

# Gradient Flows for Prediction and Control of Densities

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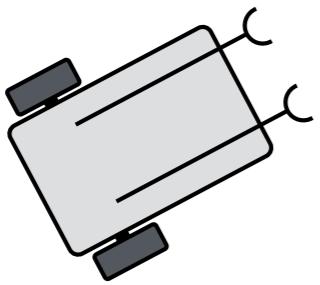
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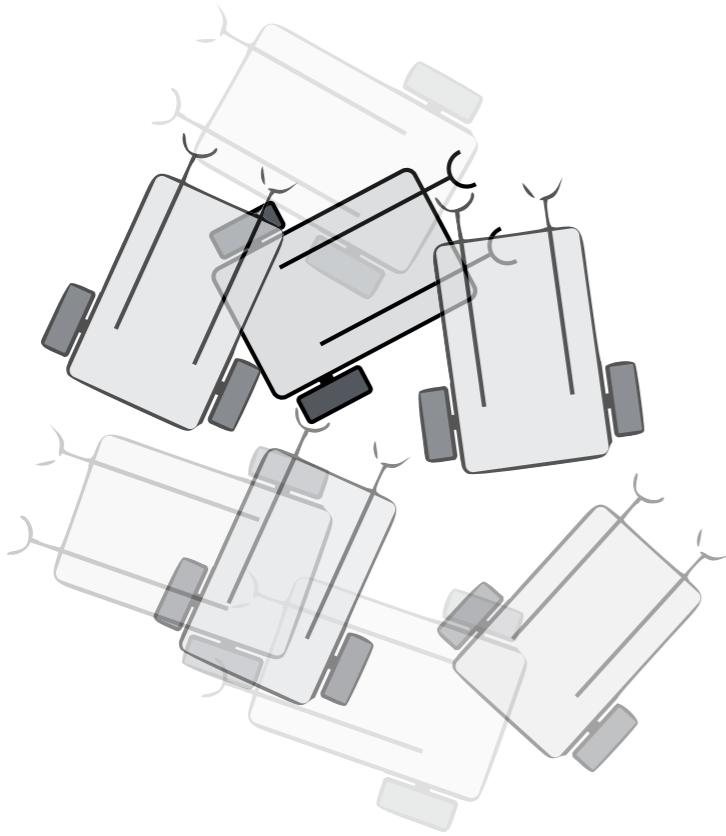
# What is density?

# Probability Density Fn.



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

# Probability Density Fn.

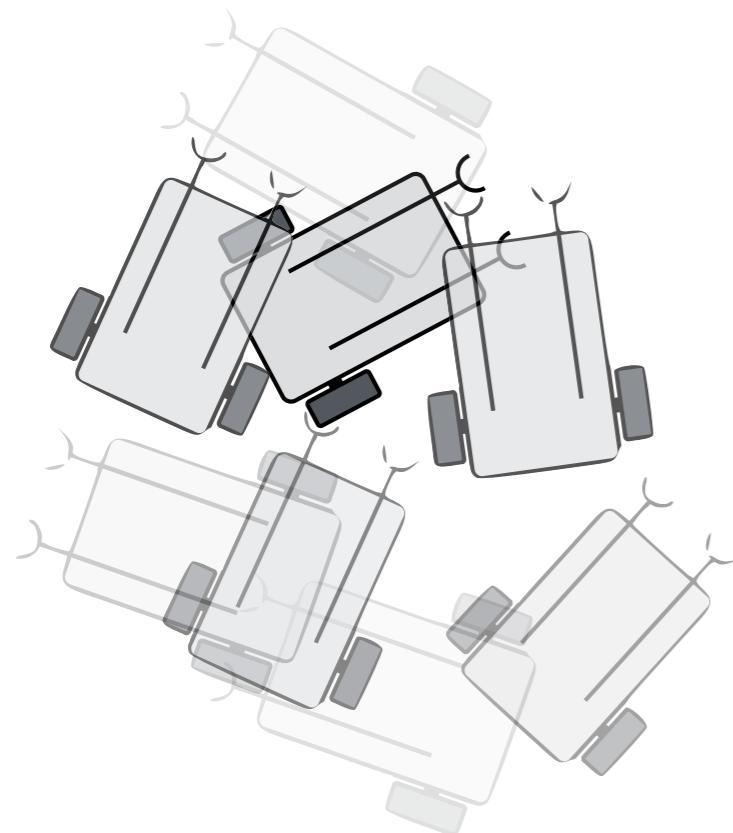


$$x(t) \in \mathcal{X} \equiv \mathbb{R}^2 \times \mathbb{S}^1$$

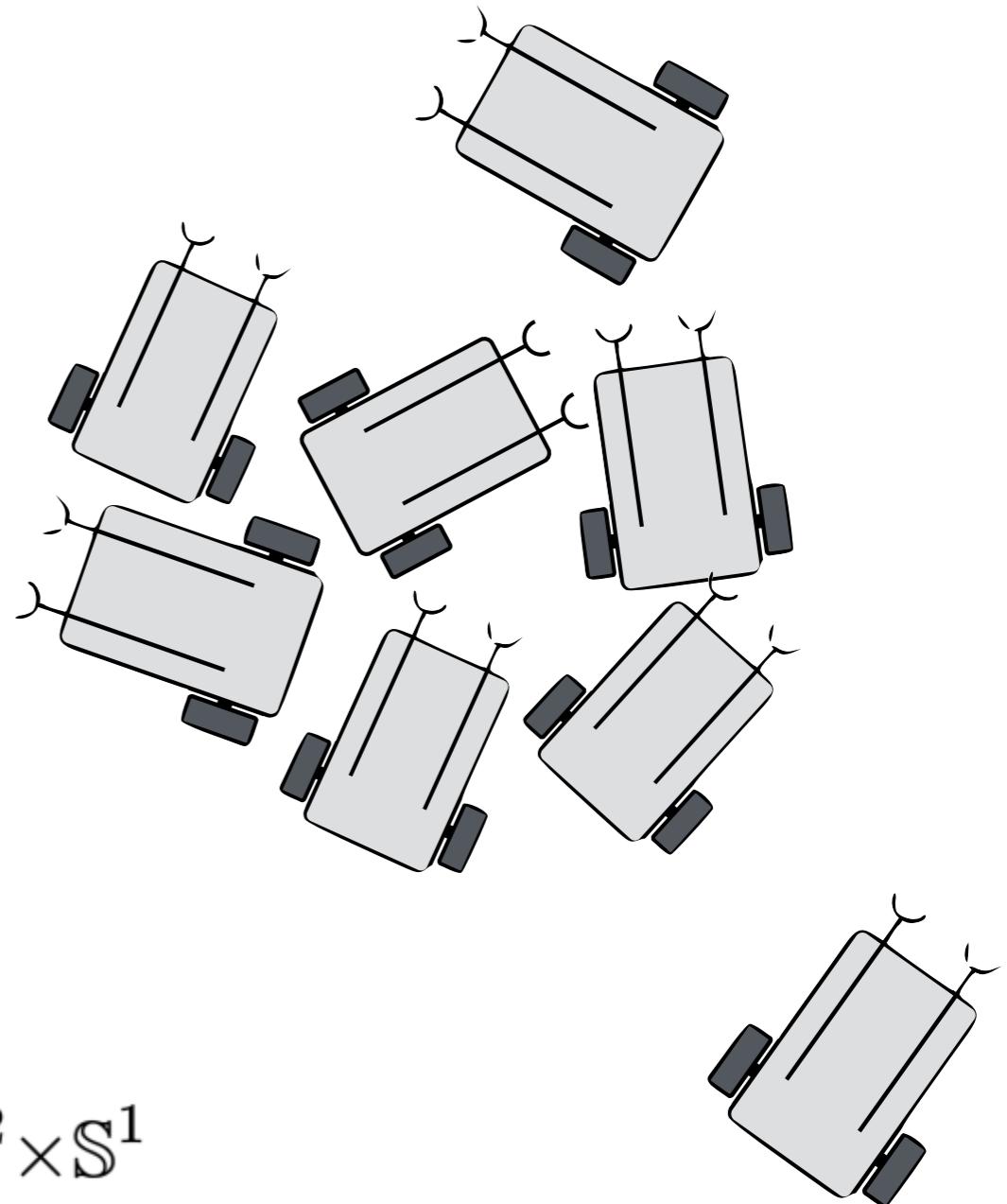
$$\rho(x, t) : \mathcal{X} \times [0, \infty) \mapsto \mathbb{R}_{\geq 0}$$

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

# Probability Density Fn.



# Population Density Fn.



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

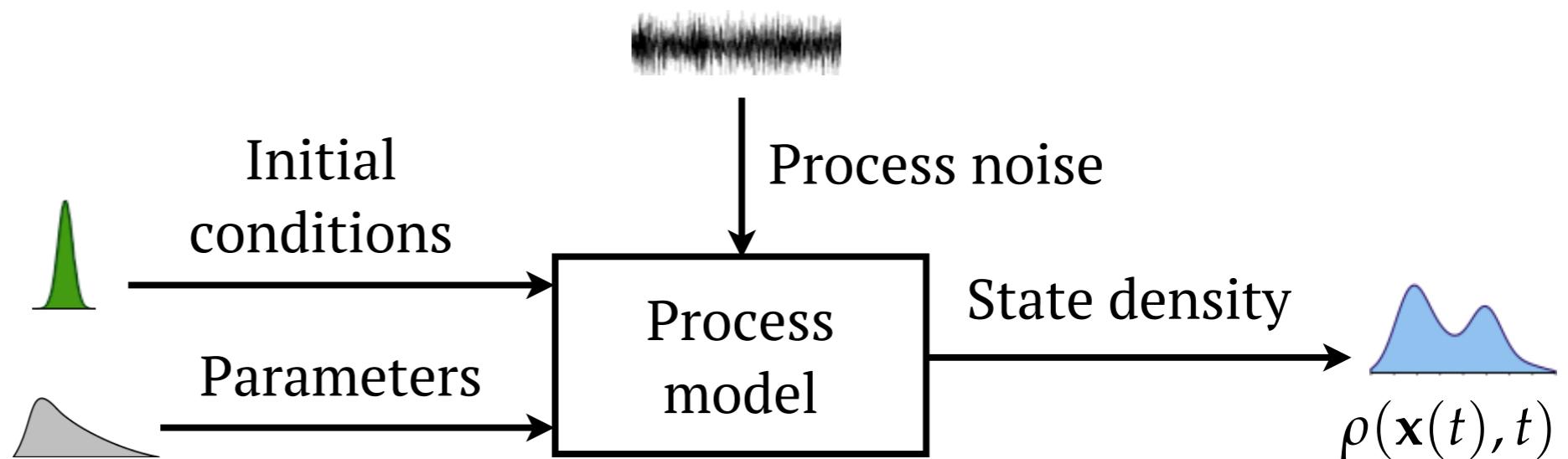
$$\rho(x, t) : \mathcal{X} \times [0, \infty) \mapsto \mathbb{R}_{\geq 0}$$

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

Why bother about densities?

# Prediction Problem

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



Trajectory flow:

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

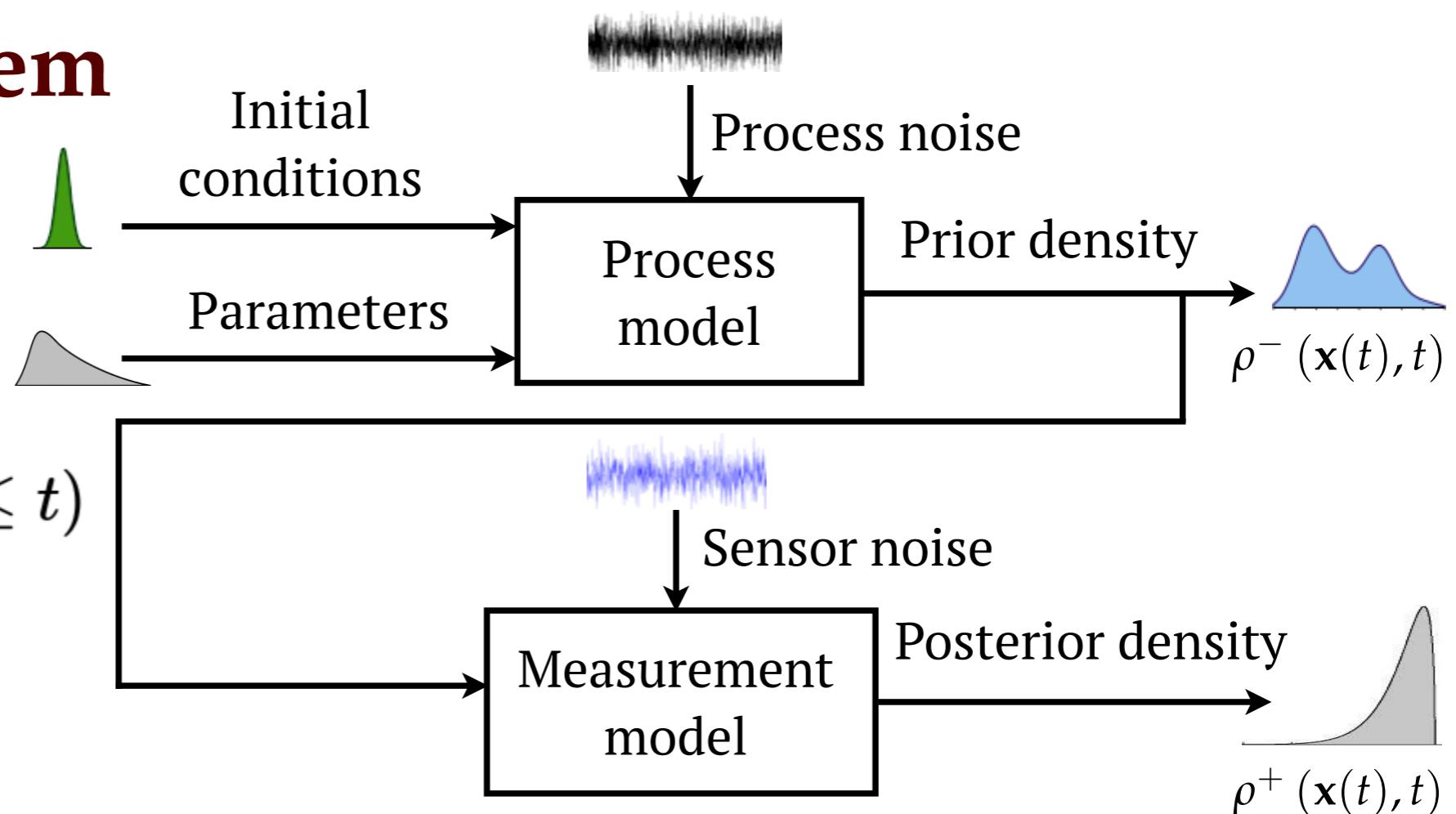
Density flow:

