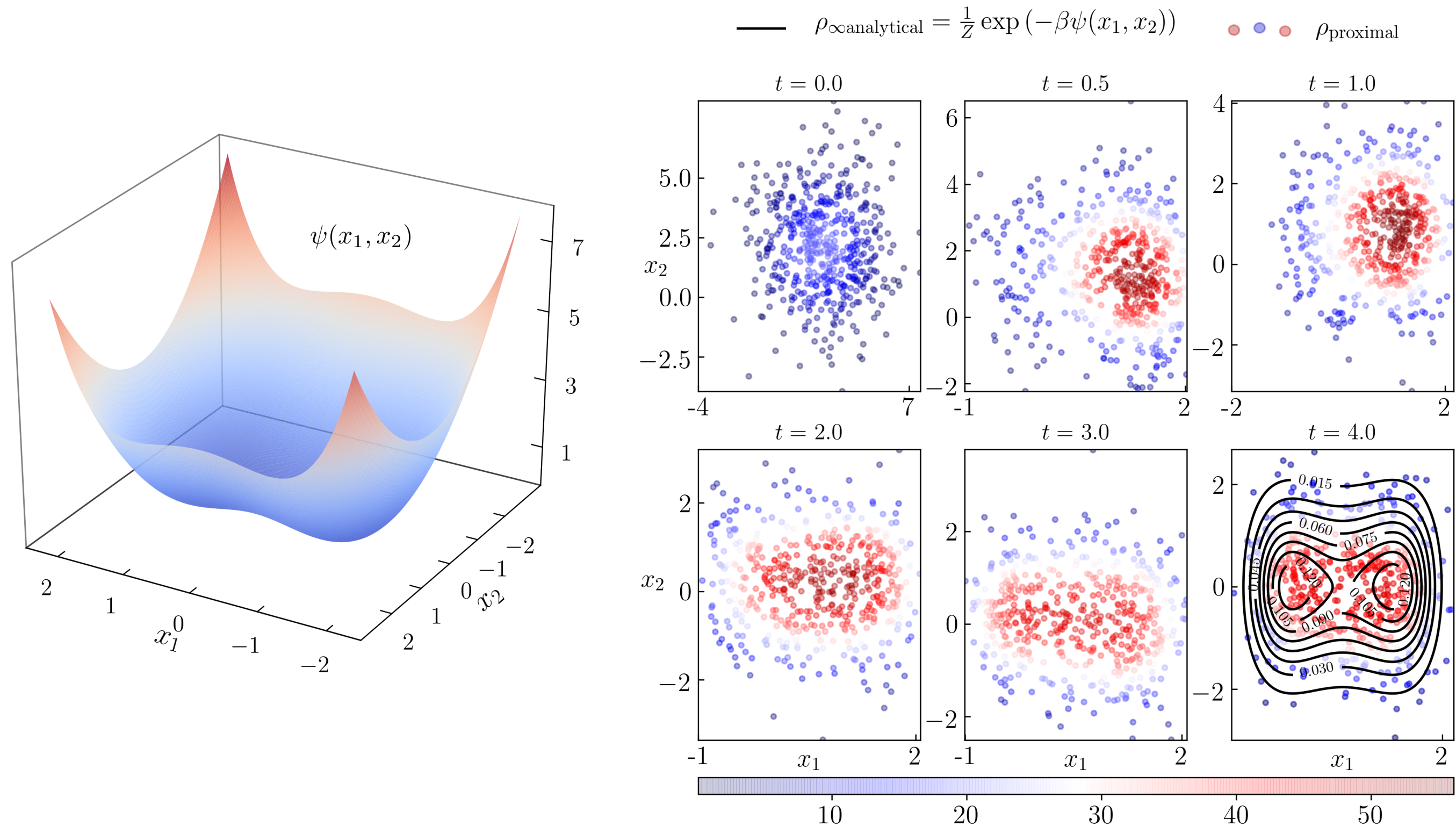


# Proximal Prediction: 2D Linear Gaussian

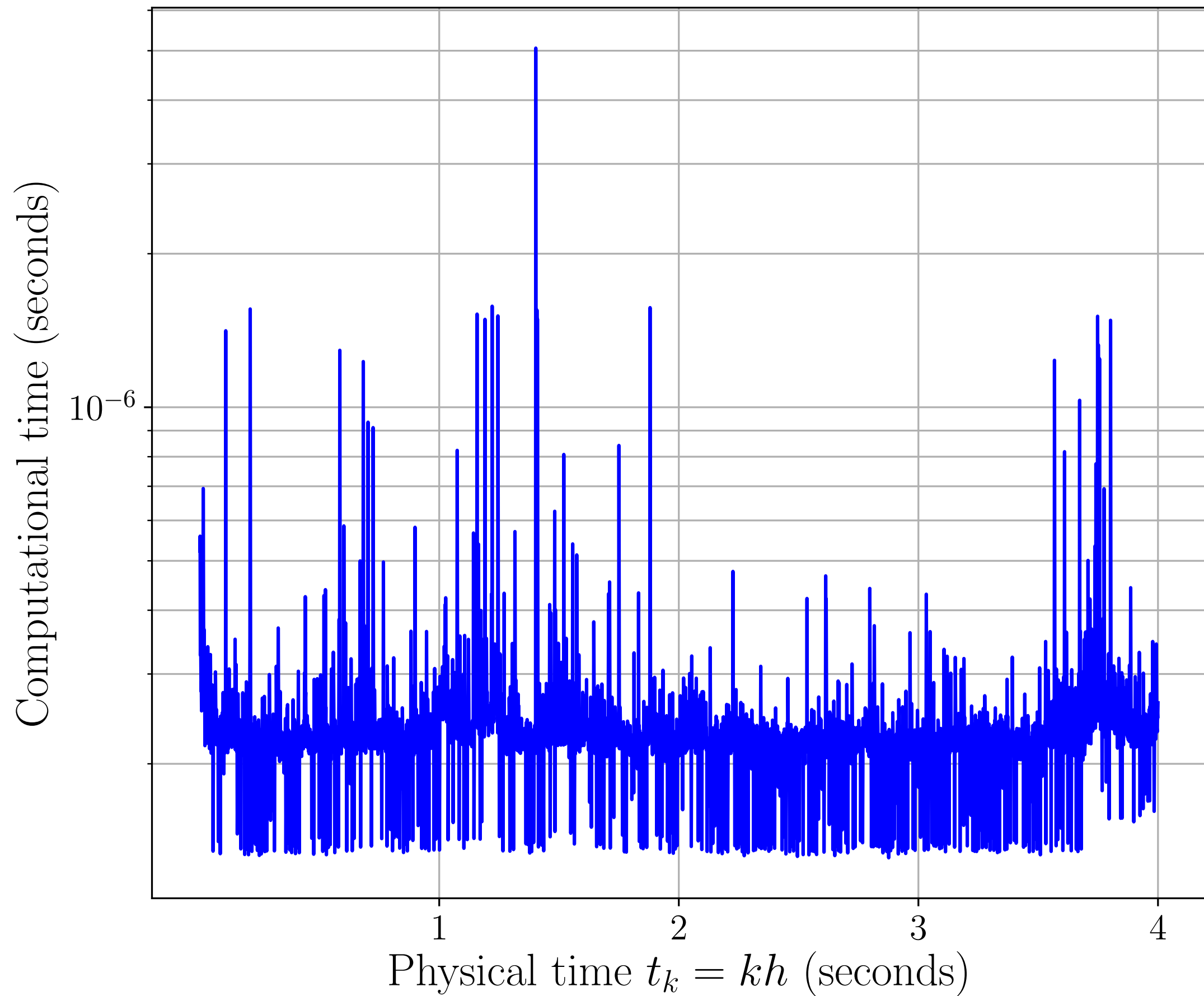




# Proximal Prediction: 2D Nonlinear Non-Gaussian



