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SCIENTIFIC MACHINE LEARNING AND TENSORFLOW TUTORIAL

Operator Learning

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February 1 - 2, 2024

Numerical PDEs: Analysis, Algorithms, and Data Challenges

ICERM

Brown University



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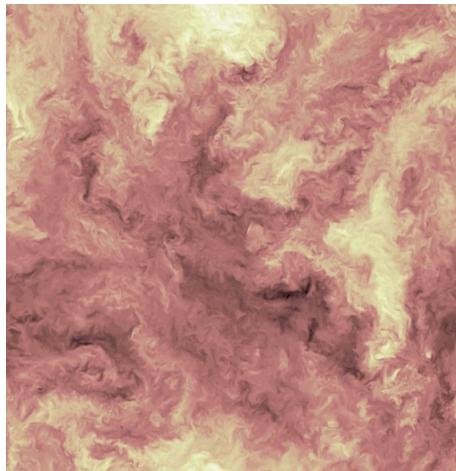
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PHYSICAL SYSTEMS ARE DESCRIBED BY PDE'S

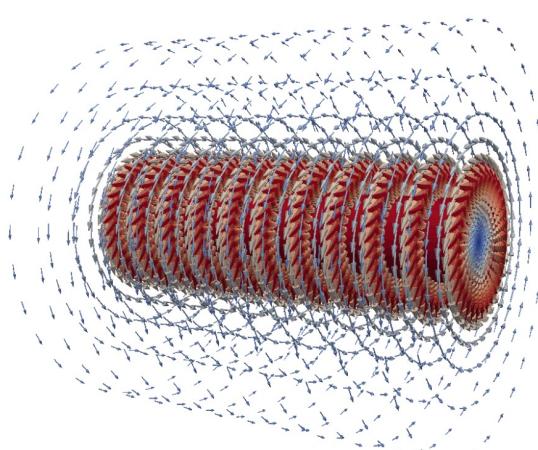


- We describe many physical systems with fields, i.e., functions over a spatio-temporal domain
- When we model field data, we're trying to find a unknown PDE
 - An equation with field valued solutions that match our data
 - Historical examples,

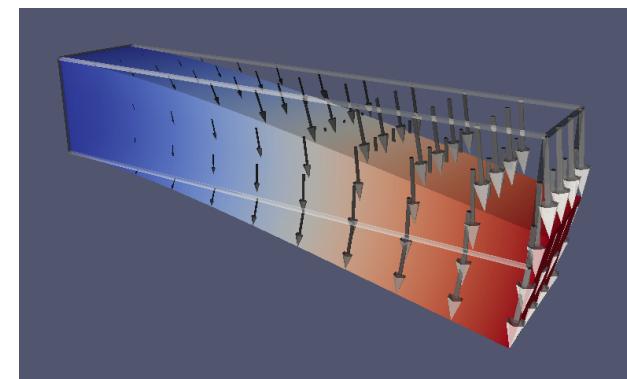
Physics	Incompressible fluid	Electromagnetism	Elasticity
Fields	Fluid velocity	Fluid velocity	Stress/strain
PDE	Navier-Stokes	Electric/magnetic	Hook's Law



