SAND2020-13253C

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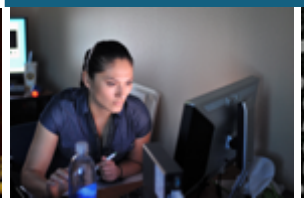
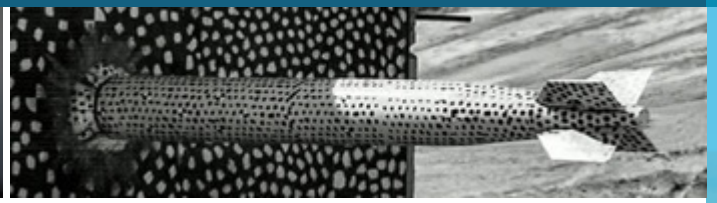
Learning continuum-scale models from micro-scale dynamics via Operator Regression





14th World Congress in Computational Mechanics

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Center for Computing Research

Sandia National Laboratories, Albuquerque, NM, USA

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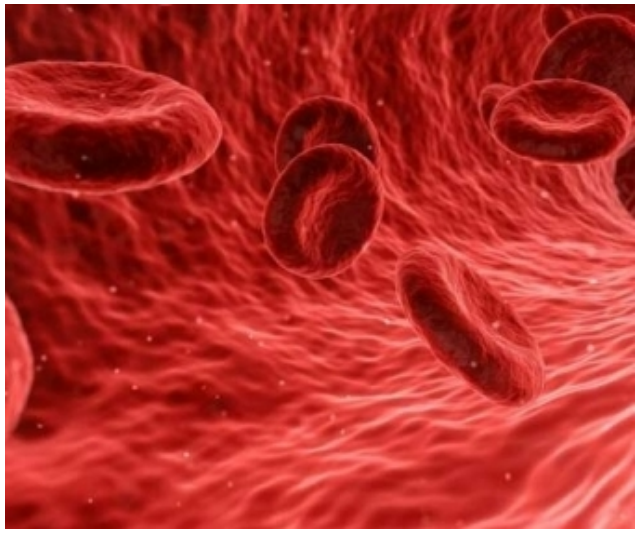
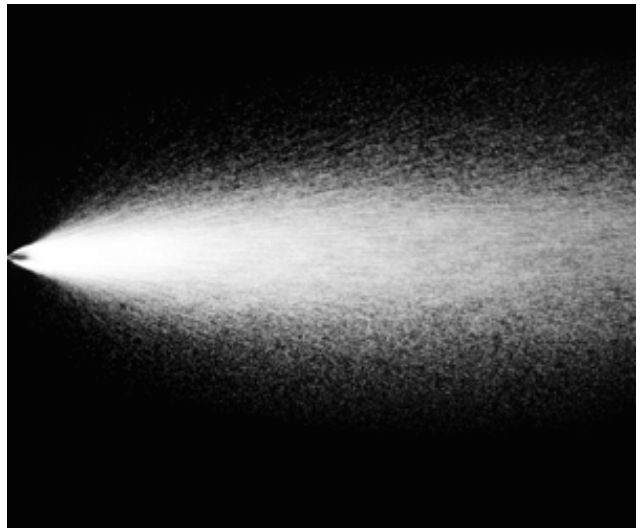
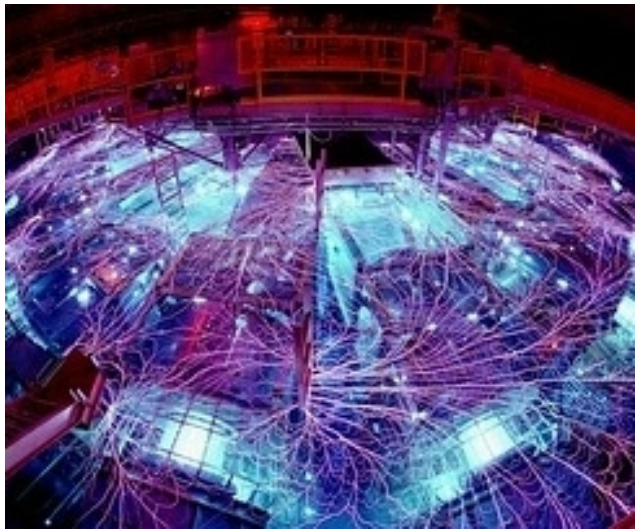
Finding models for multi-scale, multi-physics systems







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

?