# Computational Time: 2D Nonlinear Non-Gaussian



# Proximal Prediction: Satellite in Geocentric Orbit

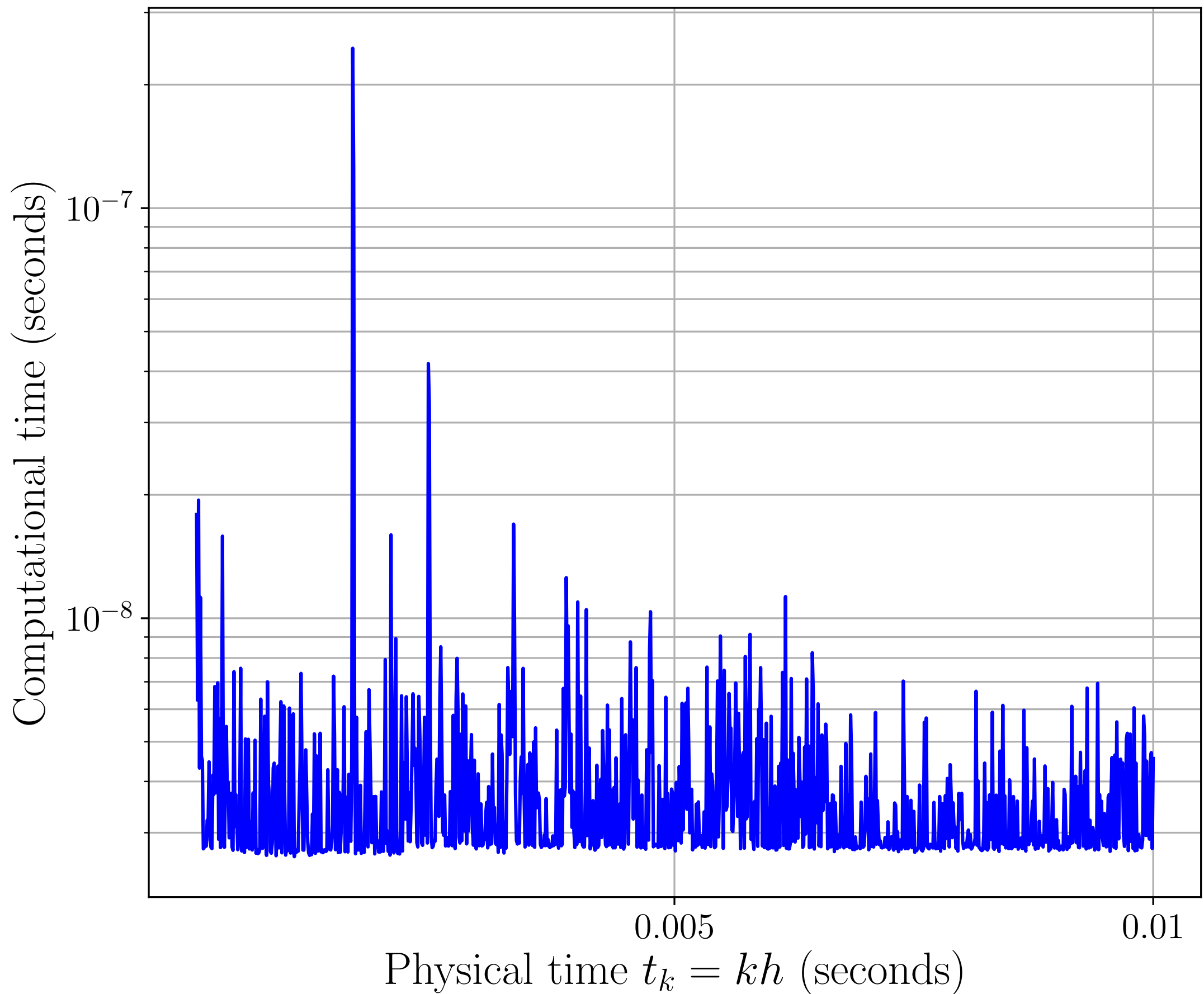
Here,  $\mathcal{X} \equiv \mathbb{R}^6$

