

Weak form SciML for Learning Models on Different Scales

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<http://github.com/MathBioCU>

IPAM

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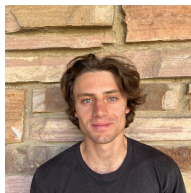
Researchers



Dr. Dan Messenger
LANL



April Tran



Seth Minor



Prof. Vanja Dukic
CU



Dr. Nora
Heitzman-Breen



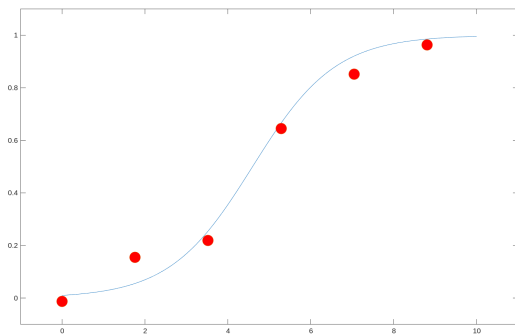
Dr. Rainey
Lyons



Dr. Cristian
López

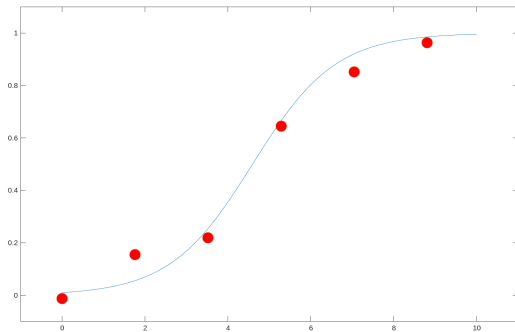
Dr. Moyi Tian
Abhi Chawla
Will Houser
Jack Krebsbach
Nic Rummel

Modeling



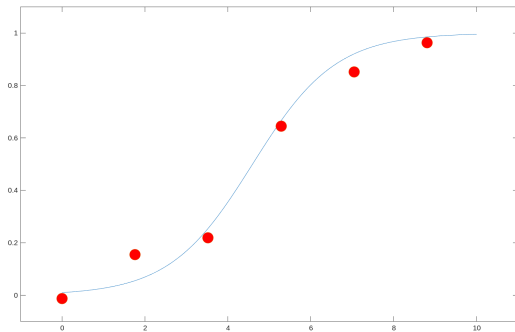
$$u(t; r, K, u_0) := \frac{e^{rt} K u_0}{K + u_0(e^{rt} - 1)}$$

Modeling



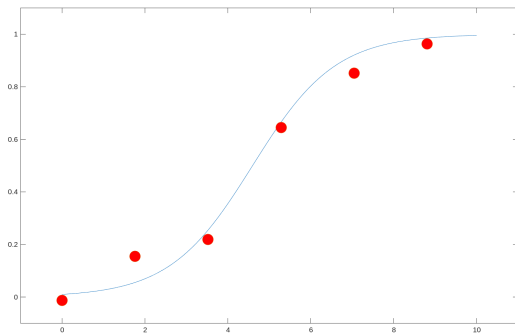
$$u(t; r, K, u_0) \approx u^N(t; r, K, u_0)$$

Modeling



$$\dot{u} = w_1 u + w_2 u^2$$

Modeling



$$-\int \dot{\phi}(t)u(t)dt = w_1 \int \phi(t)u(t)dt + w_2 \int \phi(t)u(t)^2dt$$

Data-Driven Sparse Identification & Estimation

Equation Error vs. Output/Solution Error

- Greenberg, NACA TN 2340, 1951.

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- Plug data $\mathbf{U}$ into DE

$$\partial_t u = w_1 f_1(u) + w_2 f_2(u) + \cdots$$

$$\mathbf{b} := \begin{bmatrix} \tilde{\partial}_t U_1 & \tilde{\partial}_t U_2 & \cdots & \tilde{\partial}_t U_M \end{bmatrix}^T$$

$$\mathbf{G} := [f_k(U_i)]_{i,k} = \begin{bmatrix} f_1(U_1) & f_2(U_1) & \cdots & f_K(U_1) \\ f_1(U_2) & f_2(U_2) & \ddots & \\ \vdots & \ddots & \ddots & \\ f_1(U_M) & \cdots & & f_K(U_M) \end{bmatrix}$$

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- Plug in data $\mathbf{U}$ and solve Equation-Error (EE) linear least squares problem

$$\min_{\mathbf{w}} \|\mathbf{G}\mathbf{w} - \mathbf{b}\|_2^2$$

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- FAST, but VERY sensitive to noise.
- Advances in OE methods.

SINDy: Brunton, Proctor, Kutz, PNAS (2016)

Consider a Differential Equation

$$\partial_t u = \mathbf{G}(u) \mathbf{w}^*$$

with an uber-model matrix

$$\mathbf{G}(u) = \begin{bmatrix} | & | & | & | & | & | \\ u & \partial_x u & \partial_{xx} u & \dots & u \partial_x u & u \partial_{xx} u \dots \\ | & | & | & | & | & | \end{bmatrix},$$

- 1 evaluate at $\mathbf{U}$
- 2 solve a sparse regression problem for weights $\mathbf{w}^*$:

$$\hat{\mathbf{w}} = \operatorname{argmin}_{\mathbf{w}} \|\mathbf{G}(\mathbf{U})\mathbf{w} - \partial_t \mathbf{U}\|_2^2 + \lambda \|\mathbf{w}\|_0$$

PROBLEM!

- Approximating derivatives is unstable:

$$\mathbb{E} [|\partial_x^k u - \Delta_x^k(u + \epsilon)|^2] = \mathcal{O} \left(\frac{\sigma^2}{h^{2k}} \right)$$

- True solution $u(x, t)$ may not be smooth

Consider

$$\partial_t u = \mathbf{G}(u) \mathbf{w}^\star \rightarrow \boxed{D^{\alpha^0} u = \sum_{s,j=1}^{S,J} \mathbf{w}_{s,j}^\star D^{\alpha^s} f_j(u)} \quad (1)$$

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- Interpret PDE in a weak sense: $\forall \psi \in C_c^{|\alpha|}$,

$$\left\langle (-1)^{|\alpha^0|} D^{\alpha^0} \psi, u \right\rangle = \sum_{s,j=1}^{S,J} \mathbf{w}_{s,j}^* \left\langle (-1)^{|\alpha^s|} D^{\alpha^s} \psi, f_j(u) \right\rangle \quad (2)$$

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- For test functions $(\psi_k)_{1 \leq k \leq K}$, **evaluate (2) at $\mathbf{U}$**

$$\mathbf{b}_k := \left\langle (-1)^{|\alpha^0|} D^{\alpha^0} \psi_k, \mathbf{U} \right\rangle, \quad \mathbf{G}_{k,(j-1)S+s} := \left\langle (-1)^{|\alpha^s|} D^{\alpha^s} \psi_k, f_j(\mathbf{U}) \right\rangle$$

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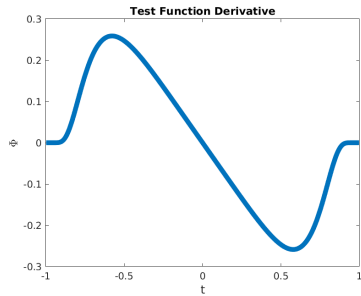
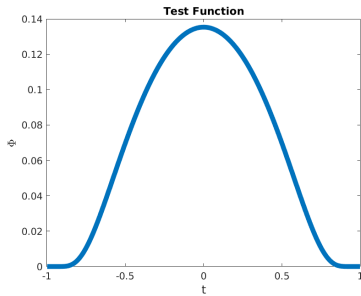
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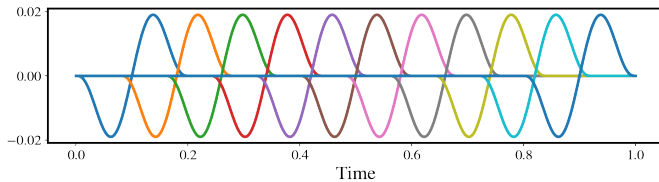
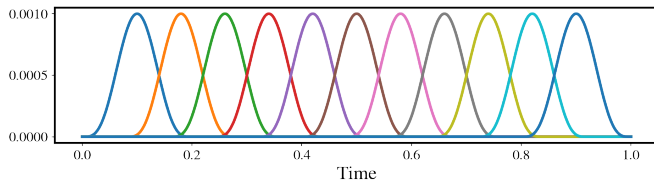
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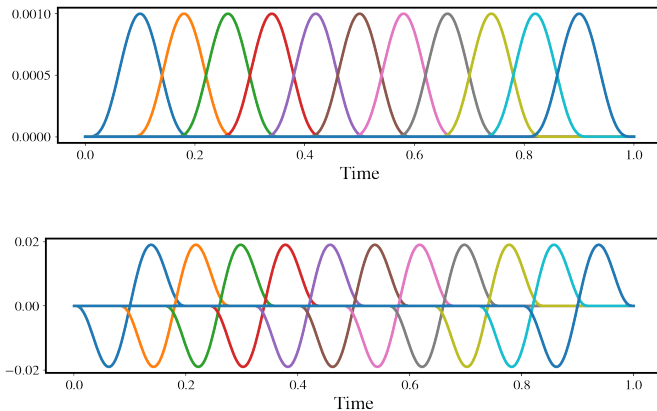
Test Functions



