

# Learning nonlinear dynamical systems from data using scientific machine learning

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[https://github.com/Romit-Maulik/UChicago\\_SummerSchool\\_2022](https://github.com/Romit-Maulik/UChicago_SummerSchool_2022)

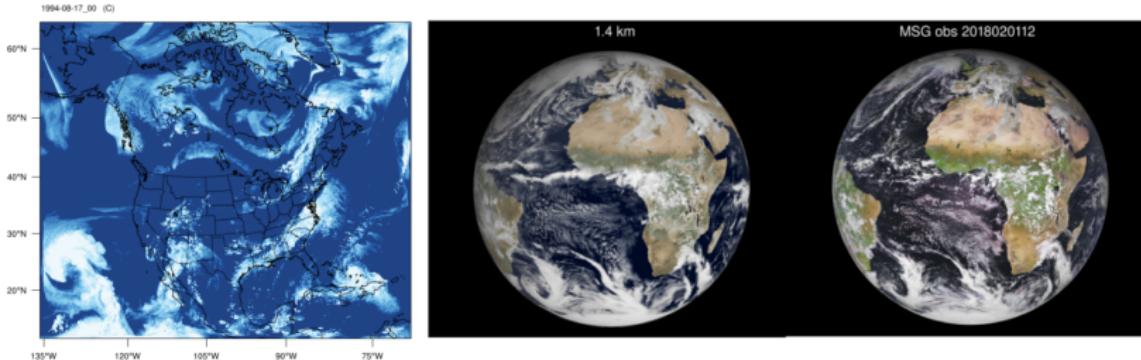
August 9, 2022

# Outline

1. Introduction and motivation.
2. Learning dynamical systems with neural ordinary differential equations.
3. Learning stochastic systems with normalizing flows.
4. Conclusions/Q&A.



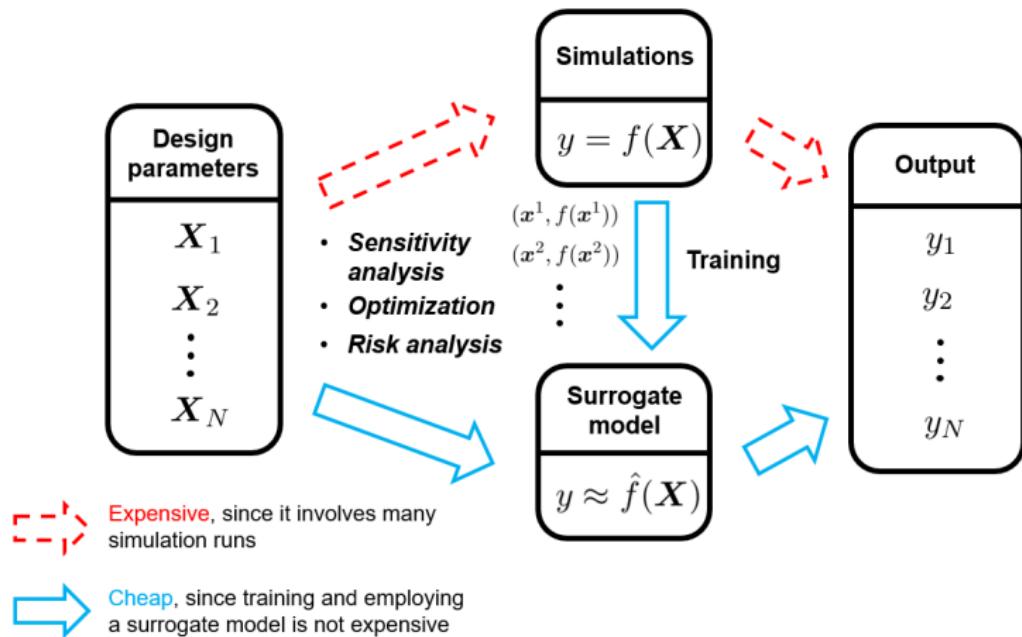
# Motivation



**Figure:** Cloud resolved weather and climate simulations are becoming a reality. 4km simulations of E3SM run over 100 forecast years require 120 million core hours (Theta-ANL) and 12 PB of storage data (250 GB/forecast day).

Image source: Jung et al., Simulations of E3SM on ANL-Theta, 2022 (top), ECMWF Simulations on ORNL-Summit, DOE E3SM All-hands meeting 2021.

# Emulating dynamical systems from data



**Figure:** Source - “An introduction to surrogate modeling” - Shuai Guo.

# Emulating dynamical systems from data

There may also be a requirement to construct ‘non-intrusive’ surrogate models - for example when dynamics are only partially understood/known - i.e., **No closed form governing laws available.**

This project is joint work with

- ▶ Prasanna Balaprakash (Argonne).
- ▶ Qi Tang, Joshua Burby (Los Alamos).
- ▶ Alec Linot, Mike Graham (Wisconsin).



## Background: Neural ordinary differential equations

$$\frac{d\mathbf{a}}{dt} = f(\mathbf{a}, \theta), \quad (\theta) \in \Theta, \quad (1)$$

where  $\Theta \subset \mathbb{R}^{N_w}$  is the space of trainable parameters of an arbitrary neural network. The NODE [3, 4, 5] approximates the latent-space evolution as a set of ordinary differential equations that can be trained through adjoint-based (i.e., continuous) backpropagation [3, 5], i.e.,

$$L(\tilde{\mathbf{a}}^T) = L(\mathbf{a}^0 + \int_{t=0}^{t=T} f(\mathbf{a}(t), \theta) dt) \quad (2)$$

$$\frac{d\mathbf{z}}{dt} = -\mathbf{z}^T \frac{\partial f(\mathbf{a}, t, \theta)}{\partial \mathbf{a}}, \quad \mathbf{z}(t) = \frac{\partial L}{\partial \mathbf{a}(t)} \quad (3)$$

$$\frac{dL}{d\theta} = - \int_{t=T}^{t=0} \mathbf{z}(t)^T \frac{\partial f(\mathbf{a}(t), \theta)}{\partial \theta} dt. \quad (4)$$



## Chaotic dynamics: The Kuramoto-Sivashinsky equation

We want to address the surrogate modeling of chaotic systems. Traditionally, most data-driven time-series modeling techniques suffer with deterministic chaos.

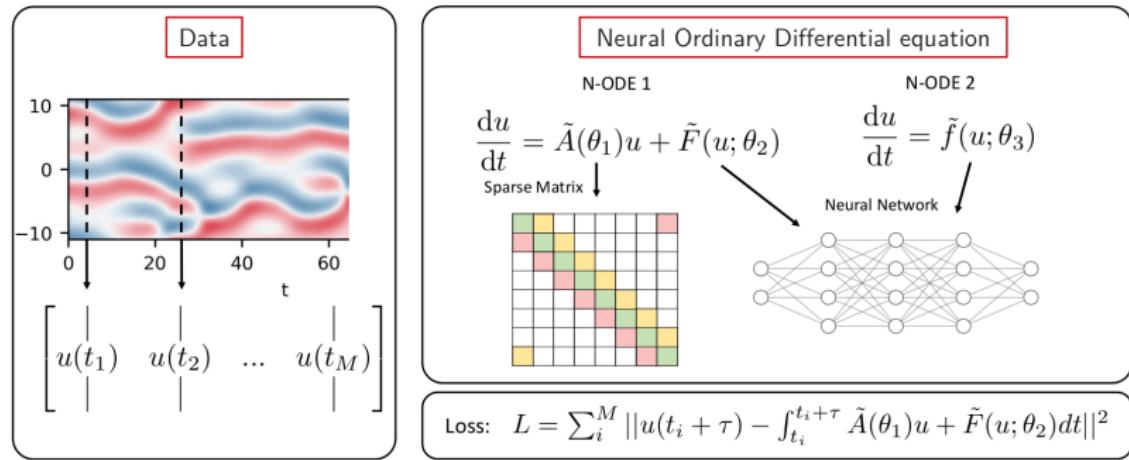
$$\frac{\partial u}{\partial t} = -u \frac{\partial u}{\partial x} - \frac{\partial^2 u}{\partial x^2} - \frac{\partial^4 u}{\partial x^4} \quad (5)$$

$$u \in \mathbb{R}^{64}; x \in [-\pi, \pi] \subset \mathbb{R}^1 \quad (6)$$

A prototypical system to study chaotic dynamics, possesses a dissipative nature (i.e., an attractor in the long-term limit), challenging for state-of-the-art black-box forecasting methods.



