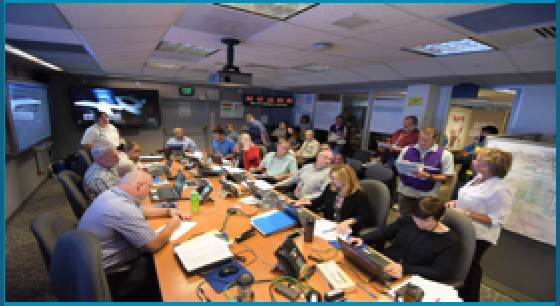
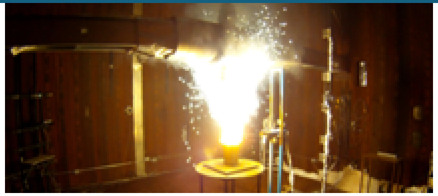
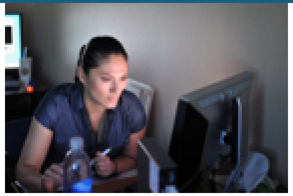
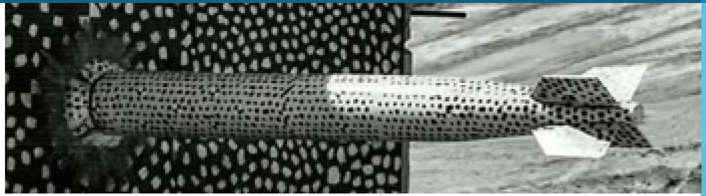
SAND2021-9189C



Modal Operator Regression for Extracting Nonlocal Continuum Models

USNCCM16

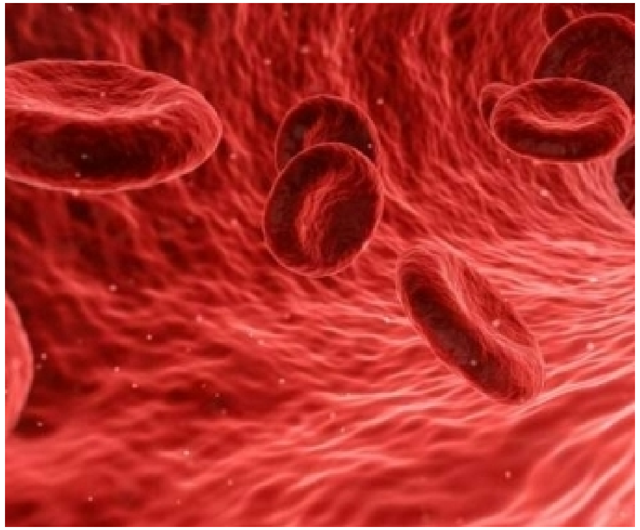
411: Nonlocal Models in Continuum Mechanics: Mathematical, Computational, Machine Learning

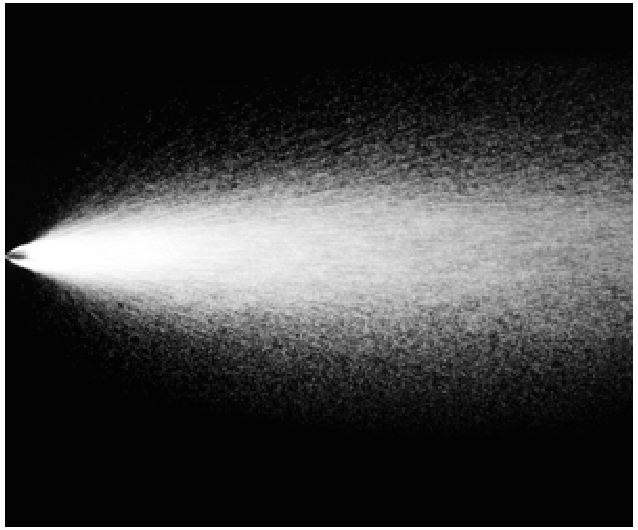
Ravi G. Patel, Nathaniel Trask, Mitchell Wood, Eric C. Cyr
Center for Computing Research

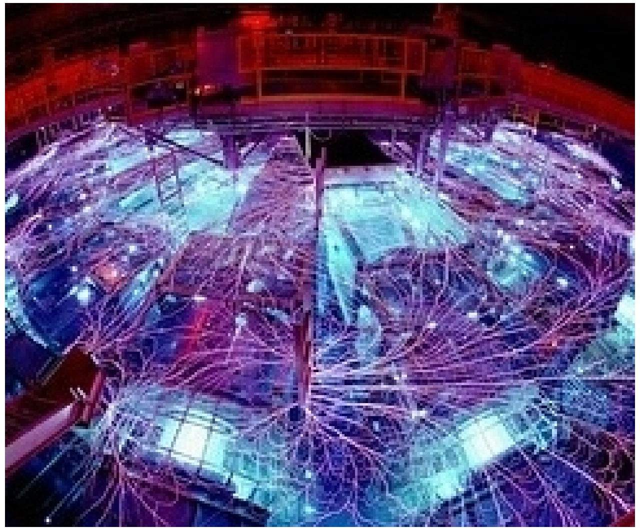
Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.
SAND No:

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

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

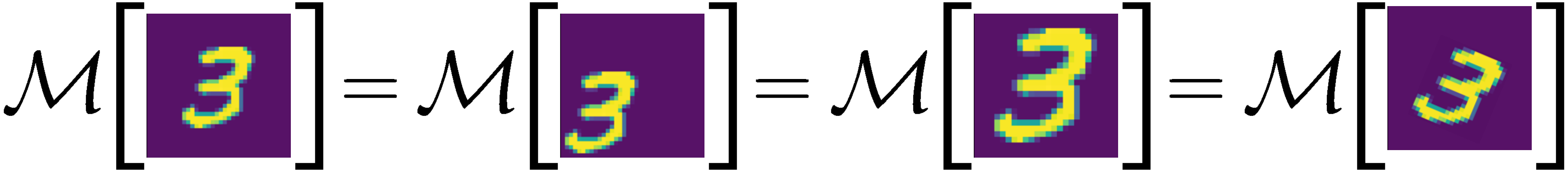
Parameter estimation

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

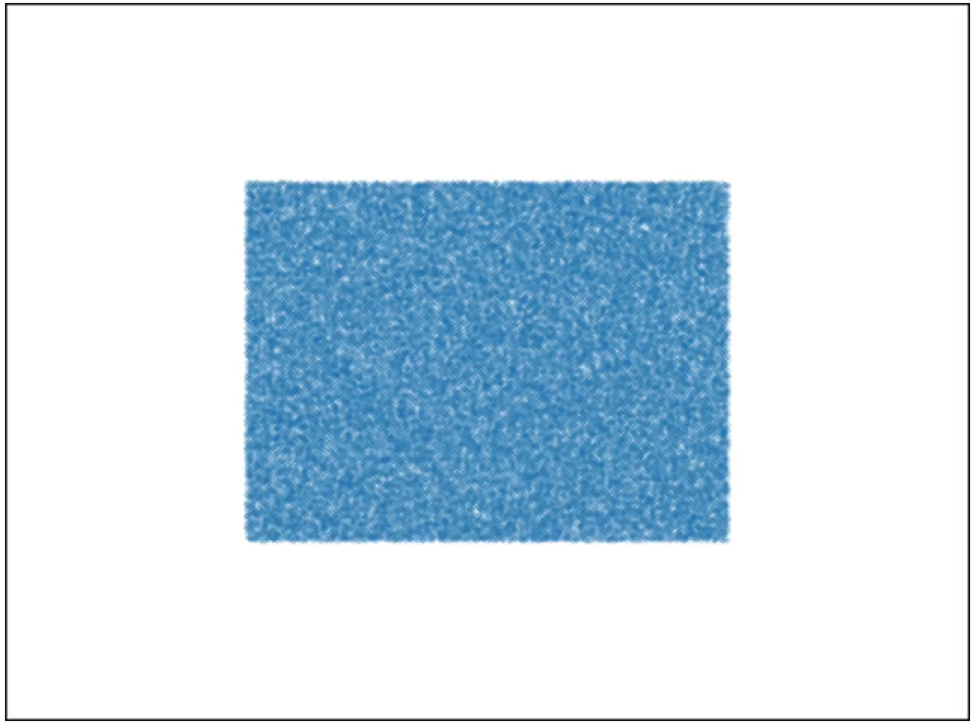
- Meltzer et al. *arXiv:1905.03046*

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

Includes Riesz derivative[1] as a special case,

$$R^\alpha u = -\mathcal{F}^{-1} |2\pi\kappa|^\alpha \mathcal{F} u$$

Optimization problem becomes,

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

[1] Bayın, *J. Math. Phys.*, 2016

MOR-Physics: motivation

For smooth functions in a periodic domain,

Physical space

$$f(x) = \sum_{\kappa} = \tilde{f}_{\kappa} e^{j\kappa x}$$

$$\partial_x^{\gamma} f(x)$$

$\mathcal{F}$ →

← $\mathcal{F}^{-1}$

Fourier space

$$f_{\kappa} = \int f(x) e^{-j\kappa x} dx$$

$$(j\kappa)^{\gamma} \tilde{f}_{\kappa}$$

Parameterization contains,

- Laplacian

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

(g points to $(-\kappa^2)$, h points to u)

- Burgers

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

(g points to $(j\kappa)$, h points to u^2)

