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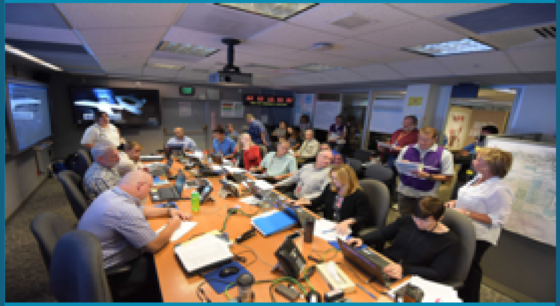
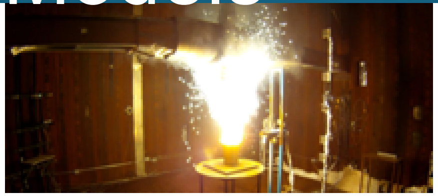
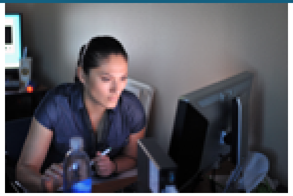
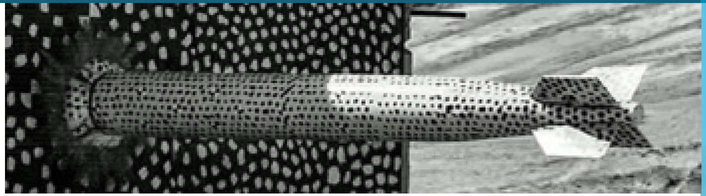
SAND2021-2315C

A Physics-Informed Operator Regression Framework for Extracting Data-Driven Continuum Models









SIAM CSE21

MS134: Machine Learning for Surrogate Model and Operator Discovery

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U.S. Department of Energy   NNSA National Nuclear Security Administration

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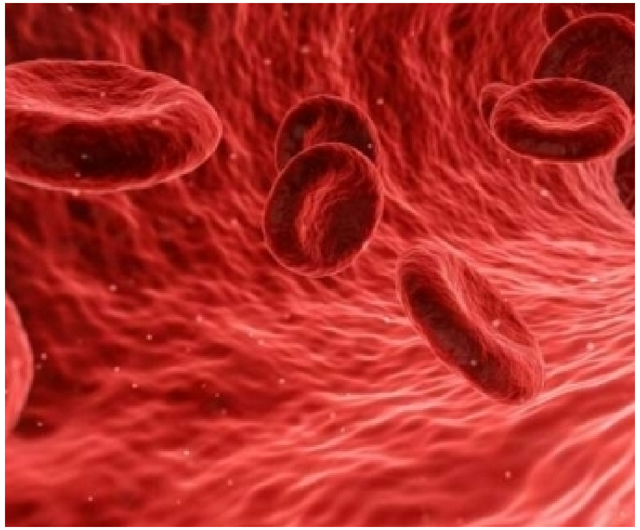
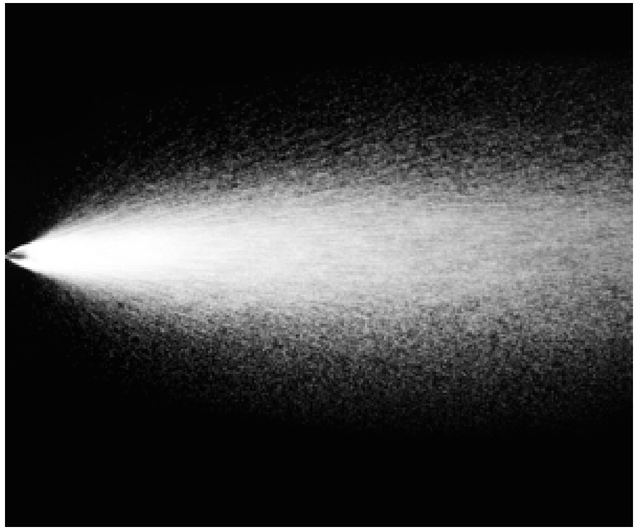
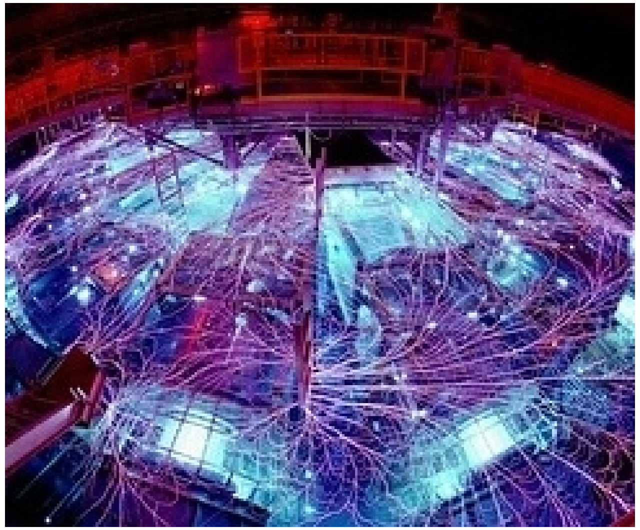
SAND No:

Finding models for multi-scale, multi-physics systems

Given experimental/high fidelity simulation data from a system,

Find a mathematical model that describes the system

Experiments/simulations generate **noisy, biased, sparse** data

Model power tradeoff

$$F(u, \dot{u}, x, t) = 0$$

$$\partial_t u + u \cdot \nabla u = -\nabla p + \nu \nabla^2 u$$

Black-box ML

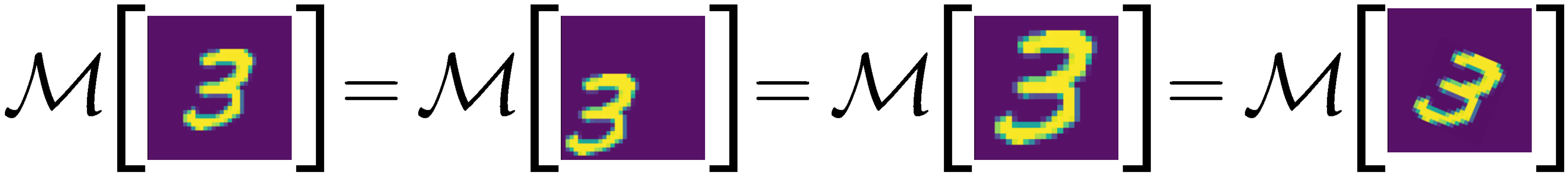
Physics constrained ML

Parameter estimation

Prone to overfitting ⟷ Strong assumptions

Case study: inductive bias in image classification

Translation, scaling, and rotation shouldn't affect an image's class



Data augmentation: train with transformed versions of training data

- How thoroughly should transformations be sampled?
- Increased cost of training

Choose model form to have desired invariance/equivariance

- E.g. ConvNets for approximate translational invariance[1]

[1] Lawrence et al. *IEEE Transactions on Neural Networks,* 1997

Other examples of inductive bias

Rotation invariant model for galaxy classification

- Dieleman et al. *Monthly Notices of the Royal Astronomical Society,* 2015

Warp invariant model

- Wong et al. *DICTA*, 2016

Permutation invariant model

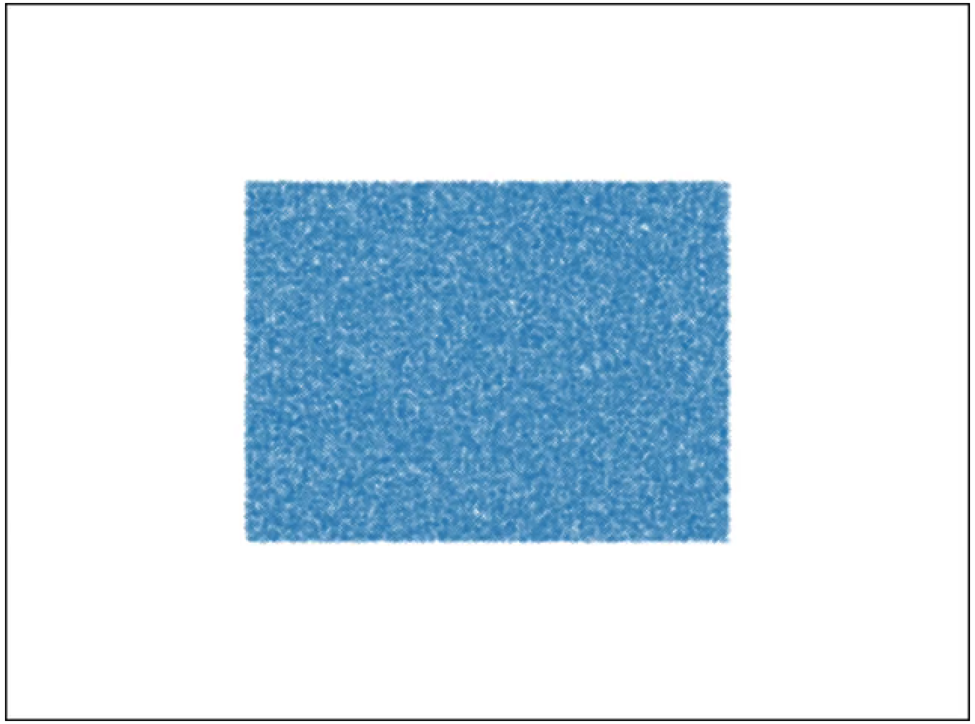
- Meltzer et al. *arXiv:1905.03046*

Rotation and translation equivariant model for 3d point cloud data

- Thomas et al. *arXiv:1802.08219*

Extracting coarse grain models

Find coarse grained dynamics, e.g. evolution of particle density for,



It may be reasonable to assume,

- Conservation
- Translational equivariance
- Rotational equivariance

Problem statement

Assume system is described by 1st order in time, autonomous PDE,

$$\partial_t u = \mathcal{N} u$$

Discretize in time,

$$u^{n+1} = u^n + \Delta t \mathcal{N} u^n = (I + \Delta t \mathcal{N}) u^n$$

Given observations, $\{v^n\}$, find,

$$\mathcal{N} = \underset{\hat{\mathcal{N}}}{\operatorname{argmin}} \sum_n \left|\left| v^{n+1} - (I + \Delta t \hat{\mathcal{N}}) v^n \right|\right|$$

More generally,

$$\mathcal{N} = \underset{\hat{\mathcal{N}}}{\operatorname{argmin}} \sum_n \left|\left| v^{n+p} - (I + \Delta t \hat{\mathcal{N}})^p v^n \right|\right|$$

Modal operator regression for physics (MOR-Physics)

For,

$$u^{n+1} = (I + \Delta t \mathcal{N}) u^n$$

Choose,

$$\mathcal{N} u = \mathcal{F}^{-1} g(\kappa; \xi_g) \mathcal{F} h(u; \xi_h)$$

Where g and h are neural networks

Optimization problem becomes,

$$\underset{\hat{\xi}_g, \hat{\xi}_h}{\operatorname{argmin}} \sum_n \left|\left| v^{n+p} - (I + \Delta t \hat{\mathcal{N}})^p v^n \right|\right|$$

