Learning Dynamical Systems from Invariant Measures

BIRS Workshop: New Ideas in Computational Inverse Problems

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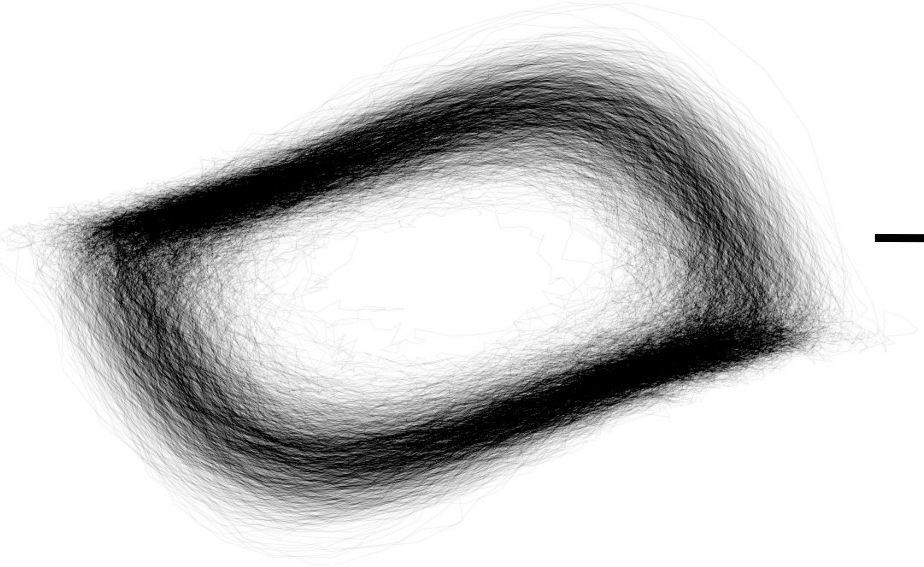
Acknowledgment: Robert Martin, U.S. Army Research Office

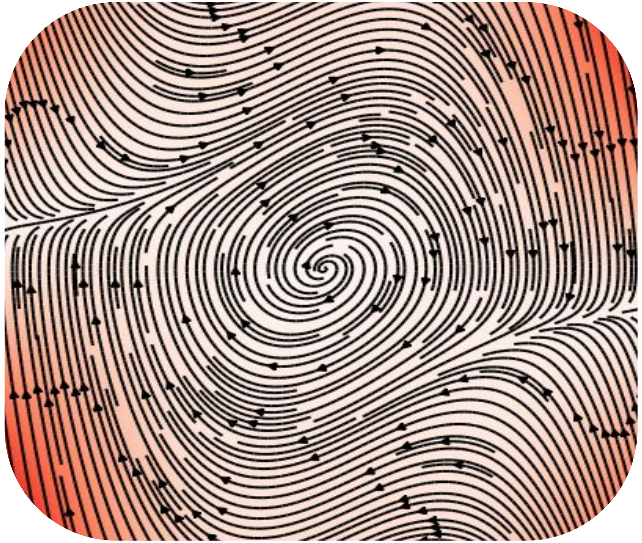
Motivation and Theory

What does it mean to learn a system?

Data



Computer Model



Imposing strict assumptions on the data quality

Noisy measurements, non-uniform in time, sampled slowly

Equations of motion with stochastic forcing

$$\{\widetilde{x}(t_i)\} \longrightarrow \dot{x} = v(x) + \omega(x,t)$$

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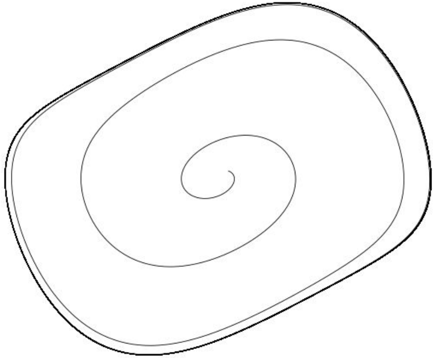
Best case scenario



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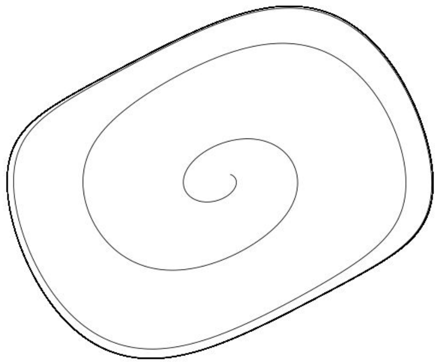
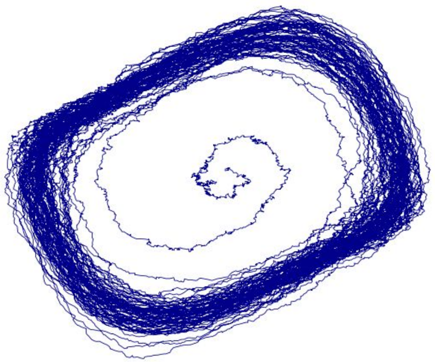


Stochastic forcing



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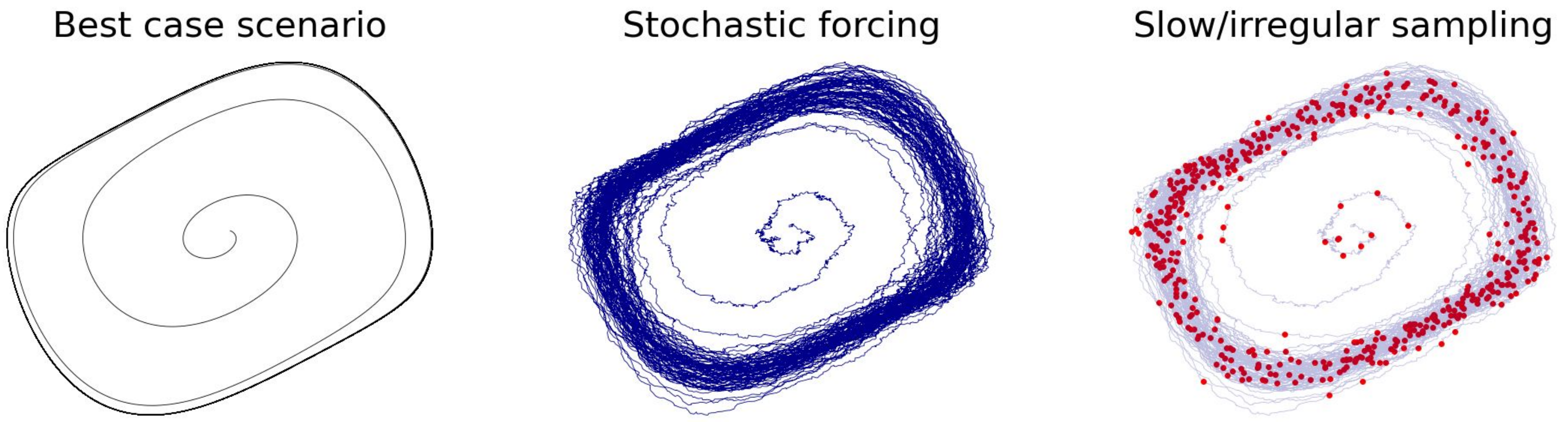
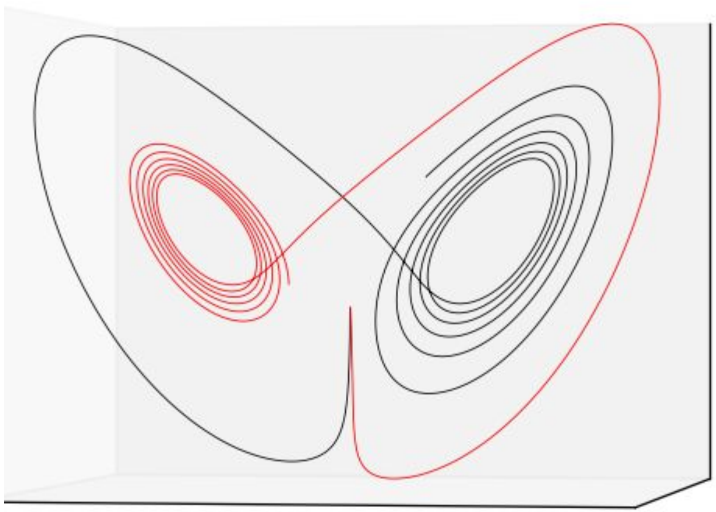