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

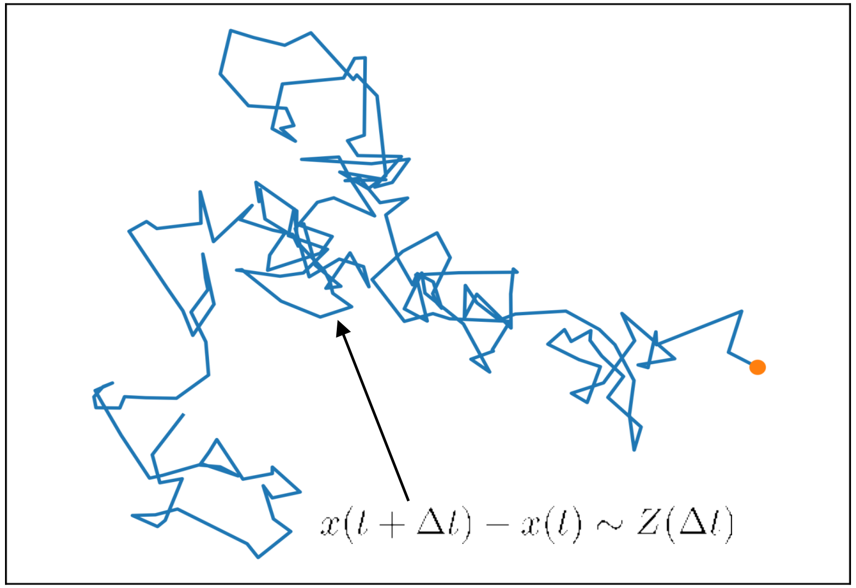
Isotropy:

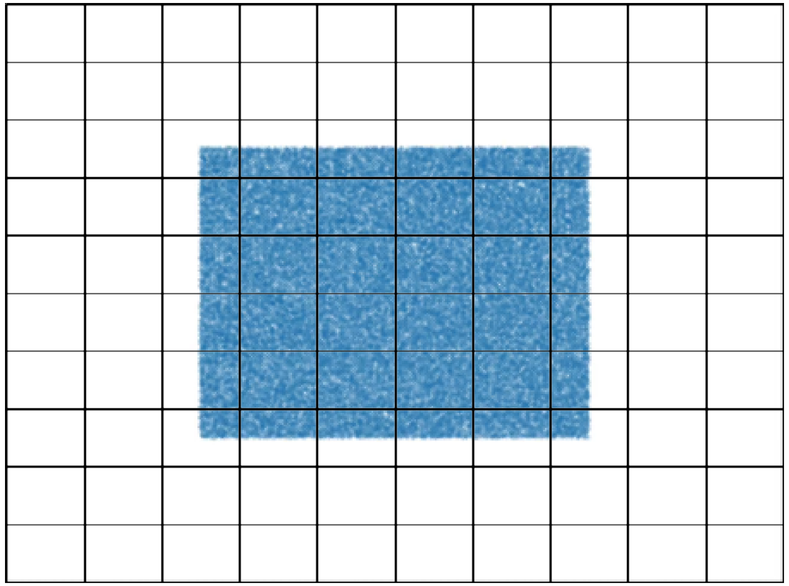
let $g(\kappa) = \tilde{g}(||\kappa||_2^2)$

Global conservation:

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

Coarse graining stochastic differential equations (SDEs)