Other modal approaches

- Wu and Xiu, *JCP*, 2020
- Li et al. *arXiv:2010.08895*

MOR-Physics: motivation

For smooth functions in a periodic domain,

Physical space		Fourier space
$f(x) = \sum_{\kappa} = \tilde{f}_\kappa e^{j\kappa x}$	$\xrightarrow{\mathcal{F}}$	$f_\kappa = \int f(x) e^{-j\kappa x} dx$
$\partial_x^\gamma f(x)$	$\xleftarrow{\mathcal{F}^{-1}}$	$(j\kappa)^\gamma \tilde{f}_\kappa$

Parameterization contains,

- Laplacian

$$\partial_x^2 u \longrightarrow \mathcal{F}^{-1}[\underbrace{(-\kappa^2)}_{g}\mathcal{F}[\underbrace{u}_{h}]]$$

- Advection

$$\partial_x u^2 \longrightarrow \mathcal{F}^{-1}[\underbrace{(j\kappa)}_{g}\mathcal{F}[\underbrace{u^2}_{h}]]$$

MOR-Physics: introducing inductive biases

Translational equivariance:

apply h point-wise, $(h \circ u)(x) = h(u(x))$

Reflective symmetry: if u solves the PDE, so does $-u$

let $h(u) = \text{sign}(u)\tilde{h}(|u|)$

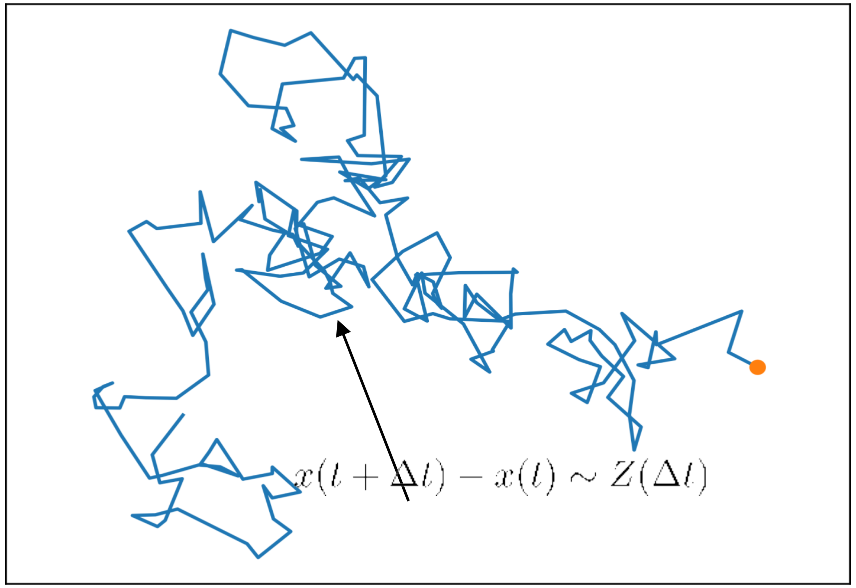
Isotropy:

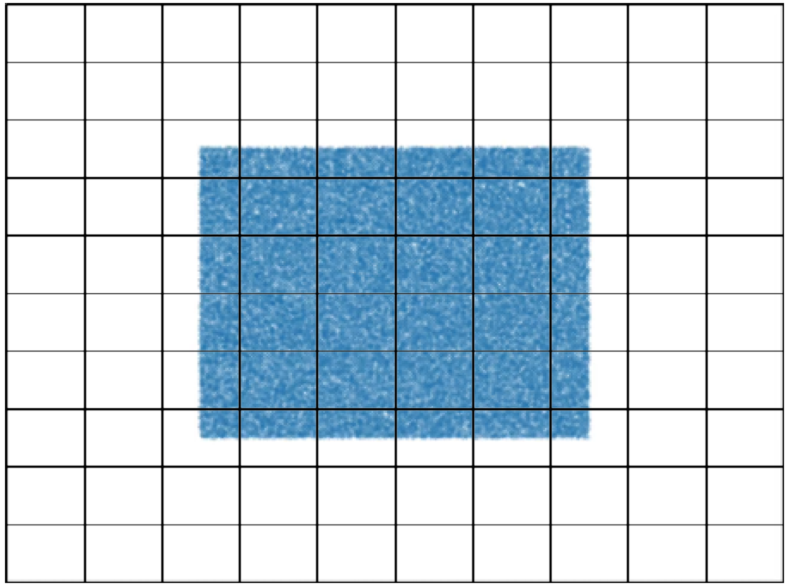
let $g(\kappa) = \tilde{g}(||\kappa||_2^2)$

Global conservation:

let $g(\kappa) = \tilde{g}(\kappa)(1 - \delta_{\kappa,0})$

Coarse graining stochastic differential equations (SDEs)