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Test Functions

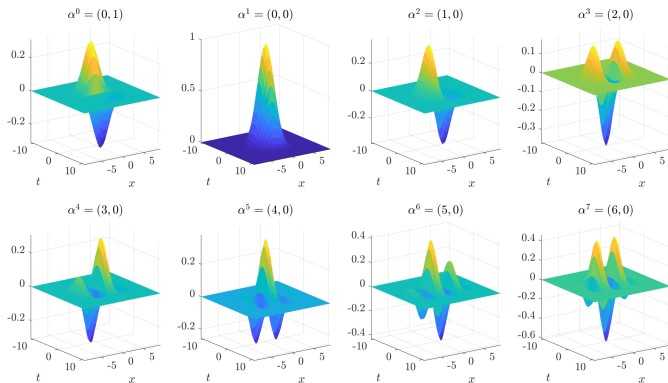


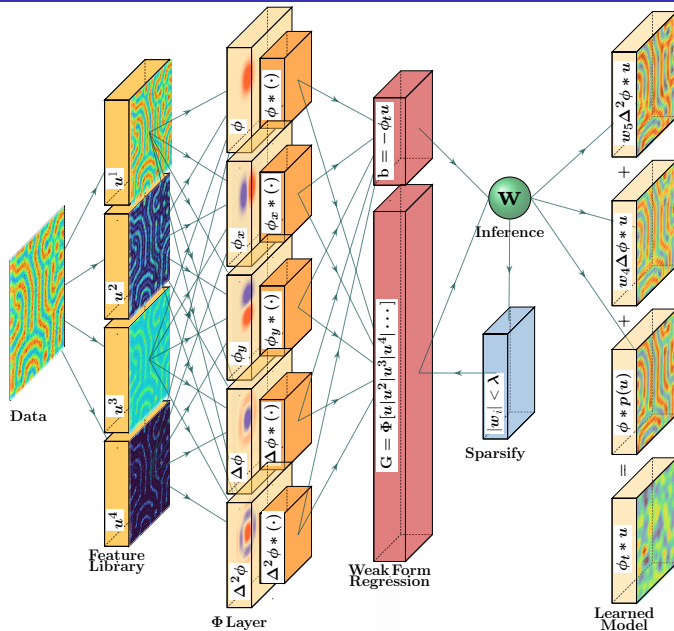
- Choose function space: radius, smoothness, shape, spectrum, ...

Test Functions

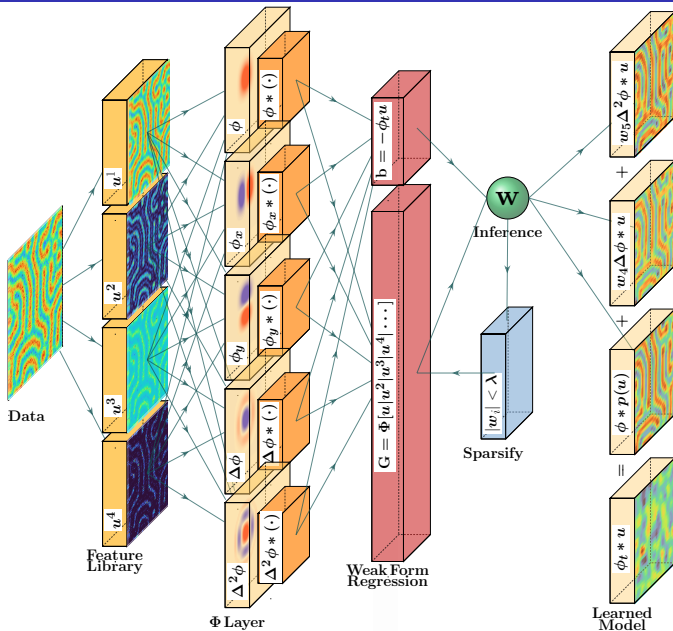
$$\phi(\bullet; a, p) = \left(1 - \left(\frac{\bullet}{a}\right)^2\right)_+^p \quad (3)$$

• $\phi \in C^{p-1}(\mathbb{R})$, $\text{supp}(\phi) = [-a, a] \rightarrow \psi = \prod \phi_i$



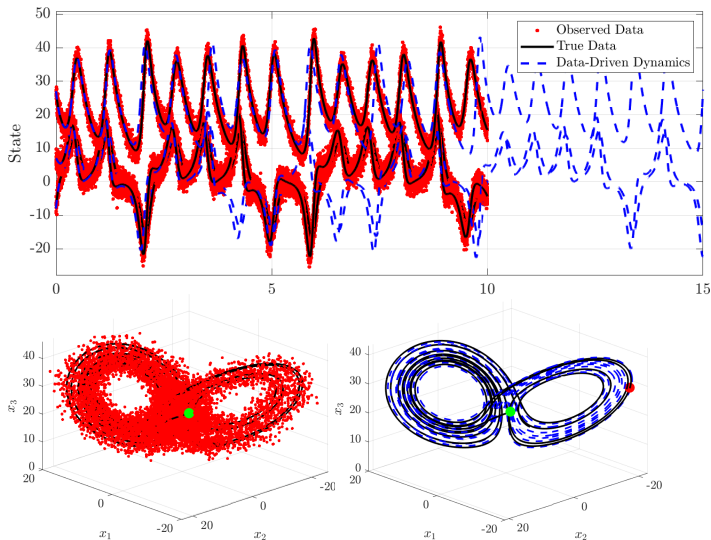


WSINDy: Interpretable AI?



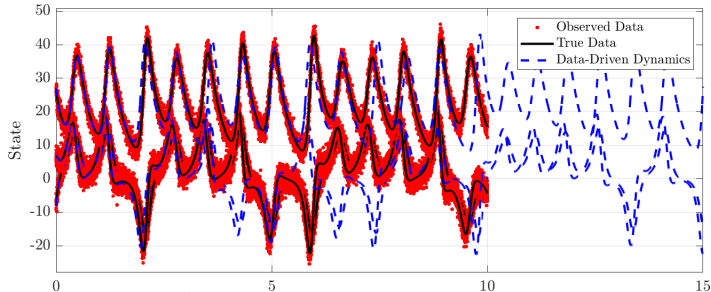
Performance

Lorenz 10% noise $\|\hat{\mathbf{w}} - \mathbf{w}^*\|_2 / \|\mathbf{w}^*\|_2 = 0.0084$

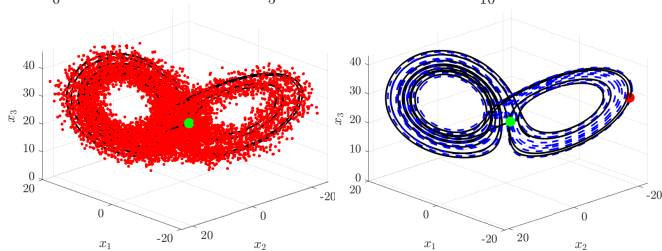


DAM & DMB, MMS 19(3):1474–1497, 2021.