Lagrangian vs. Eulerian Dynamics

Lagrangian - describes trajectories of individual particles



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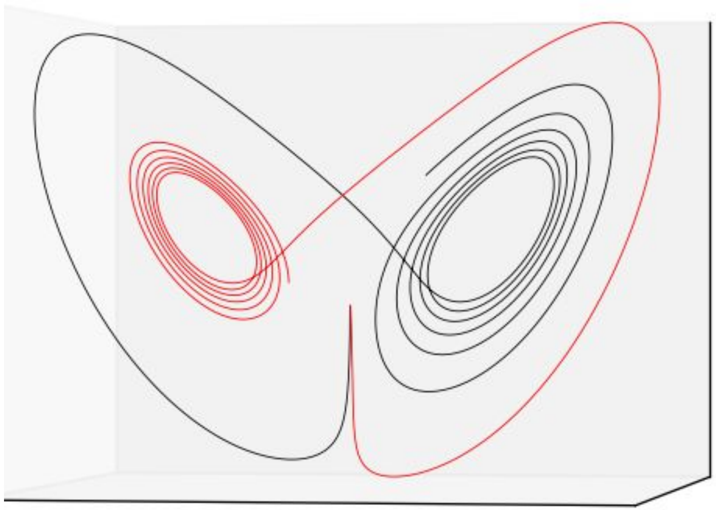

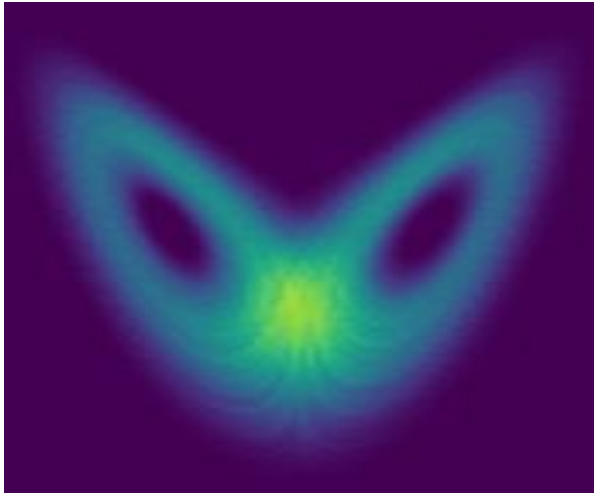

How do we go from Lagrangian to Eulerian?

Study the statistical properties of trajectories!

$$\mu_{x,N}(B) = \frac{1}{N}\sum_{k=0}^{N-1} \chi_B(T^k(x))$$

Occupation measures characterizes the the average time spent in a measurable set B for the initial condition x.

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When does this provide information about "many" trajectories?

$$m(\{x \in \Omega : \mu_{x,N} \to^* \mu\}) > 0$$

When such a measure μ exists, it is said to be physical.

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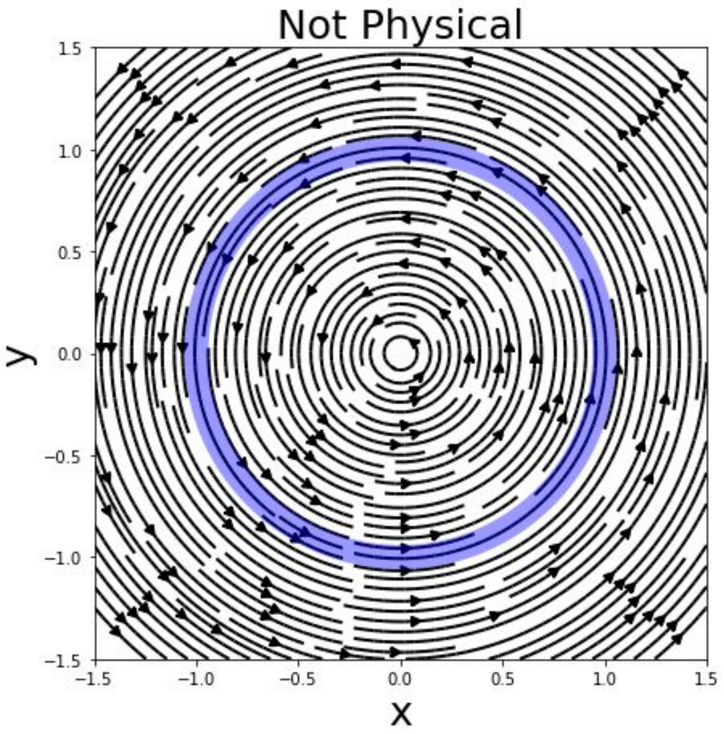
A weak-* limit of occupation measures is invariant.

$$\mu(T^{-1}(B)) = \mu(B)$$

Example and Non-Example of a Physical Measure



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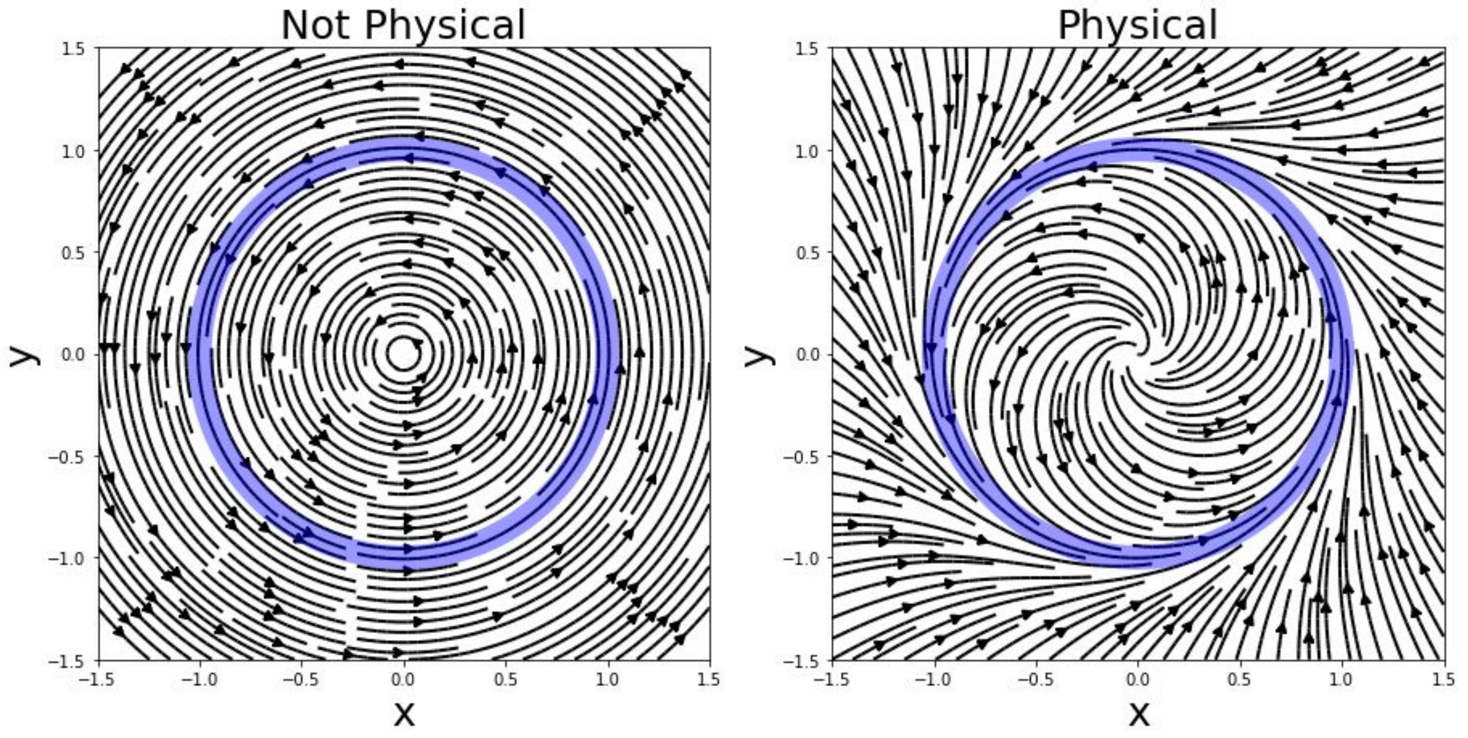