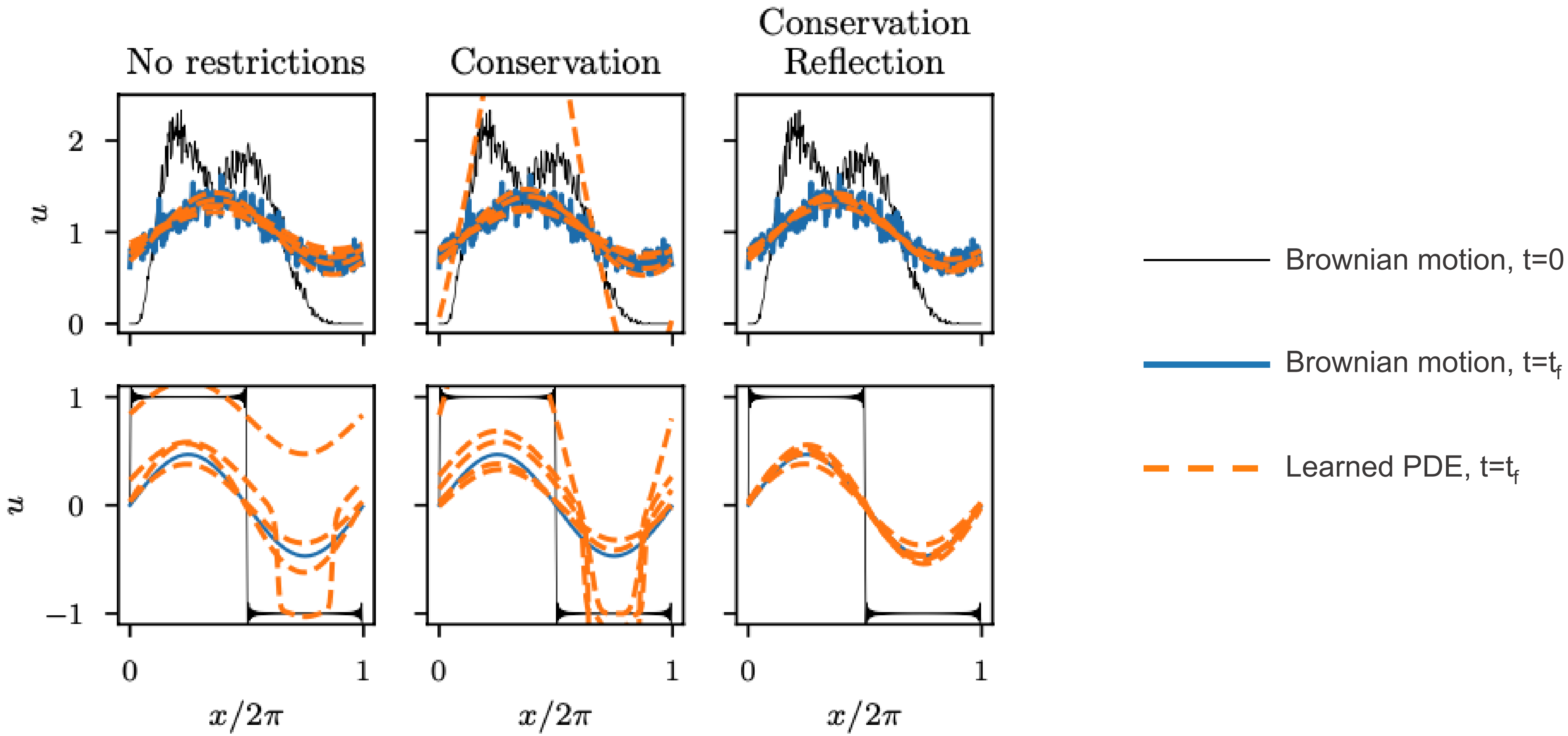


SDE for particle trajectory → PDE for particle density

1. Compute evolution of binned density from SDE trajectories
2. Fit PDE for evolution of binned density
3. Compare to analytical result

SDEs: Conservation and reflective symmetry inductive biases improves generalization

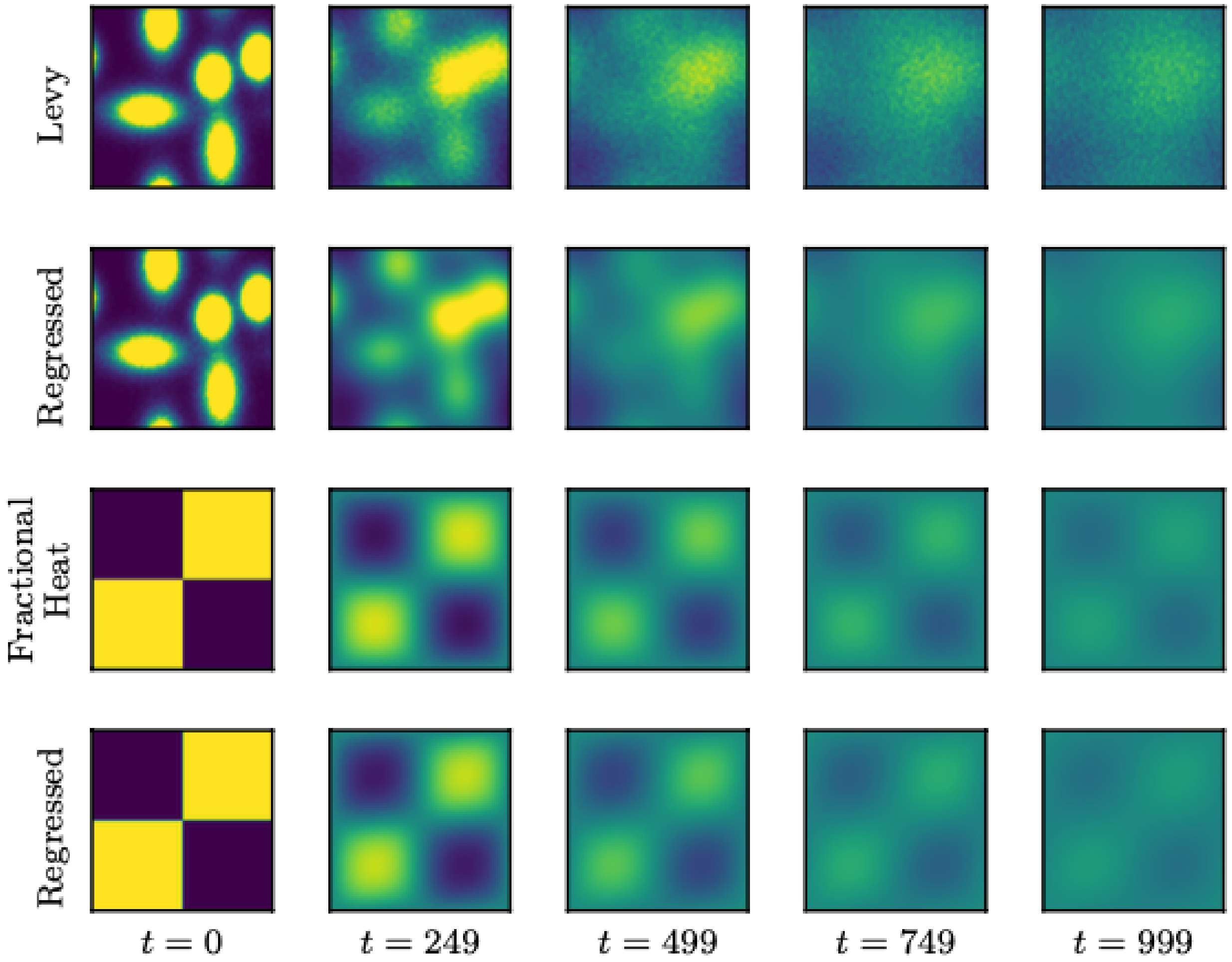
Density of Brownian data follows heat equation; $x(t + \Delta t) - x(t) \sim N(0, 2\Delta t) \rightarrow \partial_t u = \Delta u$