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

# Filtering Problem

Compute conditional joint state PDF

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



Trajectory flow:

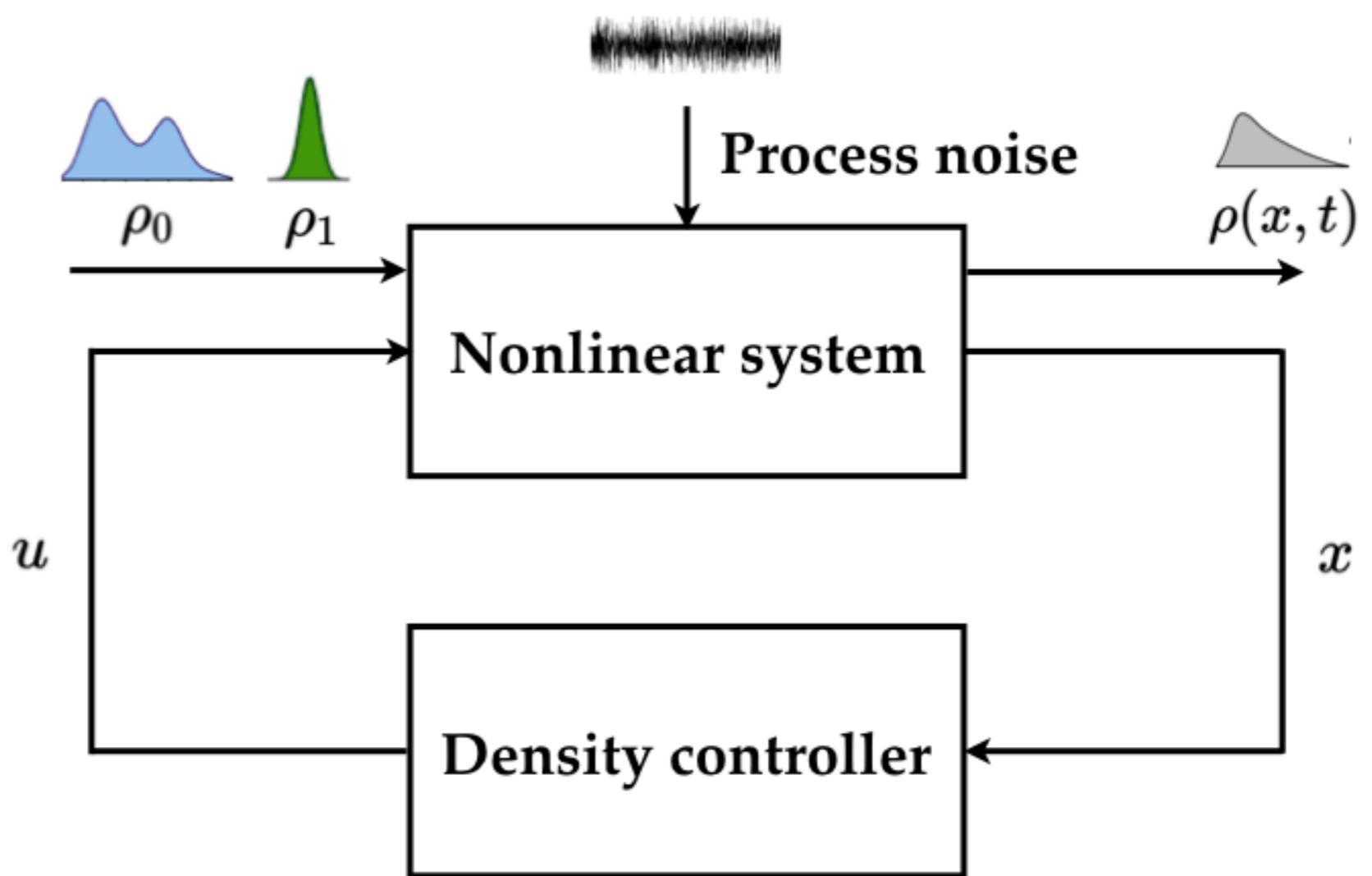
$$\begin{aligned} d\mathbf{x}(t) &= \mathbf{f}(\mathbf{x}, t) dt + \mathbf{g}(\mathbf{x}, t) dw(t), & dw(t) &\sim \mathcal{N}(0, \mathbf{Q} dt) \\ d\mathbf{z}(t) &= \mathbf{h}(\mathbf{x}, t) dt + dv(t), & dv(t) &\sim \mathcal{N}(0, \mathbf{R} dt) \end{aligned}$$

Density flow:

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

# Control Problem

Steer joint state PDF via feedback control



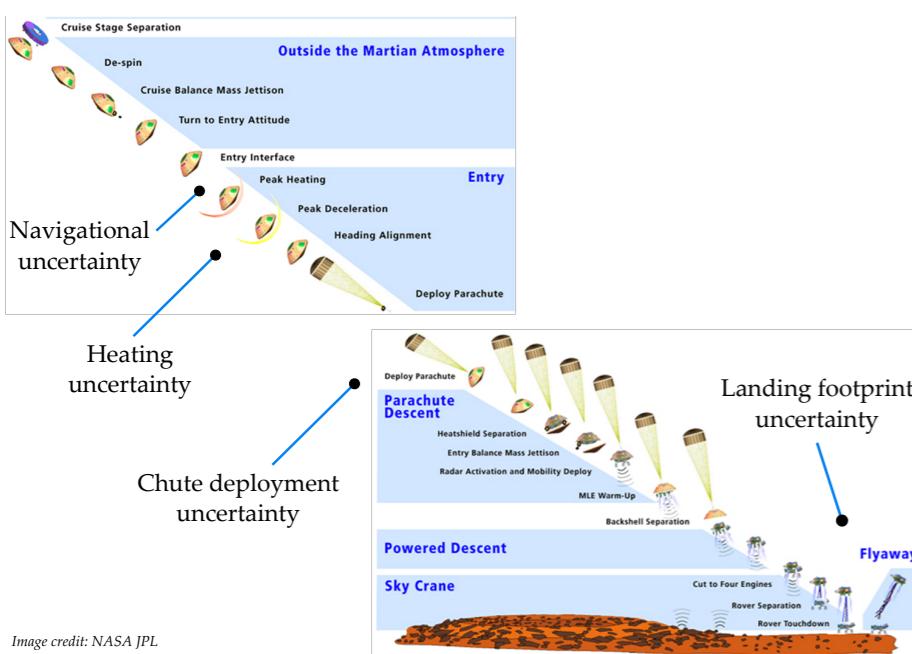
$$\underset{u \in \mathcal{U}}{\text{minimize}} \mathbb{E} \left[ \int_0^1 \|u\|_2^2 dt \right]$$

subject to

$$dx = f(x, u, t) dt + g(x, t) dw,$$
$$x(t=0) \sim \rho_0, \quad x(t=1) \sim \rho_1$$