# A novel neural ODE for capturing chaotic attractors



**Figure:** A novel neural-ODE for learning chaotic dynamics.

Linot, Burby, Tang, Balaprakash, Graham, RM. arXiv:2203.15706.



## Example: The Kuramoto-Sivashinsky equation

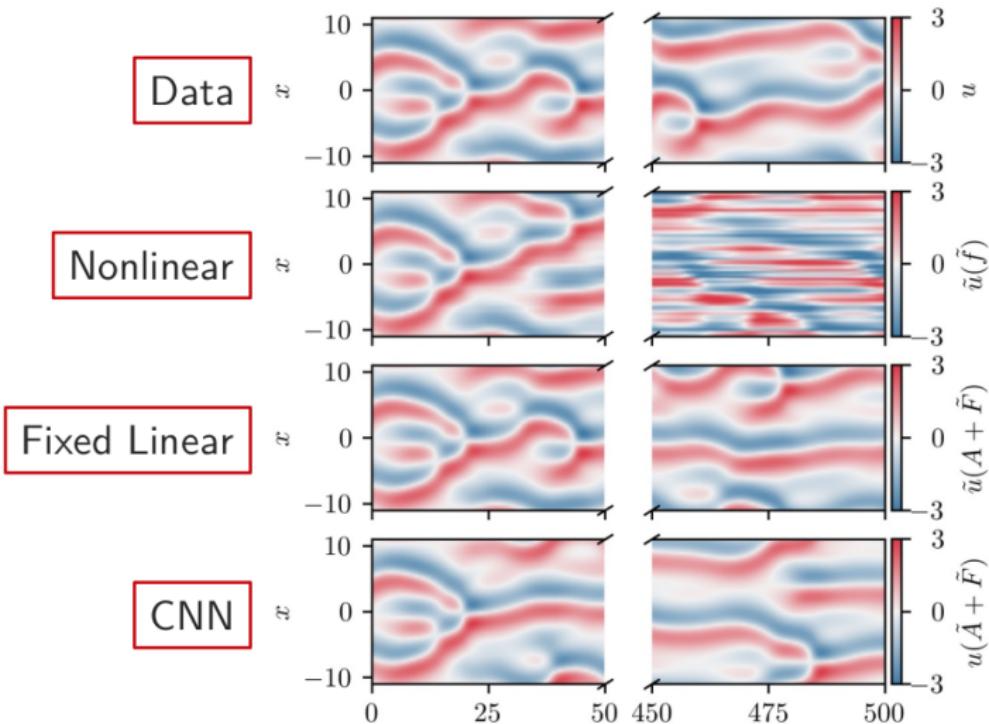
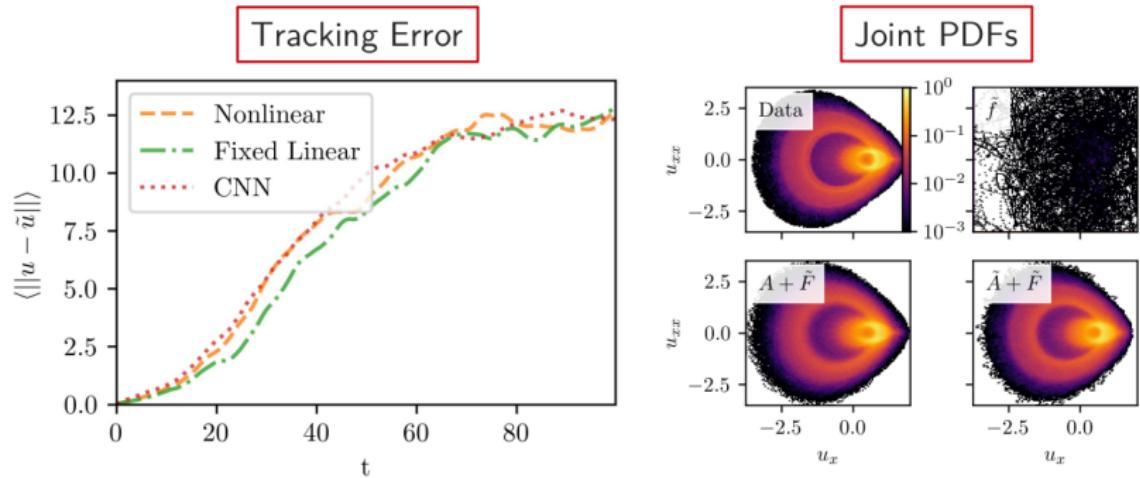


Figure: A novel neural-ODE for capturing the underlying attractors for the KS equations: Long-term stability.

# Example: The Kuramoto-Sivashinsky equation



**Figure:** A novel neural-ODE for capturing the underlying attractors for the KS equations: Attractor captured successfully!

Approximate inertial manifold theory can then be used since we have a linear term.

## Flipping the script: A reduced-order model of a surrogate

We can also reduce the order of this neural ODE a-posteriori by using the theory of approximate inertial manifolds [9]:

$$\frac{dp}{dt} = Ap + PF(p + q), \quad (7)$$

$$\frac{dq}{dt} = Aq + QF(p + q), \quad (8)$$

$$q = A^{-1}Q(p + q) \approx A^{-1}Q(p). \quad (9)$$

$$Q = I - P. \quad (10)$$

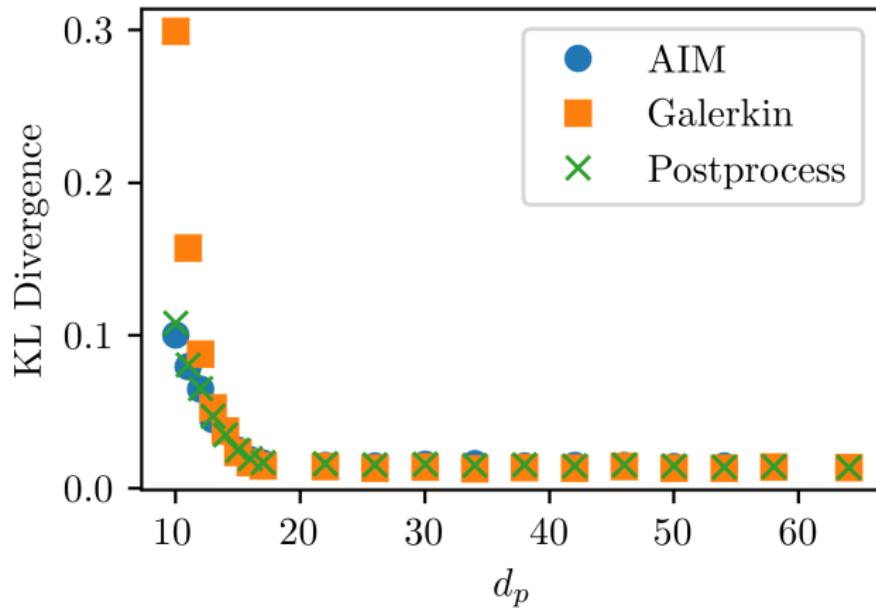
If we construct  $P$  using selected eigenvectors of the learned linear term  $A$

$$\begin{aligned} AV &= V\Lambda, \\ P &= \tilde{V}\tilde{V}^T \end{aligned} \quad (11)$$

where  $\tilde{V}$  are a truncated subset of eigenvectors that promotes  $\frac{dq}{dt} = 0$ .

Ignoring the computation of  $q$  gives us the nonlinear Galerkin ROM, computing  $q$  with  $A^{-1}Q(p)$  during the simulation gives us the AIM ROM and after the simulation gives us postprocessing ROMs.

## Example: The Kuramoto-Sivashinsky equation



**Figure:** A reduced-order model from the proposed full-order neural ODE. KL-divergence of attractor statistics - model reduced to 25% of original size.