Forced isotropic turbulence
JHTDB, turbulence.pha.jhu.edu



Magnetic field from oscillating current
Elmer FEM, elmerfem.org



Cantilever beam under gravity
FENICS, fenicsproject.org

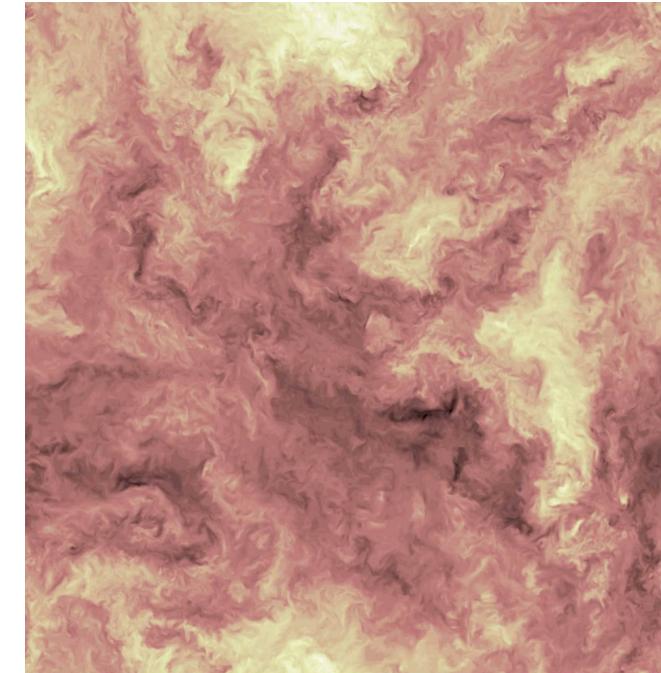
PDE MODELING IS HARD

- Multiphase, multiphysics problems
 - Can't easily model with intuition
 - Data driven methods provide an alternative

$$\begin{aligned}
 & \frac{D \langle \mathbf{u}' \otimes \mathbf{u}' \rangle}{Dt} + \nabla \cdot \left(-\nu \nabla \langle \mathbf{u}' \otimes \mathbf{u}' \rangle + \boxed{\frac{2}{3\rho} I \otimes \langle \mathbf{u}' p' \rangle + \langle \mathbf{u}' \otimes \mathbf{u}' \otimes \mathbf{u}' \rangle} \right) \\
 &= -\langle \mathbf{u}' \otimes \mathbf{u}' \rangle \cdot \nabla \mathbf{u} - \langle \mathbf{u}' \otimes \mathbf{u}' \rangle \cdot \nabla \mathbf{u} \\
 &\quad \boxed{+ \left\langle \frac{p'}{\rho} (\nabla \mathbf{u} + \nabla \mathbf{u}^T) \right\rangle} \\
 &\quad - 2\nu \left\langle (\nabla \langle \mathbf{u} \rangle)^T \cdot (\nabla \langle \mathbf{u} \rangle) \right\rangle
 \end{aligned}$$

Needs modeling

Reynolds stress modeling for single phase turbulence



Forced isotropic turbulence
JHTDB, turbulence.pha.jhu.edu

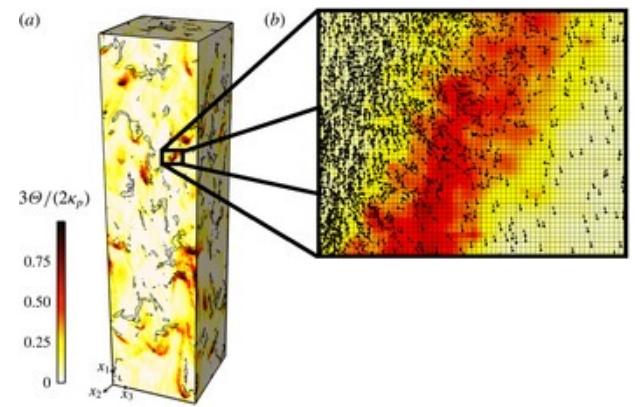
PDE MODELING IS HARD

- Multiphase, multiphysics problems
 - Can't easily model with intuition
 - Data driven methods provide an alternative