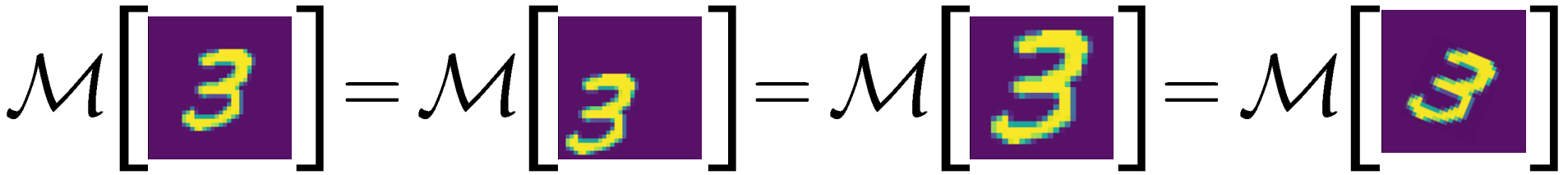
Parameter estimation

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

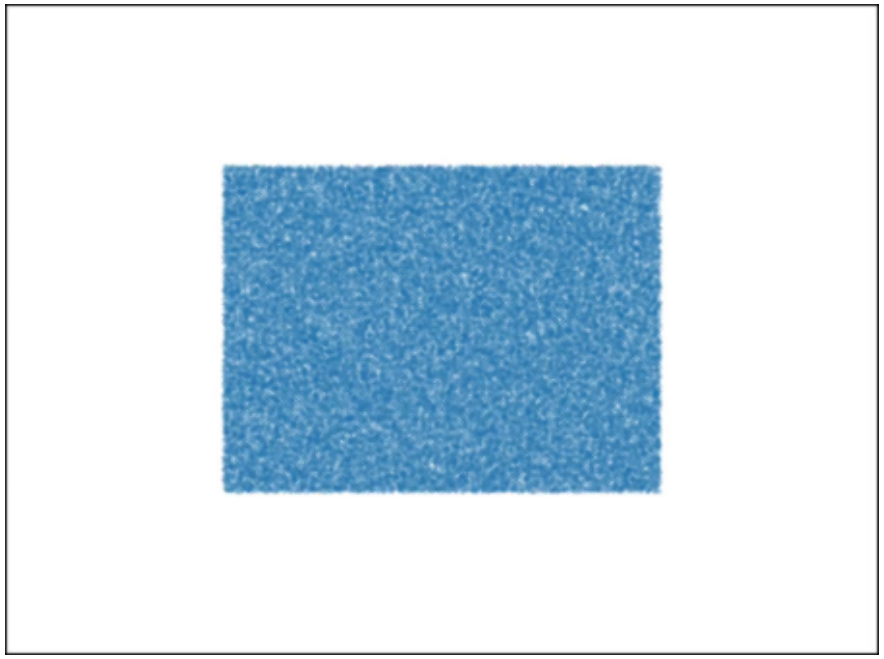
- Meltzer et al. *arXiv:1905.03046*

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,

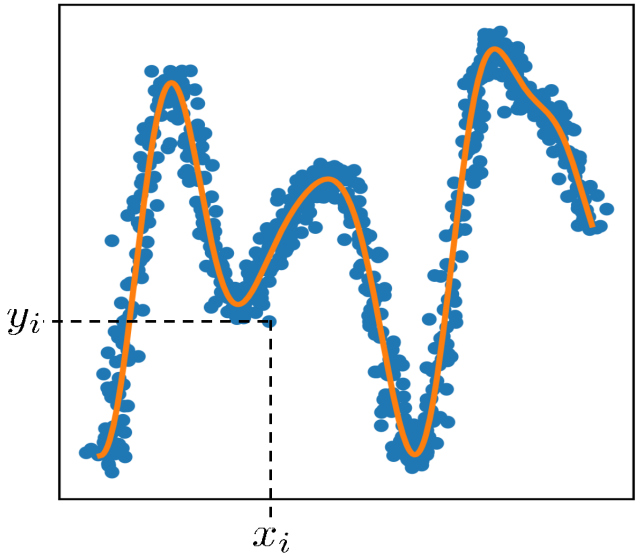
$$\mathcal{N} = \underset{\hat{\mathcal{N}}}{\operatorname{argmin}} \sum_n \left|\left| v^{n+1} - (I + \Delta t \hat{\mathcal{N}}) v^n \right|\right|$$

More generally,

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

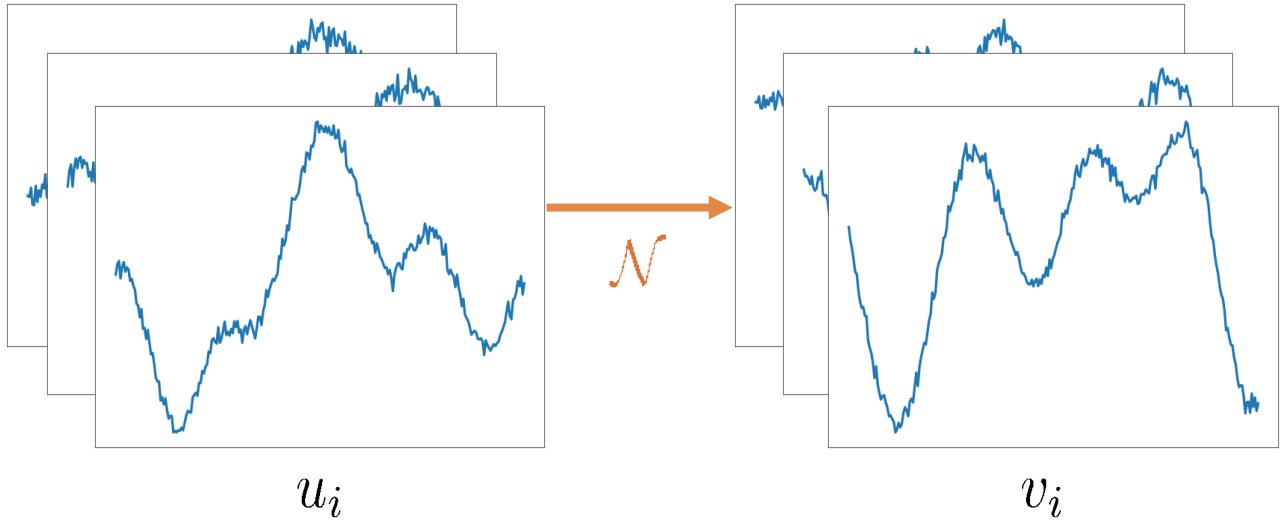
Operator regression

Fitting functions



$$\widehat{f} = \underset{f}{\operatorname{argmin}} \sum_i ||y_i - f(x_i)||$$

Fitting operators



$$\widehat{\mathcal{N}} = \underset{\mathcal{N}}{\operatorname{argmin}} \sum_i ||v_i - \mathcal{N}[u_i]||$$