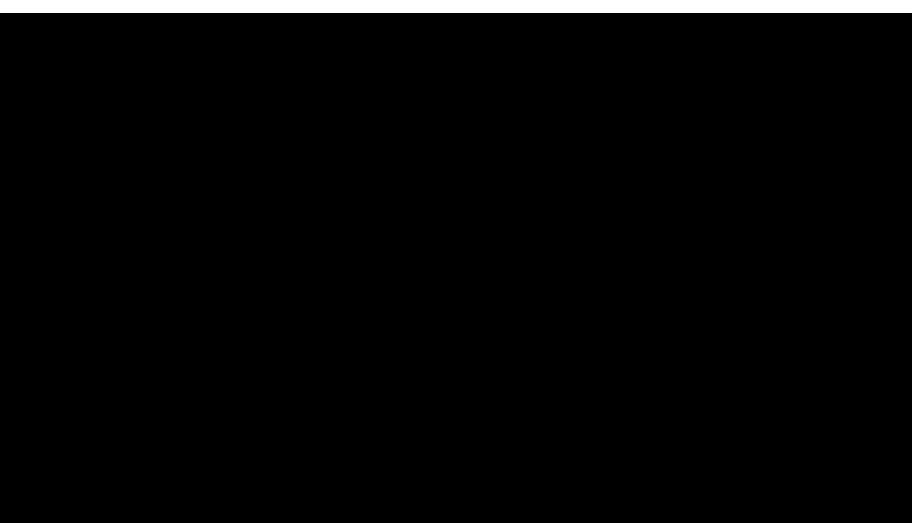
# PDFs in Mars Entry-Descent-Landing

## Prediction Problem



## Filtering Problem

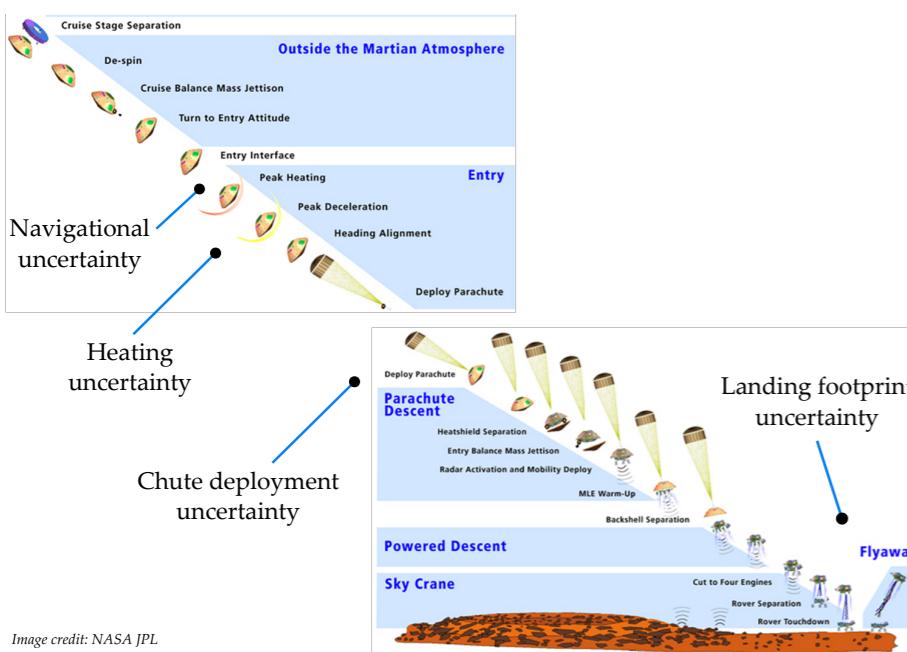
## Control Problem



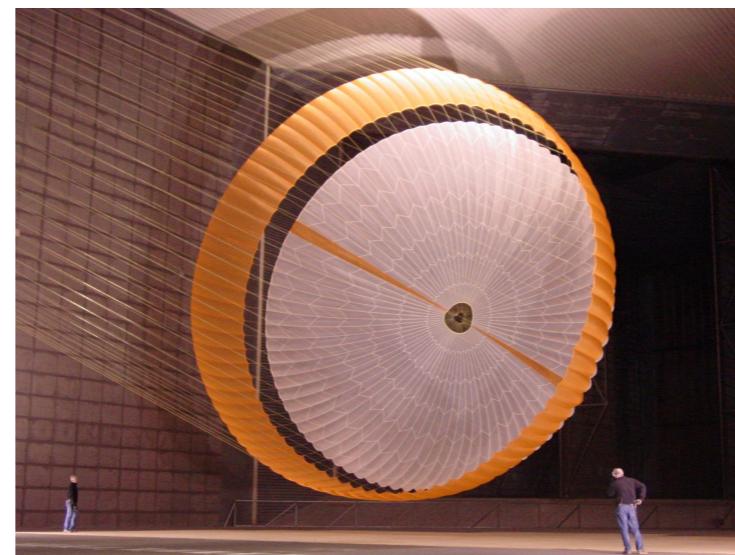
Predict heating rate uncertainty

# PDFs in Mars Entry-Descent-Landing

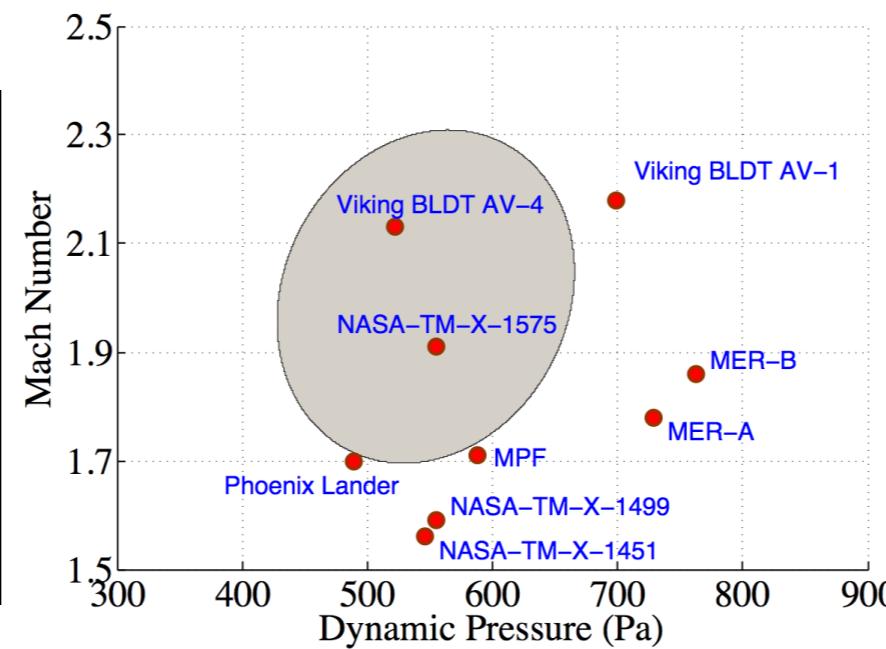
## Prediction Problem



## Filtering Problem



## Control Problem

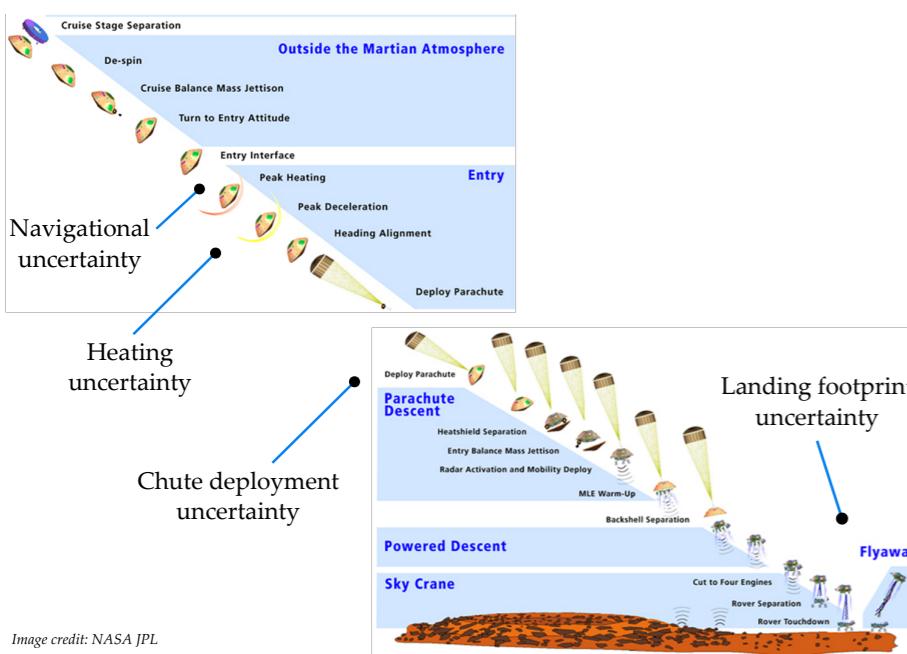


Predict heating rate uncertainty

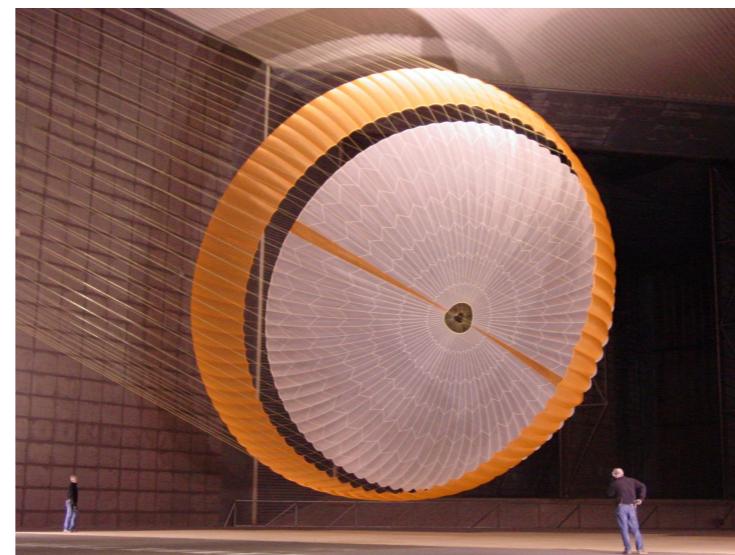
Estimate state to deploy parachute

# PDFs in Mars Entry-Descent-Landing

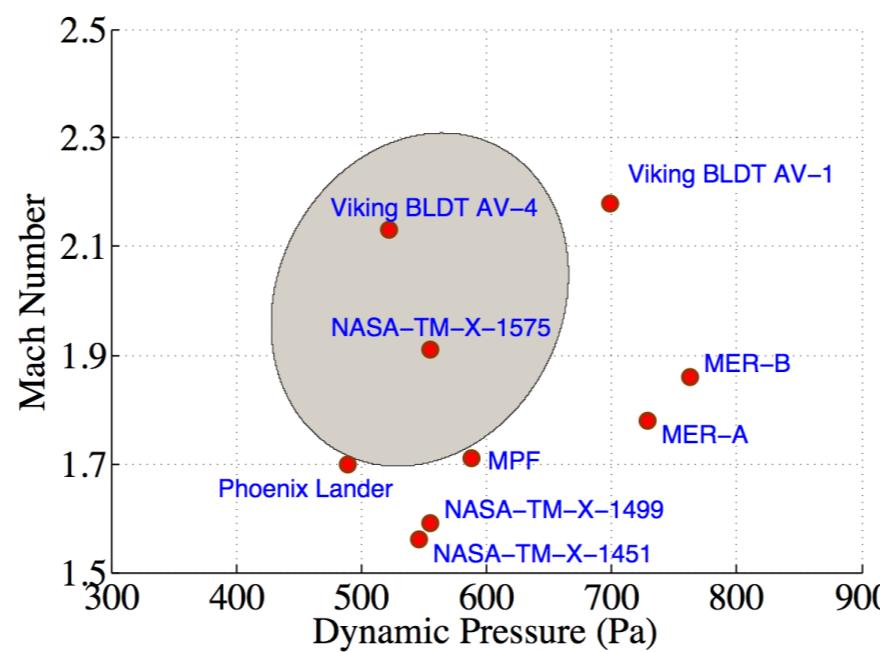
## Prediction Problem



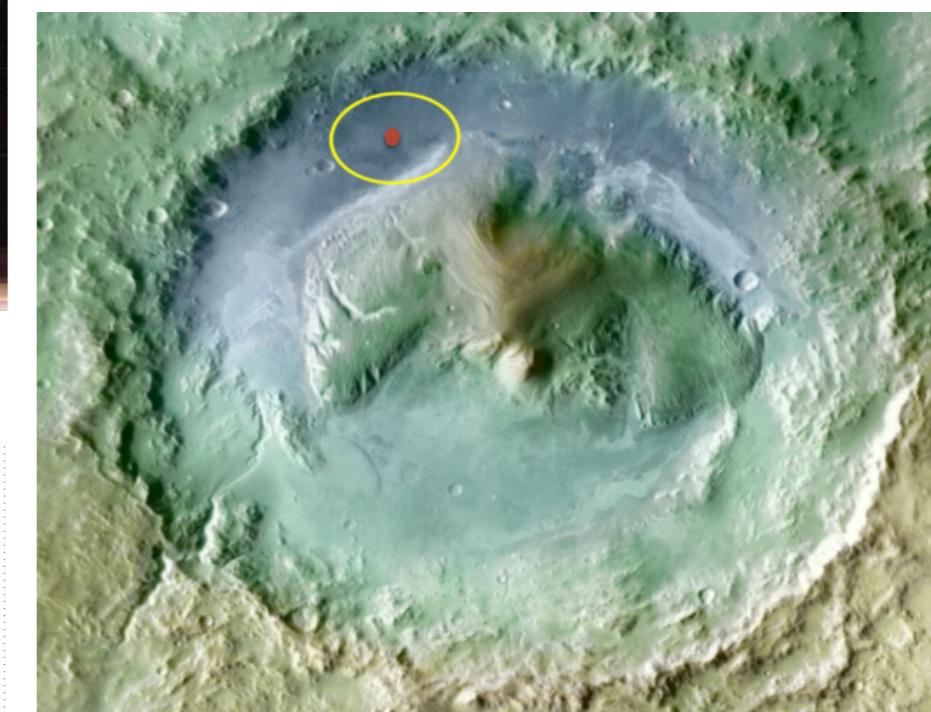
## Filtering Problem



Supersonic parachute



## Control Problem



Gale Crater (4.49S, 137.42E)

Predict heating rate uncertainty

Estimate state to deploy parachute

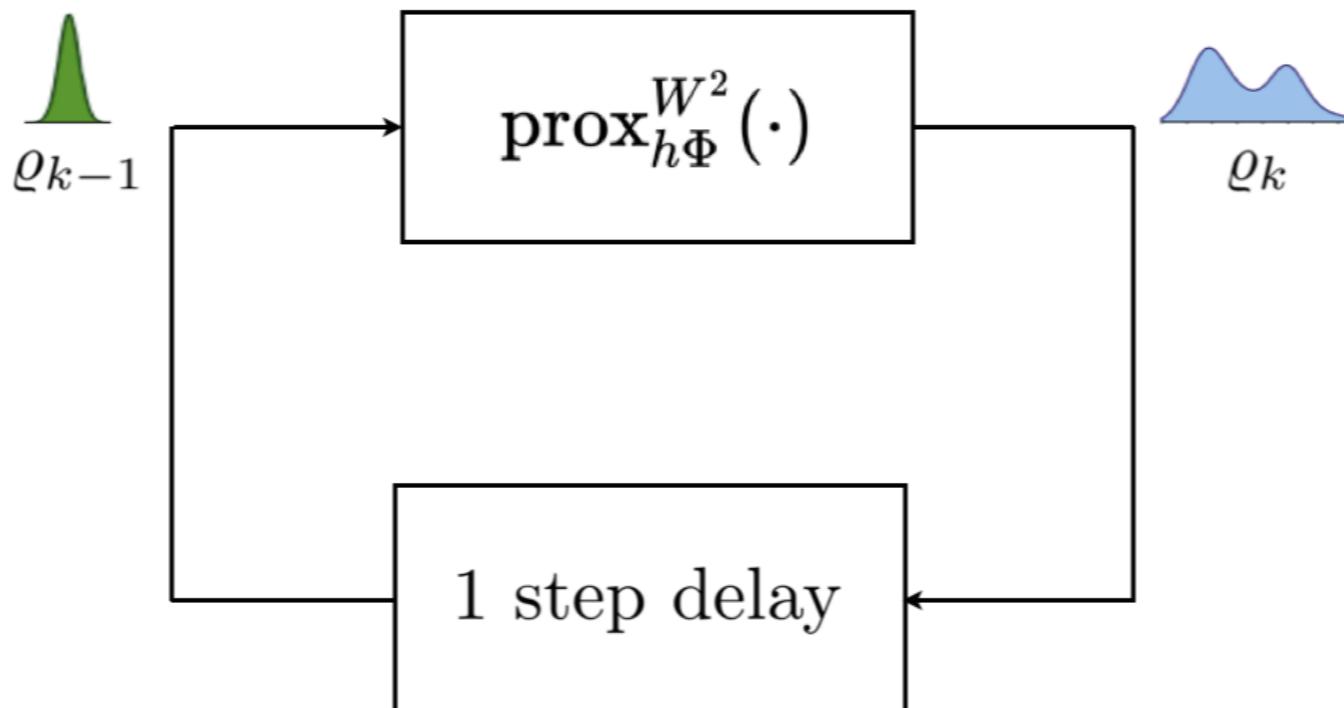
Steer state PDF to achieve desired landing footprint accuracy

# 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:  $\rho_k = \text{prox}_{h\Phi}^{W^2}(\rho_{k-1}) := \arg \inf_{\rho \in \mathcal{P}_2(\mathcal{X})} \left\{ \frac{1}{2} W^2(\rho, \rho_{k-1}) + h\Phi(\rho) \right\}$

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

Free energy functional:  $\Phi(\rho) := \int_{\mathcal{X}} \psi \rho dx + \beta^{-1} \int_{\mathcal{X}} \rho \log \rho dx$

# Gradient Flow

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

$$\frac{dx}{dt} = -\nabla \varphi(x), \quad x(0) = x_0$$

**Recursion:**

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

**Convergence:**

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

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

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

**Recursion:**

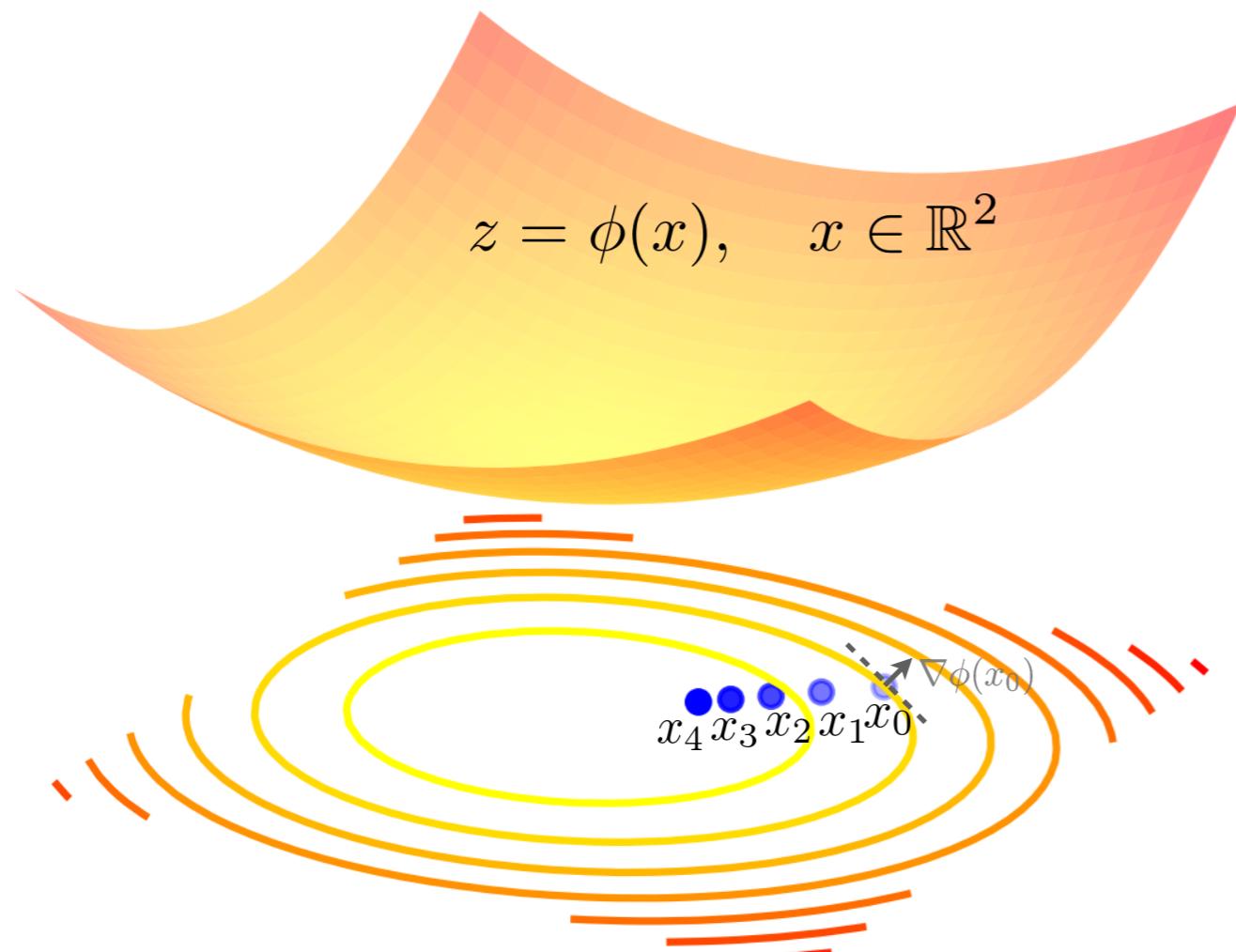
$$\begin{aligned} \rho_k &= \rho(\cdot, t = kh) \\ &= \arg \min_{\rho \in \mathcal{P}_2(\mathcal{X})} \left\{ \frac{1}{2} W^2(\rho, \rho_{k-1}) + h \Phi(\rho) \right\} \\ &=: \text{prox}_{h\Phi}^{W^2}(\rho_{k-1}) \end{aligned}$$