SDEs: Isotropy inductive bias improves generalization

Density of Levy flight data follows fractional heat equation[1],

$$x(t+\Delta t) - x(t) \sim L(\alpha, 0, \Delta t^{1/\alpha}, 0) \rightarrow \partial_t u = \Delta^{\alpha/2} u$$



[1]Lischke et al., *arXiv:1801.09767*

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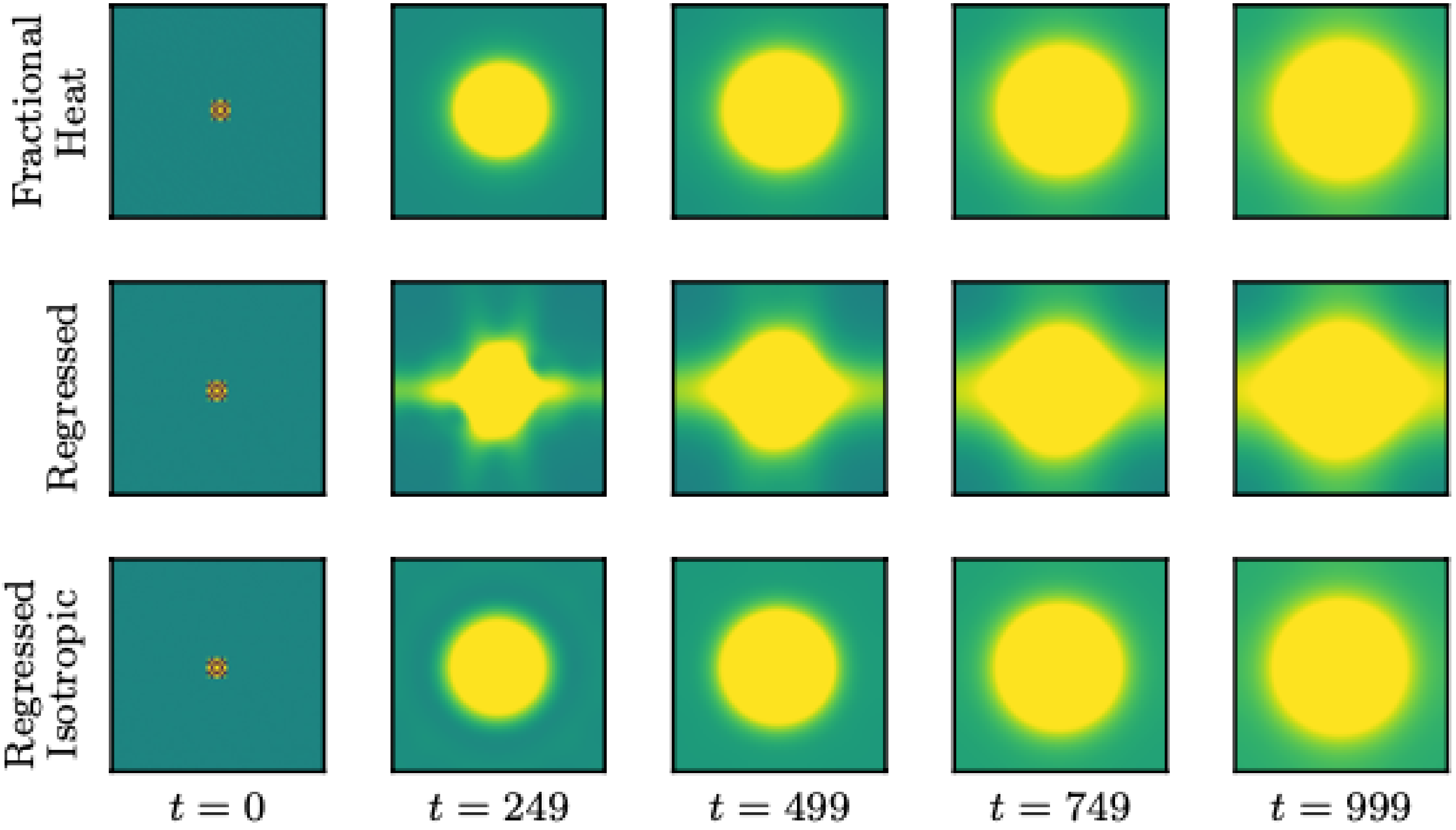
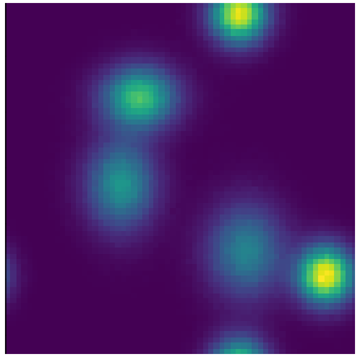