$$\begin{pmatrix} dx \\ dy \\ dz \\ dv_x \\ dv_y \\ dv_z \end{pmatrix} = \begin{pmatrix} v_x \\ v_y \\ v_z \\ -\frac{\mu x}{r^3} + (f_x)_{\text{pert}} - \gamma v_x \\ -\frac{\mu y}{r^3} + (f_y)_{\text{pert}} - \gamma v_y \\ -\frac{\mu z}{r^3} + (f_z)_{\text{pert}} - \gamma v_z \end{pmatrix} dt + \sqrt{2\beta^{-1}\gamma} \begin{pmatrix} 0 \\ 0 \\ 0 \\ dw_1 \\ dw_2 \\ dw_3 \end{pmatrix},$$

$$\begin{pmatrix} f_x \\ f_y \\ f_z \end{pmatrix}_{\text{pert}} = \begin{pmatrix} s\theta \ c\phi & c\theta \ c\phi & -s\phi \\ s\theta \ s\phi & c\theta \ s\phi & c\phi \\ c\theta & -s\theta & 0 \end{pmatrix} \begin{pmatrix} \frac{k}{2r^4} (3(s\theta)^2 - 1) \\ -\frac{k}{r^5} s\theta \ c\theta \\ 0 \end{pmatrix}, \quad k := 3J_2 R_{\text{E}}^2, \mu = \text{constant}$$



# Computational Time: Satellite in Geocentric Orbit



# Extensions: Nonlocal interactions

**PDF dependent sample path dynamics:**

$$d\mathbf{x} = - (\nabla U(\mathbf{x}) + \nabla \rho * V) dt + \sqrt{2\beta^{-1}} d\mathbf{w}$$

**McKean-Vlasov-Fokker-Planck-**

**Kolmogorov integro PDE:**

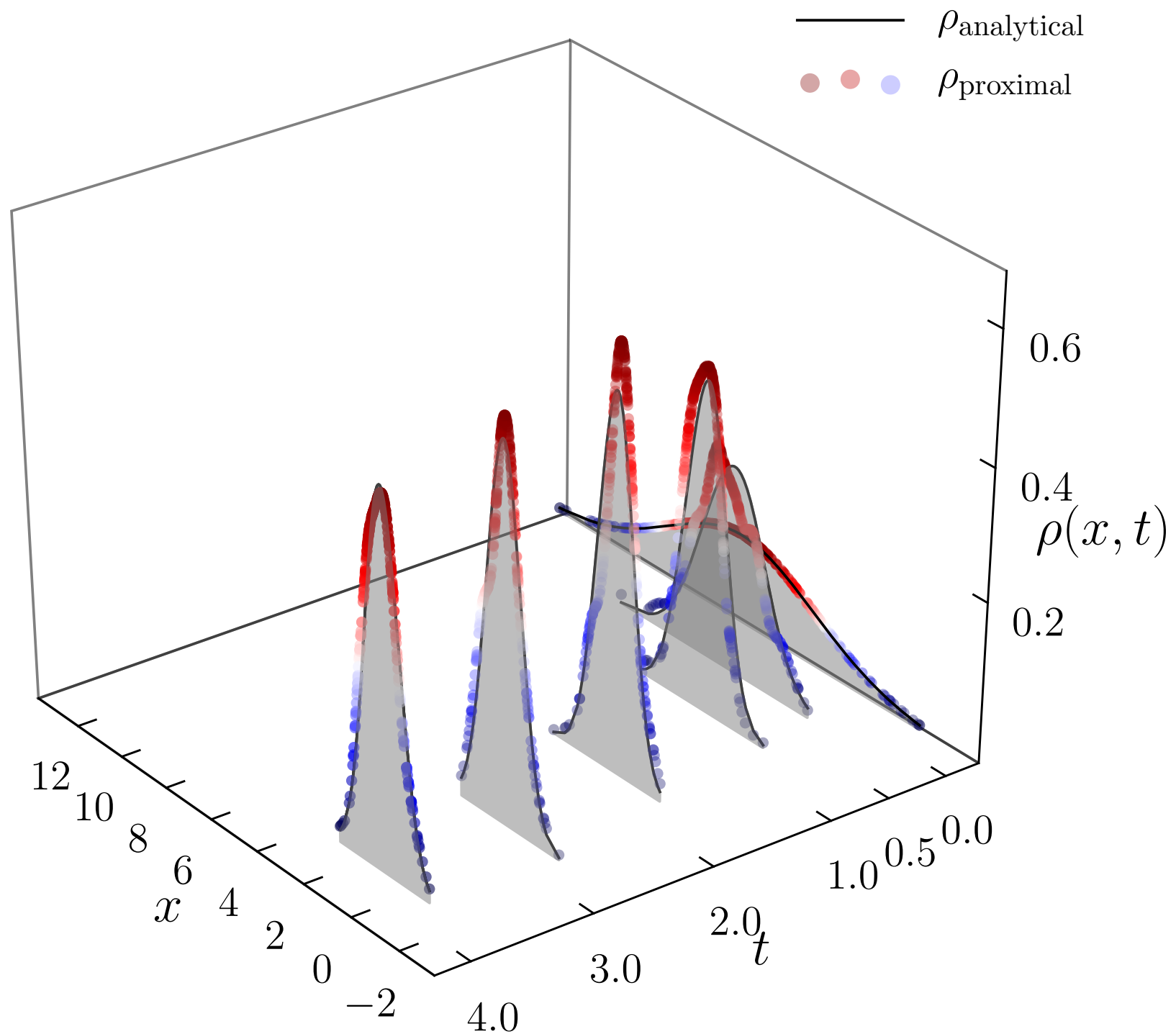
$$\frac{\partial \rho}{\partial t} = \nabla \cdot (\rho \nabla (U + \rho * V)) + \beta^{-1} \Delta \rho$$