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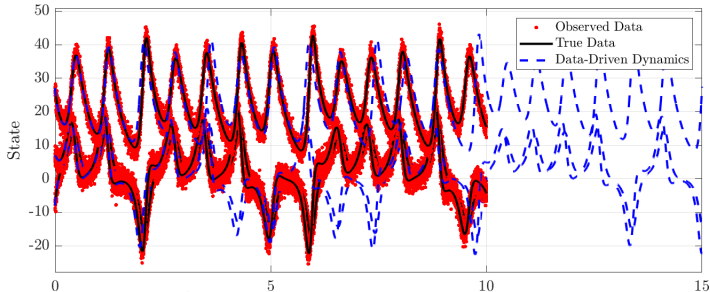


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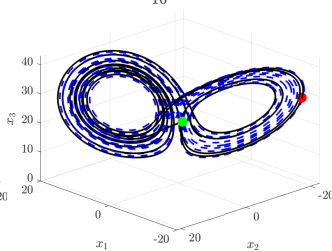
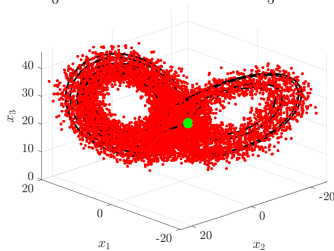
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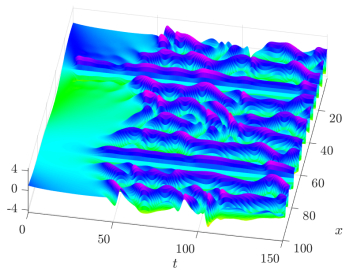
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Compare?

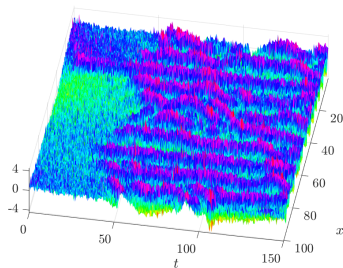


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Kuramoto Sivashinsky $u_t = -(u^2)_x - u_{xx} - u_{xxxx}$



Noise-free



50% Noise

Noise level	Max. Coefficient Error	Identification Rate
0%	8.1×10^{-7}	100%
25%	0.017	100%
50%	0.070	100%
100%	0.31	96.1%

DAM & DMB, JCompPhys, 443:110525, Oct. 2021

WSINDy Computational Cost

PDE	U (MB)	U (dim)	G (dim)	nz(w*)	Walltime (s)
IB	0.5	256×256	784×43	1	0.12
KS	0.6	256×301	$1,806 \times 43$	3	0.24
KdV	1.9	400×601	$1,443 \times 43$	2	0.39
NLS	1.0	$2 \times 256 \times 251$	$1,804 \times 190$	6	2.5
NS	233	$3 \times 324 \times 149 \times 201$	$3,872 \times 50$	4	12
PM	41	$200 \times 200 \times 128$	$4,608 \times 65$	3	16
SG	85	$129 \times 403 \times 205$	$13,000 \times 73$	3	29
RD	211	$2 \times 256 \times 256 \times 201$	$11,638 \times 181$	14	75

2011 Intel i7-2670QM CPU

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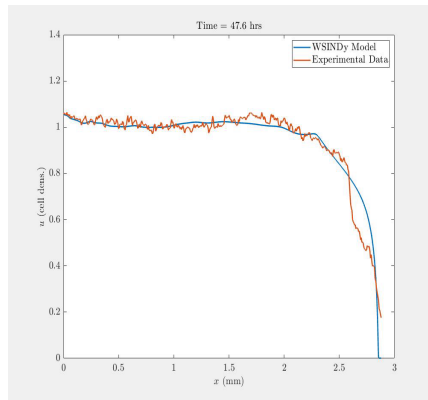
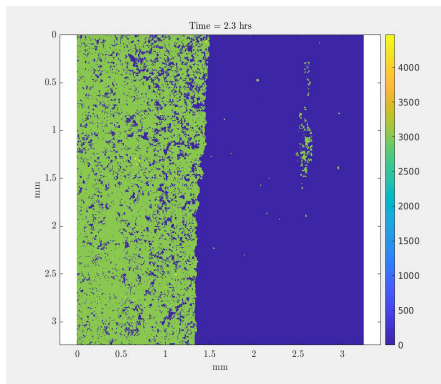
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- Comparison?

Application: Interacting Particle Systems

Wound Healing (Nardini et al., JTB, 2016)

Identified advection-diffusion PDE: $\partial_t u = \nabla \cdot (u \mathbf{a}(u)) + \Delta D(u)$

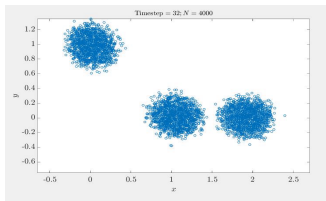


1st Order (DAM & DMB, PhysD, 2022)

Mean field equations from particle trajectory data

$$d\mathbf{x}_t^{(i)} = \left(-\frac{1}{N} \sum_{j=1}^N \nabla K(\mathbf{x}_t^{(i)} - \mathbf{x}_t^{(j)}) - \nabla V(\mathbf{x}_t^{(i)}) \right) dt + \sigma(\mathbf{x}_t^{(i)}) dB_t^{(i)}$$

Histogram for atoms B_k :



$$\int_{\mathcal{D}} G(x, y) d\mu_t^N(y)$$

$$G(x, y) = \sum_k \frac{1}{|B_k|} \mathbb{1}_{B_k}(x) \mathbb{1}_{B_k}(y)$$

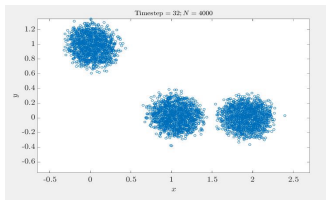
$$N \rightarrow \infty : \quad \partial_t \mu_t = \nabla \cdot (\mu_t \nabla K * \mu_t) + \nabla \cdot (\mu_t \nabla V) + \frac{1}{2} \sum_{i,j} \partial_{x_i x_j} ((\sigma \sigma^T)_{ij} \mu_t)$$

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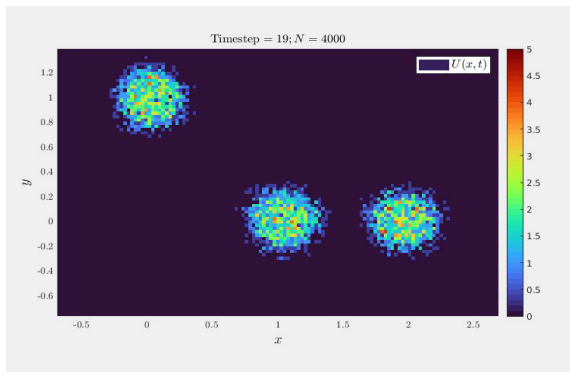
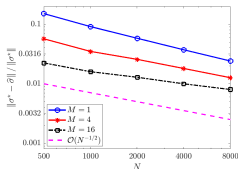
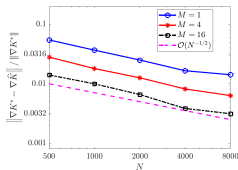
Weak form needs fewer particles and avoids problems with small bin widths.