## Example: Learning the viscous Burgers equations

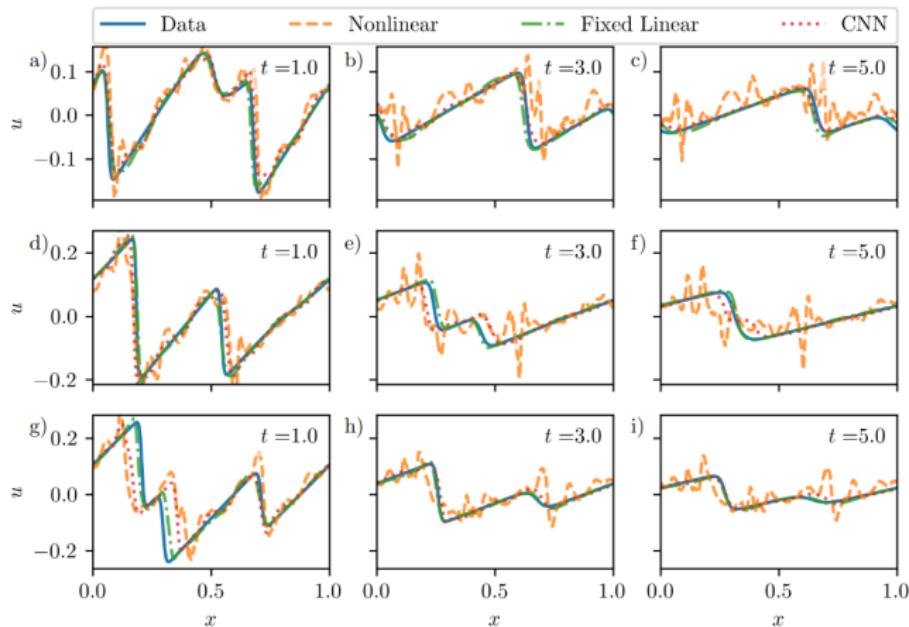
The viscous Burgers equations are given by the following system

$$\frac{\partial u}{\partial t} = -u \frac{\partial u}{\partial x} + \nu \frac{\partial^2 u}{\partial x^2} \quad (12)$$

in a domain with length  $L = 1$  and with periodic boundary conditions. Our viscosity,  $\nu = 8 \times 10^{-4}$ . Initial conditions sampled from superpositions of frequencies in Fourier space for the same viscosity. Solution discretized on 512 grid points.



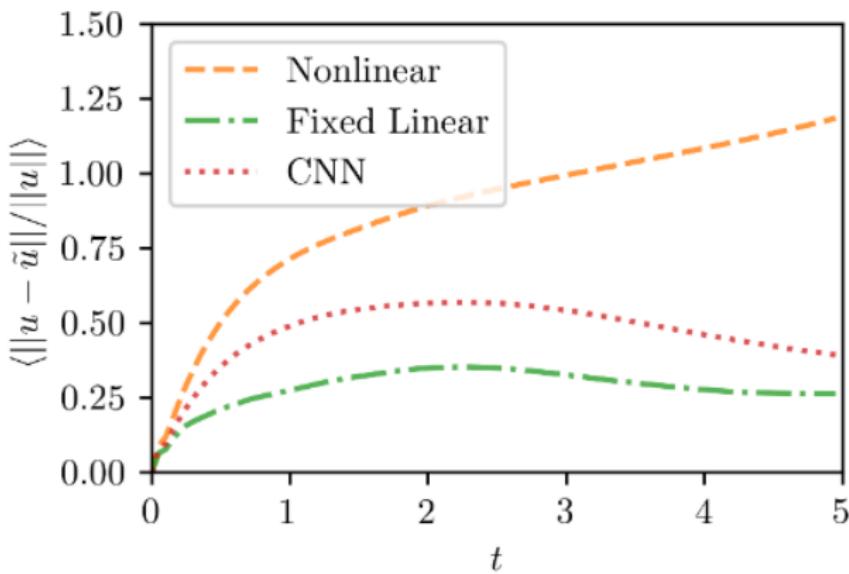
# Example: Learning the viscous Burgers equations



**Figure:** The stabilized neural ODE outperforms the standard neural ODE for learning the viscous Burgers equations.

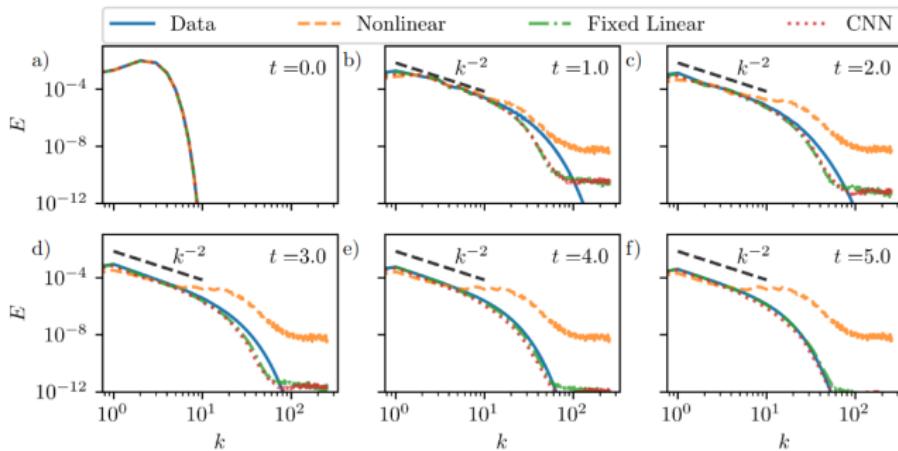


## Example: Learning the viscous Burgers equations



**Figure:** The stabilized neural ODE outperforms the standard neural ODE for learning the viscous Burgers equations - confirmed for an ensemble of test predictions.

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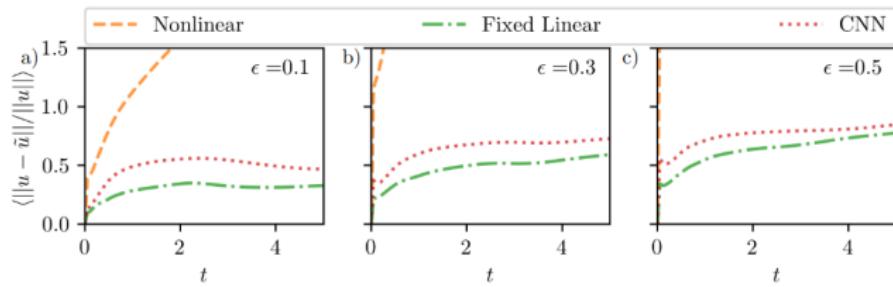
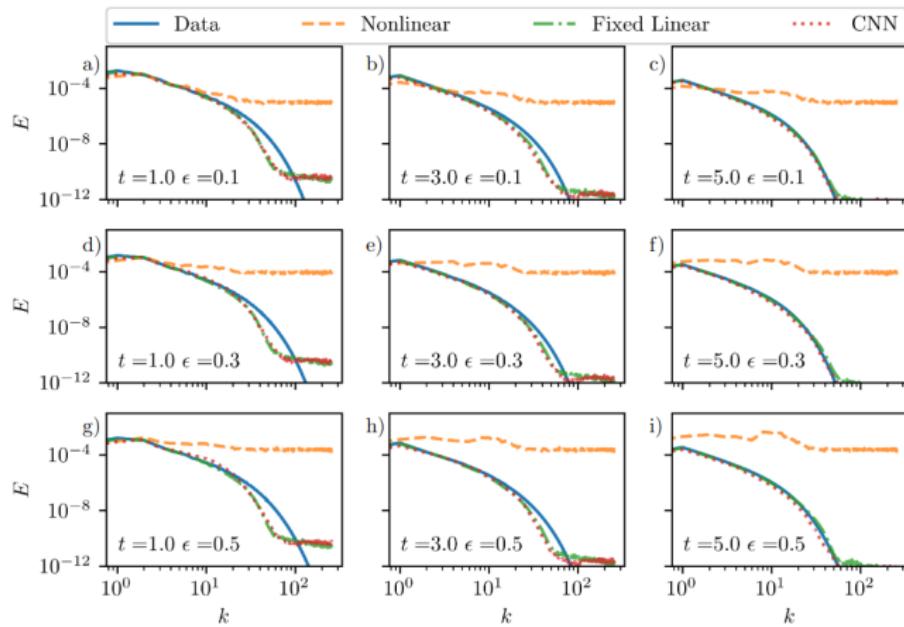