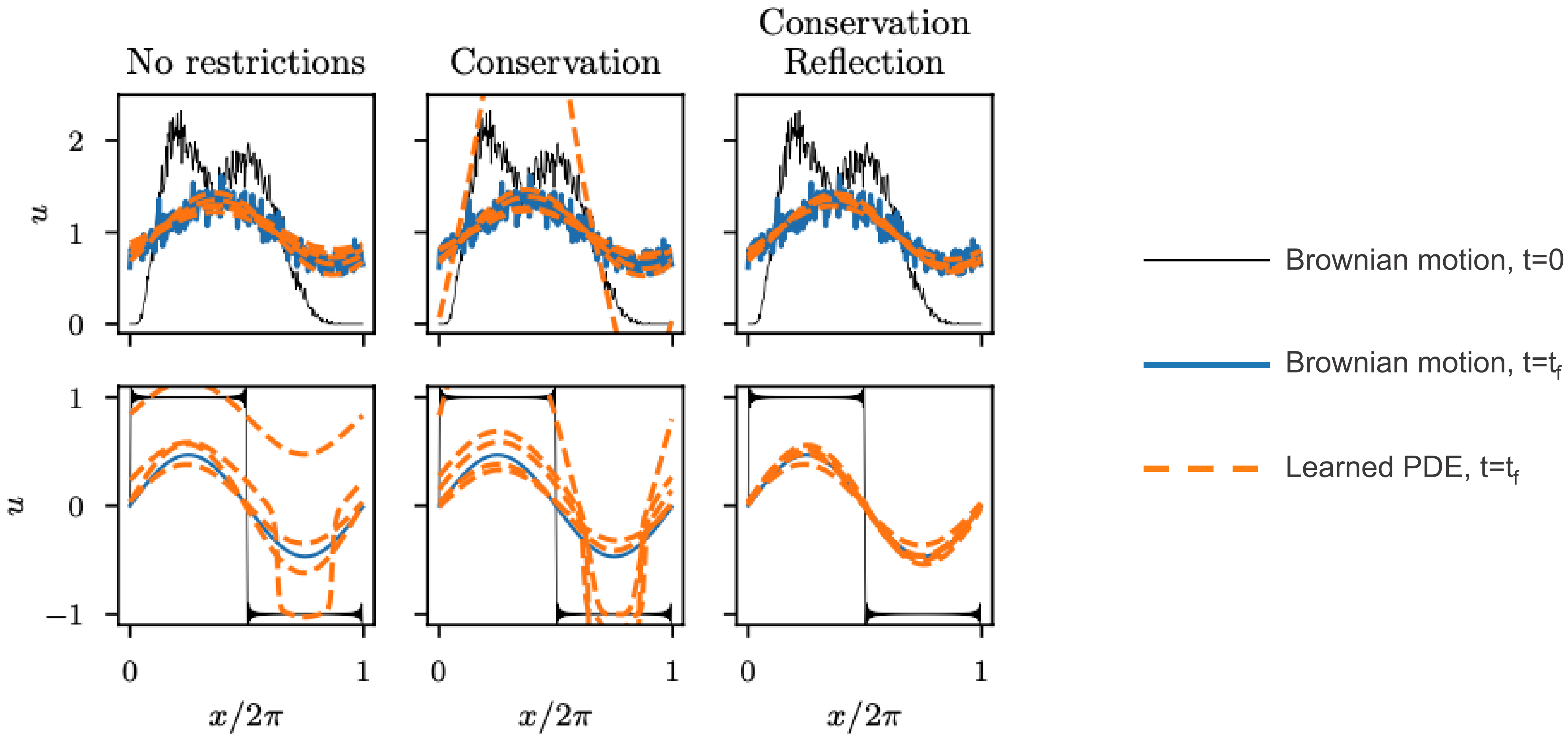


SDE for particle trajectory → PDE for particle density

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

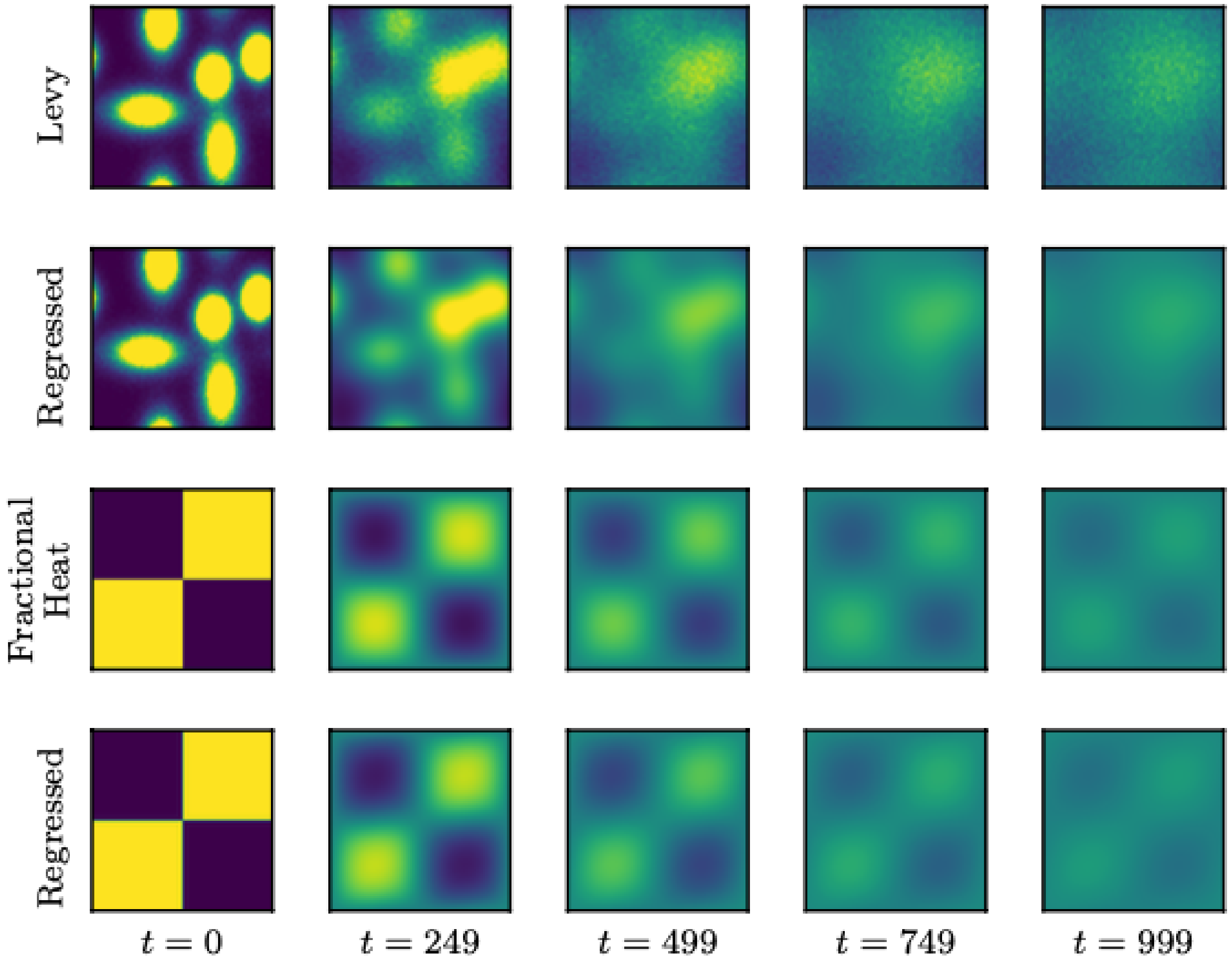
Density of Brownian data follows heat equation; $x(t+\Delta t) - x(t) \sim N(0, 2\Delta t) \rightarrow \partial_t u = \Delta u$