**Free energy:**

$$F(\rho) := \mathbb{E}_{\rho} [U + \beta^{-1} \rho \log \rho + \rho * V]$$

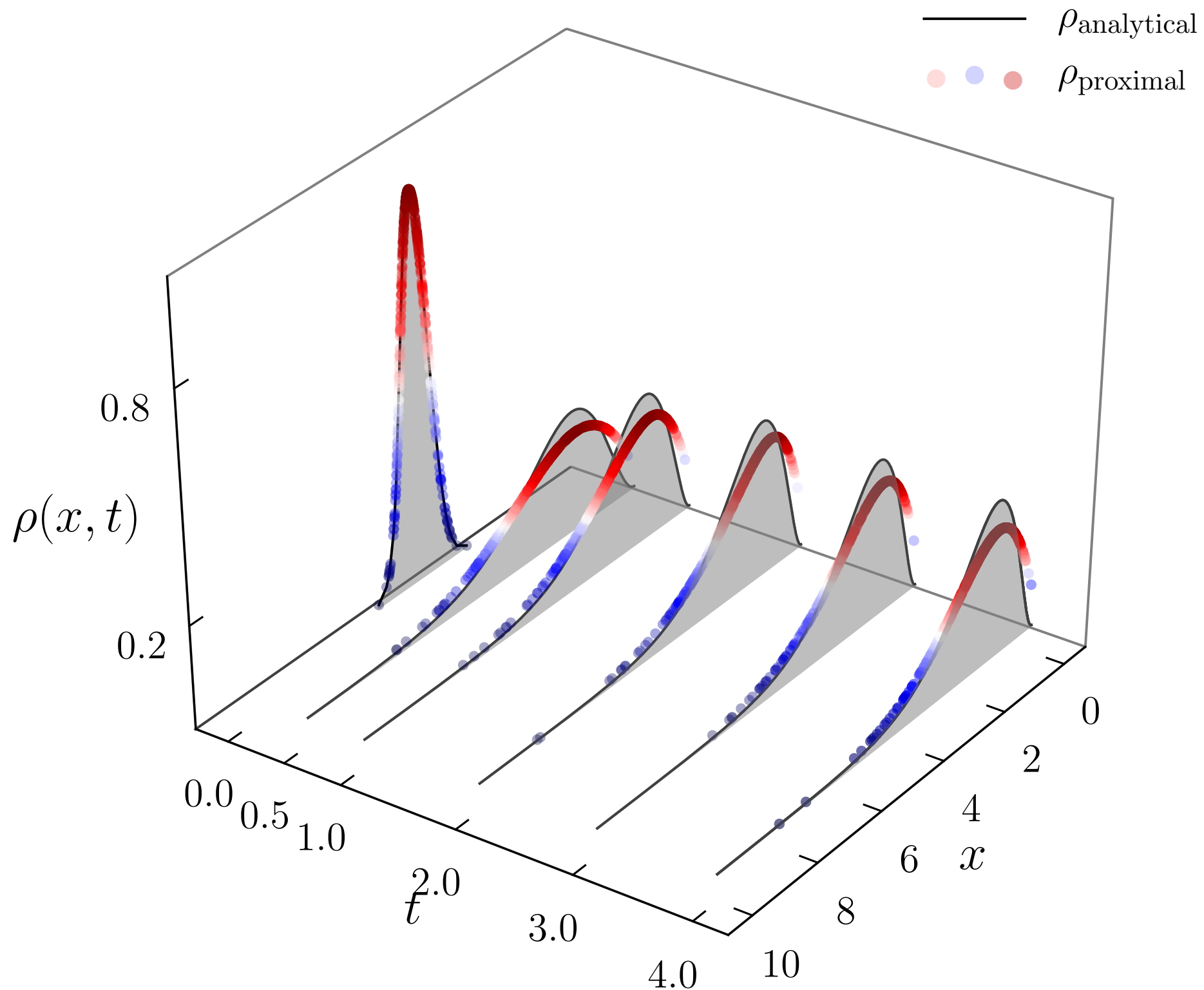
# Extensions: Nonlocal interactions (contd.)

$$U(\cdot) = V(\cdot) = \|\cdot\|_2^2$$



# Extensions: Multiplicative Noise

**Cox-Ingersoll-Ross:**  $dx = a(\theta - x) dt + b\sqrt{x} dw, 2a > b^2, \theta > 0$



# Details on Proximal Prediction

- K.F. Caluya, and A.H., Proximal Recursion for Solving the Fokker-Planck Equation, ACC 2019.
- K.F. Caluya, and A.H., Gradient Flow Algorithms for Density Propagation in Stochastic Systems, under review in TAC.

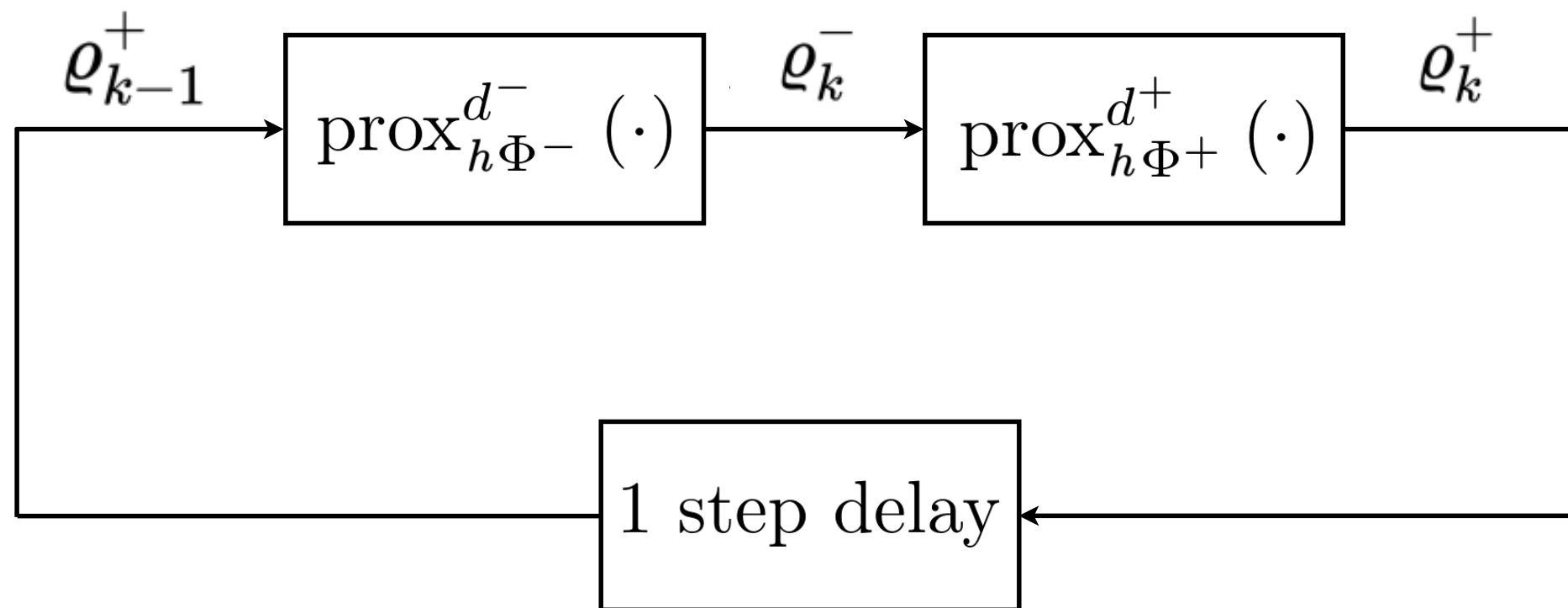
# Solving filtering problem as gradient flow