**Convergence:**

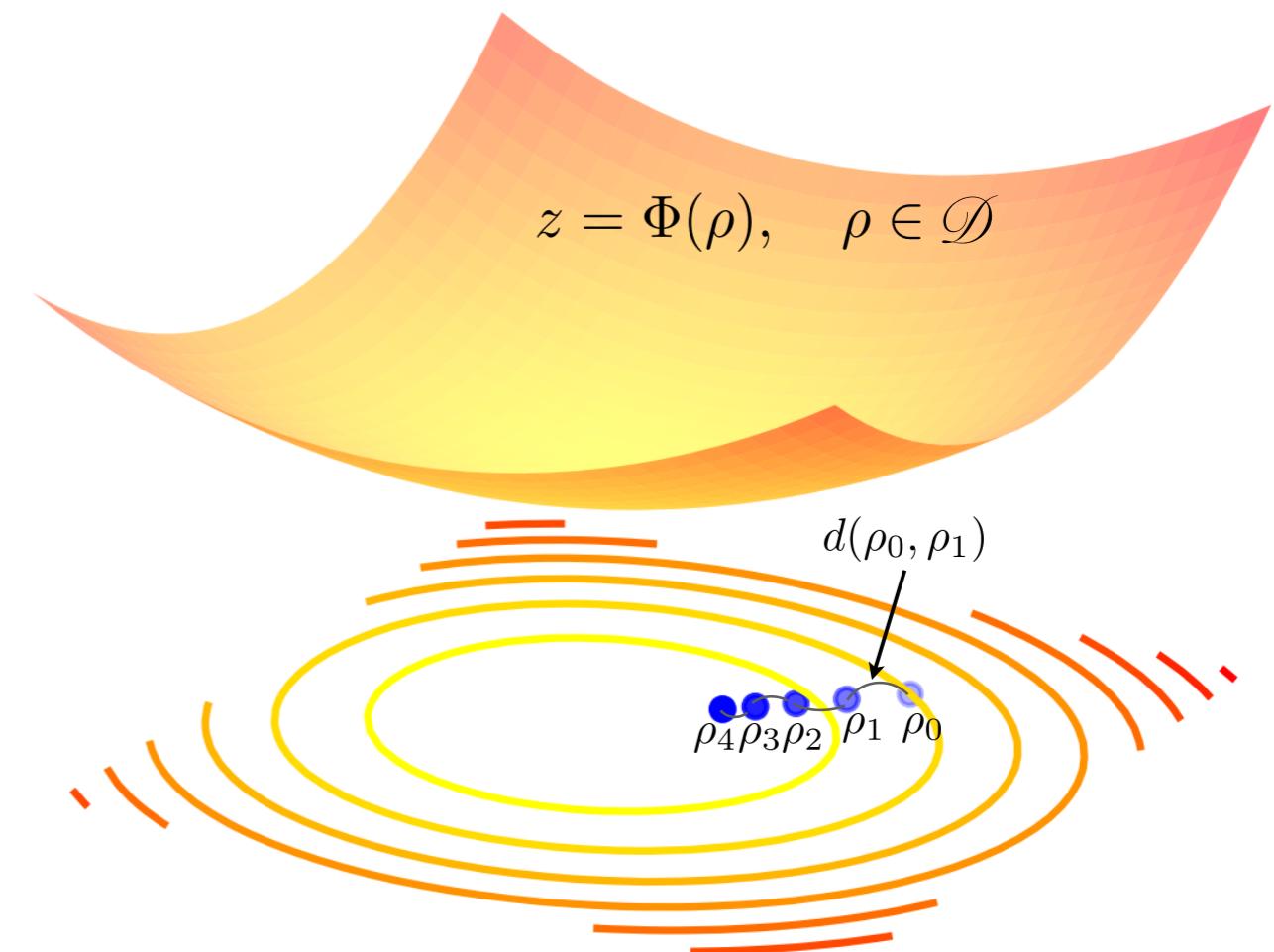
$$\rho_k \rightarrow \rho(\cdot, t = kh) \quad \text{as} \quad h \downarrow 0$$

# Gradient Flow

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

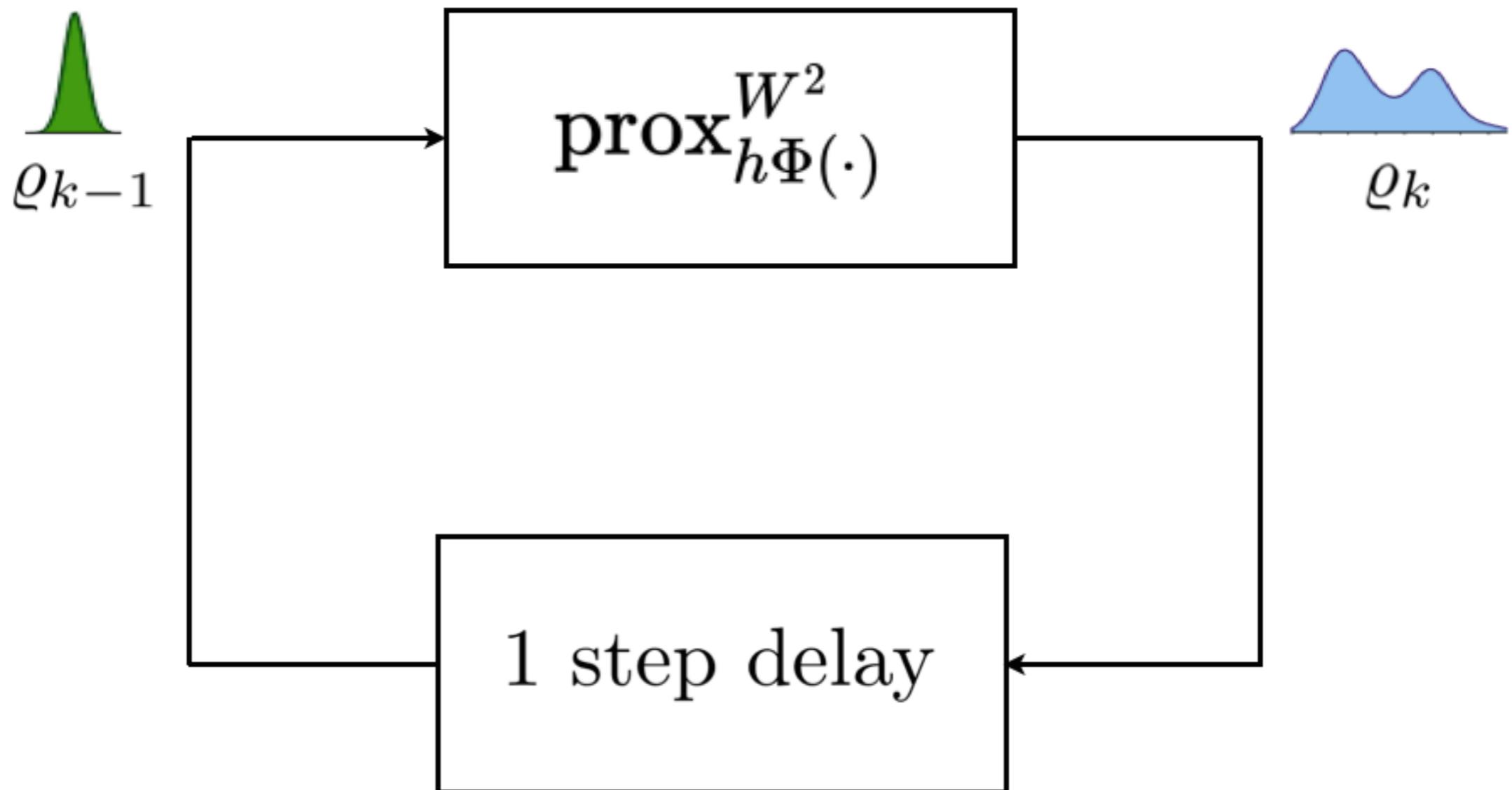


## Gradient Flow in $\mathcal{P}_2(\mathcal{X})$



# 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**

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

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$\Downarrow$     **Discrete Primal Formulation**

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

# 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**

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

# Algorithm: Gradient Ascent on the Dual Space

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$\Updownarrow$  **Dualization**

$$\begin{aligned} \lambda_0^{\text{opt}}, \lambda_1^{\text{opt}} &= \arg \max_{\lambda_0, \lambda_1 \geq 0} \left\{ \langle \boldsymbol{\lambda}_0, \varrho_{k-1} \rangle - F^*(-\boldsymbol{\lambda}_1) \right. \\ &\quad \left. - \frac{\epsilon}{h} \left( \exp(\boldsymbol{\lambda}_0^\top h/\epsilon) \exp(-\mathbf{C}_k/2\epsilon) \exp(\boldsymbol{\lambda}_1 h/\epsilon) \right) \right\} \end{aligned}$$

# Fixed Point Recursion

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

Coupled Transcendental Equations in  $y$  and  $z$

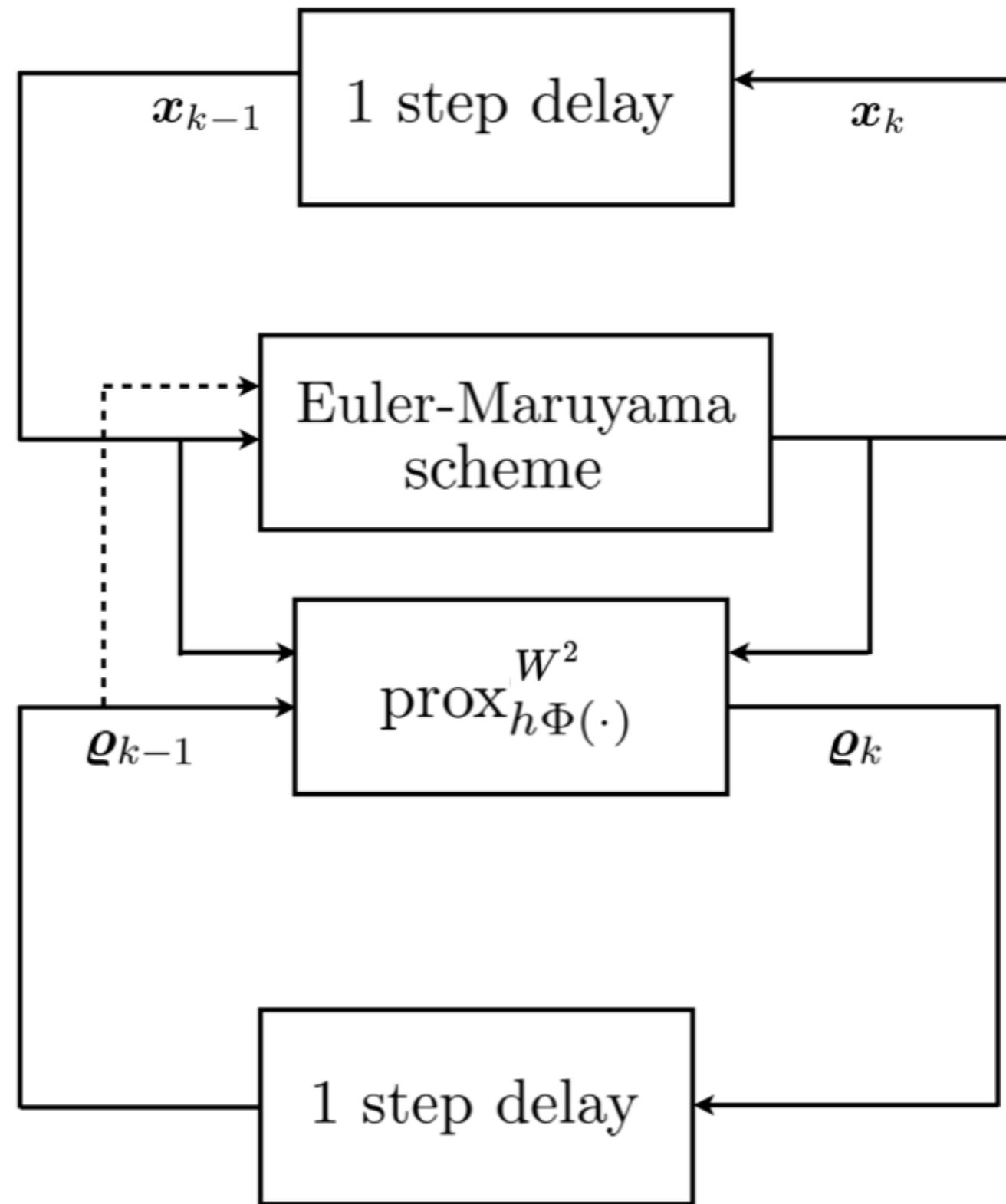
$$\begin{array}{ccc} \Gamma_k = e^{\frac{-c_k}{2\epsilon}} & \xrightarrow{\hspace{2cm}} & \\ \varrho_{k-1} & \xrightarrow{\hspace{2cm}} & \\ \xi_{k-1} = \frac{e^{-\beta\psi_{k-1}}}{e} & \xrightarrow{\hspace{2cm}} & \end{array} \boxed{y \odot \Gamma_k z = \varrho_{k-1} \\ z \odot \Gamma_k^\top y = \xi_{k-1} \odot z^{-\beta\epsilon/2h}} \rightarrow \varrho_k = z \odot \Gamma_k^\top y$$