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- 2D Local (9.2s)

$$K^*(x, y) = 0$$

$$V^*(x, y) = -x - y$$

$$\sigma^*(x, y) = \sqrt{2(1 + 0.95 \cos(\omega x) \cos(\omega y))} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

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- mean field model (FP eqn for dist of each particle):

$$\partial_t \mu_t = -\partial_x \mu_t - \partial_y \mu_t + \Delta [(1 + 0.95 \cos(\omega x) \cos(\omega y)) \mu_t]$$

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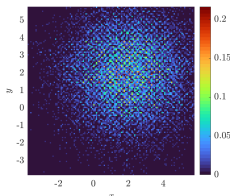
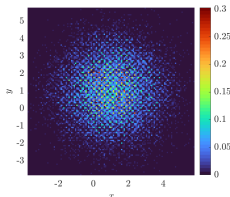
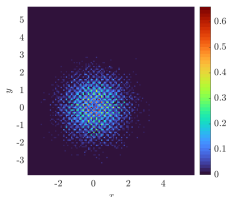
- 2D Local + Homogenization

- As $\omega \rightarrow \infty$, the WSINDy should identify the homogenized equation

$$\partial_t \mu_t = -\partial_x \mu_t - \partial_y \mu_t + \bar{\omega} \Delta \mu_t$$

$$\bar{\omega} = \left(\int_{\mathcal{D}} \frac{dx dy}{1 + 0.95 \cos(\omega x) \cos(\omega y)} \right)^{-1} \approx 0.62$$

1st Order (DAM & DMB, PhysD, 2022)



$$d\mathbf{x}_t^{(i)} = F(\mathbf{x}_t^{(i)})dt + \sqrt{2\sigma(\mathbf{x}^{(i)}, \omega\mathbf{x}^{(i)})}dB_t^{(i)}$$

N particles $\xrightarrow{N \rightarrow \infty}$ highly osc. PDE

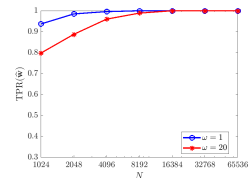
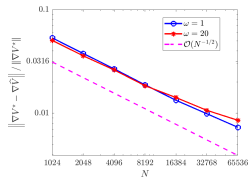
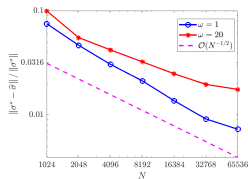
$$\partial_t \mu_t = -\nabla \cdot (F\mu_t) + \Delta(\sigma(\mathbf{x}, \omega\mathbf{x})\mu_t)$$

highly osc. PDE $\xrightarrow{\omega \rightarrow \infty}$ **homog. PDE**

$$\partial_t \bar{\mu}_t = -\nabla \cdot (F\bar{\mu}_t) + \Delta(\bar{\sigma}\bar{\mu}_t)$$

$$\bar{\sigma}(\mathbf{x}) := \left(\frac{1}{|\Omega|} \int_{\Omega} \frac{d\mathbf{y}}{\sigma(\mathbf{x}, \mathbf{y})} \right)^{-1}$$

$$F = \text{const}, \sigma(\mathbf{x}, \mathbf{y}) = 1 + 0.95 \cos(y_1) \cos(y_2) \\ \Rightarrow \bar{\sigma} \approx 0.62$$



- 1D nonlocal (**0.7s**)

$$K_{\text{QANR}}(x) = \frac{1}{2}x^2 - |x|$$

$$V(x) = 0$$

$$\sigma(x) = \left\{ 0, \sqrt{2(0.1)}, \sqrt{2(0.1)} |x - 2| \right\}$$

$$\mathbb{Y} = \mathbb{X} + \varepsilon, \varepsilon \sim \mathcal{N}(0, \epsilon^2 \|\mathbf{X}_t\|_{\text{RMS}}^2)$$

1st Order (DAM & DMB, PhysD, 2022)

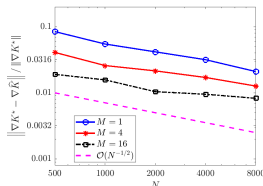
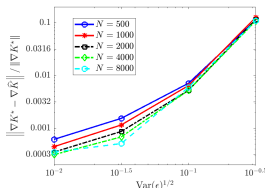
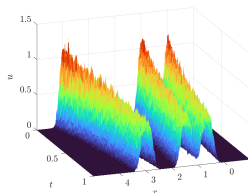
- 1D nonlocal (0.7s)

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$$V(x) = 0$$

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$$\mathbb{Y} = \mathbb{X} + \varepsilon, \varepsilon \sim \mathcal{N}(0, \epsilon^2 \|\mathbf{X}_t\|_{\text{RMS}}^2)$$



Identifies nonlocal interaction from particle trajectories

- 2D nonlocal (parabolic-elliptic Keller-Segel chemotaxis, **8.5s**)

$$K(x) = \frac{1}{2\pi} \log |x|$$

$$V(x) = 0$$

$$\sigma(x) = \{0, 0.28\}$$

$$\mathbb{Y} = \mathbb{X} + \varepsilon, \varepsilon \sim \mathcal{N}(0, \epsilon^2 \|\mathbf{X}_t\|_{\text{RMS}}^2)$$

1st Order (DAM & DMB, PhysD, 2022)

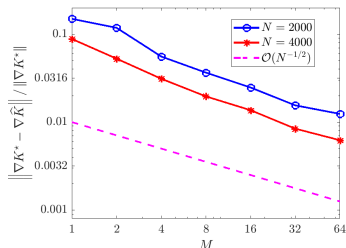
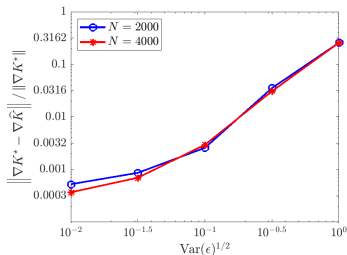
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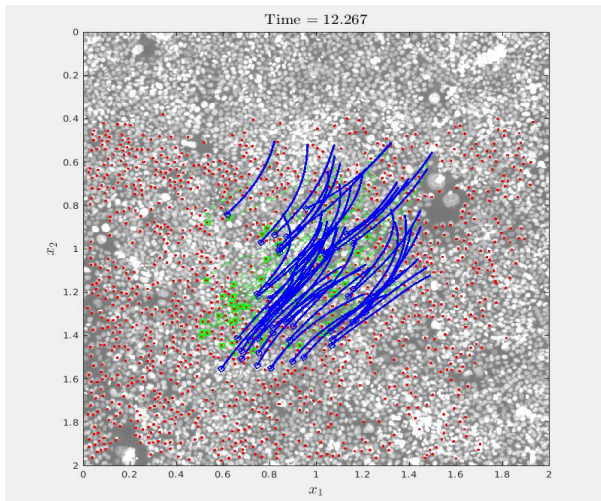
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Identifies nonlocal interaction from particle trajectories

2nd Order (DAM, Wheeler, Liu, & DMB, JRSI, 2022)

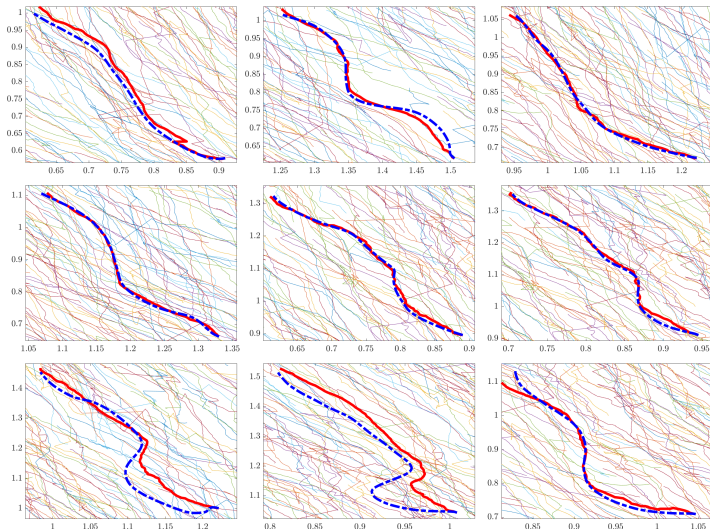
$$\ddot{x}_i = \sum_{j \neq i} f(|x_i - x_j|, \theta_{ij})(x_i - x_j) + \sum_{j \neq i} h(|x_i - x_j|, \theta_{ij})(\dot{x}_i - \dot{x}_j) + \sum_{j \neq i} d(|v_i|, \theta_{ij}) + \eta_i$$



- HaCaT cells, 2 μm EGF
- Hoechst nuclear dye
- $\Delta t = 8$ min
- 555/7106 training cells
- 264 basis functions:
 $f(r, \theta)$, $h(r, \theta)$, $d(v, \theta)$
- $\hat{w}_h \leq 0$, $\hat{w}_d \leq 0$
- Walltime 1 – 2 min.