# What's New?

**Main idea: Solve the Kushner-Stratonovich SPDE**

$$d\rho^+ = [\mathcal{L}_{\text{FP}}dt + \mathcal{L}(dz, dt, \rho^+)]\rho^+, \quad \rho(x, t=0) = \rho_0 \text{ as gradient flow in } \mathcal{P}_2(\mathcal{X})$$

**Recursion of {deterministic ◦ stochastic} proximal operators:**



**Convergence:**  $\varrho_k^+(h) \rightarrow \rho^+(x, t = kh)$  as  $h \downarrow 0$

**For prior, as before:**  $d^- \equiv W^2$ ,  $\Phi^- \equiv \mathbb{E}_{\varrho}[\psi + \beta^{-1} \log \varrho]$

**For posterior:**  $d^+ \equiv d_{\text{FR}}^2$  or  $D_{\text{KL}}$ ,  $\Phi^+ \equiv \frac{1}{2} \mathbb{E}_{\varrho^+}[(y_k - h(x))^\top R^{-1}(y_k - h(x))]$

# Explicit Recovery of Kalman-Bucy Filter

## Model:

$$d\mathbf{x}(t) = \mathbf{A}\mathbf{x}(t)dt + \mathbf{B}d\mathbf{w}(t), \quad d\mathbf{w}(t) \sim \mathcal{N}(0, \mathbf{Q}dt)$$

$$d\mathbf{z}(t) = \mathbf{C}\mathbf{x}(t)dt + d\mathbf{v}(t), \quad d\mathbf{v}(t) \sim \mathcal{N}(0, \mathbf{R}dt)$$

Given  $\mathbf{x}(0) \sim \mathcal{N}(\mu_0, \mathbf{P}_0)$ , want to recover:

$$\mathbf{P}^+ \mathbf{C} \mathbf{R}^{-1}$$

$$d\mu^+(t) = \mathbf{A}\mu^+(t)dt + \mathbf{K}(t) (d\mathbf{z}(t) - \mathbf{C}\mu^+(t)dt),$$

$$\dot{\mathbf{P}}^+(t) = \mathbf{A}\mathbf{P}^+(t) + \mathbf{P}^+(t)\mathbf{A}^\top + \mathbf{B}\mathbf{Q}\mathbf{B}^\top - \mathbf{K}(t)\mathbf{R}\mathbf{K}(t)^\top.$$

— A.H. and T.T. Georgiou, Gradient Flows in Uncertainty Propagation and Filtering of Linear Gaussian Systems, CDC 2017.

— A.H. and T.T. Georgiou, Gradient Flows in Filtering and Fisher-Rao Geometry, ACC 2018.