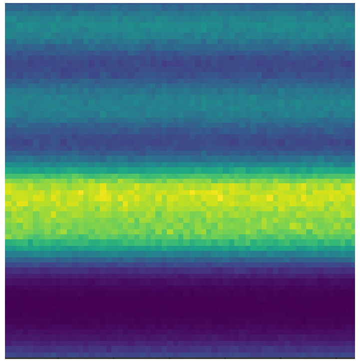
[1]Lischke et al., *arXiv:1801.09767*

Isotropy inductive bias counteracts biased data

Vary anisotropy bias in data by setting initial condition,

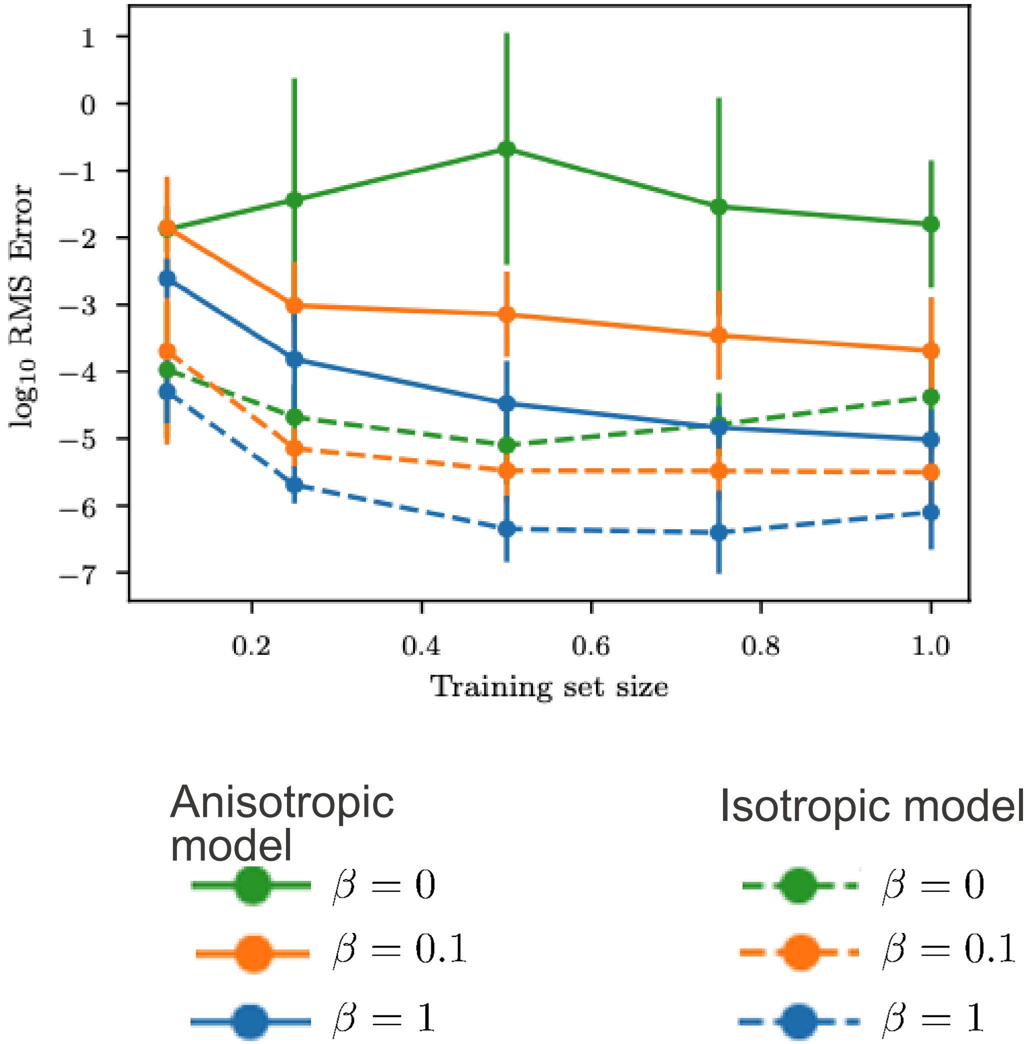


$\beta = 0$

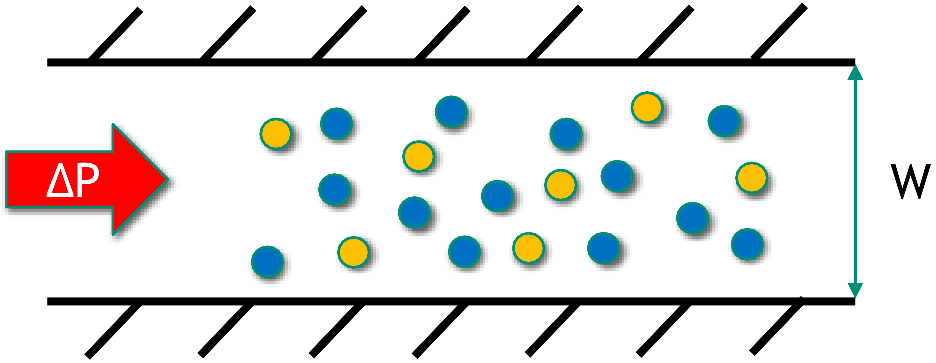


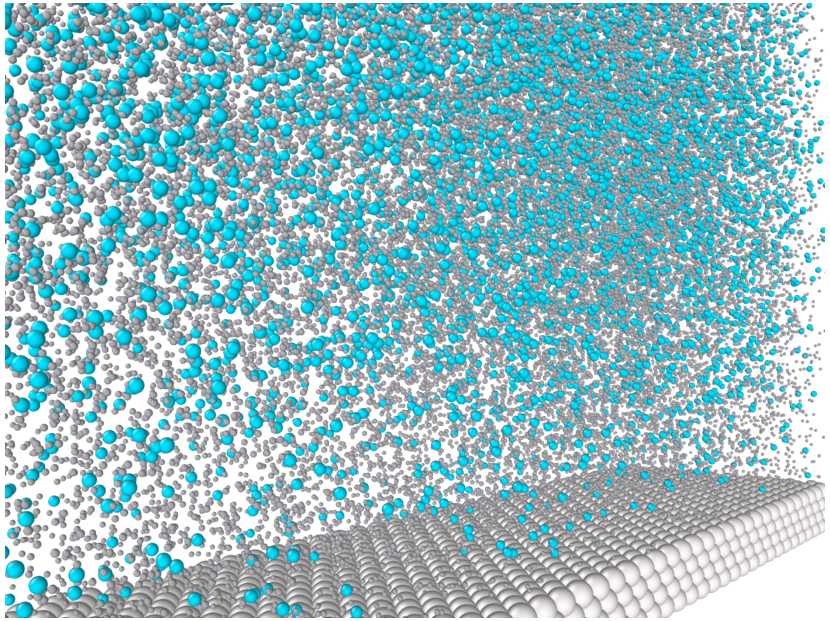
$\beta = 1$

Compare effect of isotropy inductive bias for various β



Application: coarse graining colloidal Poiseuille flow