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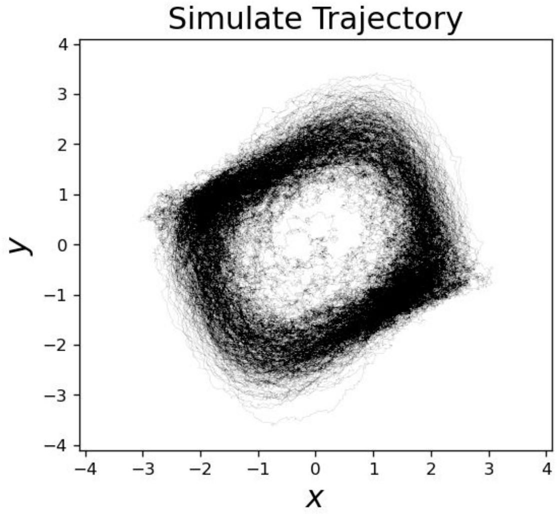

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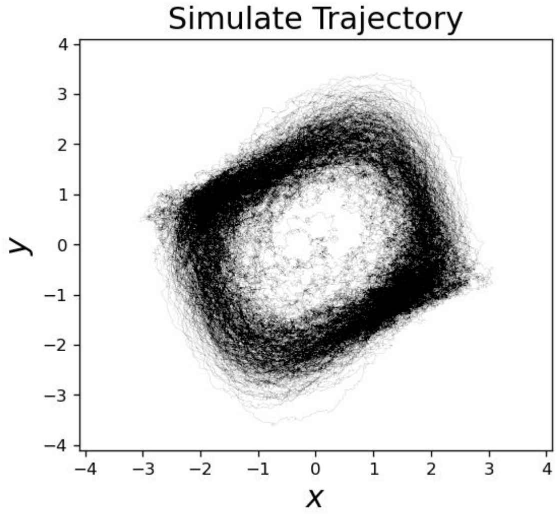

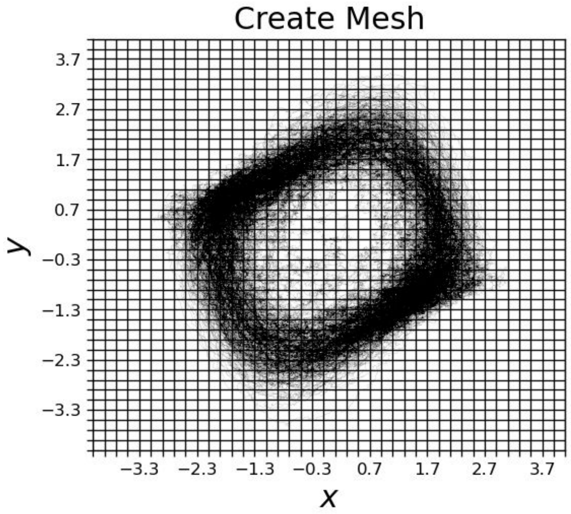

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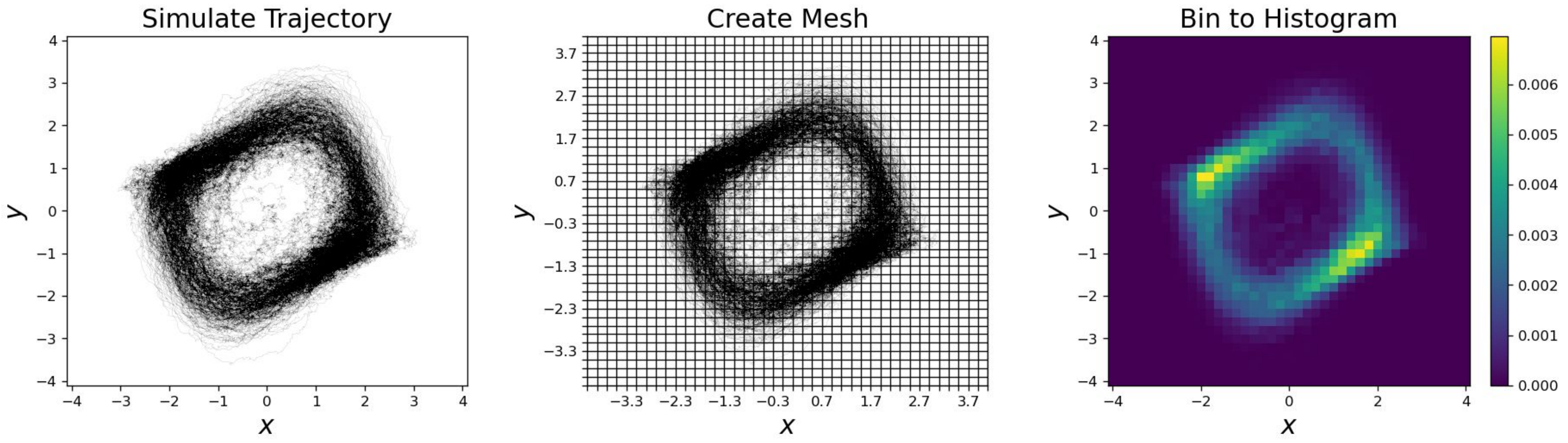

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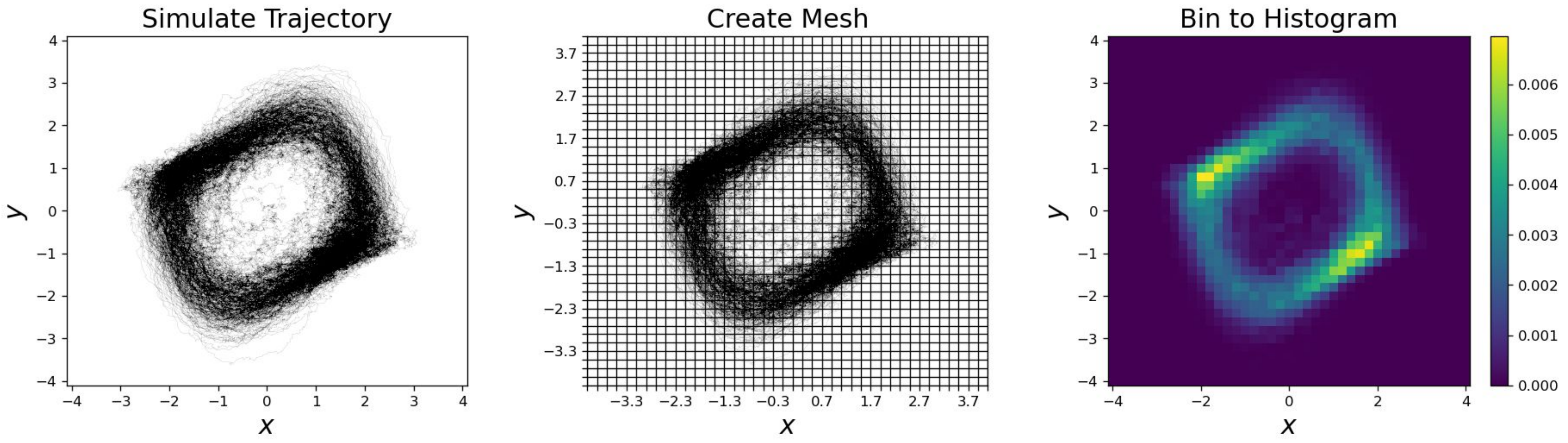

Note: this procedure does not use the sampling times of observations.

What is the goal?

Invert the mapping $v \mapsto \mu.$

If we know a physical invariant measure, can we infer the velocity field that produced it?