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

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

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

$\mathcal{F}$

$\mathcal{F}^{-1}$

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 h

- Advection

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

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

Isotropy:

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

Global conservation:

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

Validation: spatial operator regression in 1D

Given, $\{u_i, v_i = \partial_x u_i^2\}$, find,

$$\underset{\mathcal{N}}{\operatorname{argmin}} \sum_i ||\mathcal{N} u_i - v_i||^2$$

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

assuming translational equivariance

u_i

generated from low pass filtered white noise

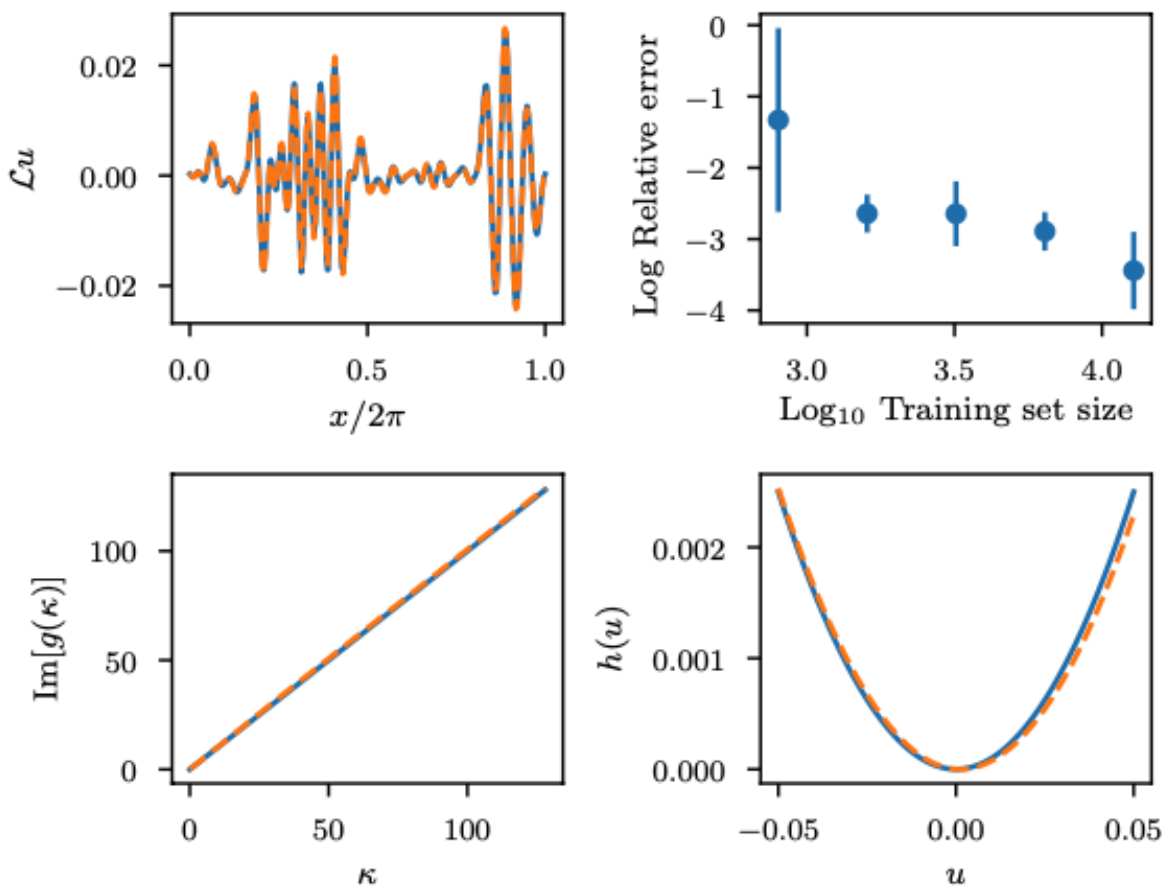


Figure 2: Application of the Burgers operator, $\partial_x u^2$, (——) and regressed operator (- - - -) to a function (*top left*). $\text{Im}[g(\kappa)]$ (*bottom left*) and $h(u)$ (*bottom right*) for both operators. Relative error, $||\mathcal{L}u - \partial_x u^2||/||\partial_x u^2||$ vs. training set size (*top right*).

Validation: spatial operator regression in 2D

Given, $\{u_i, v_i = \Delta u_i\}$, find,

$$\underset{\mathcal{N}}{\operatorname{argmin}} \sum_i ||\mathcal{N} u_i - v_i||^2$$