SDEs: Isotropy inductive bias improves generalization

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

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

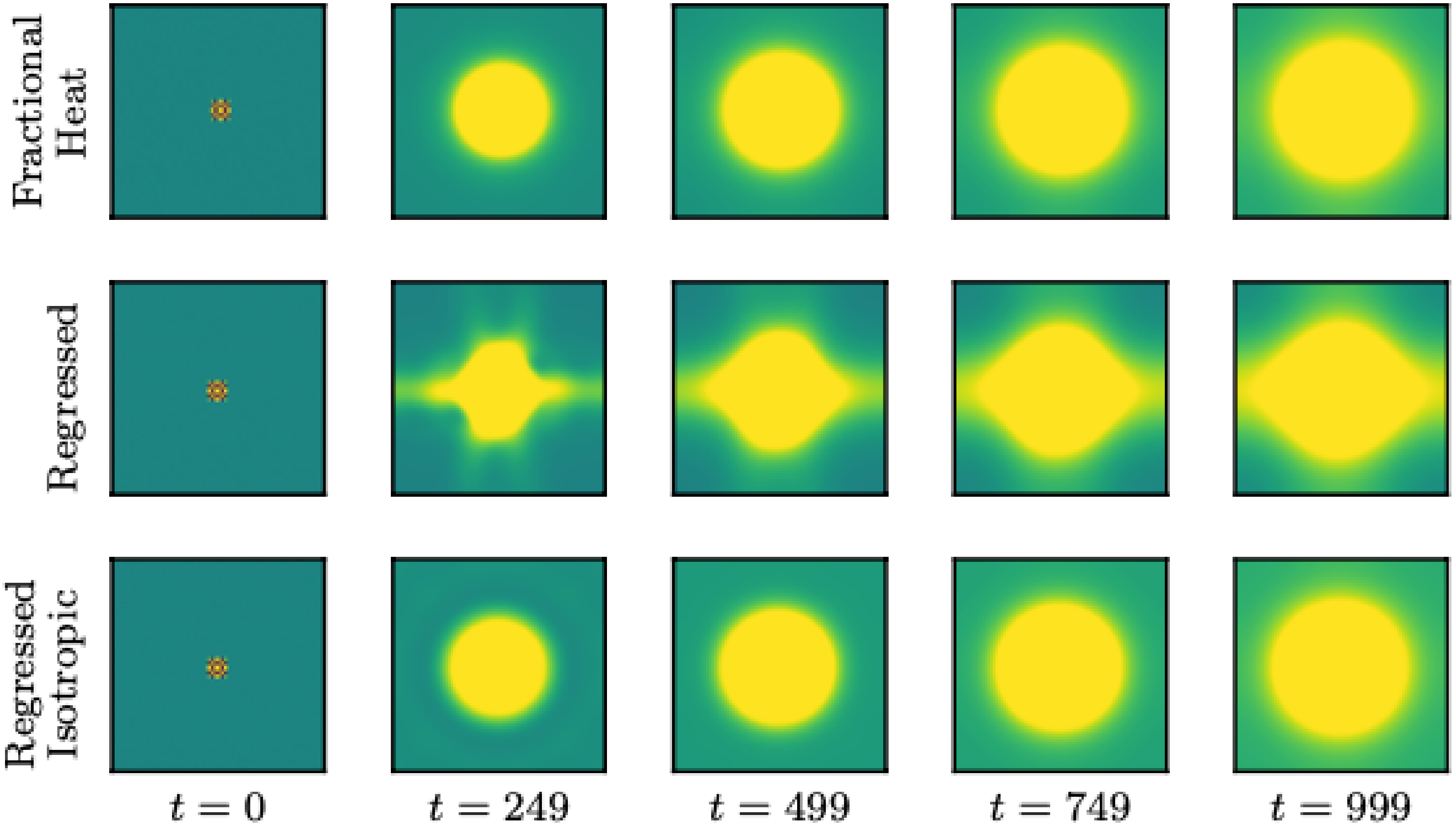


[1]Lischke et al., *arXiv:1801.09767*

SDEs: Isotropy inductive bias improves generalization

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

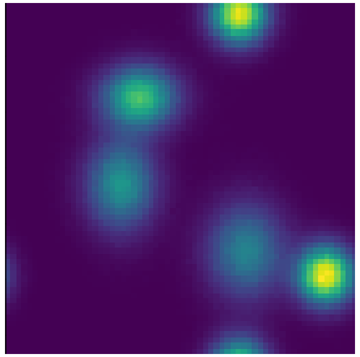
$$x(t+\Delta t) - x(t) \sim L(\alpha, 0, \Delta t^{1/\alpha}, 0) \rightarrow \partial_t u = \Delta^{\alpha/2} u$$