$$\begin{aligned}
 \frac{\partial \langle \alpha_p \rangle}{\partial t} + \nabla \cdot \langle \alpha_p \rangle \langle \mathbf{u}_p \rangle_p &= 0, \\
 \frac{\partial \langle \alpha_p'^2 \rangle}{\partial t} + \nabla \cdot \langle \alpha_p'^2 \rangle \langle \mathbf{u}_p \rangle_p + \nabla \cdot \langle \alpha_p'^2 \mathbf{u}_p'' \rangle_p &= -2 \langle \alpha_p' \mathbf{u}_p'' \rangle \cdot \nabla \langle \alpha_p \rangle - \langle \alpha_p'^2 \rangle \nabla \cdot \langle \mathbf{u}_p \rangle_p - 2 \langle \alpha_p \rangle \langle \alpha_p' \nabla \cdot \mathbf{u}_p'' \rangle - \langle \alpha_p'^2 \nabla \cdot \mathbf{u}_p'' \rangle, \\
 \frac{\partial \langle \alpha_p \rangle \langle \mathbf{u}_p \rangle_p}{\partial t} + \nabla \cdot \langle \alpha_p \rangle (\langle \mathbf{u}_p \rangle_p \otimes \langle \mathbf{u}_p \rangle_p + \langle \mathcal{P} \rangle_p) &= \langle \alpha_p \rangle (\langle \mathcal{A} \rangle_p + \mathbf{g}), \\
 \frac{\partial \langle \alpha_p \rangle \langle \mathbf{P} \rangle_p}{\partial t} + \nabla \cdot \langle \alpha_p \rangle (\langle \mathbf{u}_p \rangle_p \otimes \langle \mathbf{P} \rangle_p + \langle \mathbf{u}_p'' \otimes \mathbf{P} \rangle_p + \langle \mathbf{Q} \rangle_p) &= -\langle \alpha_p \rangle (\langle \mathbf{P} \rangle_p \cdot \nabla \langle \mathbf{u}_p \rangle_p + \langle \mathbf{P} \cdot \nabla \mathbf{u}_p'' \rangle_p)^\dagger - \frac{2}{\tau_p} \langle \alpha_p \rangle \langle \mathbf{P} \rangle_p + \frac{12 \langle \alpha_p \rangle}{\sqrt{\pi d_p}} \langle \alpha_p \Theta^{1/2} (\Delta^* - \mathbf{P}) \rangle_p, \\
 \frac{\partial \langle \alpha_p \rangle \langle \mathbf{u}_p'' \otimes \mathbf{u}_p'' \rangle_p}{\partial t} + \nabla \cdot \langle \alpha_p \rangle (\langle \mathbf{u}_p \rangle_p \otimes \langle \mathbf{u}_p'' \otimes \mathbf{u}_p'' \rangle_p + \langle \mathbf{u}_p'' \otimes \mathbf{u}_p'' \otimes \mathbf{u}_p'' \rangle_p + \langle \mathbf{P} \otimes \mathbf{u}_p'' \rangle_p^\dagger) &= -\langle \alpha_p \rangle (\langle \mathbf{u}_p'' \otimes \mathbf{u}_p'' \rangle_p \cdot \nabla \langle \mathbf{u}_p \rangle_p)^\dagger + \frac{\langle \alpha_p \rangle}{\tau_p} [\langle \mathbf{u}_f''' \otimes \mathbf{u}_p'' \rangle_p - \langle \mathbf{u}_f''' \otimes \mathbf{u}_f'' \rangle_p + \langle \mathbf{u}_f'' \otimes \mathbf{u}_p'' \rangle_p \otimes (\langle \mathbf{u}_p \rangle_p - \langle \mathbf{u}_f \rangle_p)]^\dagger \\
 &\quad + \frac{\langle \alpha_f \rangle \varphi}{\rho_f} [\langle \mathbf{u}_f''' \otimes \mathbf{u}_p'' \rangle_p - \langle \mathbf{u}_f''' \otimes \mathbf{u}_f'' \rangle_p + \langle \mathbf{u}_f'' \otimes \mathbf{u}_p'' \rangle_p \otimes (\langle \mathbf{u}_p \rangle_p - \langle \mathbf{u}_f \rangle_p)]^\dagger \\
 &\quad + \frac{\langle \alpha_f \rangle \varphi}{\rho_p} [\langle \mathbf{u}_f''' \rangle_p \otimes \nabla \langle p_f \rangle + \langle \mathbf{u}_f''' \otimes \nabla p_f' \rangle_p - \langle \mathbf{u}_f''' \rangle_p \otimes \nabla \cdot \langle \sigma_f \rangle - \langle \mathbf{u}_f''' \otimes \nabla \cdot \sigma_f' \rangle_p]^\dagger.
 \end{aligned}$$

$$\begin{aligned}
 \frac{\partial \langle \alpha_f \rangle}{\partial t} + \nabla \cdot \langle \alpha_f \rangle \langle \mathbf{u}_f \rangle_f &= 0, \\
 \frac{\partial \langle \alpha_f \rangle \langle \mathbf{u}_f \rangle_f}{\partial t} + \nabla \cdot \langle \alpha_f \rangle (\langle \mathbf{u}_f \rangle_f \otimes \langle \mathbf{u}_f \rangle_f + \langle \mathbf{u}_f''' \otimes \mathbf{u}_f''' \rangle_f) &= \frac{1}{\rho_f} (\nabla \cdot \langle \sigma_f \rangle - \nabla \langle p_f \rangle) - \langle \alpha_f \rangle \varphi \langle \mathcal{A} \rangle_p + \langle \alpha_f \rangle \mathbf{g},
 \end{aligned}$$