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

assuming translational equivariance

and compare effect of isotropy

u_i

generated from low pass filtered white noise

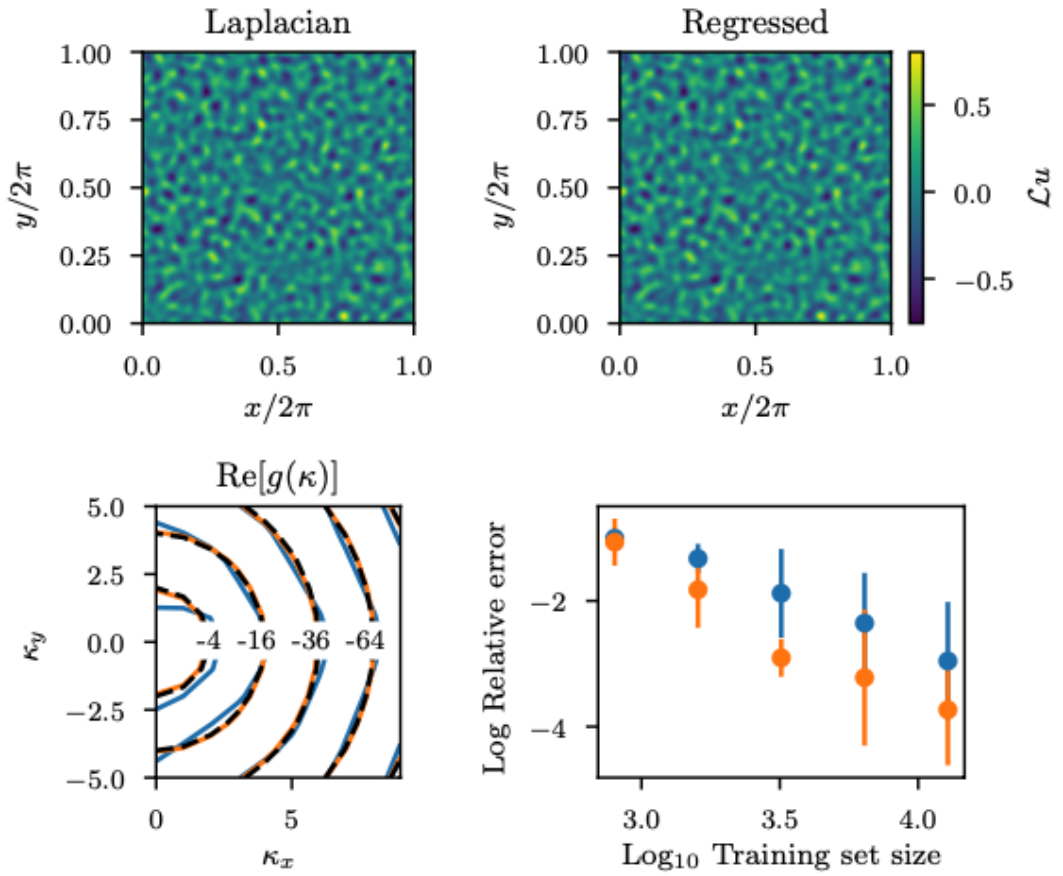
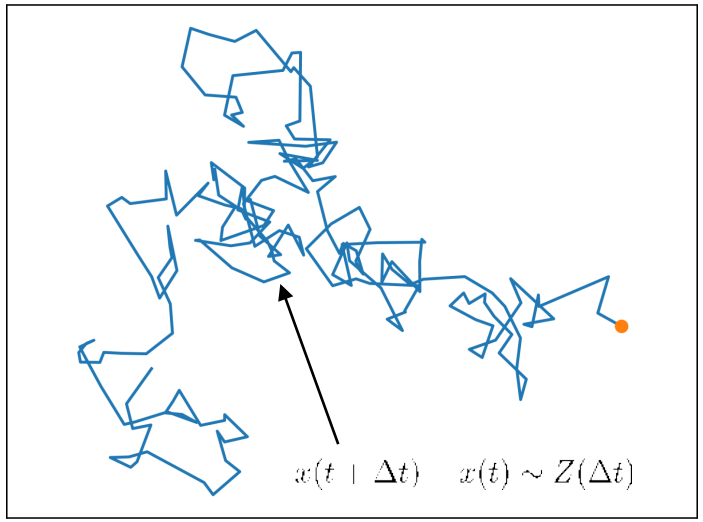
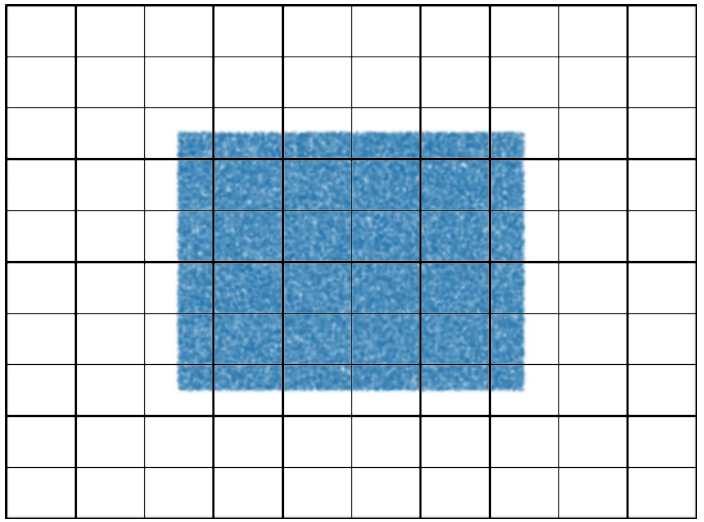


Figure 3: Application of Laplacian to a function, $\nabla^2 u$, (*top left*) and application of the regressed operator with isotropy assumption to the same function, $\mathcal{L}u$, (*top right*). Real part of the symbol of the Laplacian (----), regressed operator without isotropy assumption (——), and regressed operator with isotropy assumption (——) (*bottom left*). Relative error, $||\mathcal{L}u - \nabla^2 u||/||\nabla^2 u||$ vs. training set size (*bottom right*).