Figure: When adding noise to the initial conditions - the stabilized neural ODE performs more robustly



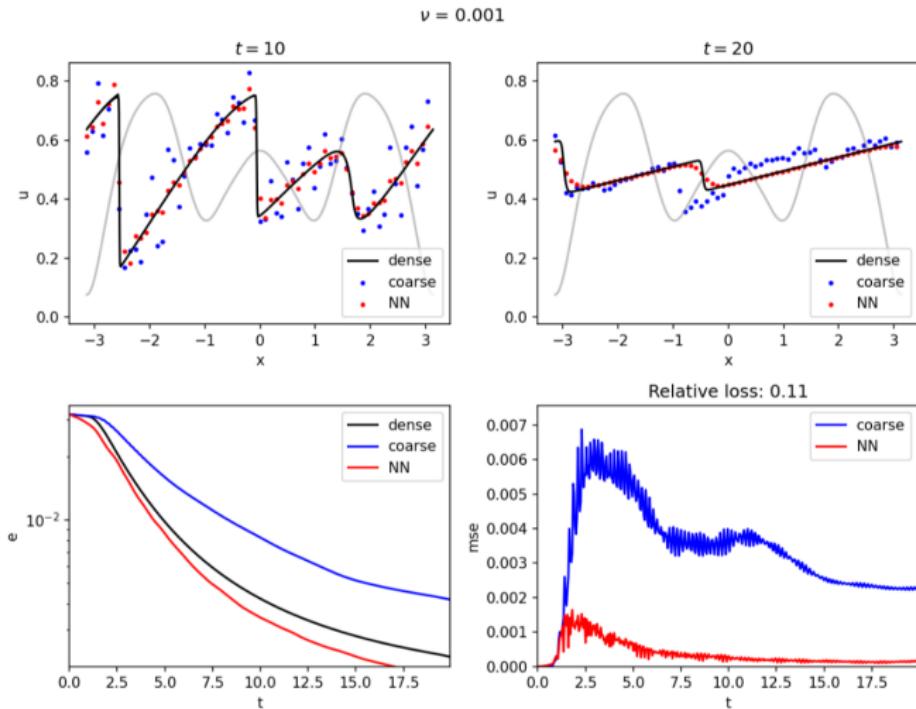
# Example: Learning the viscous Burgers equations



**Figure:** When adding noise to the initial conditions - the stabilized neural ODE performs more robustly

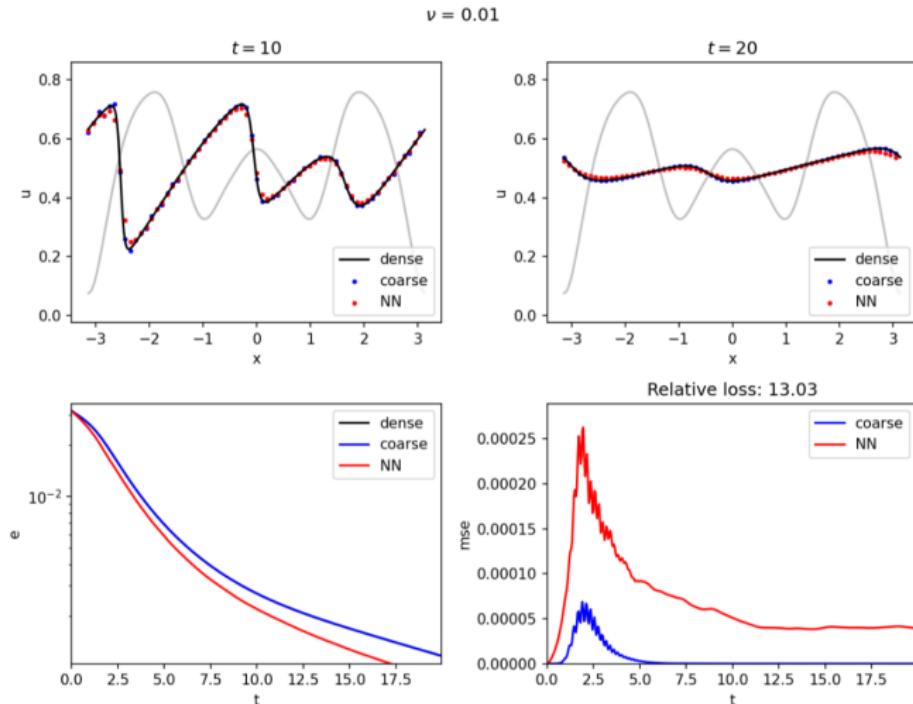


# Under-resolved snapshot data? A preview.



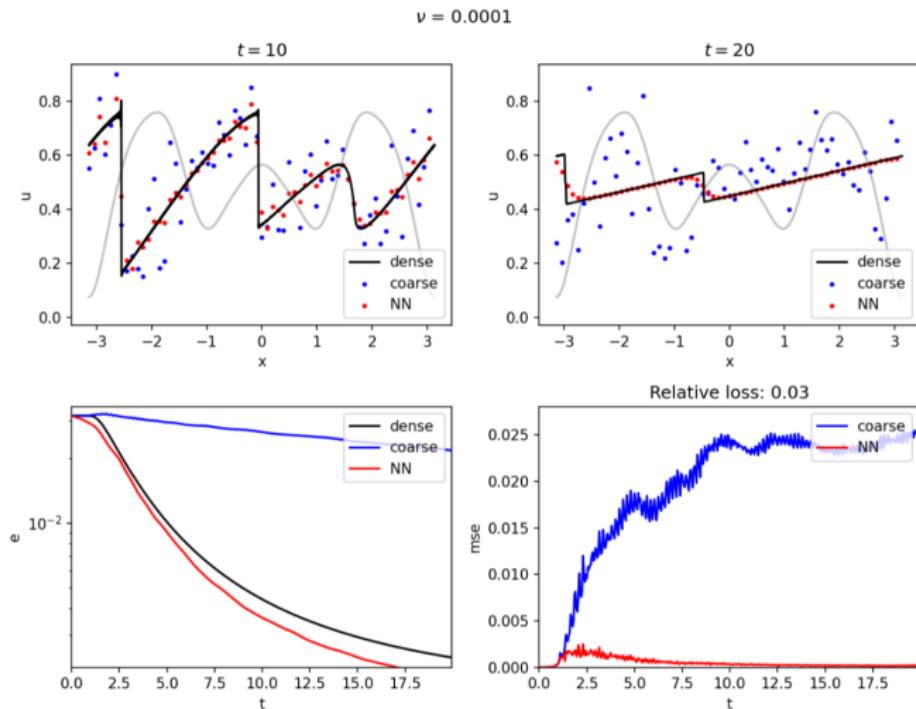
**Figure:** The stabilized NODE framework is also able to learn a stabilized coarse-grained evolution (i.e., if snapshot resolution is inadequate). Fine-grid 4096 DOF, coarse-grid 64 DOF.

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**Figure:** The stabilized NODE framework is also able to learn a stabilized coarse-grained evolution (i.e., if snapshot resolution is inadequate). Fine-grid 4096 DOF, coarse-grid 64 DOF.

# Example: Learning the invariant manifold of the sea-surface temperature

## NOAA OI SST V2 High Resolution Dataset

Data on and after 2016 is now v2.1

### Brief Description:

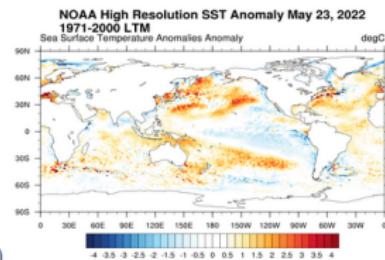
- NOAA High-resolution Blended Analysis of Daily SST and Ice. Data is from Sep 1981 and is on a 1/4 deg global grid. [More Details...](#)

### Temporal Coverage:

- Daily values from 1981/09 to present
- Sea Ice Concentration data is missing for Dec 6th 1987- Jan 10th 1988.