Reynolds averaged transport equations¹ for particle-laden turbulent flow



Granular temperature field in cluster-induced turbulence¹

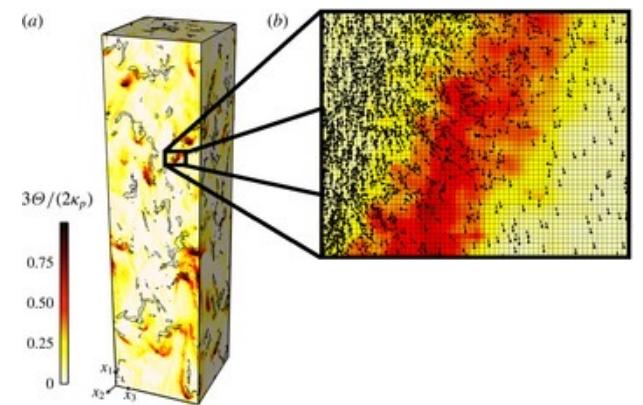
PDE MODELING IS HARD

- Multiphase, multiphysics problems
 - Can't easily model with intuition
 - Data driven methods provide an alternative

- Adding a single extra phase greatly complicates the model
- Need a scalable approach to PDE modeling

$$\begin{aligned}
 \frac{\partial \langle \alpha_p \rangle}{\partial t} + \nabla \cdot \langle \alpha_p \rangle \langle \mathbf{u}_p \rangle_p &= 0, \\
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 \frac{\partial \langle \alpha_p \rangle \langle \mathbf{P} \rangle_p}{\partial t} + \nabla \cdot \langle \alpha_p \rangle (\langle \mathbf{u}_p \rangle_p \otimes \langle \mathbf{P} \rangle_p + \langle \mathbf{u}_p'' \otimes \mathbf{P} \rangle_p + \langle \mathbf{Q} \rangle_p) &= -\langle \alpha_p \rangle (\langle \mathbf{P} \rangle_p \cdot \nabla \langle \mathbf{u}_p \rangle_p + \langle \mathbf{P} \cdot \nabla \mathbf{u}_p'' \rangle_p)^\dagger - \frac{2}{\tau_p} \langle \alpha_p \rangle \langle \mathbf{P} \rangle_p + \frac{12 \langle \alpha_p \rangle}{\sqrt{\pi d_p}} \langle \alpha_p \Theta^{1/2} (\Delta^* - \mathbf{P}) \rangle_p, \\
 \frac{\partial \langle \alpha_p \rangle \langle \mathbf{u}_p'' \otimes \mathbf{u}_p'' \rangle_p}{\partial t} + \nabla \cdot \langle \alpha_p \rangle (\langle \mathbf{u}_p \rangle_p \otimes \langle \mathbf{u}_p'' \otimes \mathbf{u}_p'' \rangle_p + \langle \mathbf{u}_p'' \otimes \mathbf{u}_p'' \otimes \mathbf{u}_p'' \rangle_p + \langle \mathbf{P} \otimes \mathbf{u}_p'' \rangle_p^\dagger) &= -\langle \alpha_p \rangle (\langle \mathbf{u}_p'' \otimes \mathbf{u}_p'' \rangle_p \cdot \nabla \langle \mathbf{u}_p \rangle_p)^\dagger + \frac{\langle \alpha_p \rangle}{\tau_p} [\langle \mathbf{u}_f''' \otimes \mathbf{u}_f'' \rangle_p - \langle \mathbf{u}_f''' \otimes \mathbf{u}_f'' \rangle_p + \langle \mathbf{u}_f'' \otimes \mathbf{u}_f''' \rangle_p \otimes (\langle \mathbf{u}_p \rangle_p - \langle \mathbf{u}_f \rangle_f)]^\dagger \\
 &\quad + \frac{\langle \alpha_f \rangle \varphi}{\tau_p} [\langle \mathbf{u}_f''' \otimes \mathbf{u}_p'' \rangle_p - \langle \mathbf{u}_f''' \otimes \mathbf{u}_f'' \rangle_p + \langle \mathbf{u}_f'' \otimes \mathbf{u}_f''' \rangle_p \otimes (\langle \mathbf{u}_p \rangle_p - \langle \mathbf{u}_f \rangle_f)]^\dagger \\
 &\quad + \frac{\langle \alpha_f \rangle \varphi}{\rho_p} [\langle \mathbf{u}_f''' \rangle_p \otimes \nabla \langle p_f \rangle + \langle \mathbf{u}_f''' \otimes \nabla p_f' \rangle_p - \langle \mathbf{u}_f''' \rangle_p \otimes \nabla \cdot \langle \sigma_f \rangle - \langle \mathbf{u}_f''' \otimes \nabla \cdot \sigma_f' \rangle_p]^\dagger.
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 \end{aligned}$$