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; $x(t+\Delta t) - x(t) \sim N(0, 2\Delta t) \rightarrow \partial_t u = \Delta u$

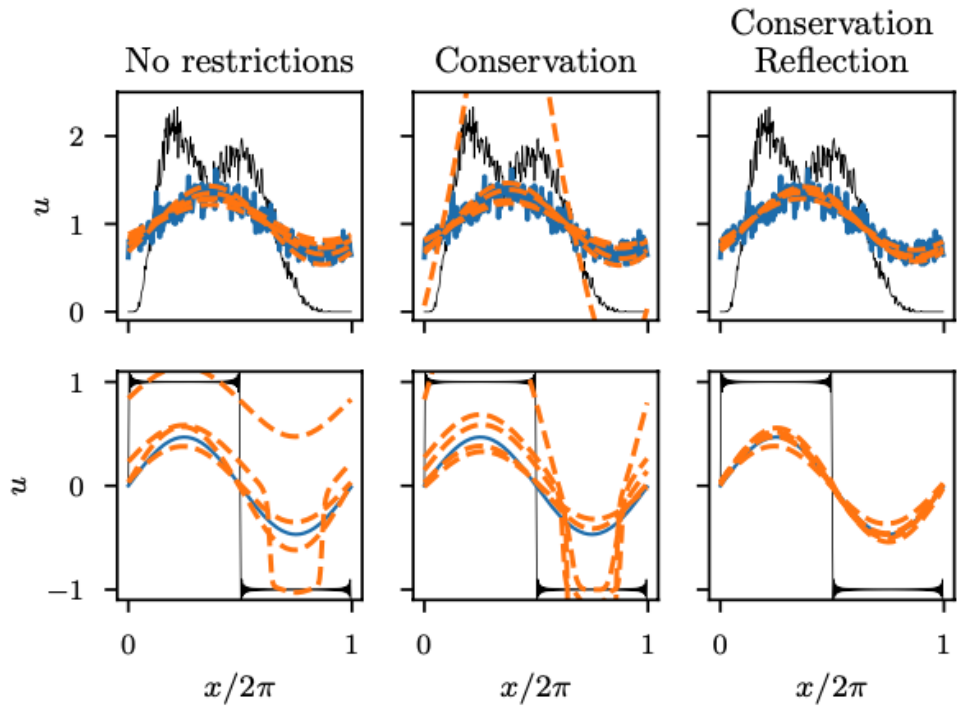


Figure 4: Evolution of the Brownian motion training data (*top row*) and the heat equation validation example (*bottom row*) from $t = 0$ (——) to $t = 1$ (——) compared to evolution of 5 realizations of the learned equation (——). Each column depicts the final learned solution with different physical assumptions yielding improved training and validation accuracy.

SDEs: Isotropy inductive bias improves generalization

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

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

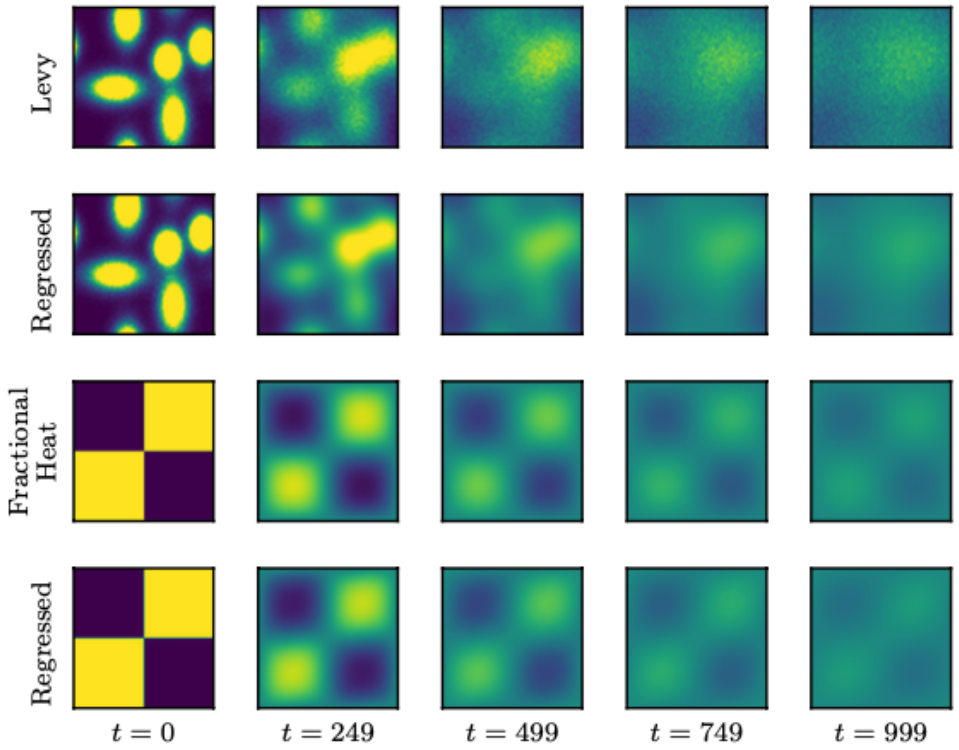


Figure 7: Histograms showing evolution of Levy flight *(first row)*. Evolution of learned operator using histogram of Brownian motion at $t = 0$ as the initial condition *(second row)*. Evolution of the fractional heat equation with square wave initial condition *(third row)*. Evolution of learned operator on square wave initial condition *(fourth row)*