# Explicit Recovery of Wonham Filter

**Model:**

$$x(t) \sim \text{Markov}(Q),$$
$$dz(t) = h(x(t)) dt + \sigma_v(t) dv(t)$$

**State space:**  $\Omega := \{a_1, \dots, a_m\}$

**Posterior**  $\pi^+(t) := \{\pi_1^+(t), \dots, \pi_m^+(t)\}$  **solves the nonlinear SDE:**

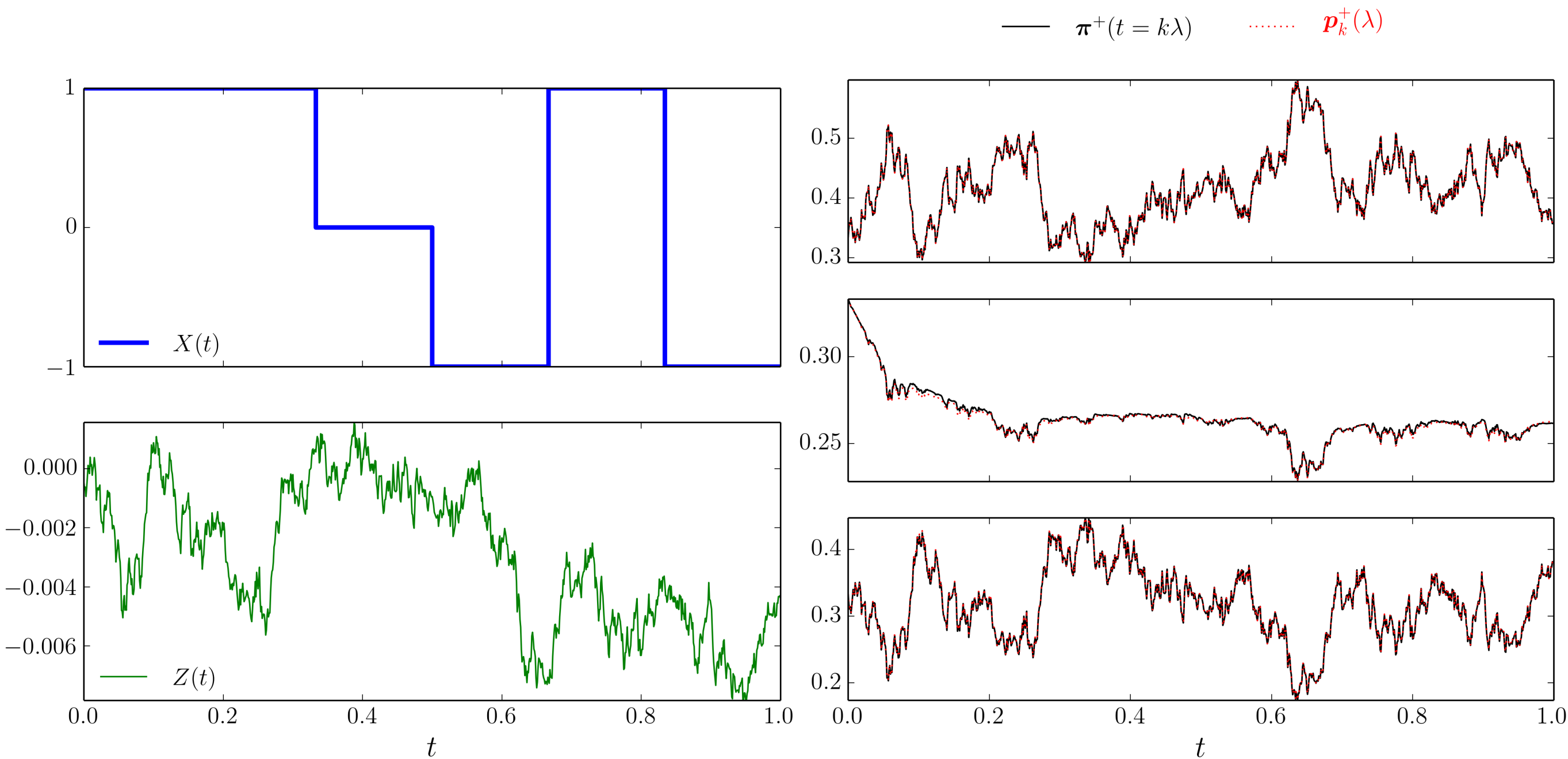
$$d\pi^+(t) = \pi^+(t)Q dt + \frac{1}{(\sigma_v(t))^2} \pi^+(t) \left( H - \hat{h}(t)I \right) \left( dz(t) - \hat{h}(t)dt \right),$$

where  $H := \text{diag}(h(a_1), \dots, h(a_m))$ ,  $\hat{h}(t) := \sum_{i=1}^m h(a_i) \pi_i^+(t)$ ,

**Initial condition:**  $\pi^+(t=0) = \pi_0$ ,

**By defn.**  $\pi^+(t) = \mathbb{P}(x(t) = a_i \mid z(s), 0 \leq s \leq t)$

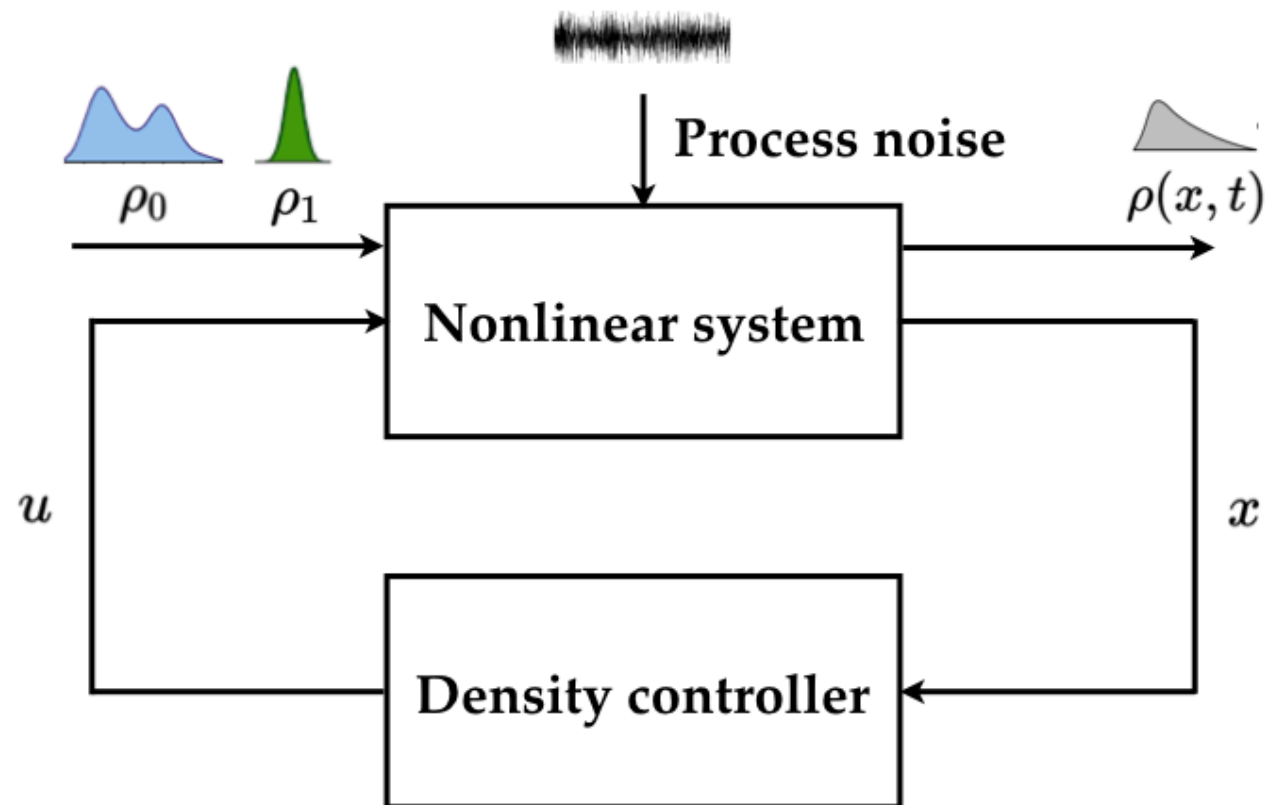
# Numerical Results for Wonham Filter



# Solving density steering using gradient flow

# Finite Horizon Feedback Density Steering

$$\begin{aligned} & \underset{u \in \mathcal{U}}{\text{minimize}} \quad \mathbb{E} \left[ \int_0^1 \|u\|_2^2 dt \right] \\ & \text{subject to} \\ & dx = f(x, u, t) dt + g(x, t) dw, \\ & x(t=0) \sim \rho_0, \quad x(t=1) \sim \rho_1 \end{aligned}$$