Granular temperature field in cluster-induced turbulence¹

Reynolds averaged transport equations¹ for particle-laden turbulent flow

OPERATOR LEARNING ENABLES PDE DISCOVERY



- PDE's are composed of operators, i.e., mappings between functions,

$$\sum_i \mathcal{N}_i(u_1, u_2, \dots) = 0$$

$$u_j \in \mathcal{U}_j : \mathbb{R}^+ \times \Omega \rightarrow \mathbb{R}^{m_j}$$

$$\mathcal{N}_i : \mathcal{U}_1 \times \mathcal{U}_2 \times \dots \rightarrow \mathcal{V}$$

- E.g., the viscous Burger's equation has three operators,

$$\partial_t u + \partial_x u^2 - \partial_x^2 u = 0$$

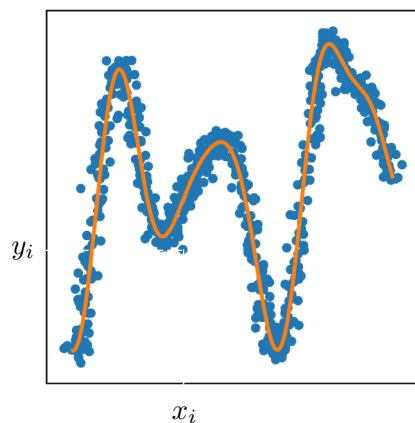
- If we're given the field data, we can find a PDE by finding it's component operators

OPERATOR LEARNING IS A GENERALIZATION OF REGRESSION

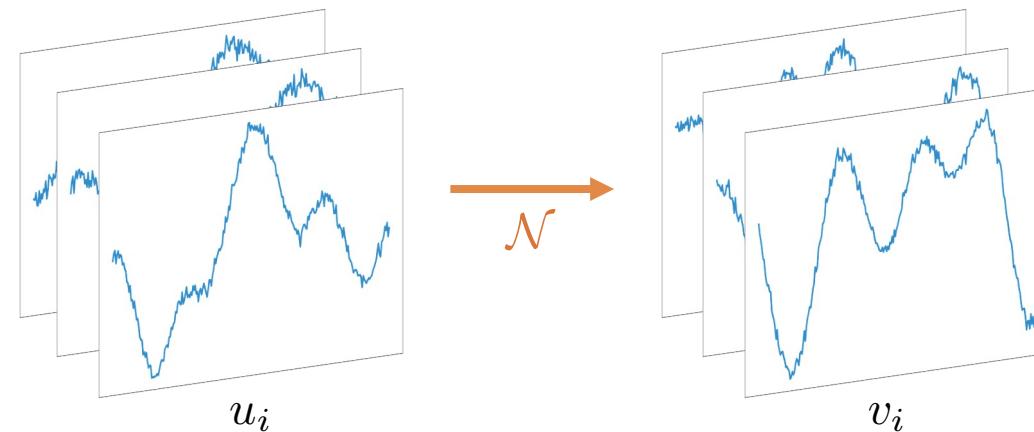


- Given pairs of functions, $\{u_i, v_i\}^{i=1,2,\dots}$, we can use regression to find the operator maps between the two, $\mathcal{N}(u_i) \approx v_i$