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

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

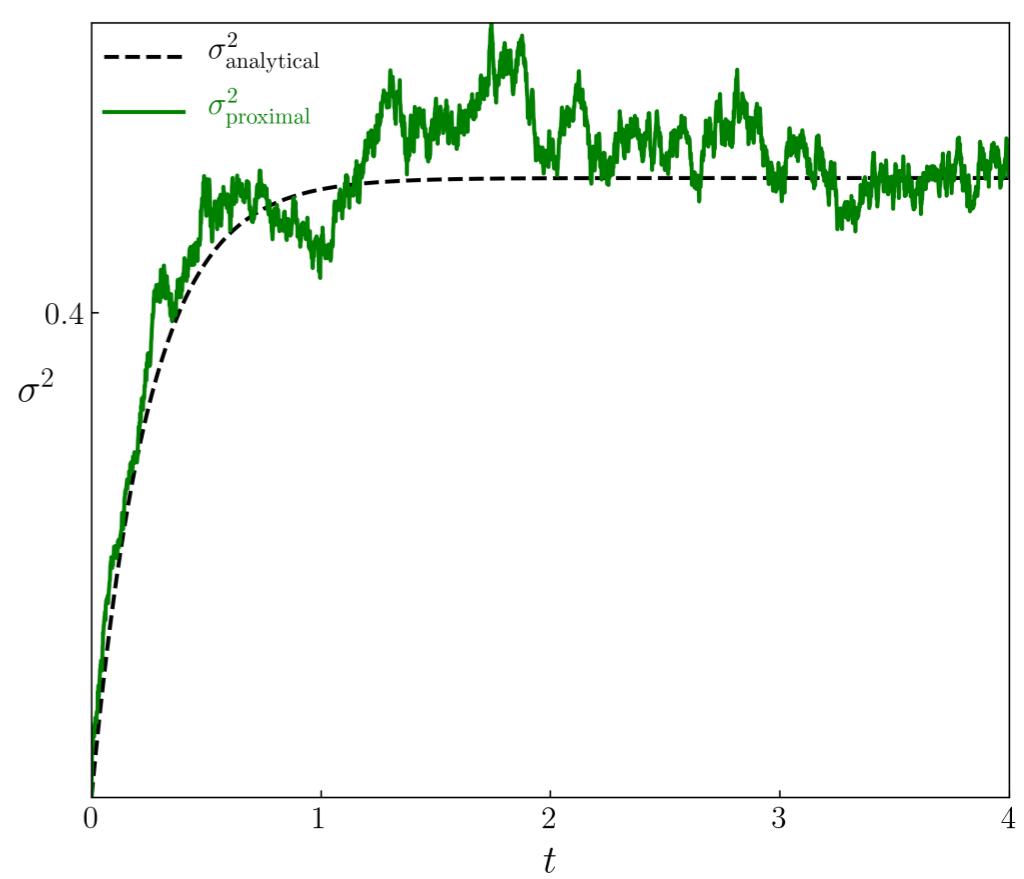
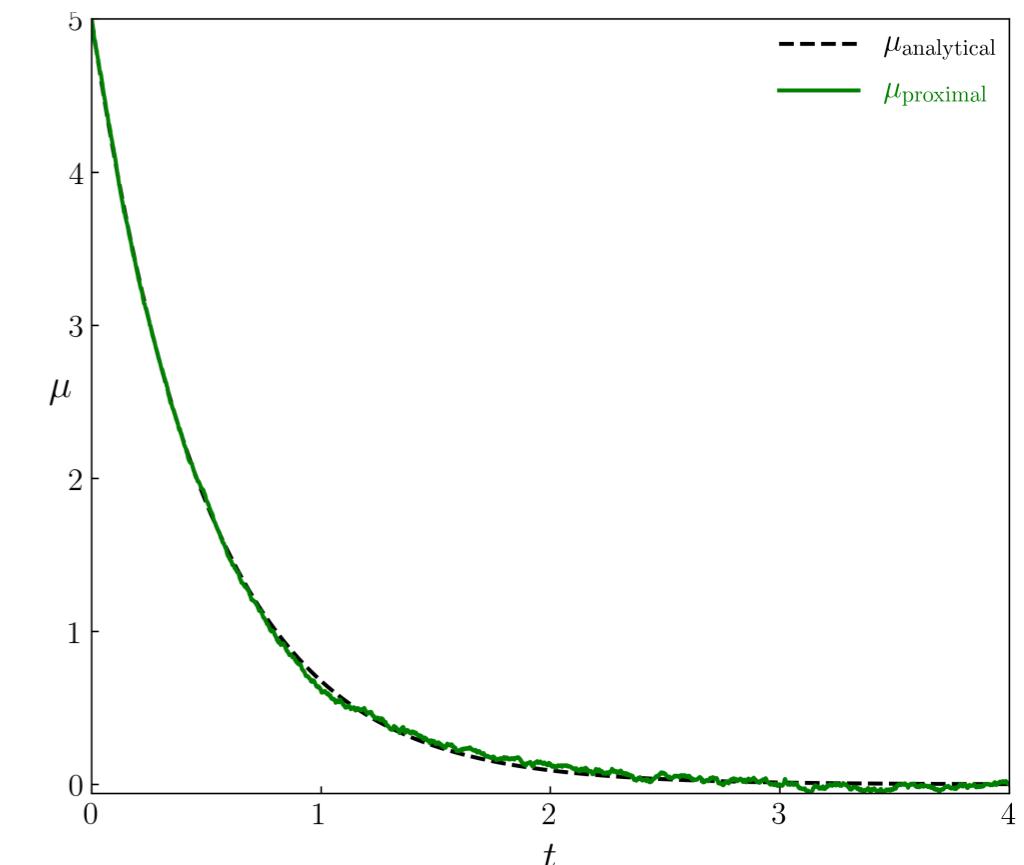
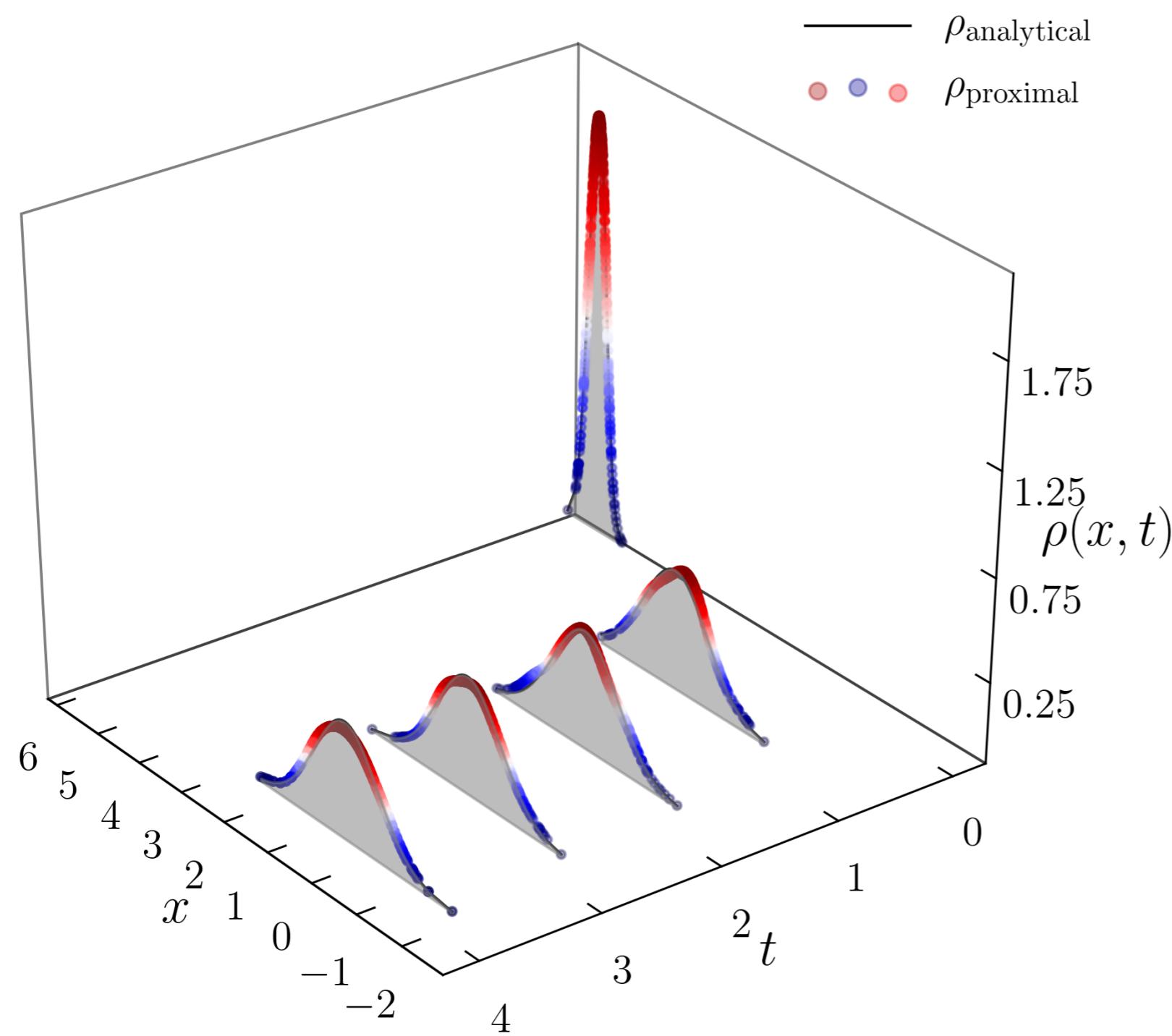
Then the solution  $(y^*, z^*)$  gives the proximal update  $\varrho_k = z^* \odot (\Gamma_k^\top y^*)$

# Algorithmic Setup

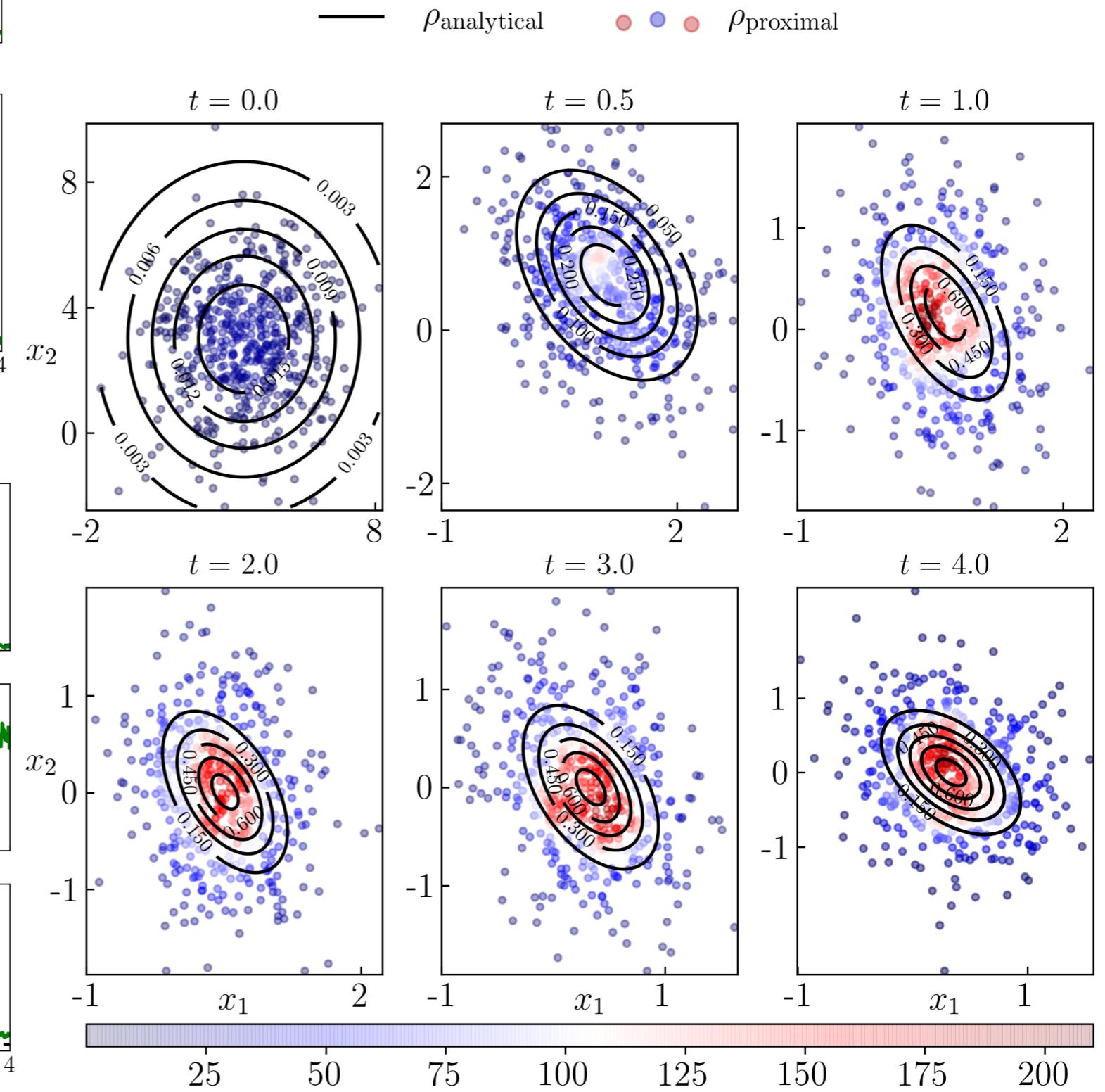
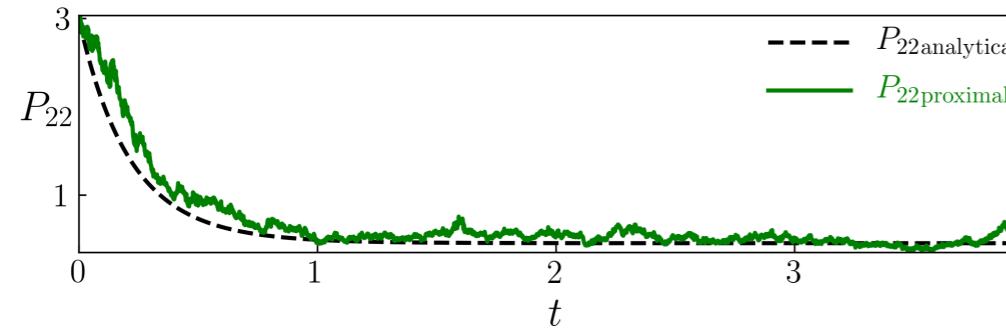
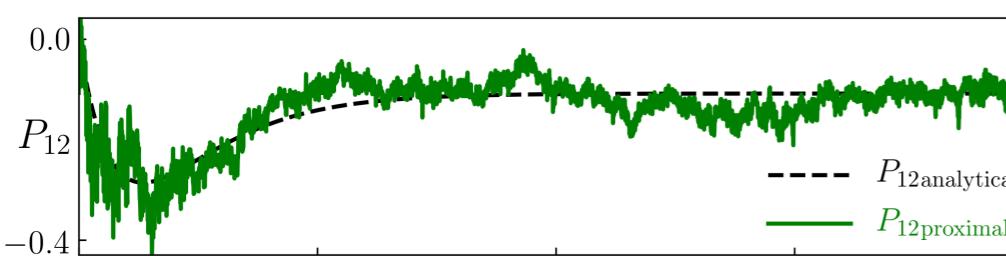
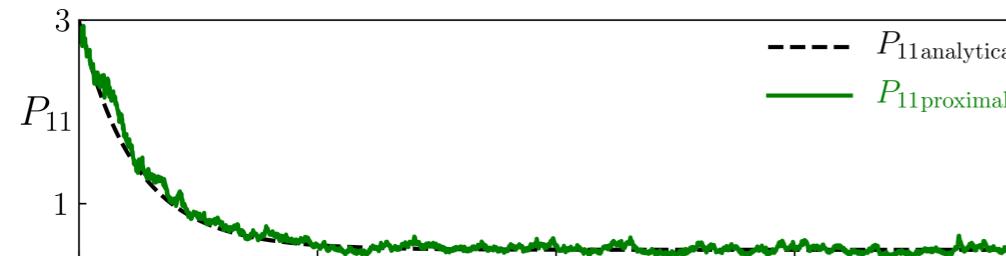
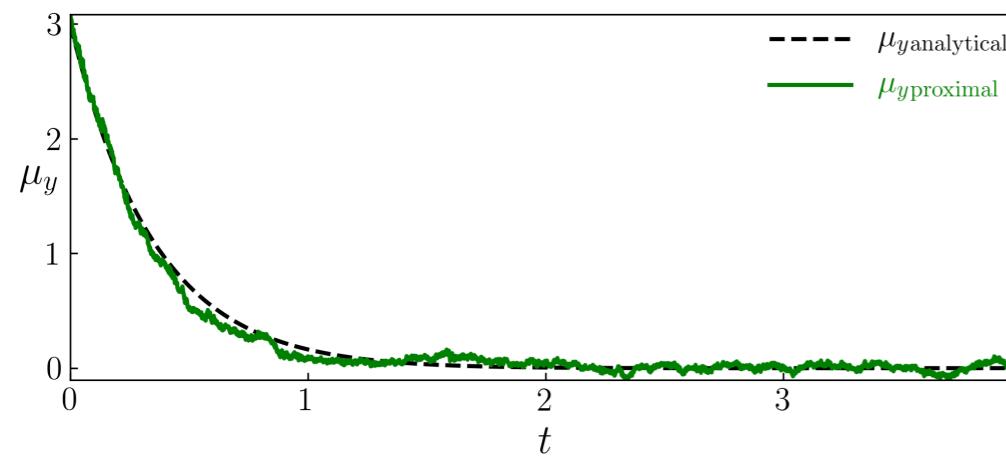
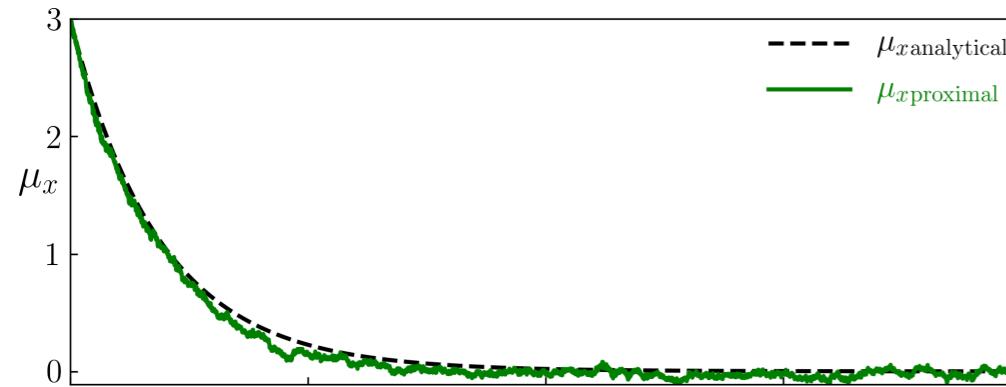