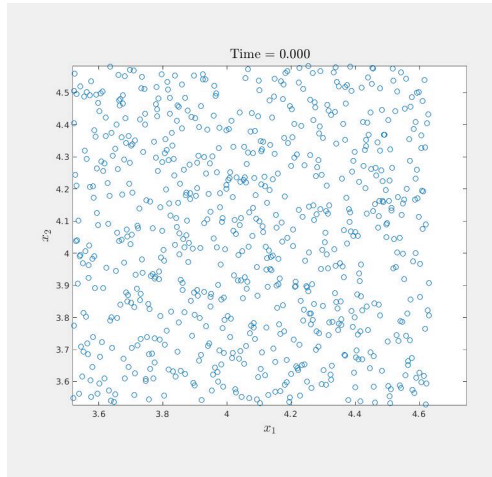
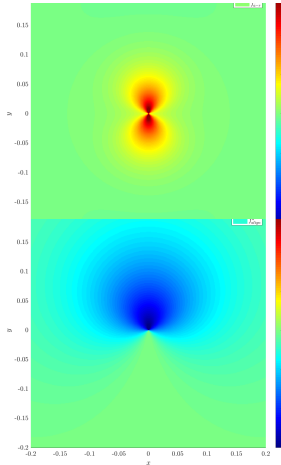
2nd Order (DAM, Wheeler, Liu, & DMB, JRSI, 2022)

$$\ddot{x}_i = \sum_{j \neq i} f(|x_i - x_j|, \theta_{ij})(x_i - x_j) + \sum_{j \neq i} h(|x_i - x_j|, \theta_{ij})(\dot{x}_i - \dot{x}_j) + \sum_{j \neq i} d(|v_i|, \theta_{ij}) + \eta_i$$



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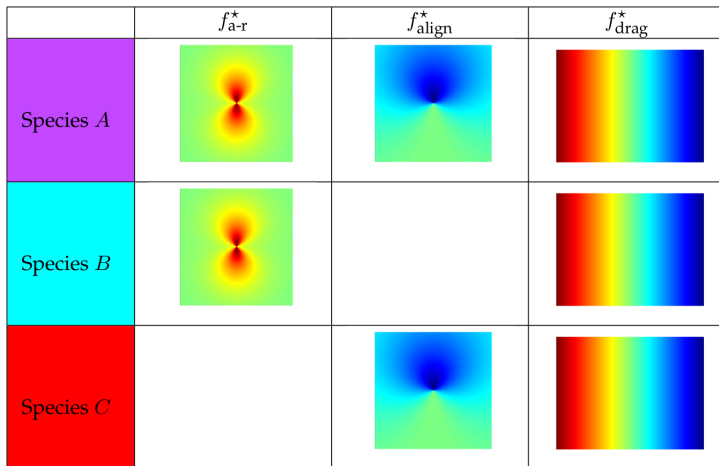
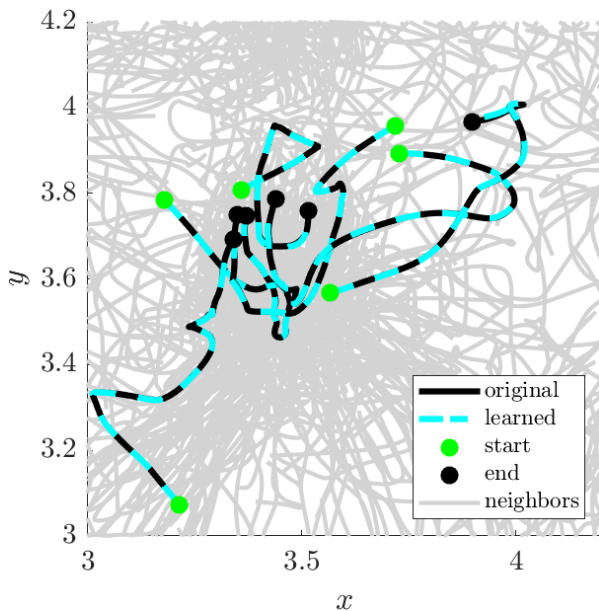
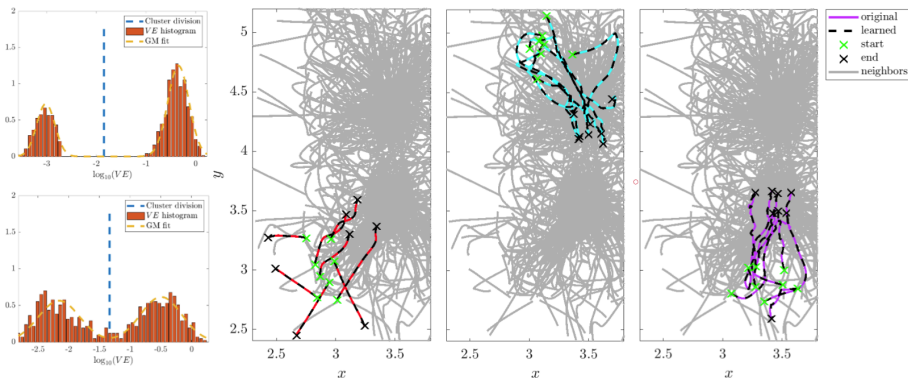


Table 1: Species delineation by active force modes.

2nd Order (DAM, Wheeler, Liu, & DMB, JRSI, 2022)



2nd Order (DAM, Wheeler, Liu, & DMB, JRSI, 2022)



- Validation errors approximately log-normally distributed
- Three-species population identified from unlabeled trajectories

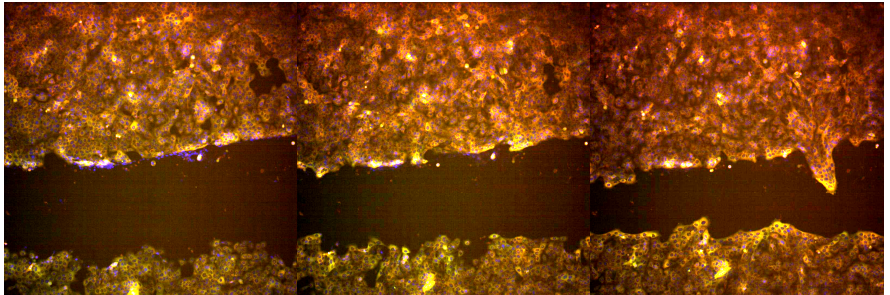


Figure: Snapshots of wound assay at $t = 0, 15, 30$ hours

Cell Migration: Lyons et al., 2025, in prep

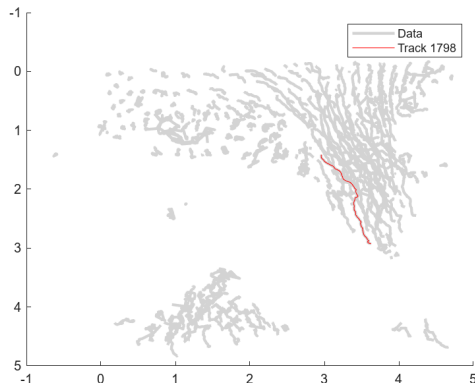
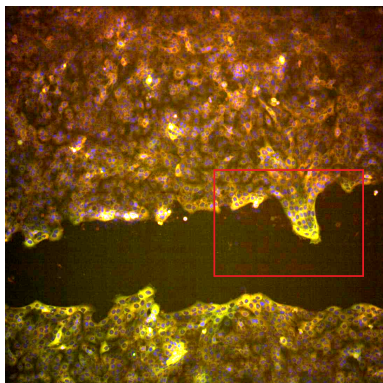
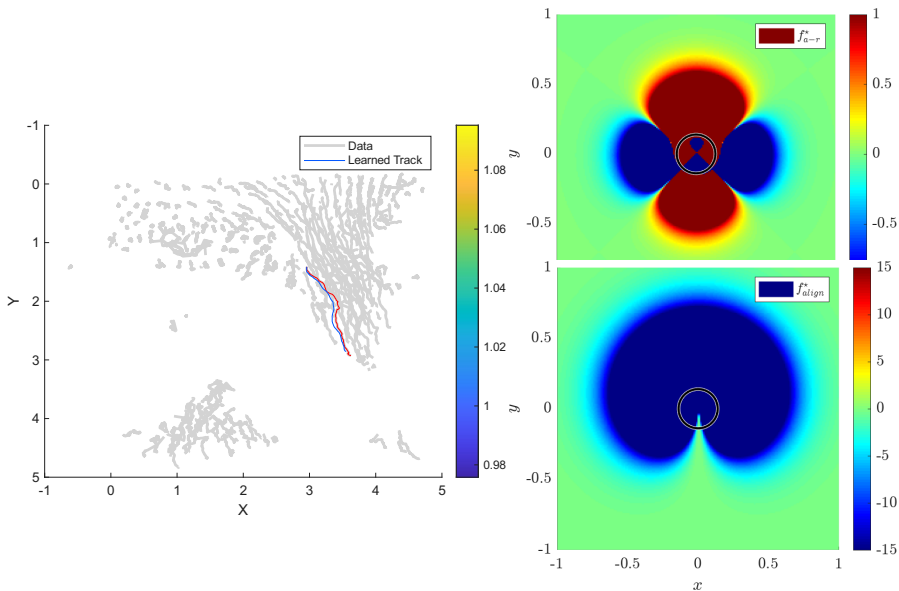