Perform molecular dynamics simulations with varying concentration (c), colloid particle size (d)

- Get time evolution of 1d profiles of

$$\boldsymbol{u} = (\boldsymbol{u_N}, \boldsymbol{u_D}) = ([\rho^L, \rho^S], [p^L, p^S],))$$

Fit continuum model assuming conservation of mass

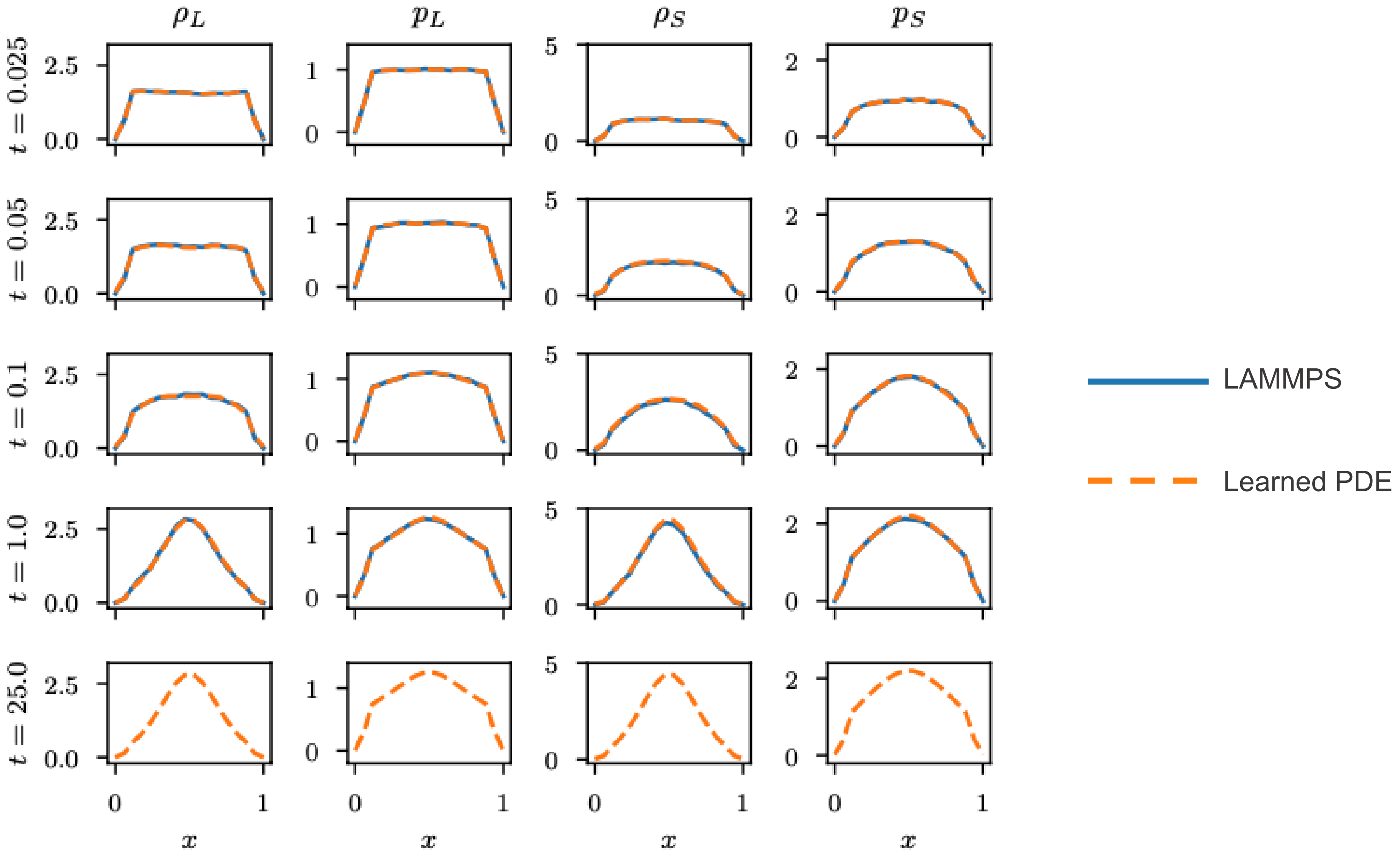
$$\partial_t u^i_N = \sum_k \mathcal{C}^{-1} g^i_k(\kappa, c, d) \mathcal{C} h^i_k(\boldsymbol{u}, c, d)$$