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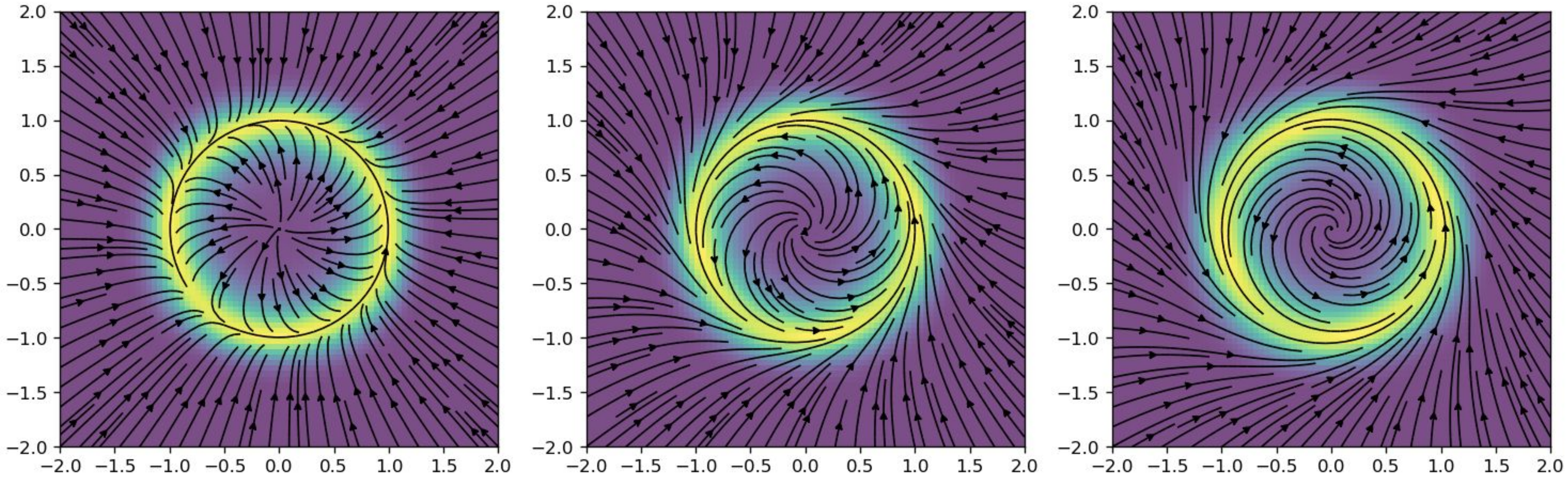
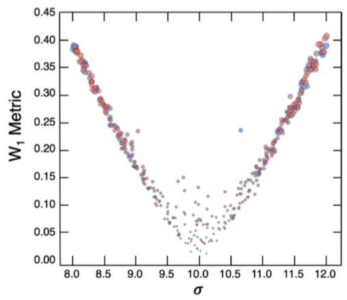
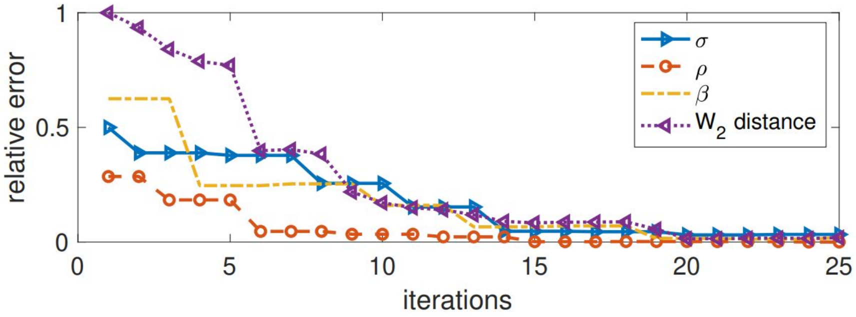


Previous Work on Learning Dynamics via Invariant Measures





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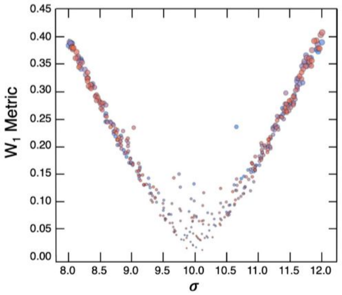

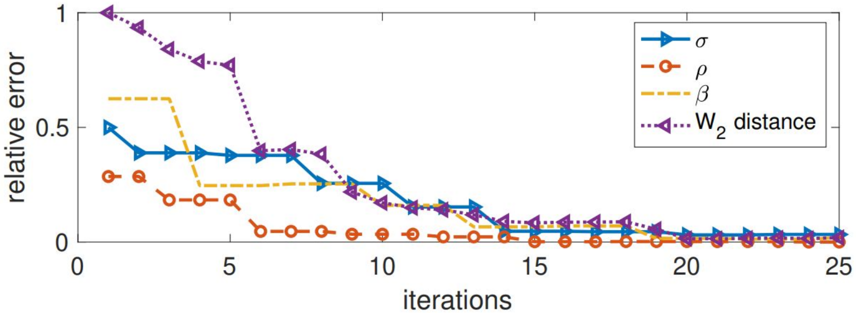

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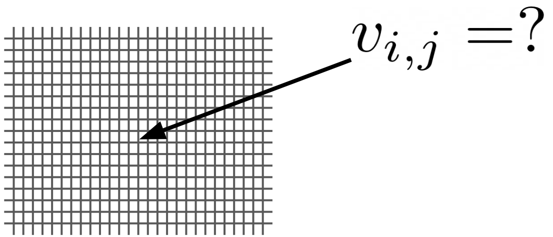
New contributions:

- Ability to model intrinsically noisy trajectories
- Large-scale parameter identification
- Learning dynamics in time-delay coordinates

Building a Forward Model

Reformulating the inversion as large-scale optimization

Discretize the velocity and "search" for a piecewise constant representation which inverts the map $v \mapsto \mu$.



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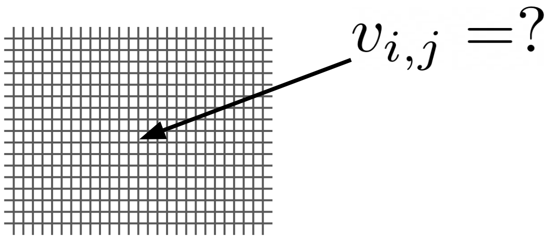
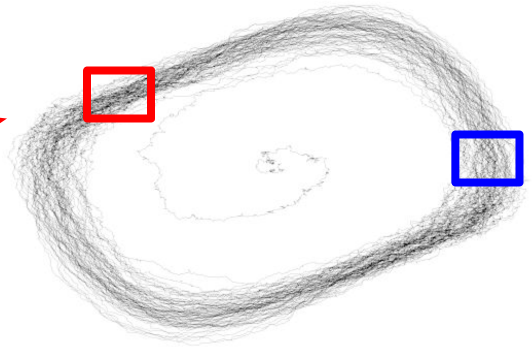


It is difficult to compute the derivative of histogram bin counts with respect to the velocity.

How does the number of particles here...



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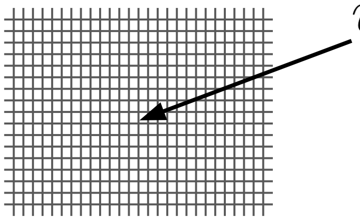

$v_{i,j} =?$

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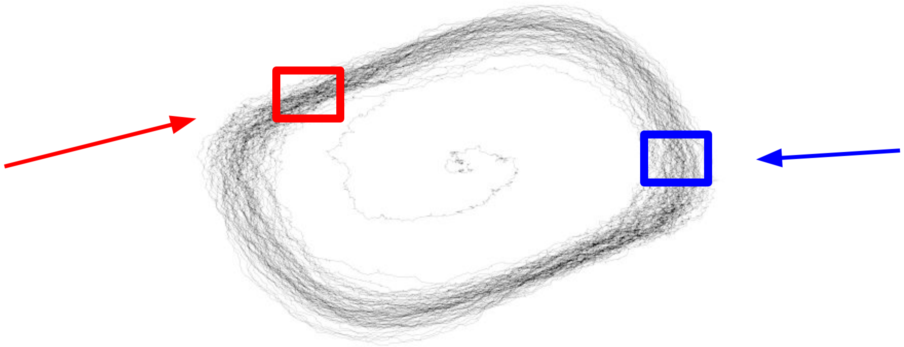

Depend on the velocity here?

We need a forward model for which the mapping $v \mapsto \mu$ is easily differentiable!

A PDE Forward Model

$$\underbrace{\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = D\nabla^2 \rho}_{\text{Eulerian}} \iff \underbrace{dX_t = v(X_t)dt + \sqrt{2D}dW_t}_{\text{Lagrangian}}$$

Physical measures describe the long term statistical behavior of Lagrangian trajectories, so we use **stationary solutions** of the Fokker-Planck Equation (FPE) as a surrogate model.