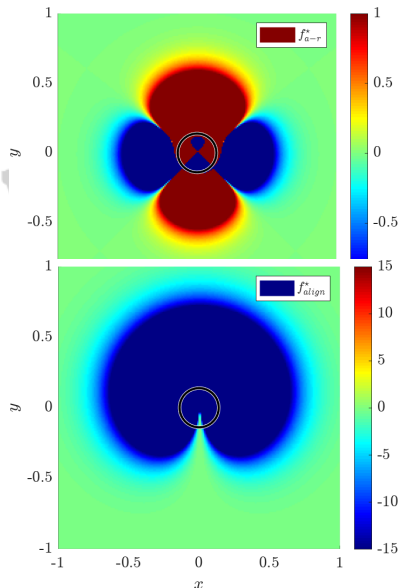
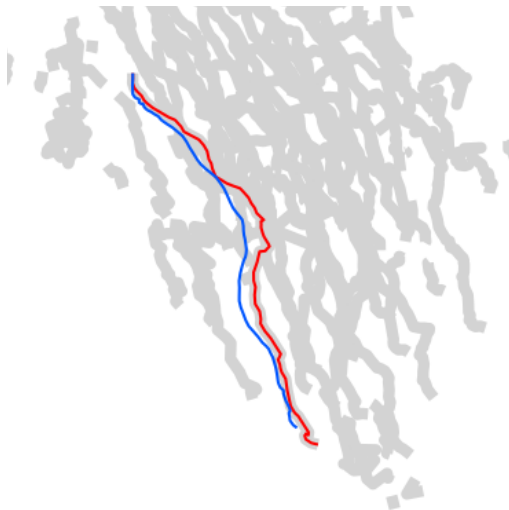
Figure: Example single cell data set

$$\left\{ \begin{aligned} \ddot{x}_i &= \frac{1}{N_{\text{tot}}} \sum_{j=1}^{N_{\text{tot}}} \textcolor{red}{f}_{\text{a-r}}(|x_i - x_j|, \theta_{ij})(x_i - x_j) \\ &+ \frac{1}{N_{\text{tot}}} \sum_{j=1}^{N_{\text{tot}}} \textcolor{blue}{f}_{\text{align}}(|x_i - x_j|, \theta_{ij})(v_i - v_j) \\ &+ \frac{1}{N_{\text{tot}}} \sum_{j=1}^{N_{\text{tot}}} \textcolor{green}{f}_{\text{drag}}(|v_i|, \theta_{ij})v_i + \eta_i. \end{aligned} \right. \quad (4)$$

Cell Migration: Lyons et al., 2025, in prep

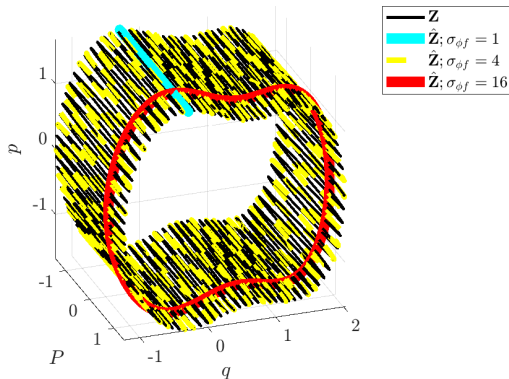


Cell Migration: Lyons et al., 2025, in prep



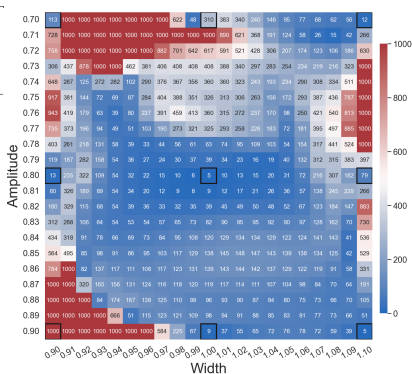
Applications: Reduced Order Modeling in Plasma Physics

Reduced Order Modeling



Nonlinear coupled oscillators

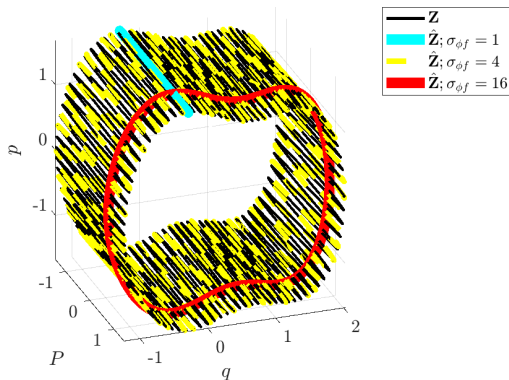
DAM, Burby, DMB, Sci Rep, 2024



Burgers' equation (WLaSDI)

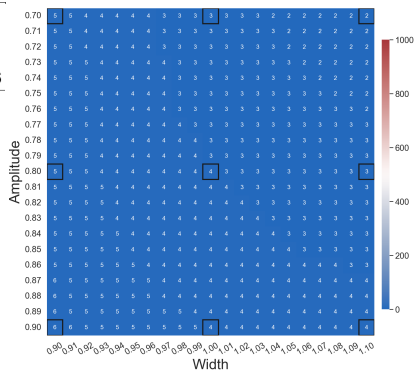
Tran et al., CMAME, 2024

Reduced Order Modeling



Nonlinear coupled oscillators

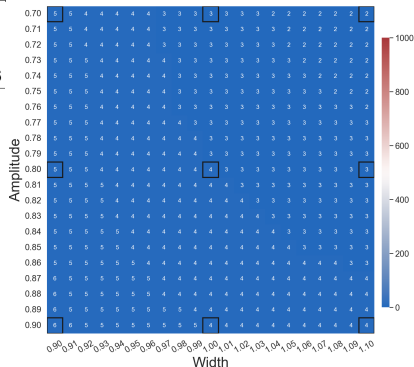
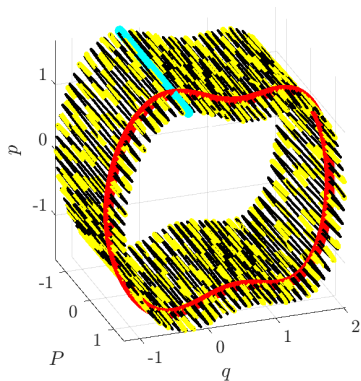
DAM, Burby, DMB, Sci Rep, 2024



50% noise $\rightarrow$ (5% error, 100X)

Tran et al., CMAME, 2024

Reduced Order Modeling



Nonlinear coupled oscillators

50% noise $\rightarrow$ (5% error, 100X)