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

SDEs: Isotropy inductive bias improves generalization

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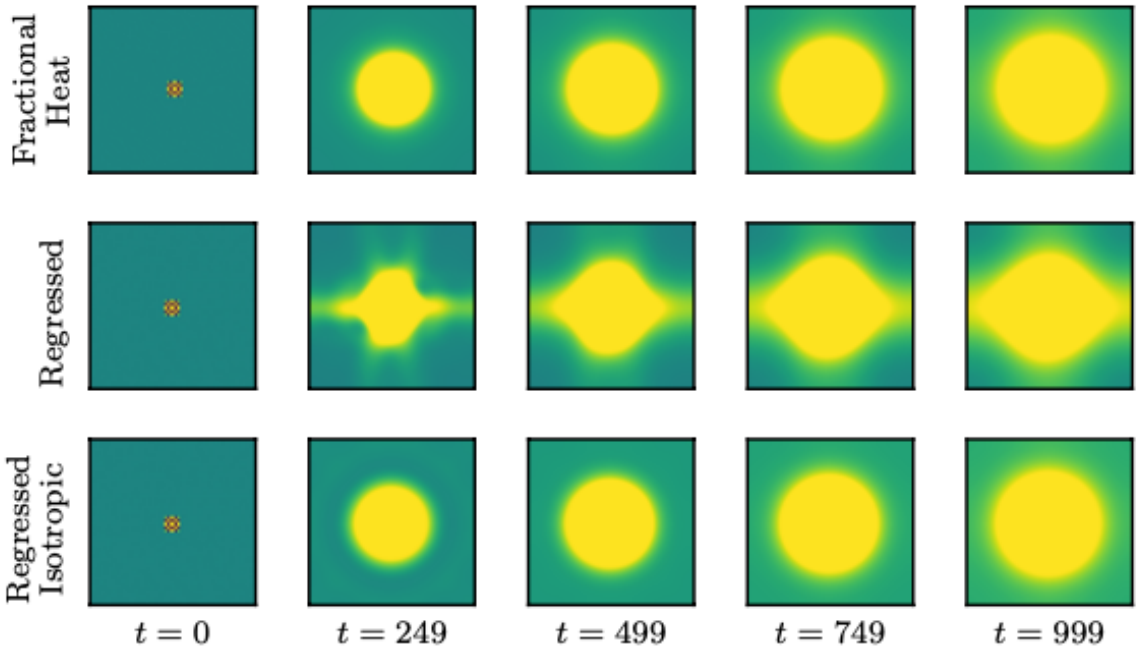
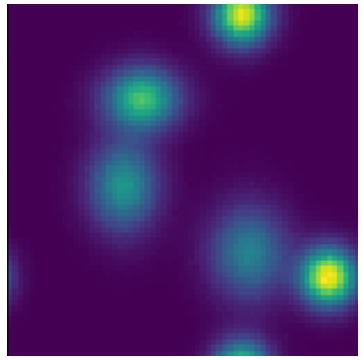


Figure 8: Evolution of the fractional heat equation with Dirac delta initial condition *(first row)*. Evolution of the learned equation without isotropy assumption with Dirac delta initial condition *(second row)*. Evolution of the learned equation with isotropy assumption with Dirac delta initial condition *(third row)*.