**Theorem:** Block co-ordinate iteration of  $(y, z)$  recursion is contractive on  $\mathbb{R}_{>0}^n \times \mathbb{R}_{>0}^n$ .

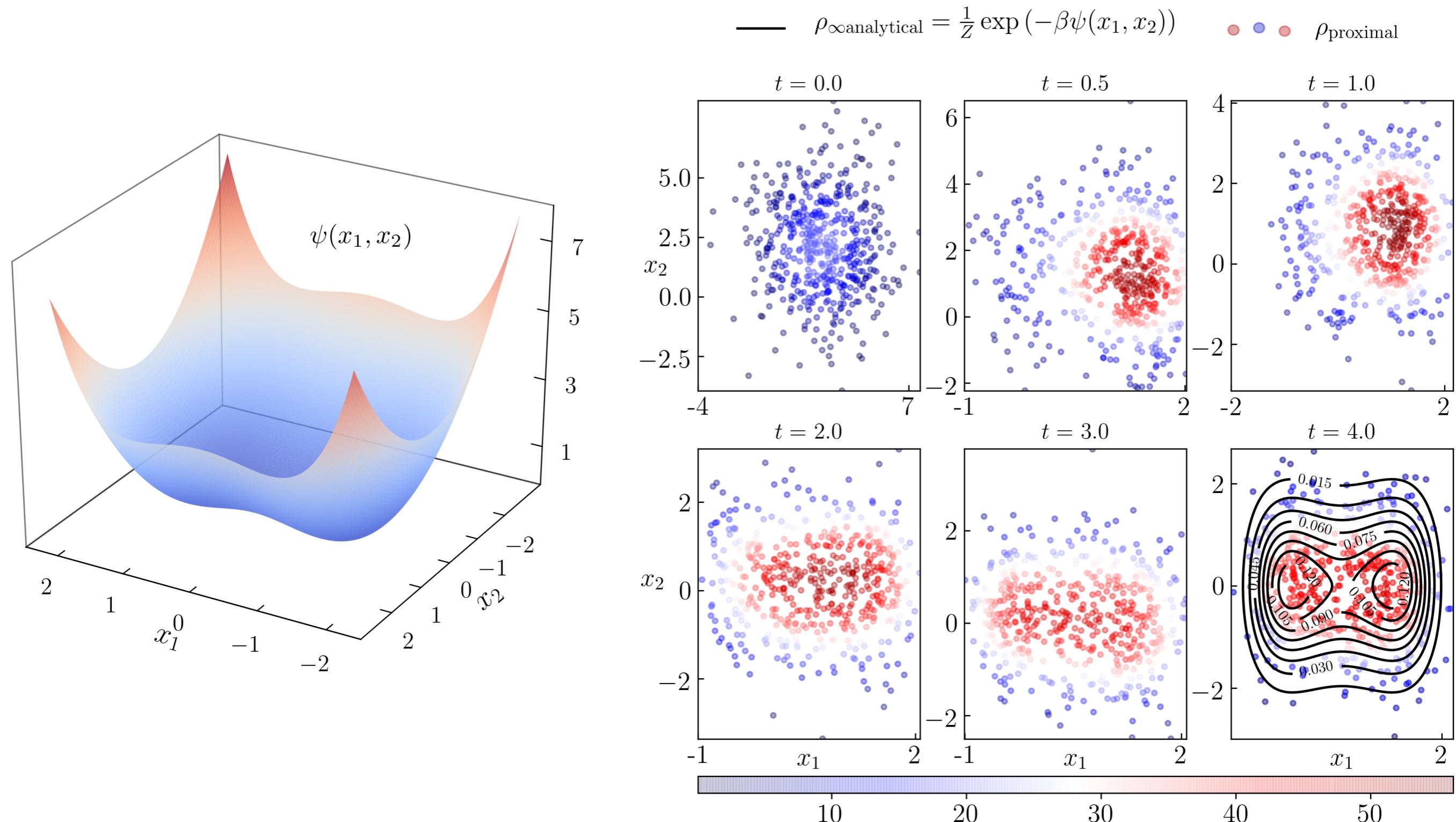
# Proximal Prediction: 1D Linear Gaussian



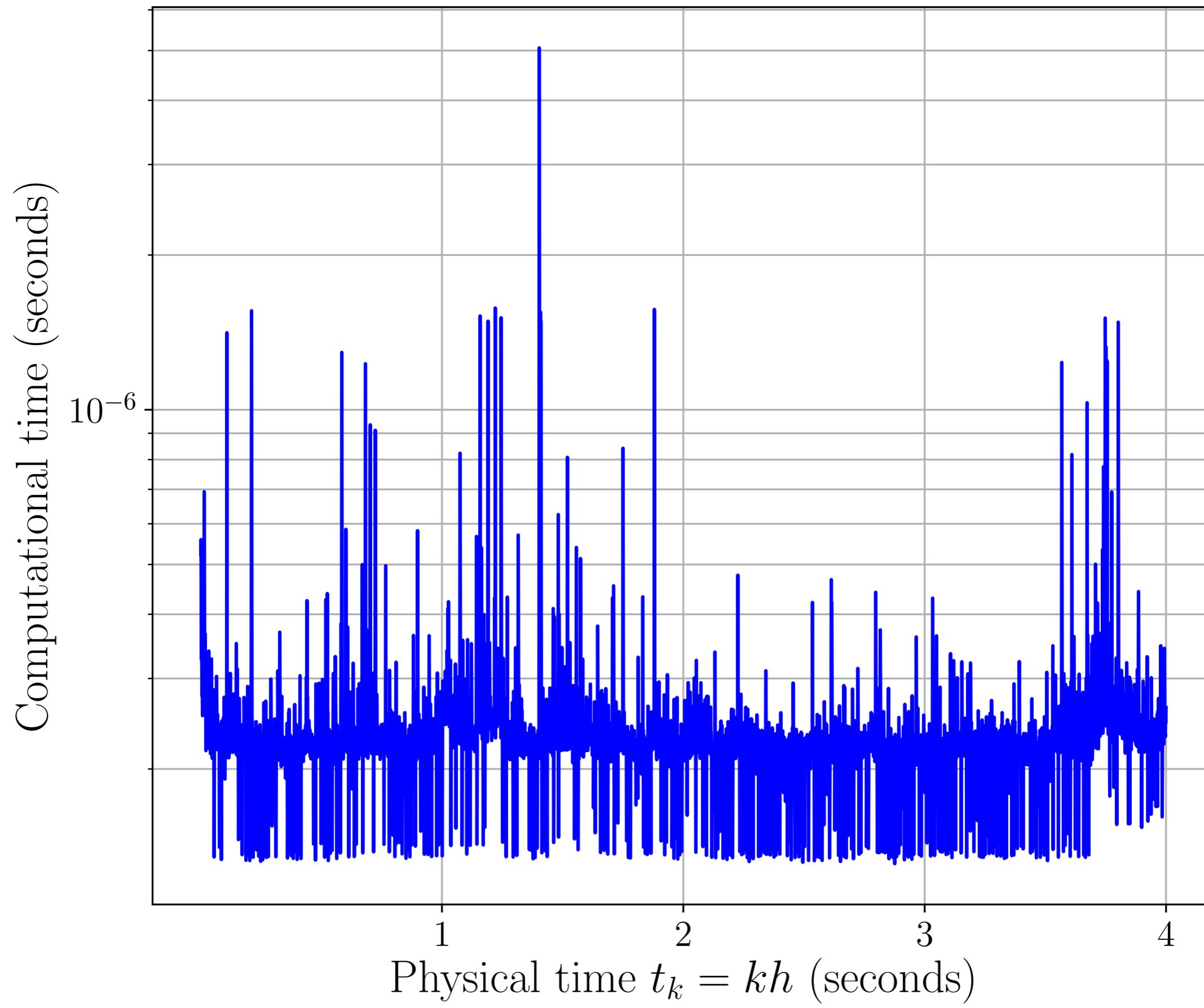
# Proximal Prediction: 2D Linear Gaussian



# Proximal Prediction: 2D Nonlinear Non-Gaussian



# Computational Time: 2D Nonlinear Non-Gaussian



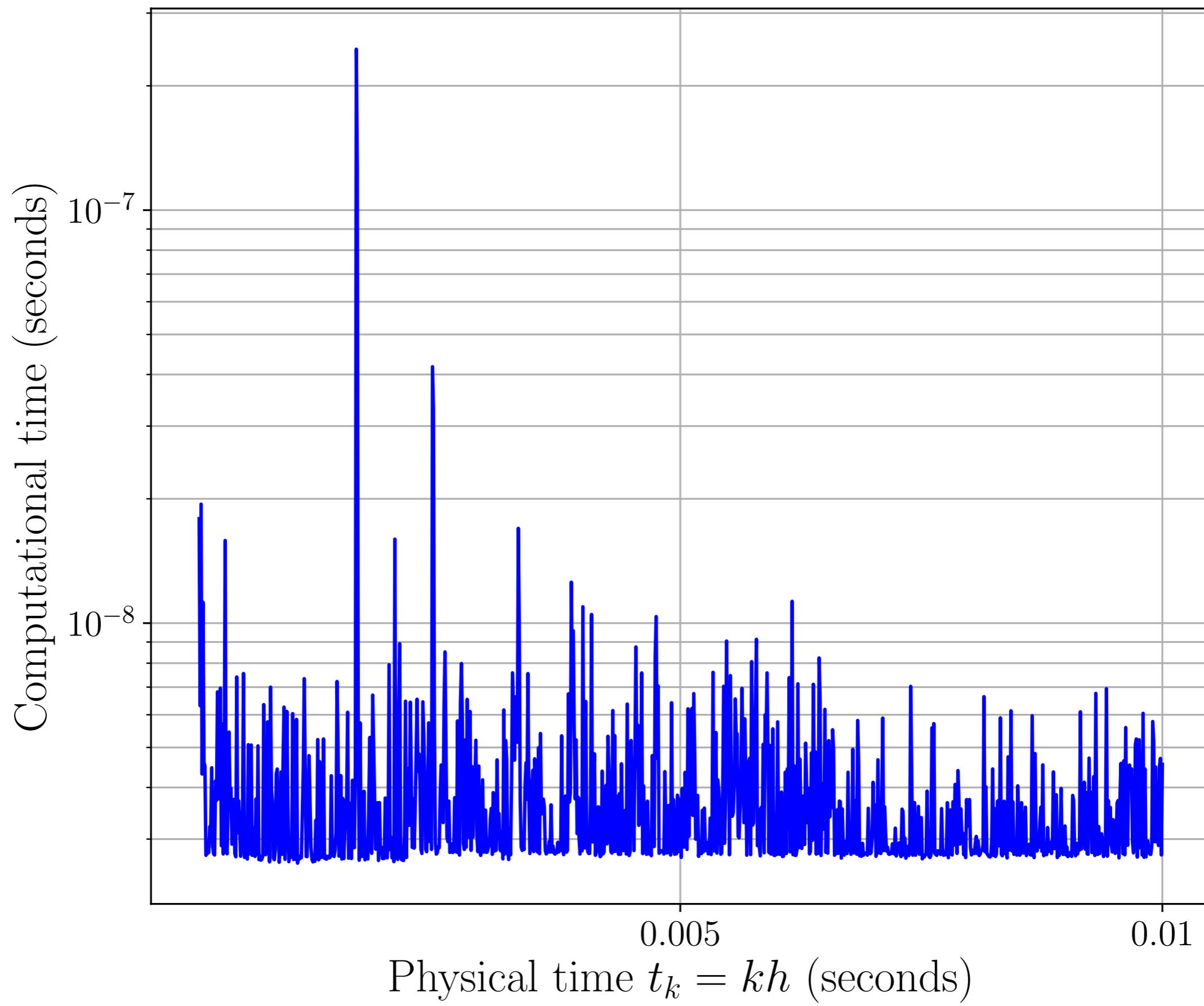
# Proximal Prediction: Satellite in Geocentric Orbit