$$\partial_t u^i_D = \sum_k \mathcal{S}^{-1} g^i_k(\kappa, c, d) \mathcal{S} h^i_k(\boldsymbol{u}, c, d)$$

where S and C are the sine and cosine transform

Find time evolution for new c, d

Application: coarse graining colloidal Poiseuille flow



Future work

Limited to simple geometries and PDEs with smooth solutions

- Alternative basis
  - Generalized moving least squares: Trask et al., *NeurIPS*, 2019

Bayesian version

Noisy data for more general problems

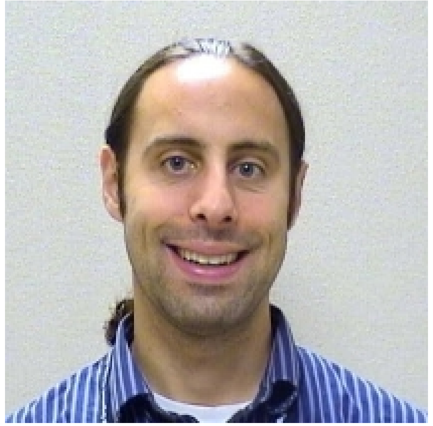
- Error-in-variables models

Applications

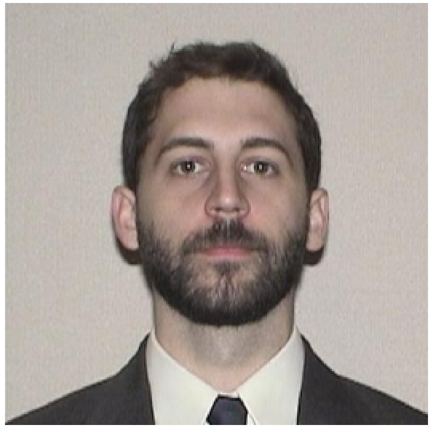
Comparisons to other operator regression methods

- Wu and Xiu, *JCP*, 2020
- Li et al. *arXiv:2010.08895*
- Graph Neural operator: Li et al., *NeurIPS*, 2020
- DeepONets: *arXiv:1910.03193*

Acknowledgements


Eric C. Cyr


Nat Trask


Mitch Wood

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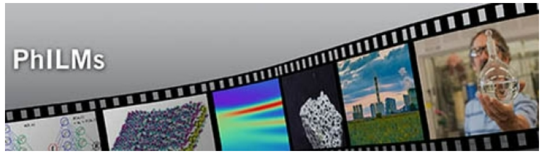
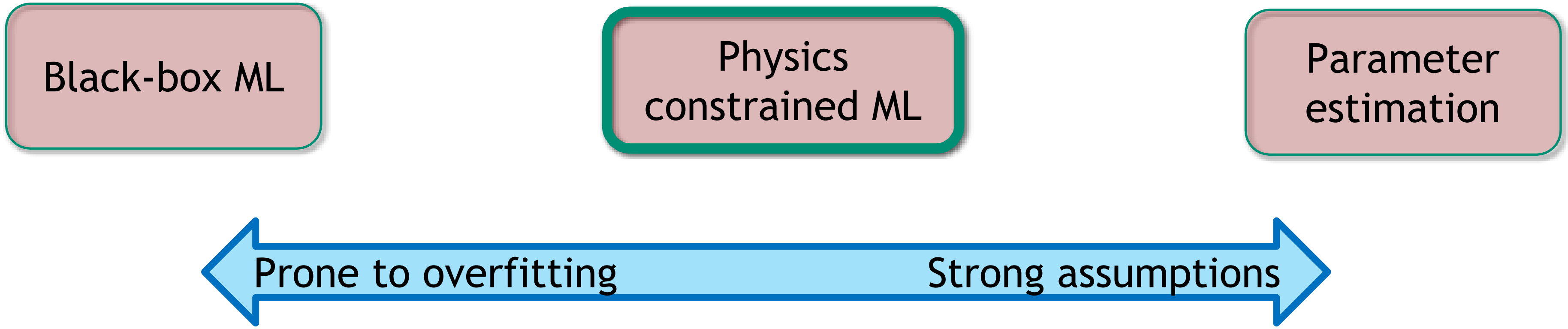


www.pnnl.gov/computing/philms

Conclusion



ML with physics informed inductive biases

- More powerful than parameter estimation
- Better generalization and extrapolation than black-box ML

Paper and code:

- Patel and Desjardins, arXiv:1810.08552
- Patel et al. *CMAME*, 2021 (arXiv:2009.11992)
- https://github.com/rgp62/MOR-Physics