### Spatial Coverage:

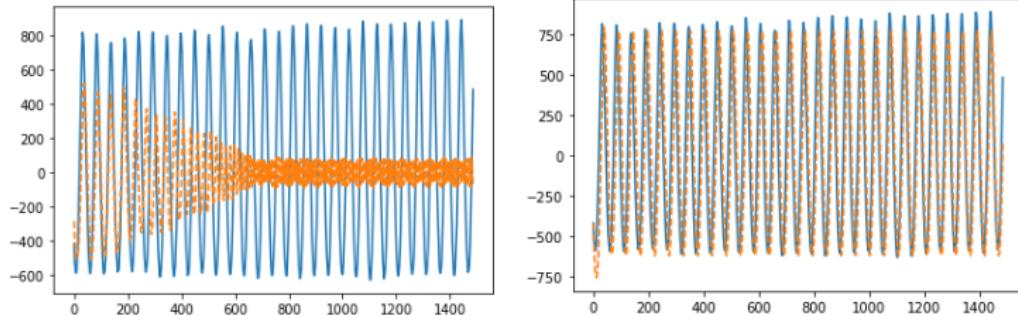
- 0.25 degree latitude x 0.25 degree longitude global grid (1440x720).
- 89.875S - 89.875N, 0.125E to 359.875E.



**Figure:** A sea-surface temperature dataset obtained from satellite and ship observations.

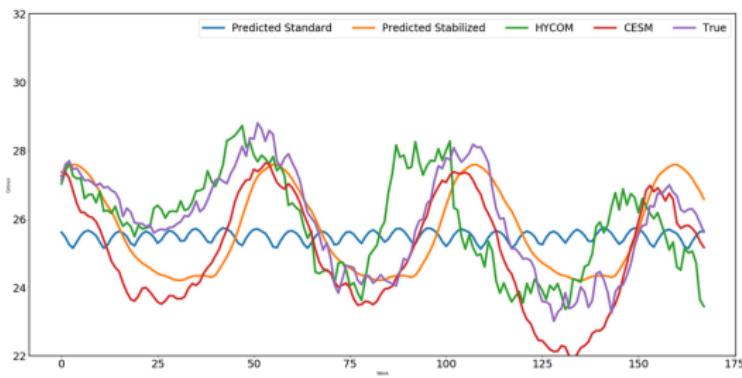


## Example: Learning the invariant manifold of the sea-surface temperature



**Figure:** Test results for learning the POD coefficients of this dataset using regular (left) and stabilized (right) neural ODEs.

## Example: Learning the invariant manifold of the sea-surface temperature



**Figure:** Preliminary results indicate that predictive dynamics do not decay to fixed point. Probe for solution at 95 degrees latitude and 250 degrees longitude.



## Example: Learning the invariant manifold of the sea-surface temperature

RMSE from stabilized NODE (ROM) over weeks 1-8:

1.189, 1.186, 1.180, 1.171, 1.171, 1.167, 1.208, 1.223

Errors from CESM (Climate model) over weeks 1-8:

1.8779, 1.867, 1.830, 1.846, 1.861, 1.869, 1.860, 1.833

Errors from HYCOM (Weather model) over weeks 1-8:

0.998, 0.994, 1.027, 1.039, 1.023, 1.046, 1.033, 1.051



## Emulating the sea-surface temperature: Worth it?

Cost to construct our NODE-ROM: 2 node hours of CPU-only laptop, cost to evaluate - negligible.

Cost to evaluate HYCOM: 44800 core hours per forecast day of Cray XC40 system.

Cost to evaluate CESM: 510 million core-hours on Yellowstone, NCAR's high-performance computing resource.

**Extensions:** Interfacing SST-ROMs as a 'boundary condition' to E3SM atmosphere.



# Intermission

Part I - finished.



# SciML for time-varying stochastic processes

Generative scientific machine learning methods can also be used to learn surrogates for stochastic dynamical systems.

This vertical is joint work with

- ▶ Jonah Botvinick-Greenhouse, Yunan Yang (Cornell University).
- ▶ Jinqiao Duan, Yubin Lu (IIT-Chicago).
- ▶ Ioannis Kevrekidis (Johns Hopkins University).



# Stochastic differential equations

The most common formulation for an Itô SDE is as follows

$$d\mathbf{x}(t) = \boldsymbol{\mu}(\mathbf{x}(t), t)dt + \boldsymbol{\sigma}(\mathbf{x}(t), t)d\mathbf{B} \quad (13)$$

where  $\mathbf{x}(t)$  is a stochastic (real) quantity,  $\mathbf{B}(t)$  is a Brownian process, and  $\boldsymbol{\sigma}(\mathbf{x}, t)$  stands for a diffusion coefficient. The PDF of  $\mathbf{x}$  is then governed by the Fokker-Planck PDE

$$\frac{\partial p(\mathbf{x}, t)}{\partial t} = - \sum_{i=1}^N \frac{\partial}{\partial \mathbf{x}_i} [\mu_i(\mathbf{x}, t)p(\mathbf{x}, t)] + \sum_{i=1}^N \sum_{j=1}^N \frac{\partial^2}{\partial \mathbf{x}_i \partial \mathbf{x}_j} [D_{ij}(\mathbf{x}, t)p(\mathbf{x}, t)] \quad (14)$$

with drift vector  $\boldsymbol{\mu} = (\mu_1, \dots, \mu_N)$  and diffusion tensor  $\mathbf{D} = \frac{1}{2}\boldsymbol{\sigma}\boldsymbol{\sigma}^\top$ , i.e

$$D_{ij}(\mathbf{x}, t) = \frac{1}{2} \sum_{k=1}^M \sigma_{ik}(\mathbf{x}, t)\sigma_{jk}(\mathbf{x}, t) \quad (15)$$

and initial condition  $p(\mathbf{x}, 0) = \delta(\mathbf{x} - \mathbf{x}_0)$ .

## Stochastic differential equations

A nonlocal Itô stochastic differential equation (SDE) may have a non-Gaussian component

$$d\mathbf{x}(t) = \boldsymbol{\mu}(\mathbf{x}(t), t)dt + \boldsymbol{\sigma}(\mathbf{x}(t), t)d\mathbf{B} + \hat{\boldsymbol{\sigma}}(\mathbf{x}(t), t)d\mathbf{L} \quad (16)$$

where  $\mathbf{L}(t)$  is a Lévy process, and  $\hat{\boldsymbol{\sigma}}(\mathbf{x}, t)$  is the anomalous diffusion coefficient. The PDF of  $\mathbf{x}$  is then governed by

$$\begin{aligned} \frac{\partial p(\mathbf{x}, t)}{\partial t} = & - \sum_{i=1}^N \frac{\partial}{\partial x_i} [\mu_i(\mathbf{x}, t)p(\mathbf{x}, t)] + \sum_{i=1}^N \sum_{j=1}^N \frac{\partial^2}{\partial x_i \partial x_j} [D_{ij}(\mathbf{x}, t)p(\mathbf{x}, t)] + \\ & \int_{\mathbb{R}^d \setminus \{0\}} \tilde{G}(x + y, x, p, \hat{\boldsymbol{\sigma}}(x)) \nu_\alpha(dy) \end{aligned} \quad (17)$$

and initial condition  $p(\mathbf{x}, 0) = \delta(\mathbf{x} - \mathbf{x}_0)$ . Here

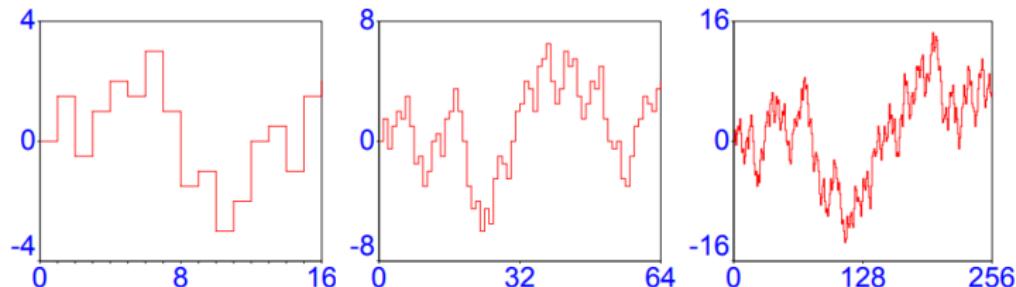
$$\nu_\alpha(dy) = \frac{C_{d,\alpha}}{|y|^{d+\alpha}} dy, \quad \text{where } C_{d,\alpha} = \frac{\alpha \Gamma((d+\alpha)/2)}{2^{1-\alpha} \pi^{d/2} \Gamma(1-\alpha/2)} \quad (18)$$

The last term in Equation 26 requires a non-local computation.