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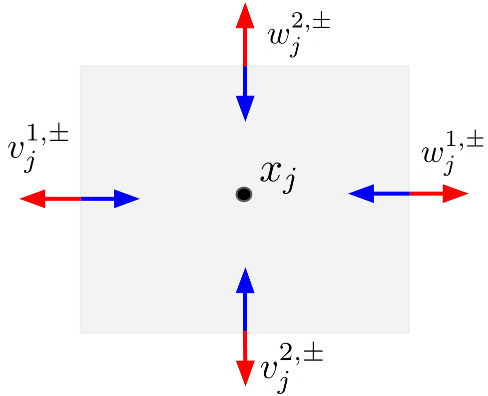
We discretize the FPE via a first order upwind finite volume method to form a Markov chain approximation of the dynamics.

$$\rho^{(\ell+1)} = M\rho^{(\ell)}, \quad M = I + K$$



Taking a closer look at the discretization…

$$K_i := \begin{array}{r} S_i \left\{ \vphantom{\begin{matrix} \ddots \\ \dfrac{D}{\Delta x_i} \\ \vdots \end{matrix}} \right. \\ \\ \\ \\ \\ \\ \\ \\ \end{array} \begin{bmatrix} \ddots & & & & \\ & -v_{j-1}^{i,-} + \dfrac{D}{\Delta x_i} & & & \\ \ddots & \vdots & & & \\ & v_{j-1}^{i,-} - w_{j-1}^{i,+} - \dfrac{2D}{\Delta x_i} & -v_j^{i,-} + \dfrac{D}{\Delta x_i} & & \\ \ddots & \vdots & \vdots & & \\ & w_{j-1}^{i,+} + \dfrac{D}{\Delta x_i} & v_j^{i,-} - w_j^{i,+} - \dfrac{2D}{\Delta x_i} & -v_{j+1}^{i,-} + \dfrac{D}{\Delta x_i} & \\ & & \vdots & \vdots & \ddots \\ & & w_j^{i,+} + \dfrac{D}{\Delta x_i} & v_{j+1}^{i,-} - w_{j+1}^{i,+} - 2\dfrac{D}{\Delta x_i} & \\ & & & \vdots & \ddots \\ & & & w_{j+1}^{i,+} + \dfrac{D}{\Delta x_i} & \\ & & & & \ddots \end{bmatrix} \in \mathbb{R}^{N \times N}.$$

Finding the Markov Chain's Stationary Distribution

We will use the Markov chain's steady state as a model for the underlying physical measure

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- If the diffusion is zero, the stationary distribution may not be unique.
- The transition matrix may be ill-conditioned.
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Solution: Teleportation regularization from Google's Pagerank algorithm.

$$M_\epsilon := (1-\epsilon)M + \frac{\epsilon}{N}\mathbf{1}\mathbf{1}^\top \in \mathbb{R}^{N\times N}, \qquad \mathbf{1} := \begin{bmatrix}1 & \dots & 1\end{bmatrix} \in \mathbb{R}^N.$$

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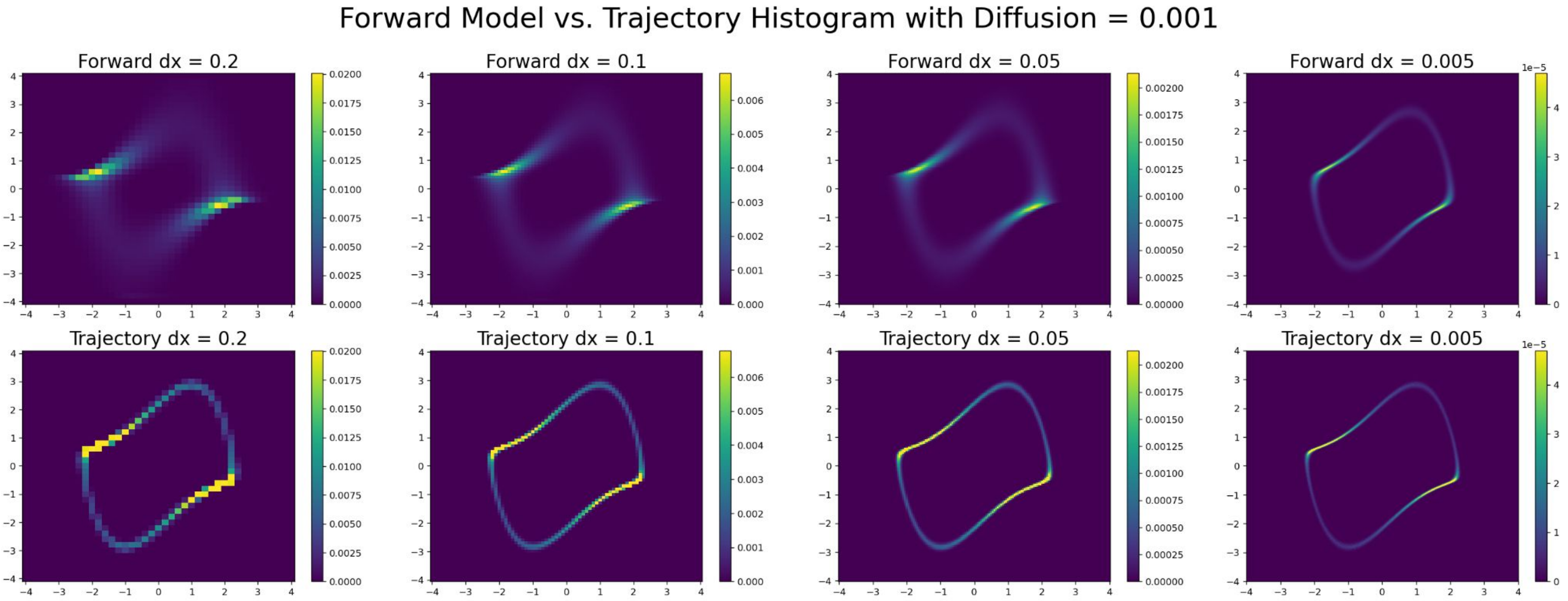
Now, the steady state can be uniquely found by solving a sparse linear system.

$$(1-\epsilon)(M-I)\rho = -\frac{\epsilon}{N}\mathbf{1}$$

Forward Model vs. Occupation Measures



Selecting an Objective Function

$$L^2(\rho, \rho^*) := \frac{1}{2}\int_\Omega (\rho(x) - \rho^*(x))^2 dx$$

Squared L2 Norm

$$D_{\mathrm{KL}}(\rho, \rho^*) := \int_{\Omega'} \rho^*(x) \log\left(\frac{\rho^*(x)}{\rho(x)}\right) dx$$

Kullback-Leibler Divergence

$$D_{\mathrm{JS}}(\rho, \rho^*) = \frac{1}{2} D_{KL}(\rho, \rho') + \frac{1}{2} D_{KL}(\rho^*, \rho')$$

Jenson-Shannon Divergence

$$W_2^2(\rho, \rho^*) := \inf_{T_{\rho,\rho^*} \in \mathcal{M}} \int_\Omega |x - T_{\rho,\rho^*}(x)|^2 d\rho(x)$$

Quadratic Wasserstein Distance

Computing the Gradient

Using the Adjoint State Method

Compute the Fréchet derivative of the objective function with respect to the current density

$$\boxed{\frac{\partial L_2}{\partial \rho} = \rho - \rho^*.}$$

$$\boxed{\frac{\partial D_{\mathrm{KL}}}{\partial \rho} = -\frac{\rho^*(x)}{\rho(x)}.}$$

$$\boxed{\frac{\partial D_{\mathrm{JS}}}{\partial \rho} = \frac{1}{2}\log\left(\frac{2\rho}{\rho+\rho^*}\right)}$$

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Solve the adjoint equation

$$(M_\epsilon - I)^T \lambda = -\left(\frac{\partial \mathcal{J}}{\partial \rho} - \frac{\partial \mathcal{J}}{\partial \rho} \cdot \rho \mathbf{1}\right)^T$$

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Compute gradient with respect to the piecewise constant velocities used in the Markov matrix.

$$\frac{\partial \mathcal{J}}{\partial v_i} = \lambda \cdot \frac{\partial M_\epsilon}{\partial v_i} \rho$$

Velocity Parameterization

$$v = v(\theta) \implies \frac{\partial \mathcal{J}}{\partial \theta_k} = \frac{\partial \mathcal{J}}{\partial v} \cdot \frac{\partial v}{\partial \theta_k}$$

The first term comes from the adjoint state method and the second is easy to compute when the functional form of the paramaterization is known.