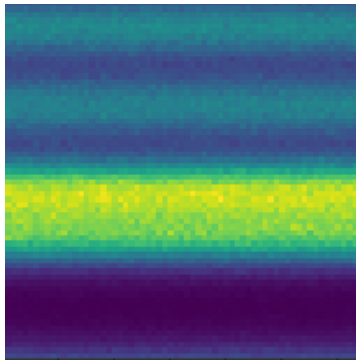
[1]Lischke et al., *arXiv:1801.09767*

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

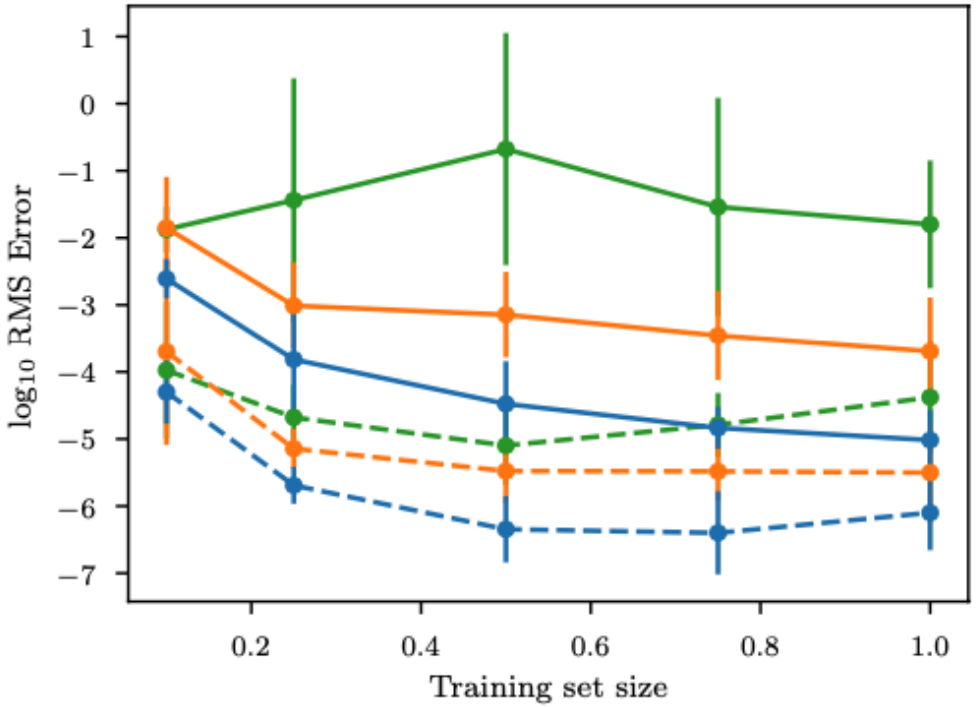
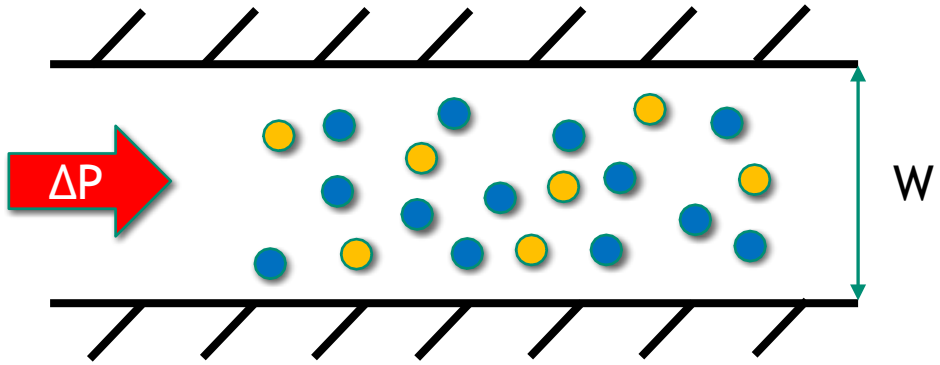
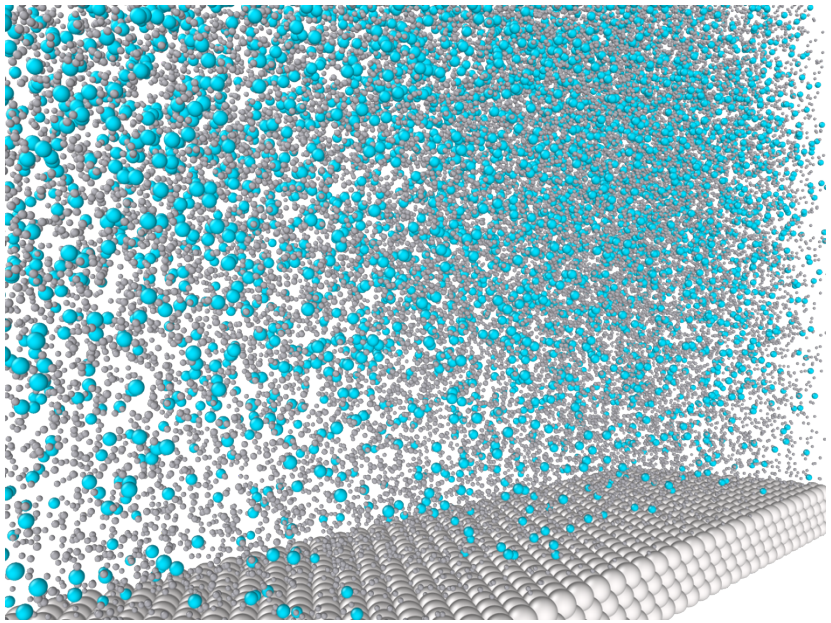


Figure 10: Test error vs. size of training set for anisotropic model trained on data with degree of anisotropy, $\beta = 0.0$ (—●—), $\beta = 0.1$ (—●—), and $\beta = 1.0$ (—●—); and for isotropic model trained on data with $\beta = 0.0$ (- -●- -), $\beta = 0.1$ (- -●- -), and $\beta = 1.0$ (- -●- -). (statistically isotropic: $\beta = 0$; statistically 1D : $\beta = 1$)