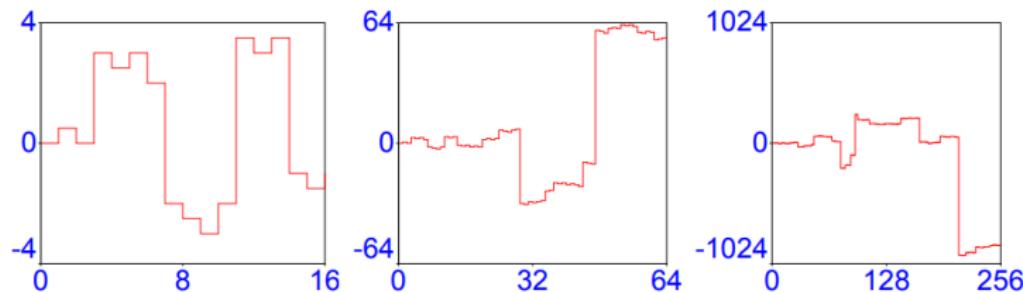


# Stochastic differential equations

Brownian process



Lévy process



## Using SciML for a ‘Fokker-Planck surrogate’

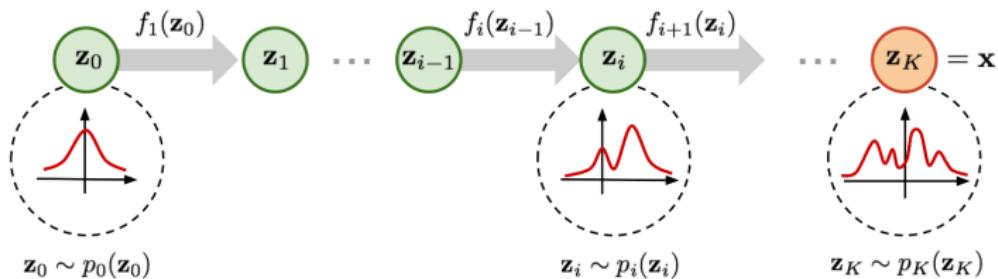
Can we learn a time-varying density directly from data? Existing work broadly falls into following themes:

- ▶ The use of neural-ODE analogs for the stochastic differential equations (Duvenaud, Ruthotto, Jia).
- ▶ Use of generative adversarial networks for learning the sampler of these densities (Karniadakis).
- ▶ Direct solution of a ‘Fokker-Planck’ physics-informed neural network.



# Normalizing flows

Normalizing flows provide a general way to express probability distributions, only requiring a base distribution and a series of bijective transformations. Given  $\mathbf{z}$  as a  $D$ -dimensional real vector sampled from a prior (or latent) density  $p_{\mathbf{z}}(\mathbf{z})$ .



<sup>9</sup><https://lilianweng.github.io/lil-log/2018/10/13/flow-based-deep-generative-models.html>

## Normalizing flows

Given  $\mathbf{z}$  as a  $D$ -dimensional real vector sampled from a prior (or latent) density  $p_z(\mathbf{z})$ , we find a transformation  $T$  such that:

$$\mathbf{z} = T(\mathbf{x}), \quad \text{where } \mathbf{z} \sim p_z(\mathbf{z}) \quad (19)$$

When the transformation  $T$  is invertible and both  $T$  and  $T^{-1}$  are differentiable, the density of  $\mathbf{x}$  is well-defined and can be obtained by a change of variables:

$$p_{\mathbf{x}}(\mathbf{x}) = p_z(T(\mathbf{x})) |\det J_T(\mathbf{x})|, \quad \text{where } \mathbf{z} = T(\mathbf{x}) \quad (20)$$

and  $J_T(\mathbf{z})$  is the Jacobian of  $T$ . Consider a set of samples  $\{\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_n\}$  taken from an unknown distribution  $p_{\mathbf{x}}(\mathbf{x})$ , we can minimize the negative log-likelihood,

$$\mathcal{L} = - \sum_{i=1}^n \log p_z(T(\mathbf{x}_i)) + \log |\det J_T(\mathbf{x})|_{\mathbf{x}=\mathbf{x}_i}. \quad (21)$$

## Normalizing flows

Given two invertible and differentiable transformations  $T_1$  and  $T_2$ , we have the following properties:

$$\begin{aligned}(T_2 \circ T_1)^{-1} &= T_1^{-1} \circ T_2^{-1} \\ \det J_{T_2 \circ T_1}(\mathbf{z}) &= \det J_{T_2}(T_1(\mathbf{z})) \cdot \det J_{T_1}(\mathbf{z}).\end{aligned}\tag{22}$$

Consequently, we can build complex transformations by composing  $K$  simpler transformations, i.e.,  $T = T_K \circ T_{K-1} \circ \dots \circ T_1$ . Each  $T_K$  transforms  $\mathbf{z}_{K-1}$  into  $\mathbf{z}_K$ , assuming

$$\mathbf{z}_0 = \mathbf{x} \text{ and } \mathbf{z}_K = \mathbf{z}\tag{23}$$

Consider a set of samples  $\{\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_n\}$  taken from an unknown distribution  $p_{\mathbf{x}}(\mathbf{x})$ , we can minimize the negative log-likelihood,

$$\mathcal{L} = - \sum_{i=1}^n \log p_{\mathbf{z}}(T(\mathbf{x}_i)) + \log |\det J_T(\mathbf{x})|_{\mathbf{x}=\mathbf{x}_i}.\tag{24}$$



## Multivariate temporal normalizing flows (TNFs)

The hard part about constructing a normalizing flow is proposing a functional form for  $T$ . In this study, we propose

$$\begin{aligned} z_{1:d} &= x_{1:d} \\ z_{d+1:D} &= x_{d+1:D} \odot e^{\mu(\mathbf{x}_{1:d}, t)} + \nu(\mathbf{x}_{1:d}, t), \end{aligned} \tag{25}$$

where the notation  $\odot$  is Hadamard product,  $\mu$  and  $\nu$  are neural networks. Here  $d$  is a hyperparameter and  $\mathbf{x}_{1:d} = (x_1, x_2, \dots, x_d)$ . The determinant of the Jacobian becomes

$$\det J_T = e^{\mu(\mathbf{x}_{1:d}, t)} \tag{26}$$

Members of the audience who are familiar with normalizing flows will recognize this as a ‘time-varying’ version of Dinh et als., RealNVP.



## TNF Example

Consider a two-dimensional stochastic differential equation with pure jump Lévy motion, (i.e., only anomalous diffusion)

$$\begin{aligned} dX_1(t) &= (8X_1(t) - X_1^3(t)) dt + dL_1^\alpha(t) \\ dX_2(t) &= -(8X_2(t) - X_2^3(t)) dt + dL_2^\alpha(t) \\ (X_1(0), X_2(0)) &\sim \mathcal{N}(0, I_{2 \times 2}) \end{aligned} \tag{27}$$

where  $L_1^\alpha$  and  $L_2^\alpha$  are two disjoint independent scalar real-value  $\alpha$ -stable Lévy motion with triple  $(0, 0, \rho)$ . Sampling a dataset  $\mathcal{D}$  from the solution of the SDE as our training data, where

$t_1 = 0$ ,  $t_m = 0.95$ ,  $\Delta t = 0.05$ ,  $m = 20$  and  $n = 500$ .

This example leads to a multimodal distribution evolution.