Consider simple case:  $f(x, u, t) \equiv f(x, t) + u$ ,  $g = \sqrt{2\epsilon}$

Coupled Nonlinear PDE system (Fokker-Planck + Hamilton-Jacobi-Bellman):

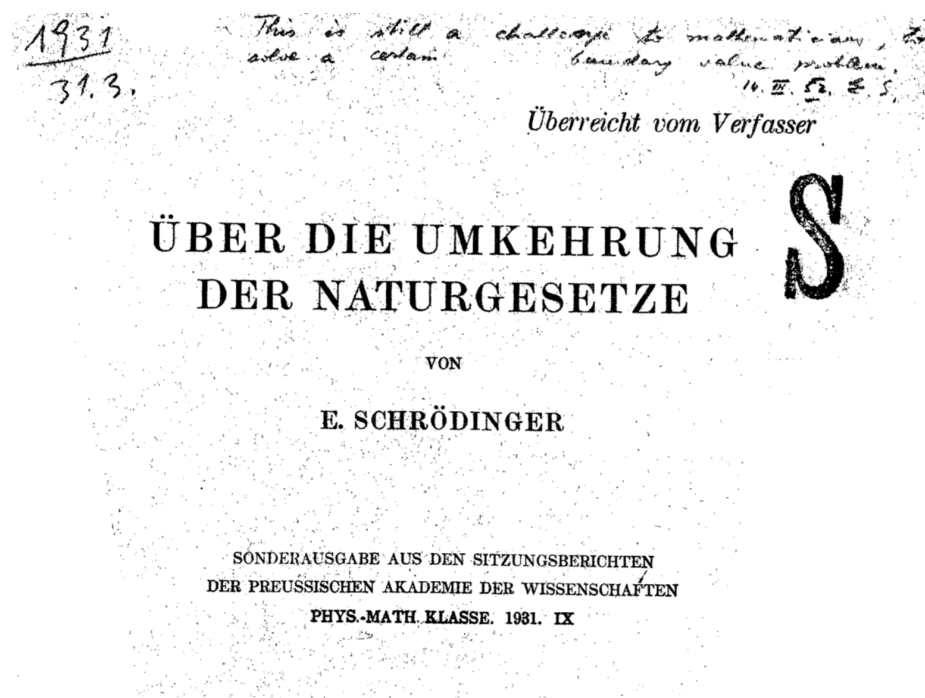
$$\begin{aligned} \frac{\partial \rho}{\partial t} &= -\nabla \cdot (\rho(f + \nabla \psi)) + \epsilon \Delta \rho, \\ \frac{\partial \psi}{\partial t} &= -\langle f, \nabla \psi \rangle - \frac{\|\nabla \psi\|_2^2}{2} - \epsilon \Delta \psi. \end{aligned}$$

LTV case is solved (boundary coupled system of Riccati ODEs):

— Y. Chen, T.T. Georgiou, and M. Pavon, Optimal Transport Over a Linear Dynamical System, TAC 2017 [George S. Axelby Outstanding Paper Award]

# Solution via Schrödinger Bridge

Schrödinger's (until recently) forgotten papers:



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.



Schrödinger's contribution:

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

For  $f = -\nabla U$ :

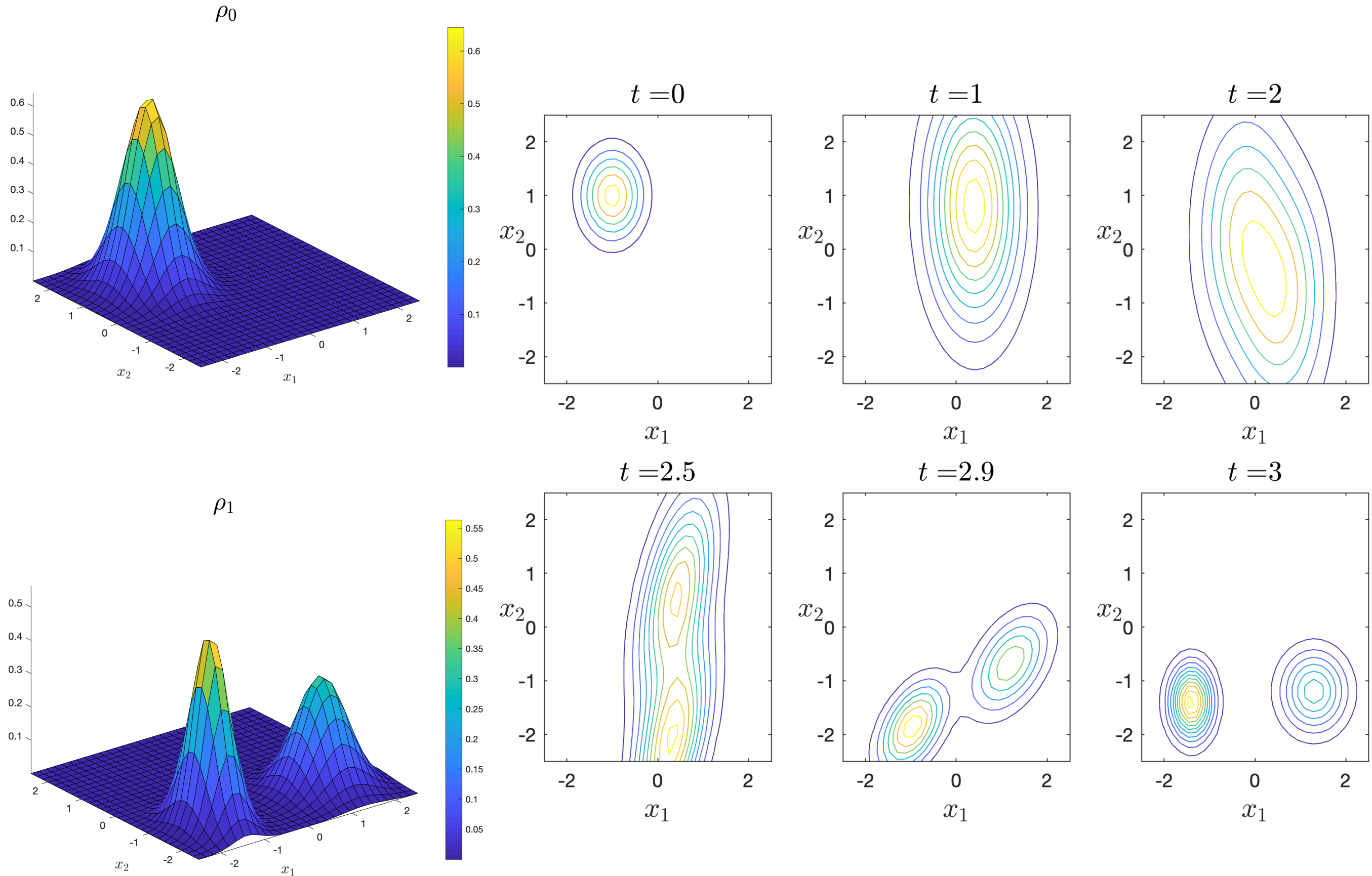
$$\frac{\partial \hat{\varphi}}{\partial t} = \nabla \cdot (\hat{\varphi} \nabla U) + \epsilon \Delta \hat{\varphi}, \quad \hat{\varphi}(x, t = 0) = \hat{\varphi}_0,$$