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

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

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

where S and C are the sine and cosine transform

Find time evolution for new c, d

Application: coarse graining colloidal Poiseuille flow

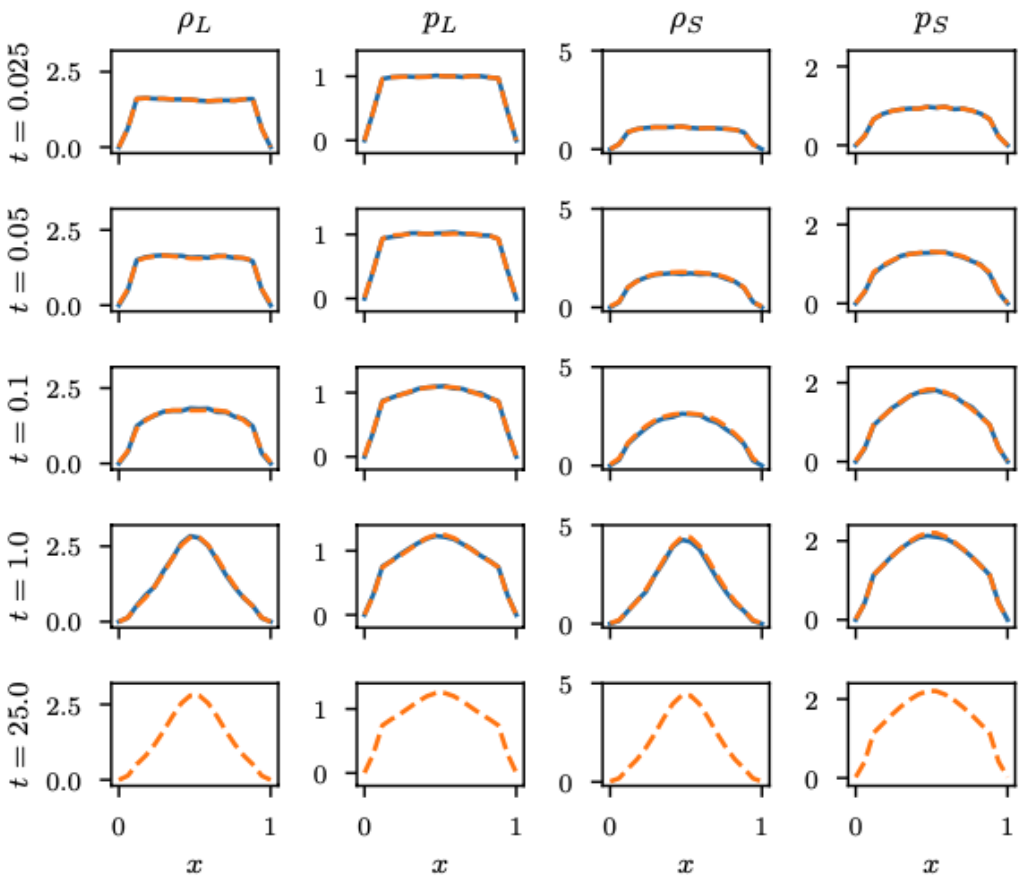


Figure 15: Colloidal system with $(c, d) = (0.15, 2.5)$. Evolution of LAMMPS simulation (——) and regressed 4 equation model (- - - -). Small particle density (*first column*), small particle momentum (*second column*), large particle density (*third column*), and large particle momentum (*fourth column*) is shown for increasing time (*rows*).

Future work

Limited to simple geometries and PDEs with smooth solutions
- Alternative basis
  - Generalized moving least squares: Trask et al., *NeurIPS*, 2019

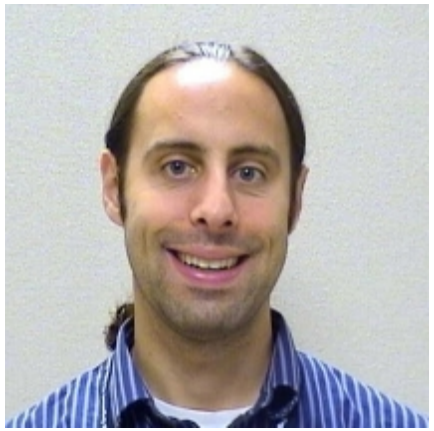
Bayesian version

Noisy data for more general problems
- Error-in-variables models

Applications

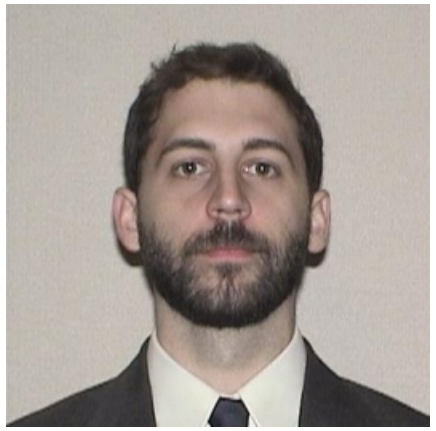
Comparisons to other operator regression methods
- Wu and Xiu, *JCP*, 2020
- Li et al. *arXiv:2010.08895*
- Graph Neural operator: Li et al., *NeurIPS*, 2020
- DeepONets: *arXiv:1910.03193*

Acknowledgements



Eric C. Cyr

Nat Trask



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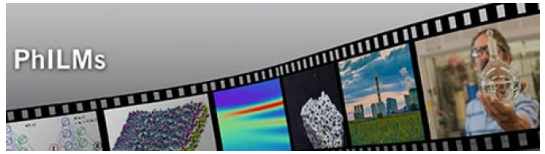

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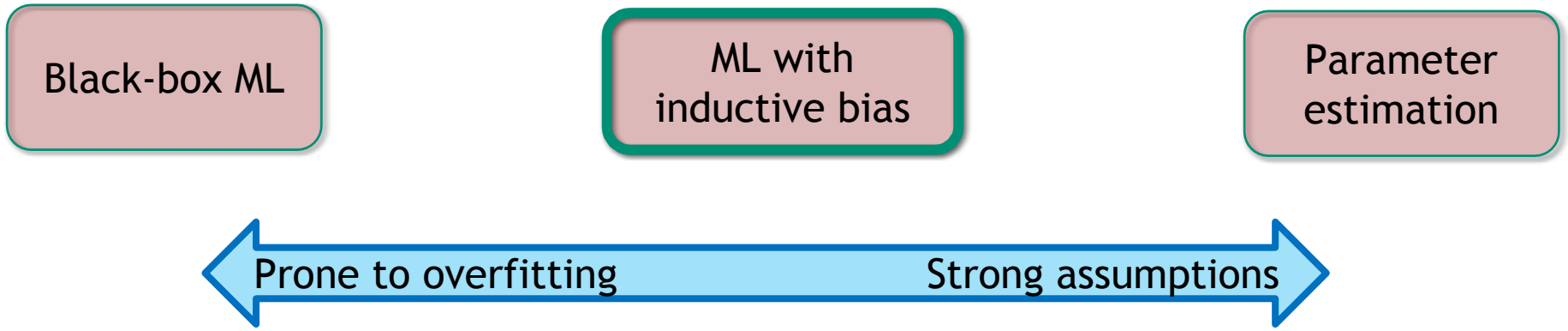
Conclusion



ML with physics informed inductive biases

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

Paper and code:

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