DAM, Burby, DMB, Sci Rep, 2024

Tran et al., CMAME, 2024

Automated discovery of models on different scales

Applications: Parameter Estimation

Weak form Parameter Estimation

- Minimize the residual

$$\|[\mathbf{G}(\mathbf{U})] \mathbf{w} + \mathbf{b}(\mathbf{U})\|_2^2$$

- The OLS solution is

$$\hat{\mathbf{w}} := (\mathbf{G}^T \mathbf{G})^{-1} \mathbf{G}^T \mathbf{b}$$

$$\mathbf{G} := [\mathbb{I}_d \otimes (\Phi \Theta(\mathbf{U}))]$$

$$\mathbf{b} := -\text{vec}(\Phi(\dot{\mathbf{U}}))$$

Weak form Parameter Estimation

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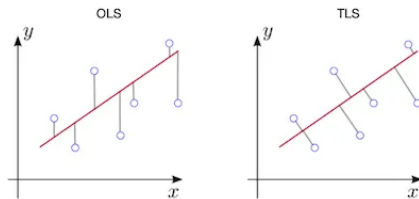
$$\mathbf{b} := -\text{vec}(\Phi(\dot{\mathbf{U}}))$$

- **But, this is a GLS problem:**

$$\|[\mathbf{G}(\mathbf{u}^* + \varepsilon)] \mathbf{w} + \mathbf{b}(\mathbf{u}^* + \varepsilon)\|_2^2$$

Weak form Parameter Estimation

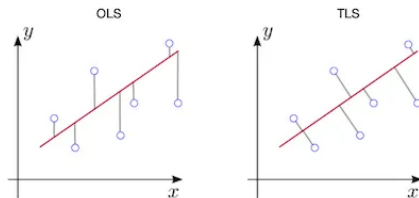
- Specifically, it's an Errors-in-Variables problem:



<https://towardsdatascience.com/>

Weak form Parameter Estimation

- Specifically, it's an Errors-in-Variables problem:



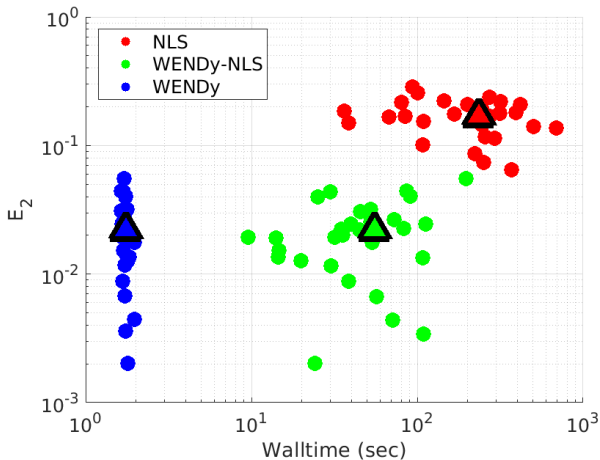
<https://towardsdatascience.com/>

- Solve via iterative reweighting of covariance:

$$\mathbf{G}\mathbf{w}^* - \mathbf{b} \sim \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{L}_{\mathbf{w}^*} (\mathbf{L}_{\mathbf{w}^*})^T)$$

$$\mathbf{L}_{\mathbf{w}} := [\text{mat}(\mathbf{w})^T \otimes \Phi] \nabla \Theta \mathbf{K} + [\mathbb{I}_d \otimes \dot{\Phi}].$$

FitzHugh-Nagumo: Parameter Estimation (5% noise)



DMB, DAM, VD, WENDy, Bull. Math. Biol., 2023

FitzHugh-Nagumo: Parameter Inference

	w_1	w_2	w_3	w_4	w_5	w_6
w_1	1.000	-0.984	0.850	0.233	-0.202	-0.186
w_2		1.000	-0.813	-0.178	0.203	0.135
w_3			1.000	0.411	-0.306	0.003
w_4				1.000	-0.551	-0.136
w_5					1.000	-0.183
w_6						1.000

(Scaled) Covariance Matrix for FN with 20% noise, 128 timepoints

DMB, DAM, VD, WENDy, Bull. Math. Biol., 2023

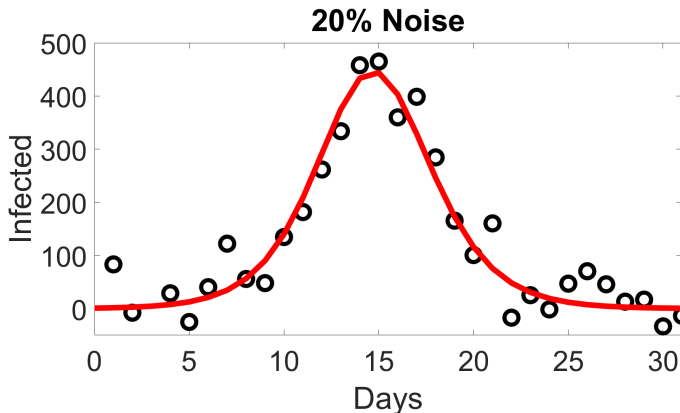
Parameter Estimation: All Variables Measured?

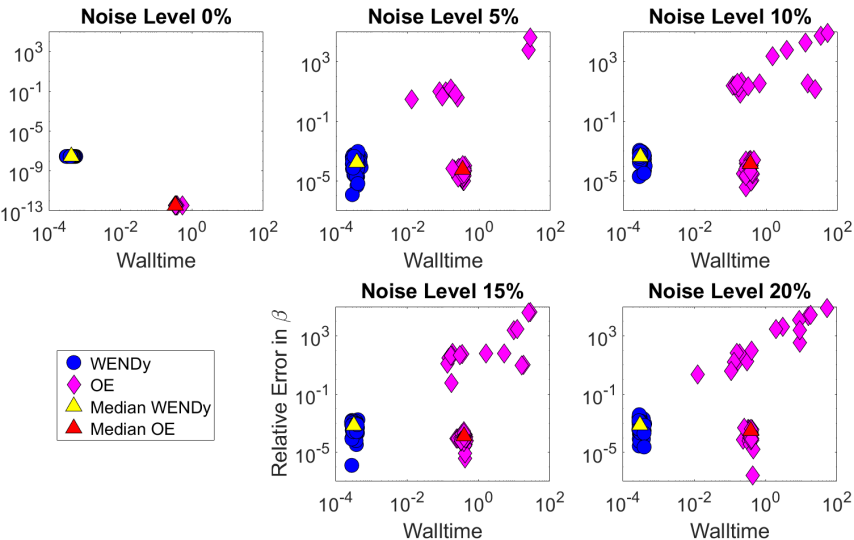
- SIR ODE $N = S + I + R = 10,000$, $\beta = 5.5/N$

$$\dot{S} = -\beta SI$$

$$\dot{I} = \beta SI - 5I$$

$$\dot{R} = 5I$$

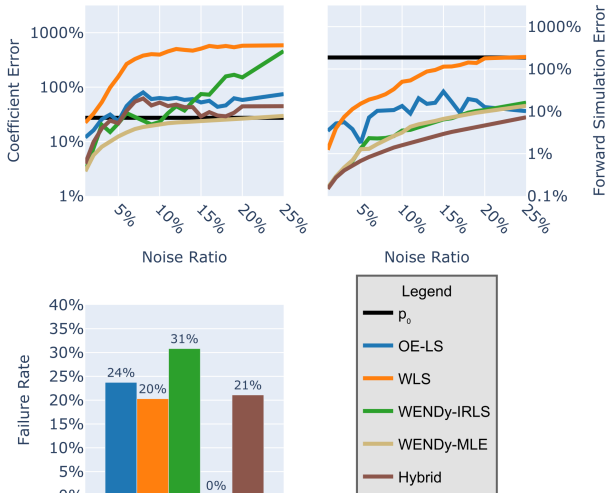




Parameter Estimation: Nonlinear in Parameters? Non-Gaussian Errors?