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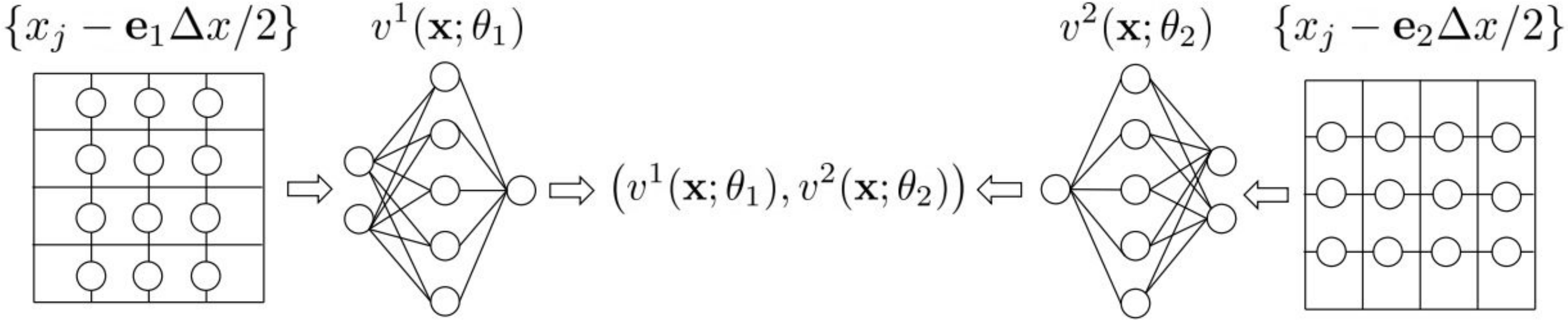


The Optimization Framework

1.) Solve the forward problem $$M_\epsilon \rho = \rho$$

2.) Evaluate the cost $$\mathcal{J}(\rho, \rho^*)$$

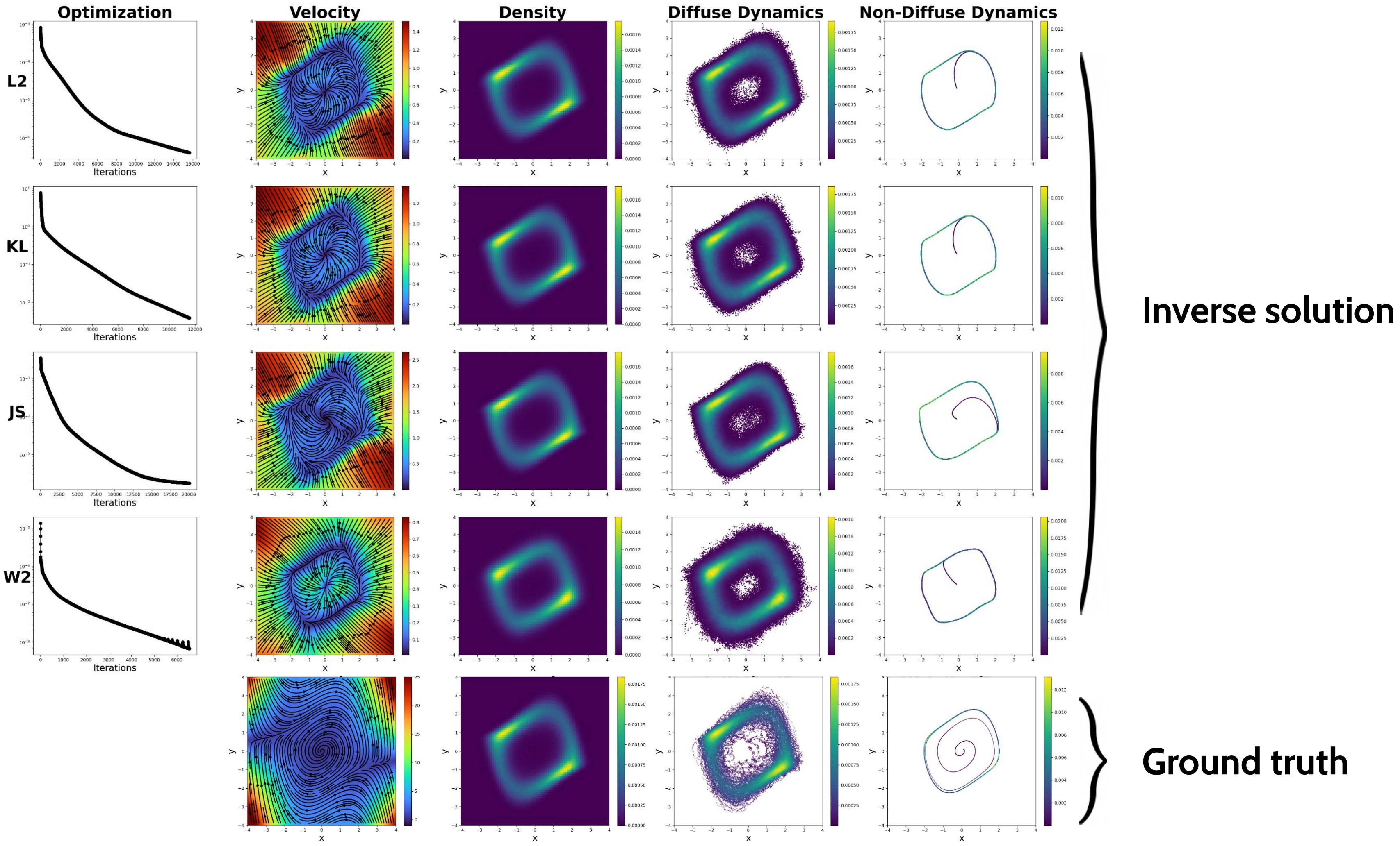
3.) Compute the Frechet derivative $$\phi = \frac{\partial \mathcal{J}}{\partial \rho}$$

4.) Solve the adjoint equation $$(M_\epsilon^T - I)\lambda = -\phi + \phi \cdot \rho \mathbf{1}$$

5.) Compute the gradient $$\frac{\partial \mathcal{J}}{\partial v_i} = \lambda \cdot \frac{\partial M_\epsilon}{\partial v_i} \rho \qquad \frac{\partial \mathcal{J}}{\partial \theta_k} = \frac{\partial \mathcal{J}}{\partial v} \cdot \frac{\partial v}{\partial \theta_k}$$

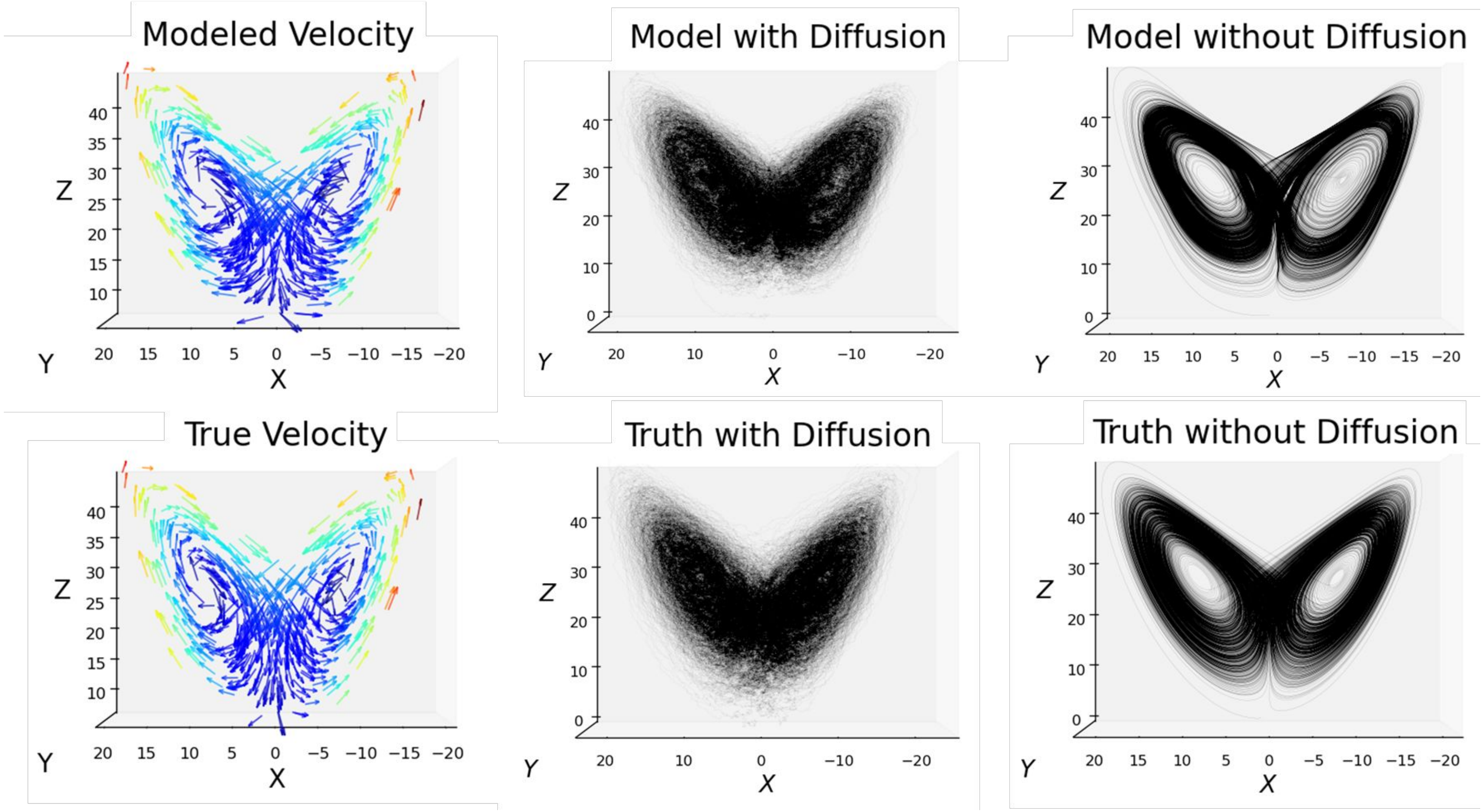
6.) Descend Adam, L-BFGS-B, CG, etc.