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

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

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

# Computational Time: Satellite in Geocentric Orbit



# Extensions: Nonlocal interactions

PDF dependent sample path dynamics:

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

McKean-Vlasov-Fokker-Planck-Kolmogorov integro PDE:

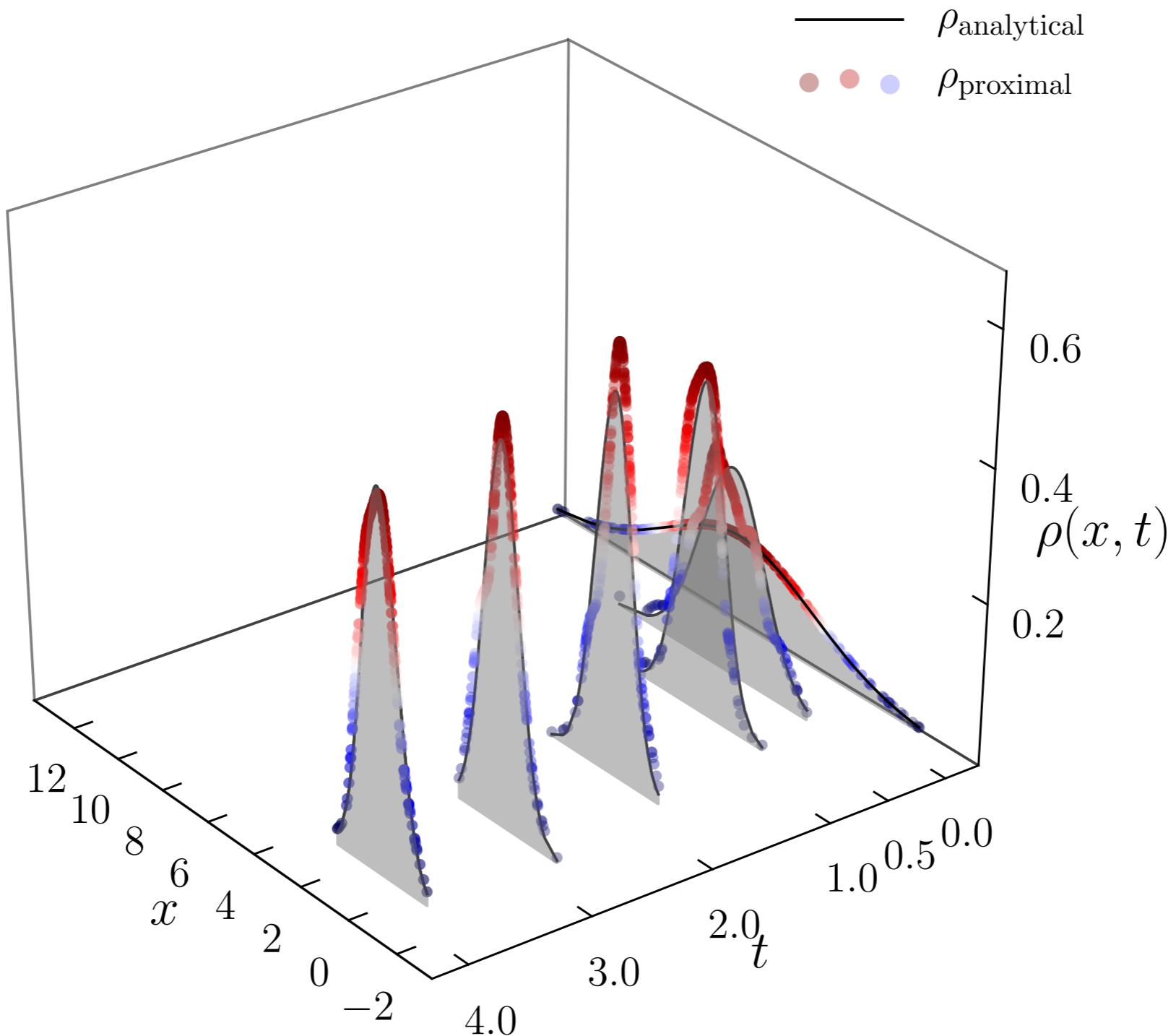
$$\frac{\partial \rho}{\partial t} = \nabla \cdot (\rho \nabla (U + \rho * V)) + \beta^{-1} \Delta \rho$$

Free energy:

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

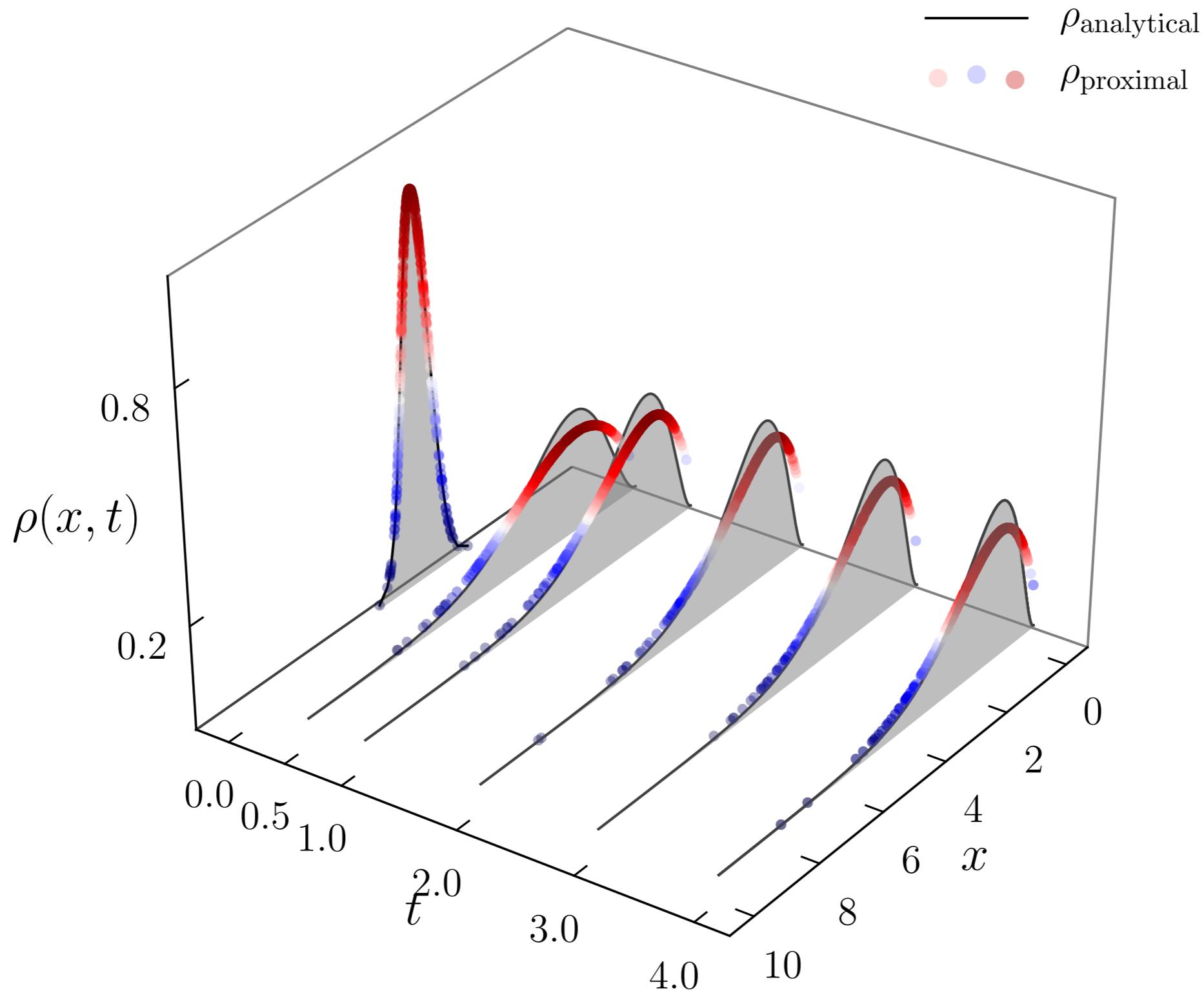
# Extensions: Nonlocal interactions (contd.)

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



# Extensions: Multiplicative Noise

Cox-Ingersoll-Ross:  $\mathrm{d}x = a(\theta - x) \, \mathrm{d}t + b\sqrt{x} \, \mathrm{d}w, 2a > b^2, \theta > 0$



# 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.

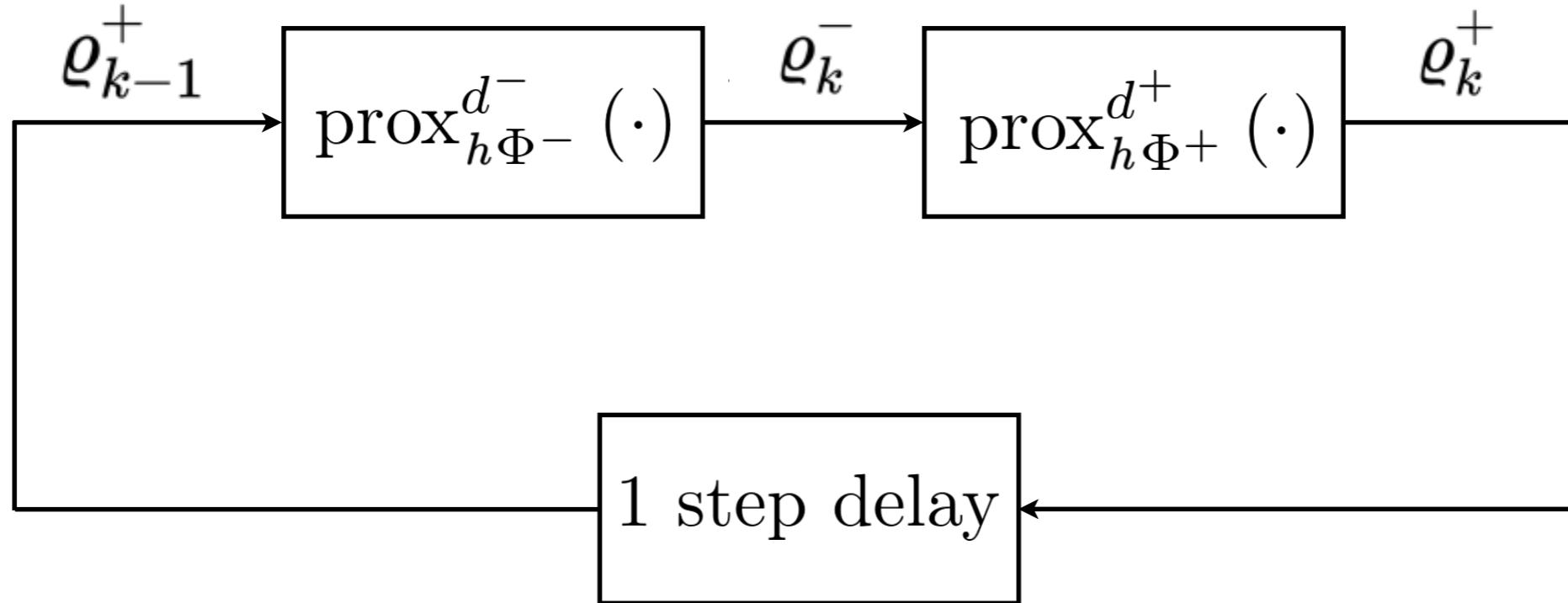
# Solving filtering problem as gradient flow

# 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  $\circ$  stochastic} proximal operators:



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

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

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

# 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:

$$\begin{matrix} \mathbf{P}^+ \mathbf{C} \mathbf{R}^{-1} \\ | \end{matrix}$$

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

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

— 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:**

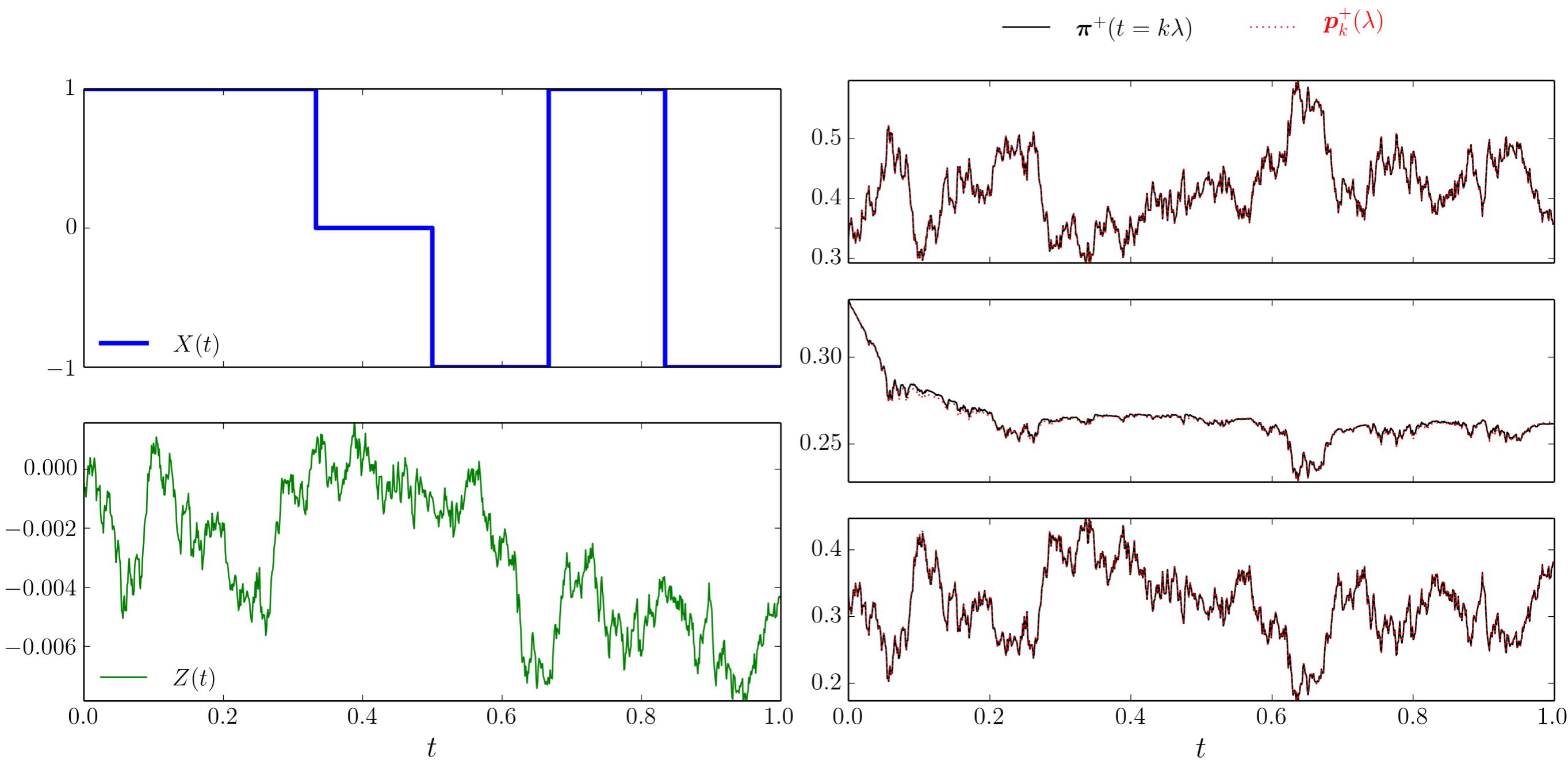
$$d\pi^+(t) = \pi^+(t)Q dt + \frac{1}{(\sigma_v(t))^2} \pi^+(t) \left( H - \hat{h}(t)I \right) \left( dz(t) - \hat{h}(t)dt \right),$$