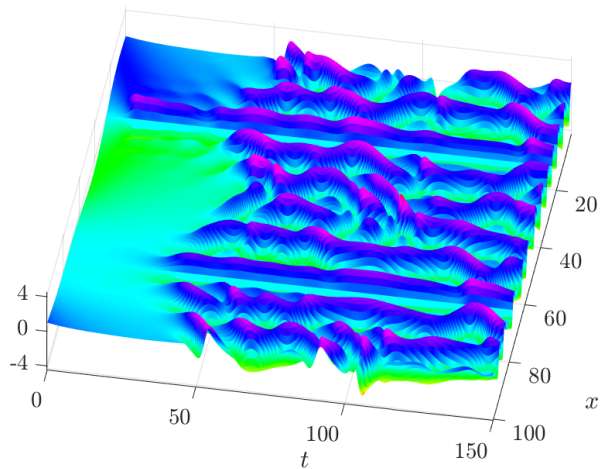
$$\dot{u}_1 = \frac{p_1}{36 + p_2 u_2} - p_3 \quad \dot{u}_2 = p_1 u_1 - p_5$$

Goodwin

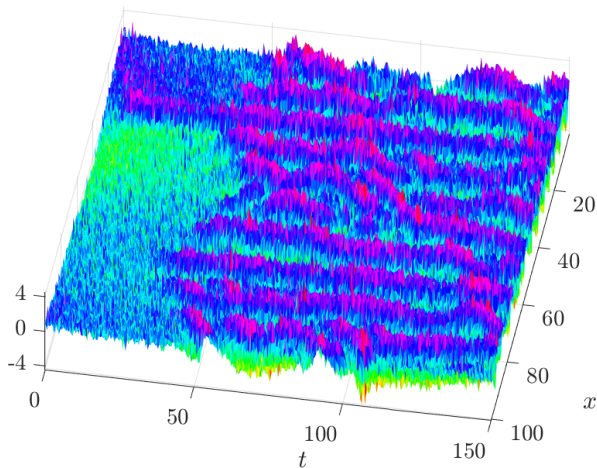


Parameter Estimation: PDE?

PDEs? KS $u_t = - (u^2)_x - u_{xx} - u_{xxxx}$



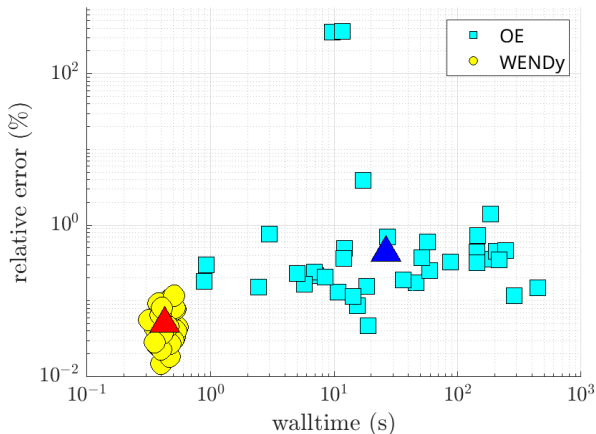
PDEs? KS $u_t = - \left(u^2\right)_x - u_{xx} - u_{xxxx}$



Infer parameters from noisy data

$$\mathbf{w} = (-1, -1, -1)$$

Parameter Estimation Performance (20% noise)



OE - Output Error

DMB, DAM, VD, WENDy for PDEs, 2025, in prep.

Theory

WSINDy Asymptotic Discoverability Class

$$\mathbf{U}^{(n)} = u^*(\mathbf{X}^{(n)}, \mathbf{t}^{(n)}) + \varepsilon, \quad \widehat{\mathbf{w}}^{(n)} = \text{WSINDy}(\mathbf{U}^{(n)}), \quad \Delta x^{(n)} \rightarrow 0$$

In what sense does $\widehat{\mathbf{w}}^{(n)} \rightarrow \mathbf{w}^*$?

Theorem

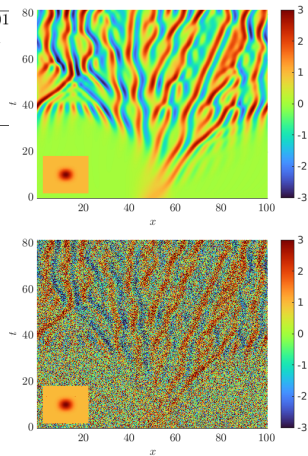
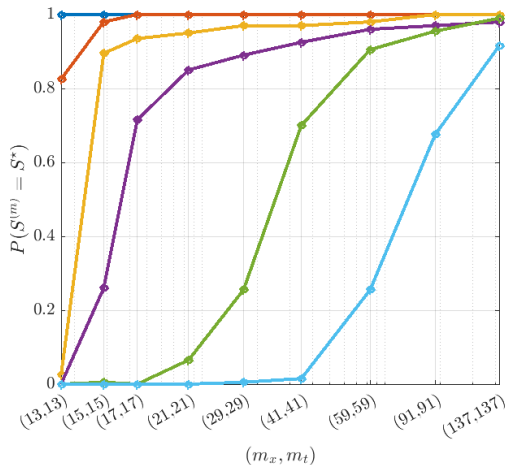
*Under reasonable assumptions (subGaussian ε , poly-trig Θ), there exists a **critical noise level** $\sigma_c > 0$ and a stability tolerance θ_* such that for all $\sigma < \sigma_c$, all $\theta \in (0, \theta_*)$, and sufficiently large n ,*

$$\text{supp}(\widehat{\mathbf{w}}^{(n)}) = \text{supp}(\mathbf{w}^*) \quad \text{and} \quad \|\widehat{\mathbf{w}}^{(n)} - \mathbf{w}^*\|_\infty < C(\theta + \sigma^2) \quad (5)$$

with probability exceeding $1 - 4K(\mathfrak{J} + 1) \exp\left(-\frac{c}{2} (m_n \theta)^{2/p_{\max}}\right)$ for any $\theta > 0$, where $m_n = |\text{supp}(\psi) \cap (\mathbf{X}^{(n)}, \mathbf{t}^{(n)})|$.

WSINDy Asymptotic Discoverability Class

$$\partial_t u = (1)\partial_x^4 u + (0.75)\partial_x^6 u + (-0.5)\partial_x(u^2) + (0.1)\partial_x^3(u^2)$$



DAM & DMB, IMA J. Num. Ana., 2024

Summary

Summary

- Equation Learning: WSINDy

Summary

- Equation Learning: WSINDy
- Parameter Inference: WENDy

Summary

- Equation Learning: WSINDy
- Parameter Inference: WENDy
- <http://github.com/MathBioCU>

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- Equation Learning: WSINDy
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- <http://github.com/MathBioCU>
 - Matlab
 - Python
 - Julia
 - R (in development)

Related Work

- Fasel, Kutz, Brunton, & Brunton. Ensemble-SINDy..., PRSA, 2022.
 - E-WSINDy
- Bertsimas & Gurnee, ...mixed-integer optimization, Nonlin. Dyn., 2023
 - WSINDy + MIO
- Tang et al., WeakIdent, J. Comp. Phys., 2023.
 - Narrow fits + Trimming beats sequential least squares
- Russo & Laiu, ... WSINDy Surrogate Models, SIADS 2024
 - Reproducing Kernel Hilbert Space
- Woodall et al., ... MRI ..., APL Bioeng., 2024
 - Perfusion dynamics from DCE-MRI images
- López et al., Weak-Form Modified Sparse Identification of Nonlinear Dynamics. J. Comp. Phys., Sep. 2025, 114410.

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2022-2027 DOE MMICC DE-SC0023346

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- Seth Minor (2028)

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- Dr. Cristian López

- Dr. Moyi Tian

- Cassidy All

- Peter Burke

- Abhi Chawla

- Mitali Desai

- Will Houser

- Jack Krebsbach

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- IPS #2 DAM, Wheeler, Liu, & DMB. WSINDy for migration, JSRI, 2022
- Online DAM, Dall'Anese & DMB Online WSINDy MSML 2022
- ParEst #1 DMB, DAM, VD, WENDy, BMB, 2023
- ROM #1 AT et al., WLaSDI, CMAME, 2024
- ROM #2 DAM, Burby, DMB, Coarse-graining... Sci Rep 2024.
- Theory #1 DAM & DMB, Asymptotics..., IMA JNumAna 2024
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- Cold Atoms Wang & DAM, PRA, 2025
- ROM #3 He et al., WgLaSDI, IJNME, 2025.
- MHD Vasey et al., JCP, 2025

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- MHD Vasey et al., JCP, 2025
- ROM #3 Bonneville, et al., arXiv2403.10748 2024.
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- ParEst #2 Rummel et al., WENDy-MLE, arXiv:2502.08881, 2025.

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