Numerical Results



Optimization
Velocity
Density
Diffuse Dynamics
Non-Diffuse Dynamics
L2
KL
JS
W2
Iterations
Inverse solution
Ground truth

Lorenz-63 System - Inverting V1



What if we only have partial observations?

$$\underbrace{\dot{x} = v(x)}_{\text{full dynamics}} \qquad \underbrace{y : \mathcal{M} \to \mathbb{R}}_{\text{observation function}} \qquad \underbrace{\{y(x(t_i))\}_{i=1}^{N}}_{\text{available data}}$$

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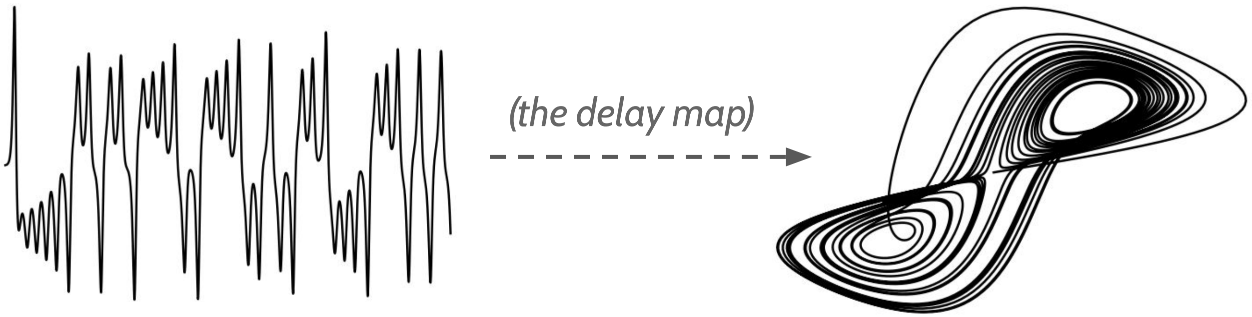
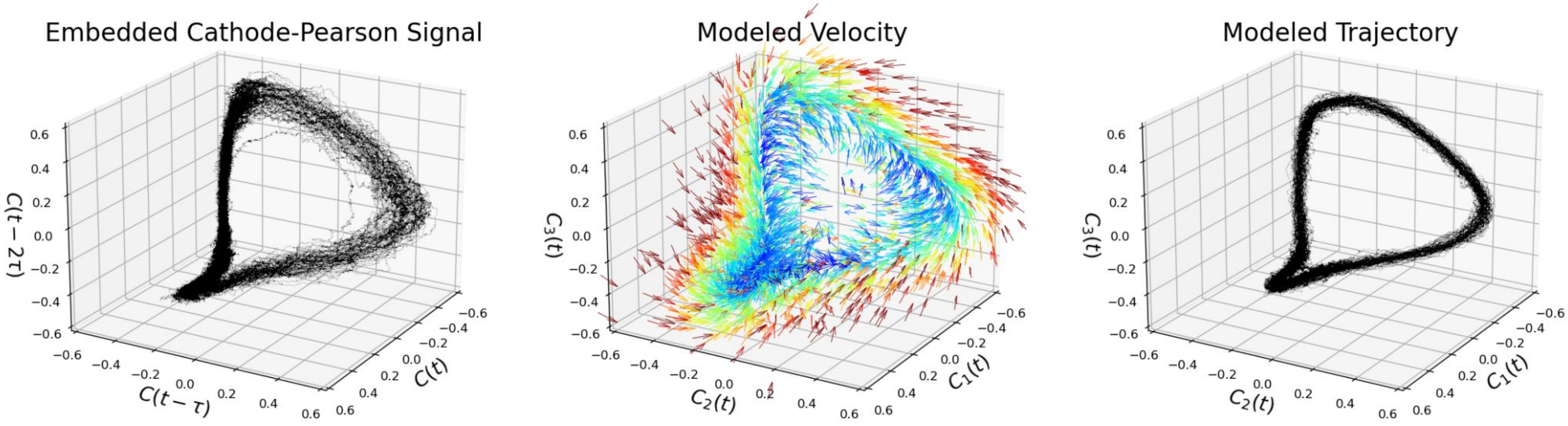
Motivated by Takens' Theorem (1981), we can instead learn the dynamics in delay coordinates.

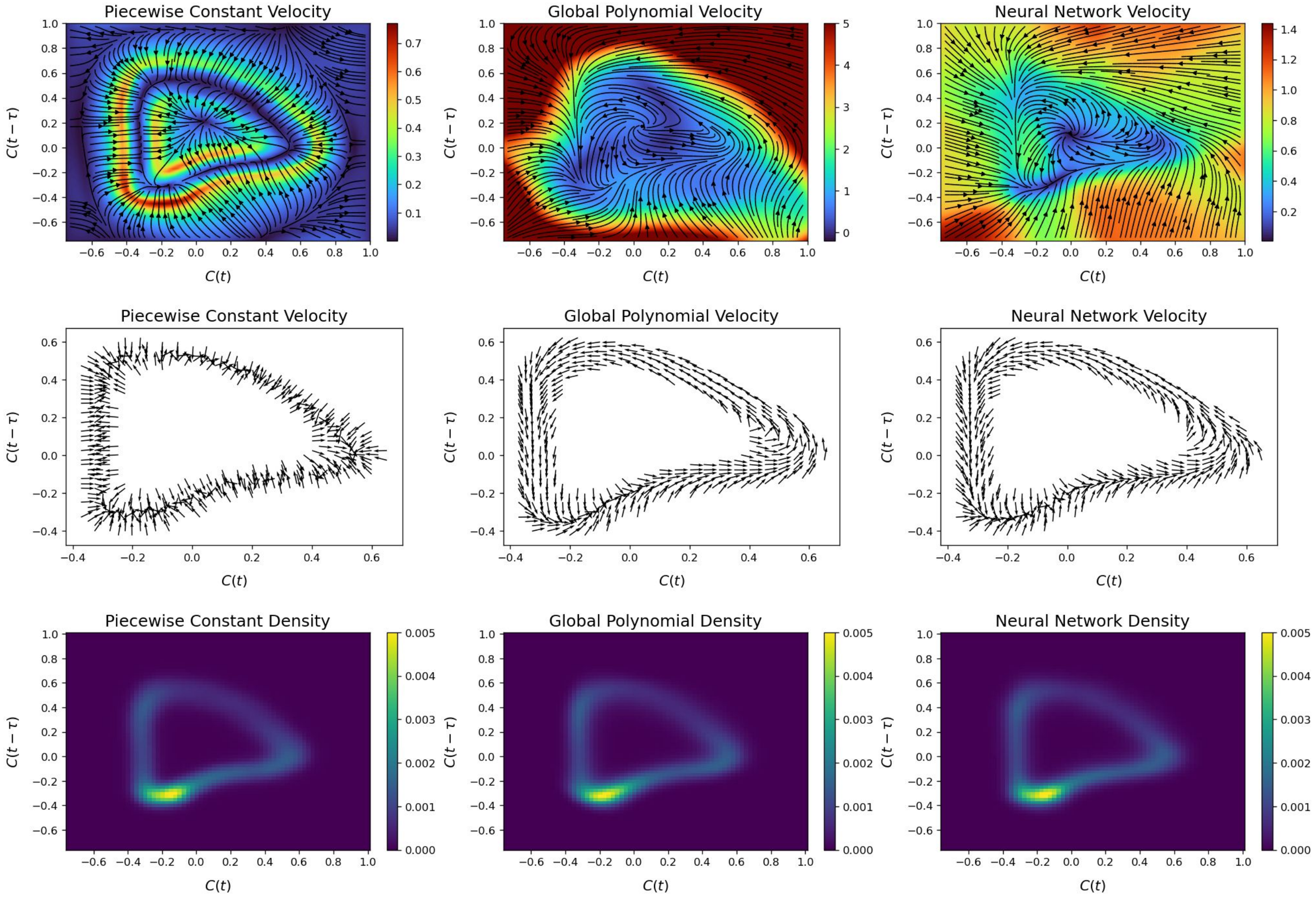
$$\exists \underbrace{\Phi : \mathcal{M} \to \mathbb{R}^d}_{\text{diffeomorphism}} \text{ with } \Phi(x(t)) = (y(t), y(t-\tau), \ldots, y(t-2d\tau))$$