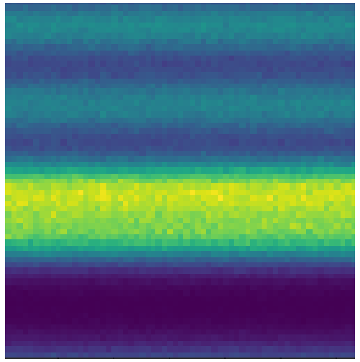
[1]Lischke et al., *arXiv:1801.09767*

Isotropy inductive bias counteracts biased data

Vary anisotropy bias in data by setting initial condition,

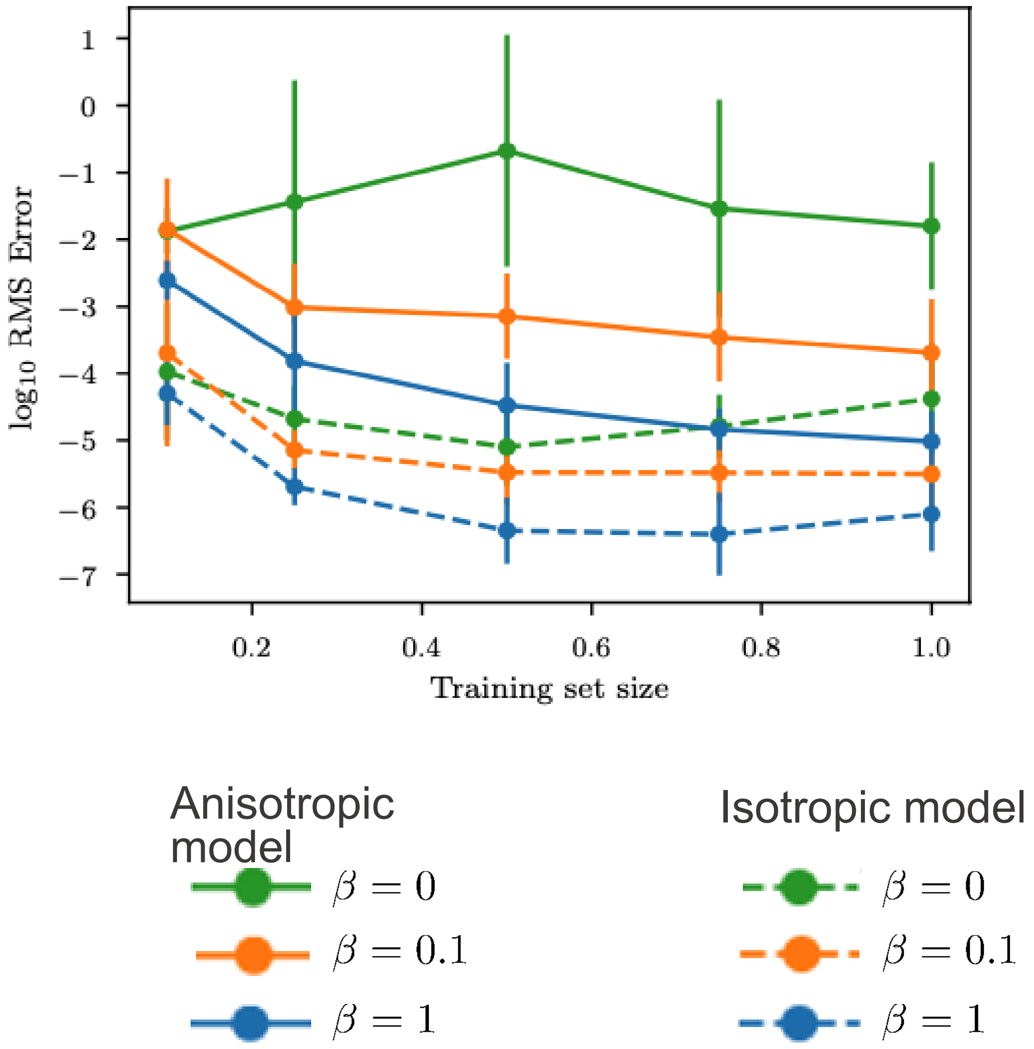


$\beta = 0$

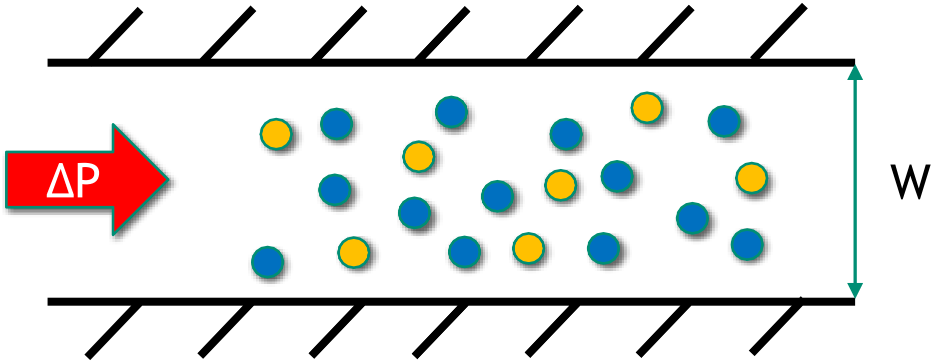


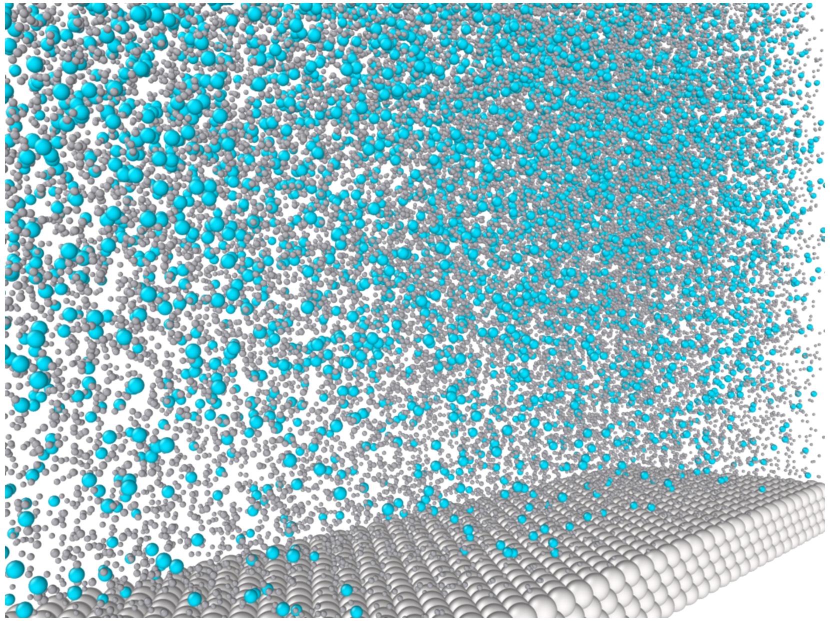
$\beta = 1$