$$\frac{\partial \varphi}{\partial t} = \nabla U \cdot \nabla \varphi - \epsilon \Delta \varphi, \quad \hat{\varphi}(x, t = 1) = \varphi_1,$$

Optimal controlled joint state PDF:  $\rho^*(x, t) = \hat{\varphi}(x, t)\varphi(x, t)$



# Feedback Density Steering: Proximal Algorithms



# Details on Feedback Density Control for Nonlinear Systems

- K.F. Caluya, and A.H., Finite Horizon Density Control for Static State Feedback Linearizable Systems, under review in TAC.
- K.F. Caluya, W. Li, and A.H., Schrodinger Bridge with Nonlinear Drift, working draft.

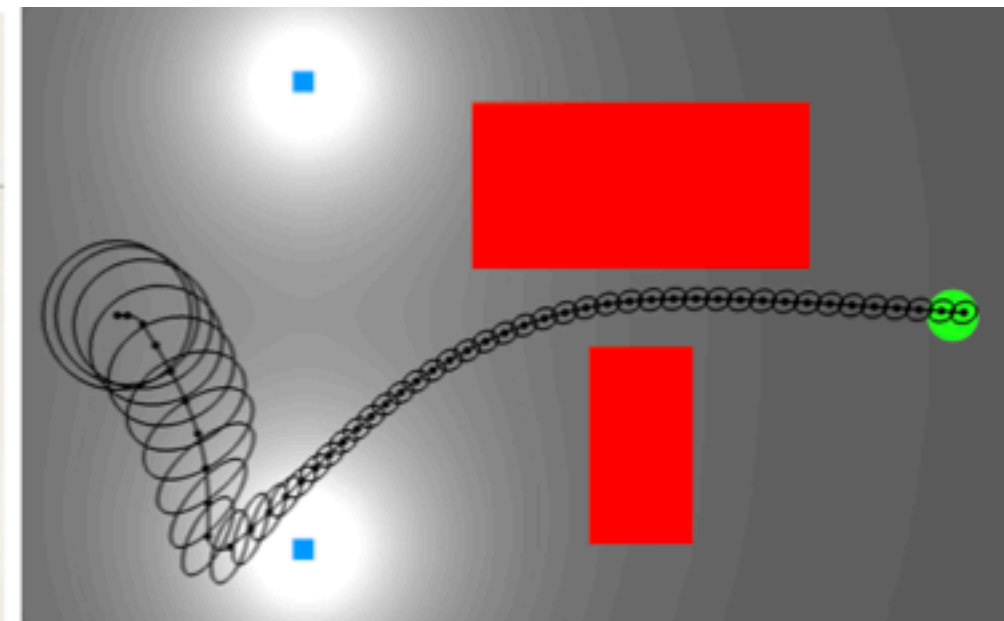
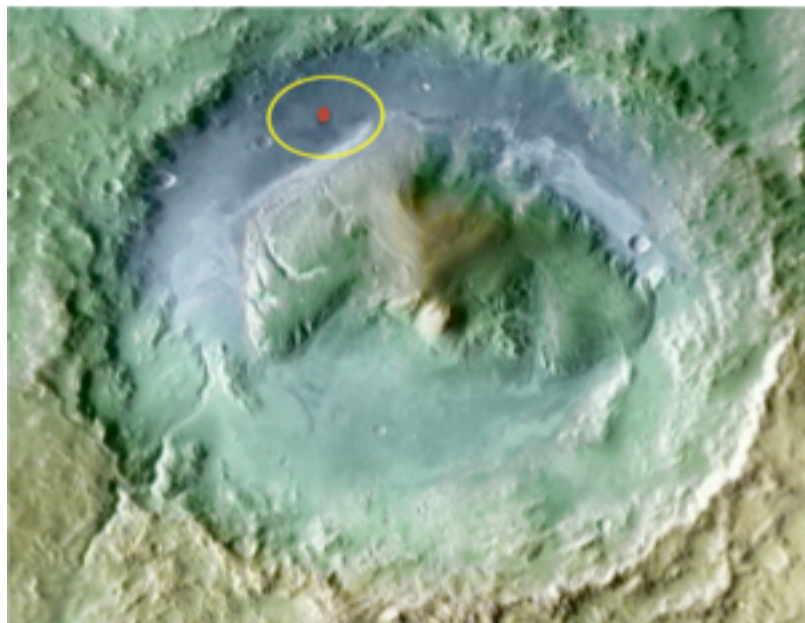
# Take Home Message

Emerging systems-control theory of PDFs

Three problems involving PDFs: prediction, filtering, control

One unifying framework: proximal recursion on the manifold of PDFs

Many applications:





**Thank You**