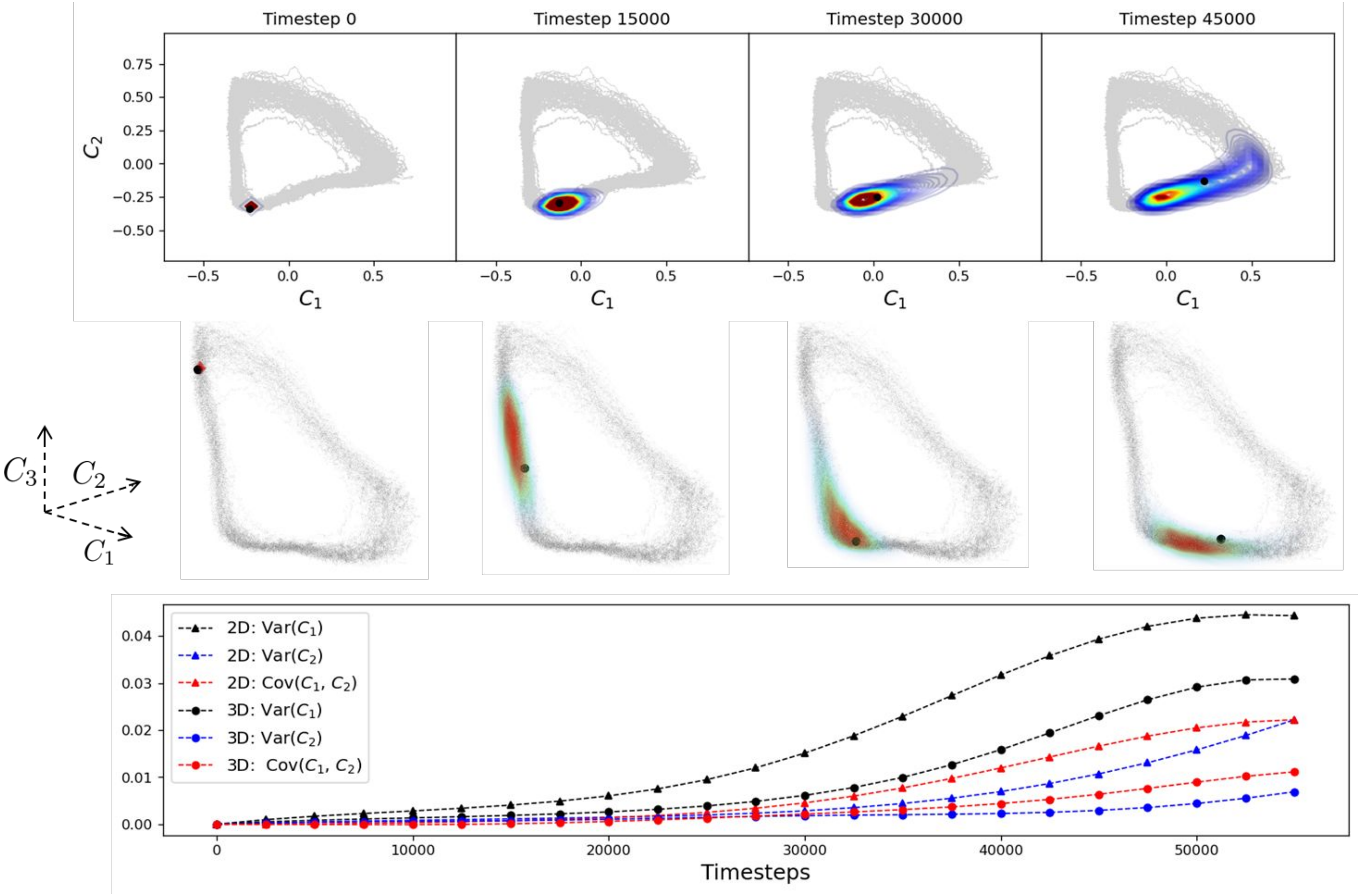
Application to a Hall-Effect Thruster (HET)



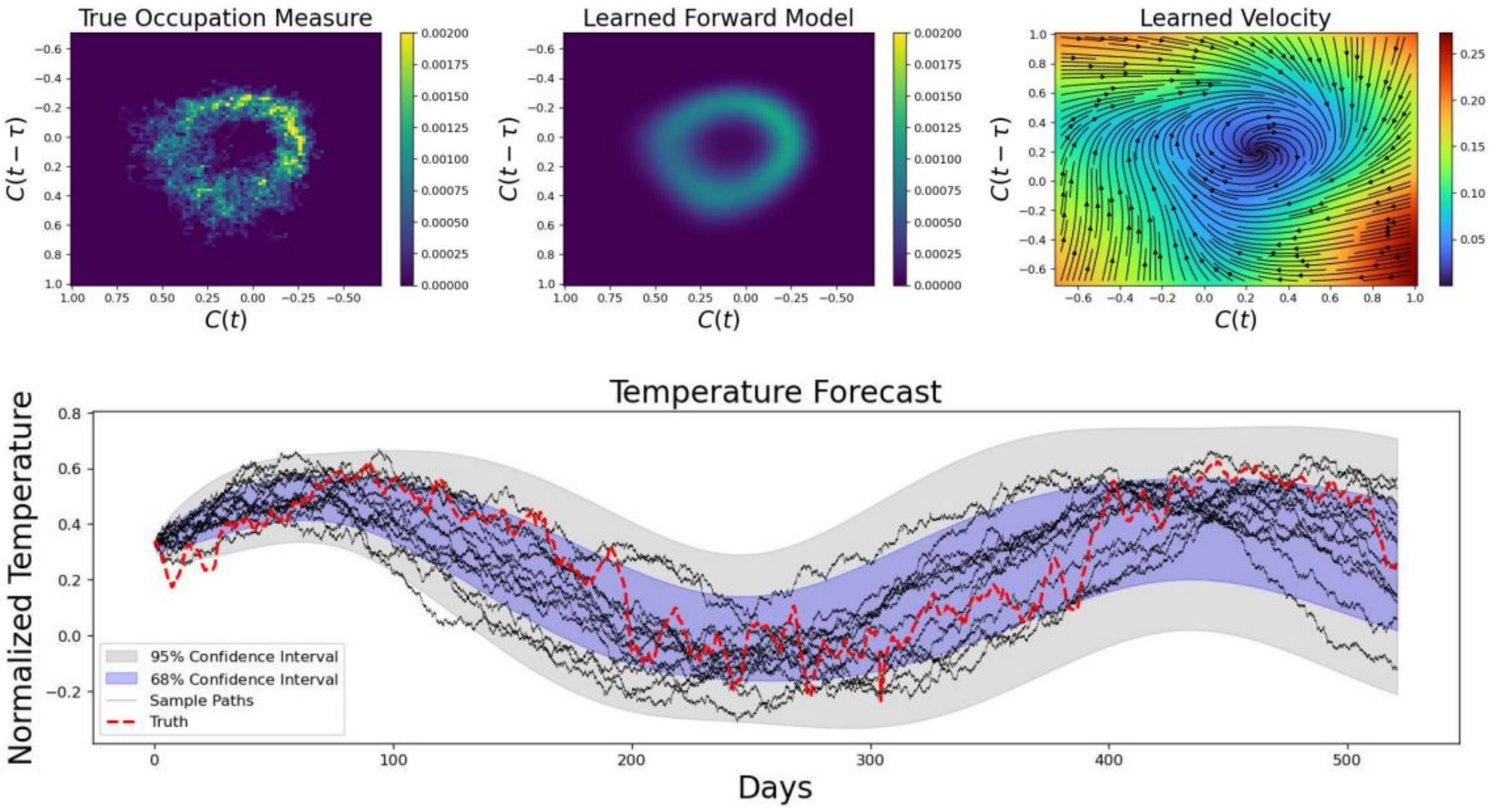
Varying the Paramaterization



Quantifying Model Uncertainty



Temperature Prediction with Uncertainty Quantification



Future Directions

- Dimension-free and mesh-free approaches
- Unstructured Mesh
- Higher order finite volume method
- Study inverse problem regularity
- The case of multiple attractors
- Learning an anisotropic diffusion

Thank you!

Questions?