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

**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



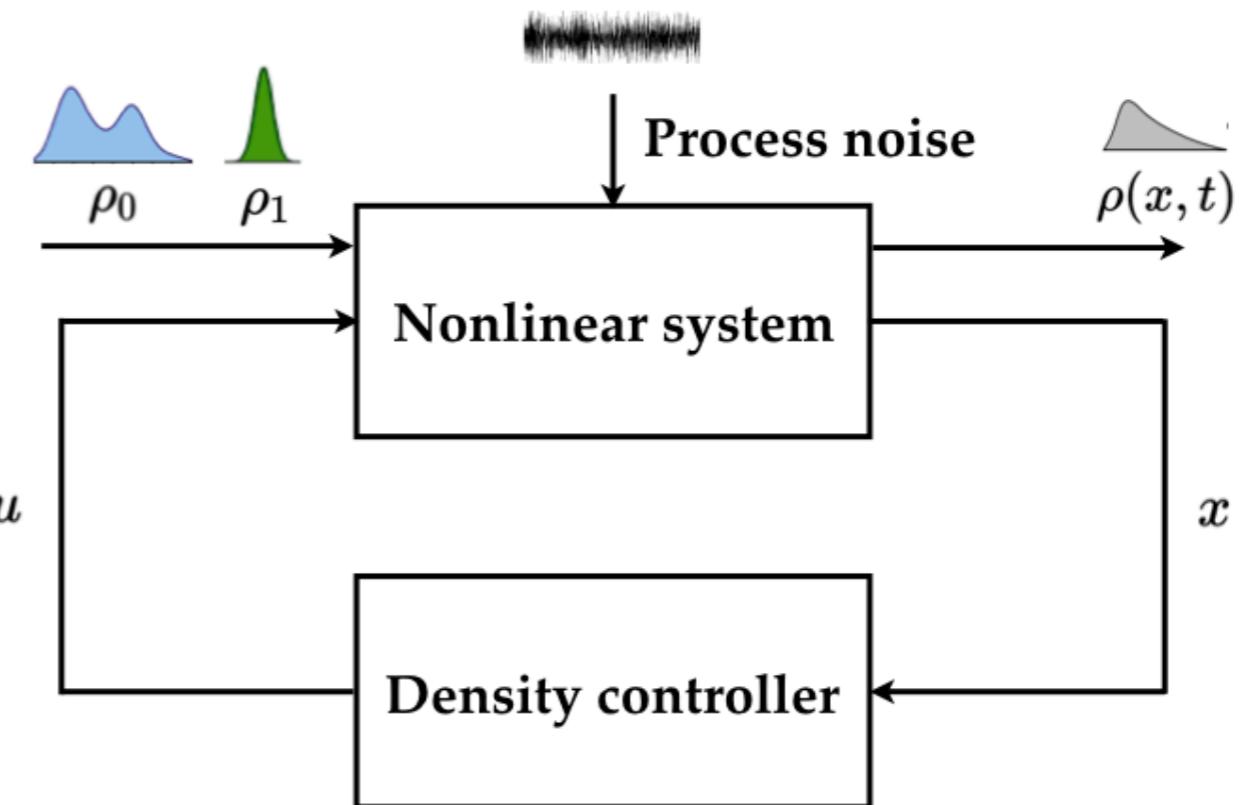
# Solving density steering using gradient flow

# Finite Horizon Feedback Density Steering

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

subject to

$$dx = f(x, u, t) dt + g(x, t) dw, \quad u \\ x(t=0) \sim \rho_0, \quad x(t=1) \sim \rho_1$$



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):

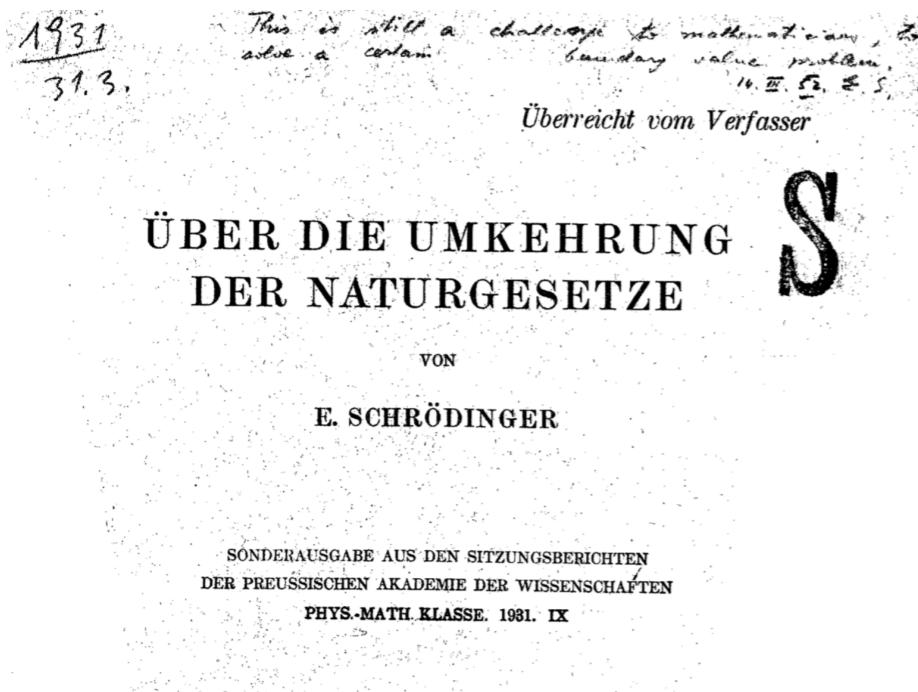
$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho(f + \nabla \psi)) + \epsilon \Delta \rho,$$

$$\frac{\partial \psi}{\partial t} = -\langle f, \nabla \psi \rangle - \frac{\|\nabla \psi\|_2^2}{2} - \epsilon \Delta \psi.$$

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

# 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:

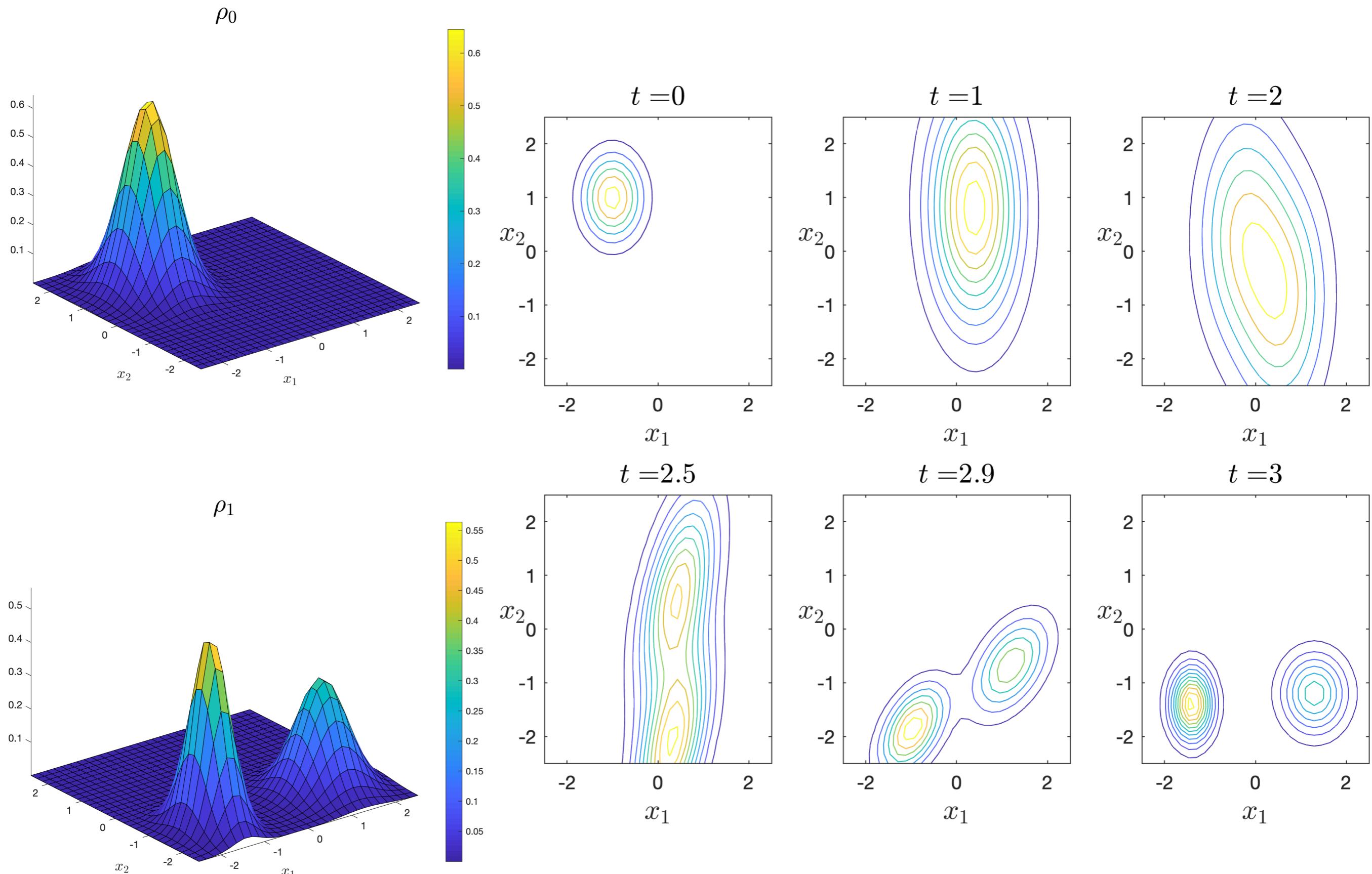
2 coupled nonlinear PDEs → boundary-coupled linear PDEs!!

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.

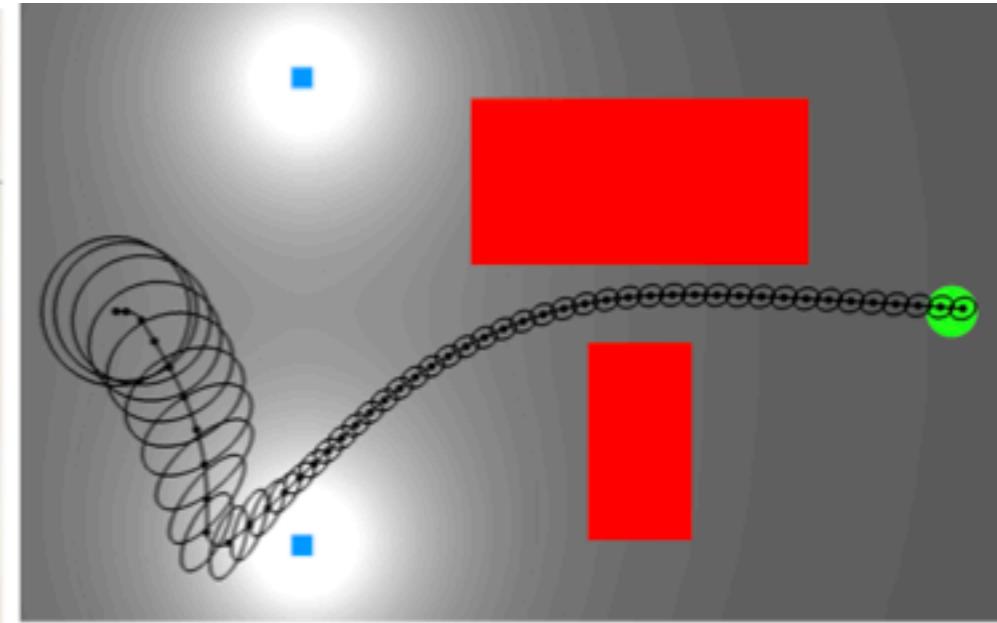
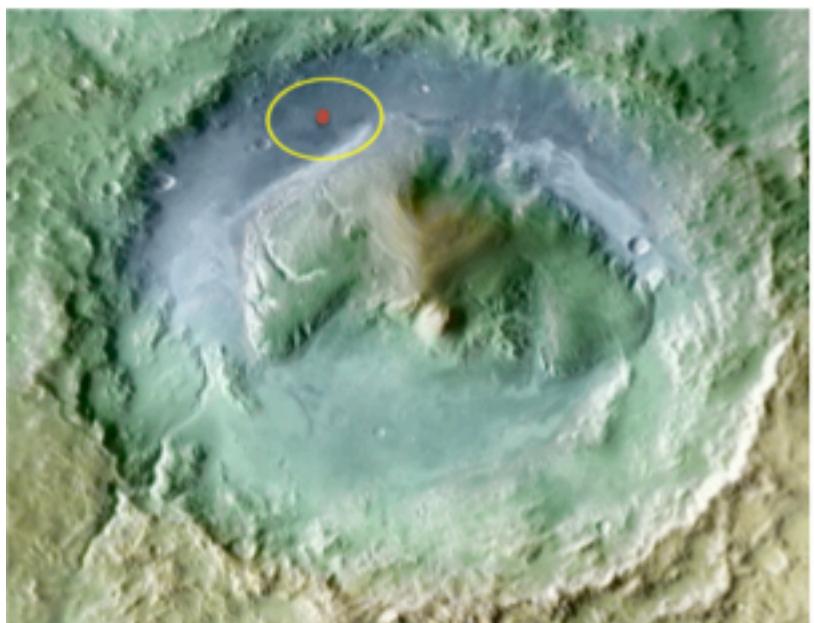
# Take Home Message

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