Compare effect of isotropy inductive bias for various β



Application: coarse graining colloidal Poiseuille flow





Perform molecular dynamics (MD) 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,

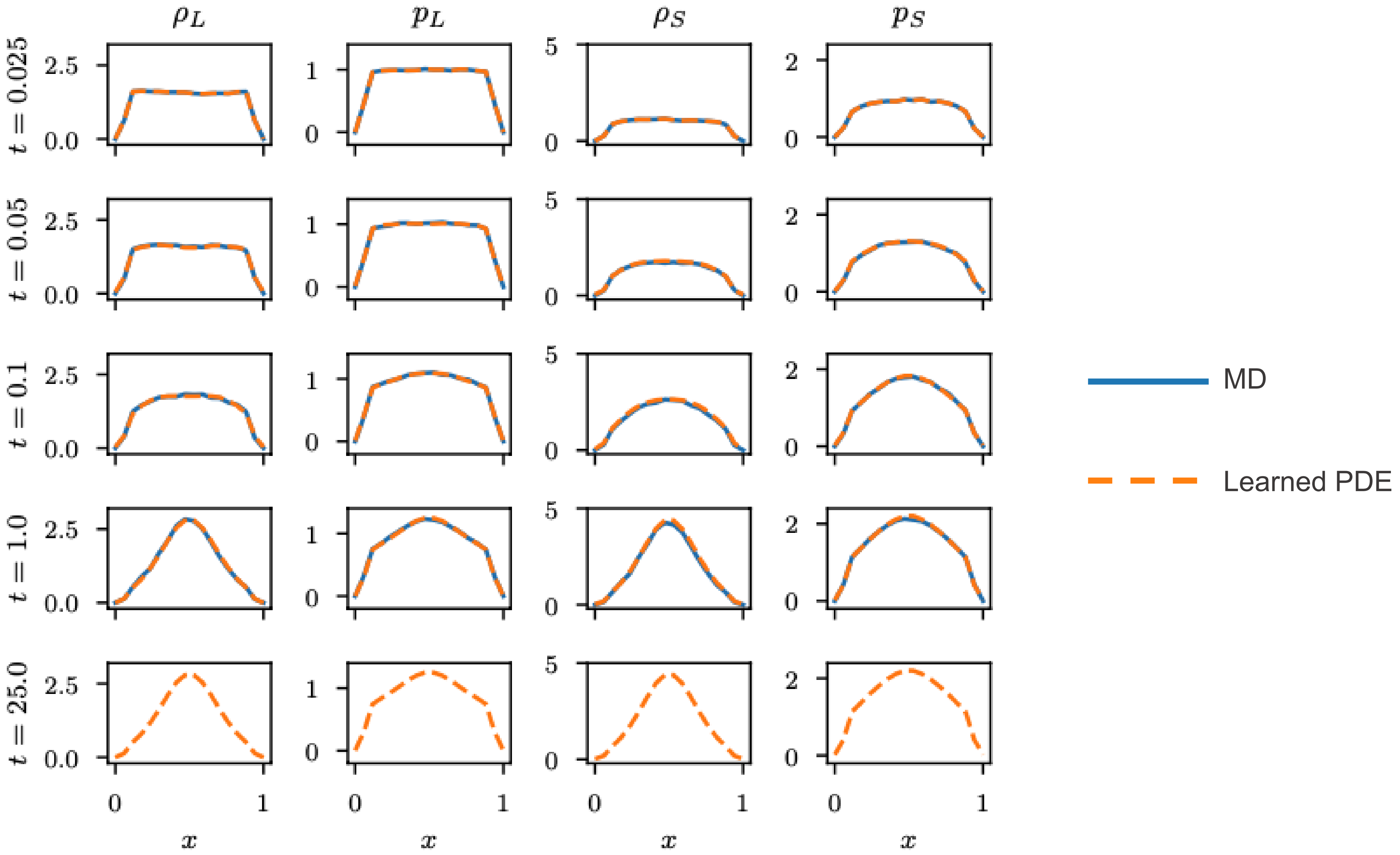
$$\partial_t u_N^i = \sum_k \mathcal{C}^{-1} g_k^i(\kappa, c, d)\mathcal{C} h_k^i(\boldsymbol{u}, c, d)$$