# TNF Example

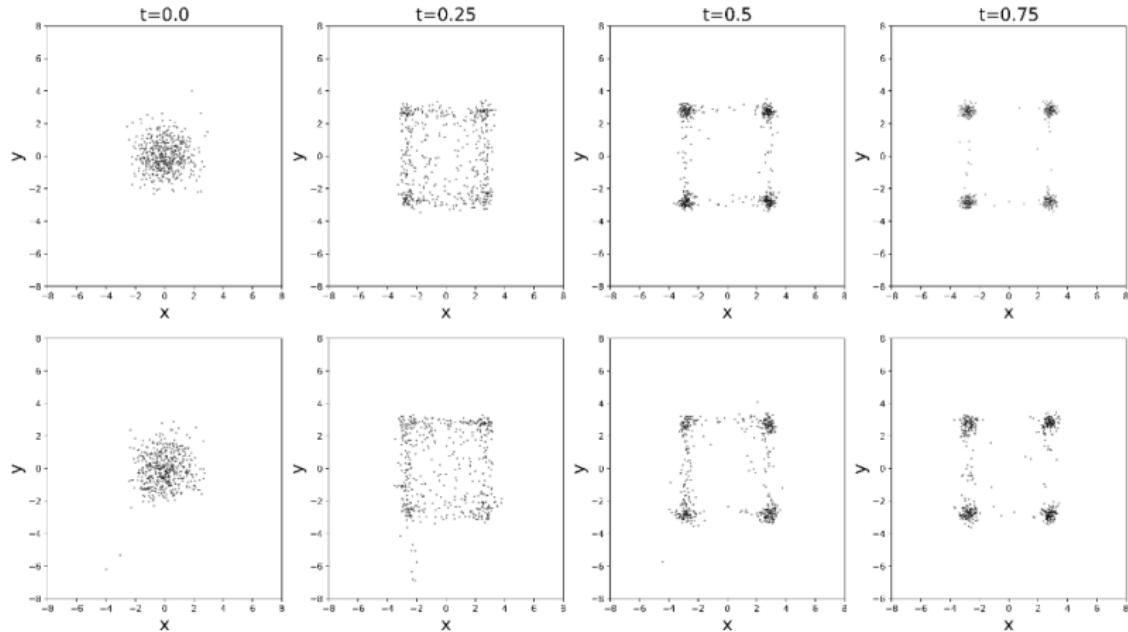
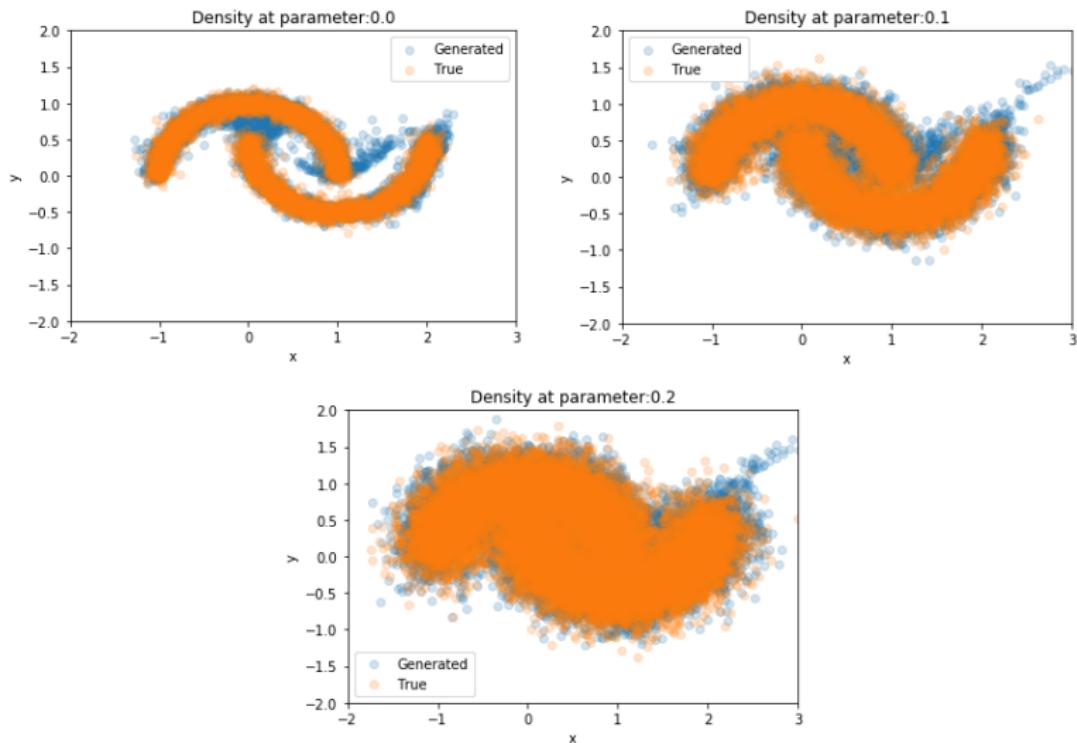


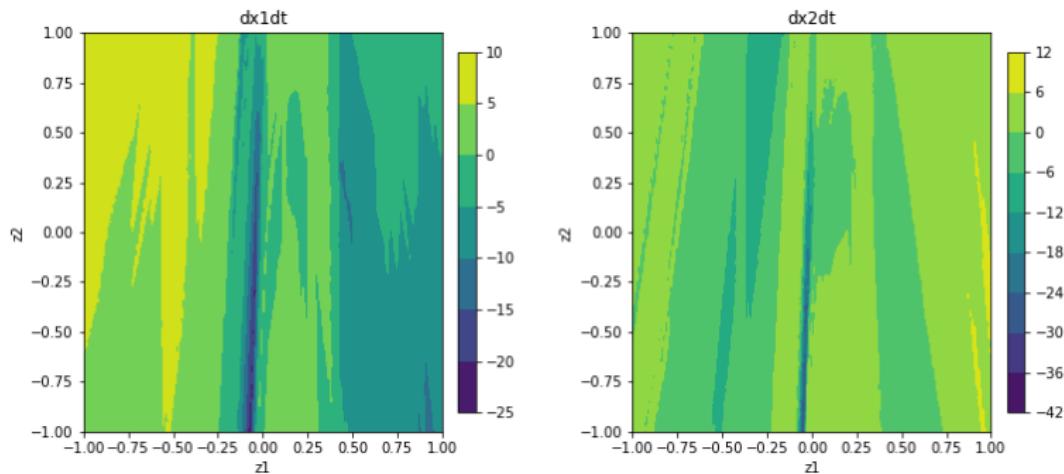
Figure: True - top and predicted - bottom. For different locations in time.

# Half moons example



**Figure:** Learning the half-moon densities parameterized by noise.

## Half moons example



**Figure:** Extracting the ‘learned’ half-moon flow map for no noise.  
Connection to discovering physical systems? Work underway.

$$\frac{d\mathbf{x}}{dt} = \frac{\partial T^{-1}}{\partial t}(\mathbf{z}, t) \quad (28)$$



## Use case: Attractor reconstruction

We can construct partially observed periodic systems, given training data for full state observations. Given a time delayed embedding

$$\Psi(\mathbf{x}(t); \tau, d) := (\psi(\mathbf{x}(t)), \psi(\mathbf{x}(t - \tau)), \dots, \psi(\mathbf{x}(t - (d - 1)\tau))), \quad (29)$$

for a suitable embedding dimension of  $d \geq 1$  and delay parameter  $\tau > 0$ .

By Takens' Theorem, we have that  $\Psi : \mathcal{M} \rightarrow \mathcal{M}_\psi$  is a diffeomorphism - where  $\mathcal{M}$  is the manifold generated by the true dynamics  $\mathbf{x}(t)$  and by  $\mathcal{M}_\psi$  is the manifold generated by the delayed observable. Here  $\psi(\mathbf{x}_t)$  is a partial observable of the full-state. We want to learn  $\Psi^{-1} : \mathcal{M}_\psi \rightarrow \mathcal{M}$ .



# Use case: Attractor reconstruction

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**Algorithm 5:** Deterministic Attractor Reconstruction with Conditional Normalizing Flows

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**Input:** Full state measurements  $\{\mathbf{x}(t_i)\}_{i=1}^K$ , where  $t_i \leq T$  and the partial observations  $\{\psi(\mathbf{x}(t_i))\}_{i=1}^{K+M}$

**Data Preparation:**

Select an embedding dimension  $d$  and a time-delay  $\tau$ .

Compute the points  $\Psi(\mathbf{x}(t_i); \tau, d)$ .

Accumulate the noise-inflated observations  $\mathcal{O}$ .

**Training:**

For  $\ell = 1, \dots, L$

Form the  $r$ -point random sample  $R := \{\mathbf{x}(t_i) + \epsilon_{ij}\}$ .

Compute the log-likelihood that  $\Phi(\Psi(\mathbf{x}(t_i)); \theta)^{-1}(R) \sim \mathcal{N}(0, I)$ .

Update  $\theta$ .