$$\partial_t u_D^i = \sum_k \mathcal{S}^{-1} g_k^i(\kappa, c, d)\mathcal{S} h_k^i(\boldsymbol{u}, c, d)$$

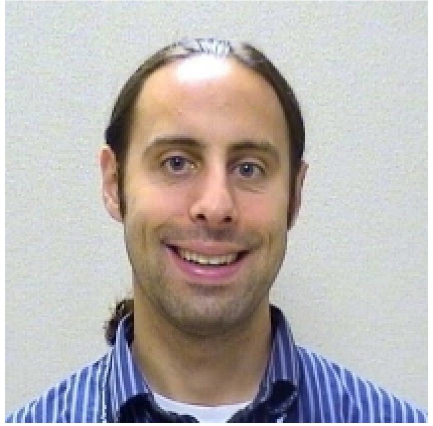
where S and C are the sine and cosine transform

Find time evolution for new c, d

Application: coarse graining colloidal Poiseuille flow

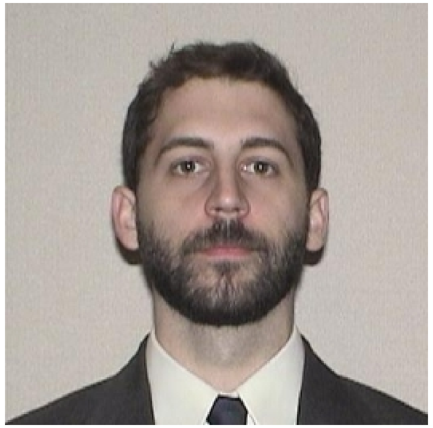


Acknowledgements



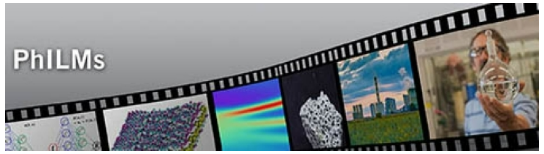
Eric C. Cyr

Nat Trask



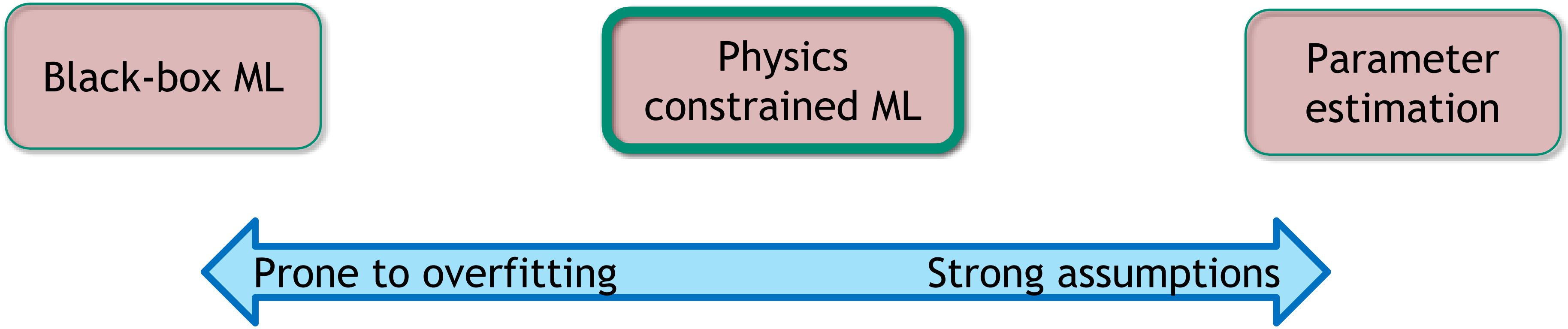
Mitch Wood

U.S. DEPARTMENT OF ENERGY | Office of Science



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, Trask, Wood, Cyr. *CMAME*, 2021 (arXiv:2009.11992)
- https://github.com/rgp62/MOR-Physics