Return

**Testing:**

For  $m = K + 1, \dots, K + M$

Sample  $s$  points  $\{p_i\}_{i=1}^s \sim \mathcal{N}(0, I)$

Evaluate  $P := \Phi(\Psi(\mathbf{x}(t_m)); \theta) \# \{p_i\}_{i=1}^s$

Assign  $\mathbf{x}(t_m) \leftarrow \text{mean}(P)$ .

Return

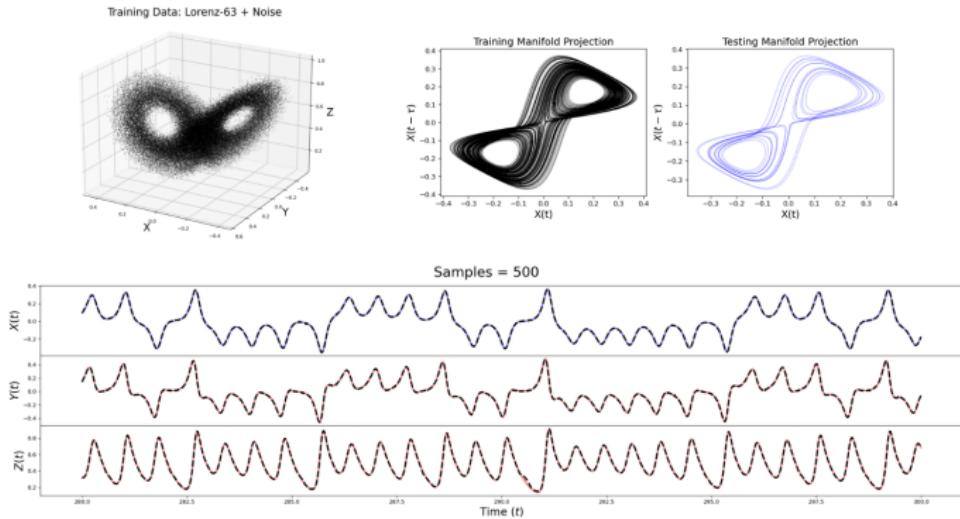
**Output:** The reconstructed full states  $\{\mathbf{x}(t_i)\}_{i=1}^{K+M}$ .

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**Figure:** Algorithm for state reconstructions using conditional normalizing flows.



# Use case: Attractor reconstruction



**Figure:** Reconstructing the Lorenz-63 attractor.

Note that the current formulation of this approach assumes partial observations of the current timestep. Extensions to a pure ‘forecast’ paradigm underway.

<sup>0</sup>Botvinick-Greenhouse, Yang, and Maulik, in-preparation.

## Use case: Brownian-SDE identification

Recall, also, that the generator of the SDE is given by

$$Af(\mathbf{x}(t)) = \boldsymbol{\mu}(\mathbf{x}(t), t) \cdot \nabla f(\mathbf{x}(t)) + \frac{1}{2} \operatorname{Tr} (\boldsymbol{a}(\mathbf{x}(t)) \boldsymbol{H}_f(\mathbf{x}(t))) \quad (30)$$

where  $\boldsymbol{a} = \boldsymbol{\sigma} \boldsymbol{\sigma}^T$ . After some algebra, the SDE extraction boils down to setting  $f(\mathbf{x}(t)) = \mathbf{x}$  which gives us

$$\begin{aligned} Af(\mathbf{x}(t)) &= \boldsymbol{\mu}(\mathbf{x}(t)) \cdot \nabla f + \frac{1}{2} \operatorname{Tr} (\boldsymbol{a}(\mathbf{x}(t)) \boldsymbol{H}_f(\mathbf{x}(t))) \\ &= \boldsymbol{\mu}(\mathbf{x}(t)) \cdot \mathbf{e}_i + \frac{1}{2} \operatorname{Tr} (\boldsymbol{a}(\mathbf{x}(t)) \mathbf{0}) \\ &= \boldsymbol{\mu}_i(\mathbf{x}(t)) \cdot s \end{aligned} \quad (31)$$

where  $\boldsymbol{\mu}_i$  obtained on some suitable discretization of  $\mathbf{x}(t)$ .

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<sup>10</sup> Lu et al., Physica D, 417, 132830, 2021

## Use case: Brownian-SDE identification

Furthermore we can set  $f(\mathbf{x}(t)) = \mathbf{x}(t)^2$  to get

$$\begin{aligned} Af(\mathbf{x}(t)) &= \mu(\mathbf{x}(t)) \cdot \nabla f(\mathbf{x}(t)) + \frac{1}{2} \operatorname{Tr}(f(\mathbf{x}(t)) H_f(\mathbf{x}(t))) \\ &= \mu(\mathbf{x}(t)) \cdot 2\mathbf{x}(t)_i \mathbf{e}_i + \frac{1}{2} \operatorname{Tr}(a(\mathbf{x}(t)) H_{f(\mathbf{x}(t))}(\mathbf{x}(t))) \quad (32) \\ &= 2\mathbf{x}(t)_i \mu_i(\mathbf{x}(t)) + a_{ii}(\mathbf{x}(t)) \end{aligned}$$

This gives us diagonal terms of  $\sigma(\mathbf{x}(t))$  (and the problem ends here if  $\sigma(\mathbf{x}(t))\sigma(\mathbf{x}(t))^T$  is diagonal). In case they're not - we need to set  $f(\mathbf{x}(t)) = x_i(t)x_j(t)$  where  $i \neq j$  to obtain off-diagonal terms.

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<sup>10</sup> Lu et al., Physica D, 417, 132830, 2021

## Use case: Brownian-SDE identification

We begin with the one-dimensional double-well system (with Brownian motion)

$$dX_t = [-X_t^3 + 4X_t] dt + [0.2X_t^3 + 0.6] dB_t \quad (33)$$



Figure: Double well system



## Use case: Brownian-SDE identification

We obtain drift and diffusion approximations that are similar to the SDE terms - we may couple this to a sparse regression to obtain functional forms (with William McClure, ex-Master's student at IIT-Chicago).

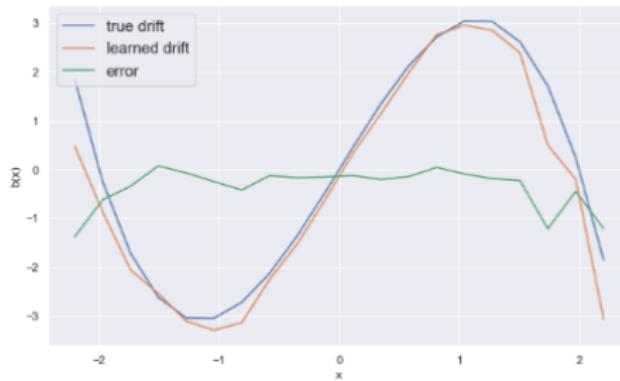


Figure: Learning the drift



## Use case: Brownian-SDE identification

We obtain drift and diffusion approximations that are similar to the SDE terms - we may couple this to a sparse regression to obtain functional forms (with William McClure, ex-Master's student at IIT-Chicago).

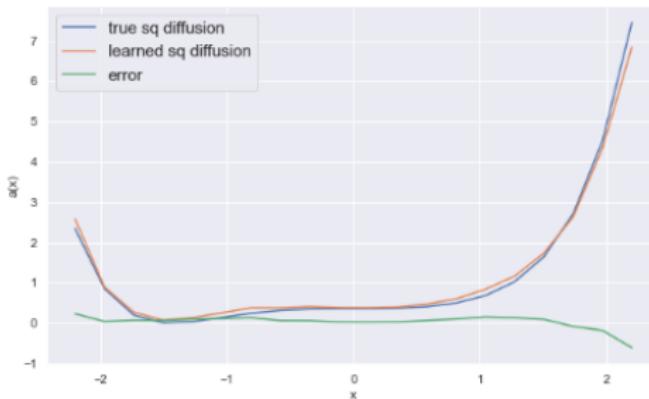


Figure: Learning the diffusion



# Big picture applications

## Applications:

- ▶ Elegant particle/continuum coupling for various multiscale, multiphysics problems.
- ▶ Subgrid scale modeling for complex systems.
- ▶ Synthetic boundary condition generators (inflow turbulence).



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[romit-maulik.github.io](https://romit-maulik.github.io)



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