Fitting functions



Fitting operators



$$\hat{f} = \operatorname{argmin}_{\mathbf{f}} \sum_i \|y_i - \mathbf{f}(x_i)\|_2^2$$

$$\hat{\mathcal{N}} = \operatorname{argmin}_{\mathcal{N}} \sum_i \|v_i - \mathcal{N}[u_i]\|_{\mathcal{V}}$$

THREE COMPONENTS OF AN OPERATOR LEARNING METHOD



1. A discretization for functional data
 - To run on computers, we need to work with some discretization
 - Usually implicit in the dataset we receive
 - Often taken to be point evaluations of the functions
2. An interpolation scheme
 - Even though we only work with discretizations, we should be able to evaluate the functions anywhere they're defined
 - Can be learned or fixed
3. A parameterized mapping between discretizations
 - We'll use gradient based methods to optimize these parameters against the error norm

OPERATOR LEARNING PARAMETERIZATIONS



Modal operator regression for physics (MOR-Physics^{1,2})

- Given pairs of functions, $(u_i, v_i)^{i=1,2,\dots}$, let's find a Poisson-like PDE,

$$\mathcal{N}(u) = v$$

- Let's assume they're given as point-wise evaluations on a regular, periodic grid
- We parameterize the unknown operator as,

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

Where g and h are neural networks. \mathcal{F} is the Fourier transform

- Optimization problem becomes,

$$\xi_g, \xi_h = \operatorname{argmin}_{\hat{\xi}_g, \hat{\xi}_h} \sum_i \left\| v_i - \mathcal{N}(u_i; \hat{\xi}_g, \hat{\xi}_h) \right\|_2^2$$

¹R.G. Patel and Desjardins, *arxiv: 1810.08552* (2018)

²R.G. Patel et al., *CMAME* (2021)

MOR-PHYSICS: MOTIVATION



For smooth functions in a periodic domain,

Physical space

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

$$\begin{array}{c} \xrightarrow{\mathcal{F}} \\ \xleftarrow{\mathcal{F}^{-1}} \end{array}$$

Fourier space

$$\begin{aligned} f_{\kappa} &= \int f(x) e^{-j\kappa x} dx \\ (j\kappa)^{\gamma} \tilde{f}_{\kappa} \end{aligned}$$

Parameterization contains,

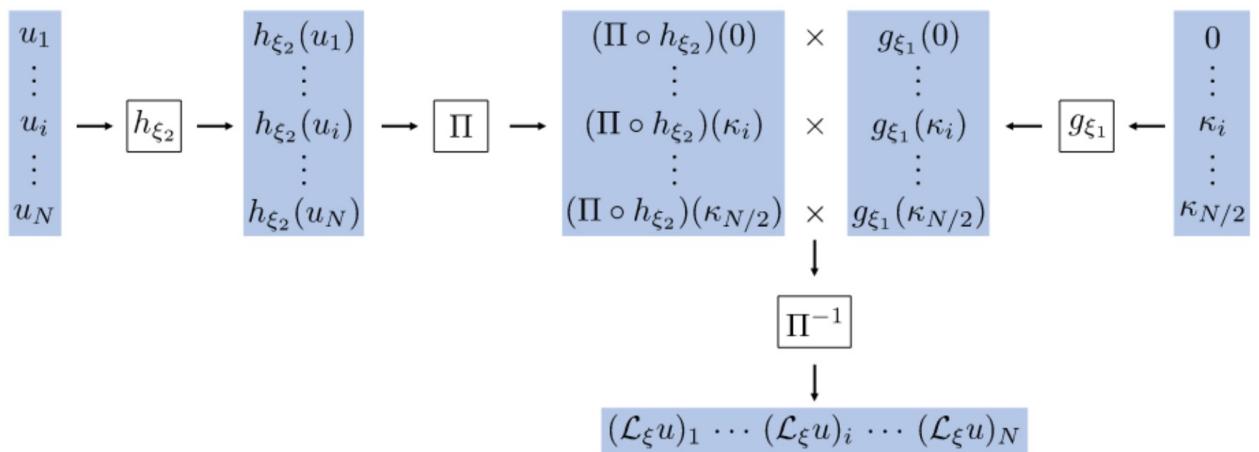
- Laplacian

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

- Burgers operator

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

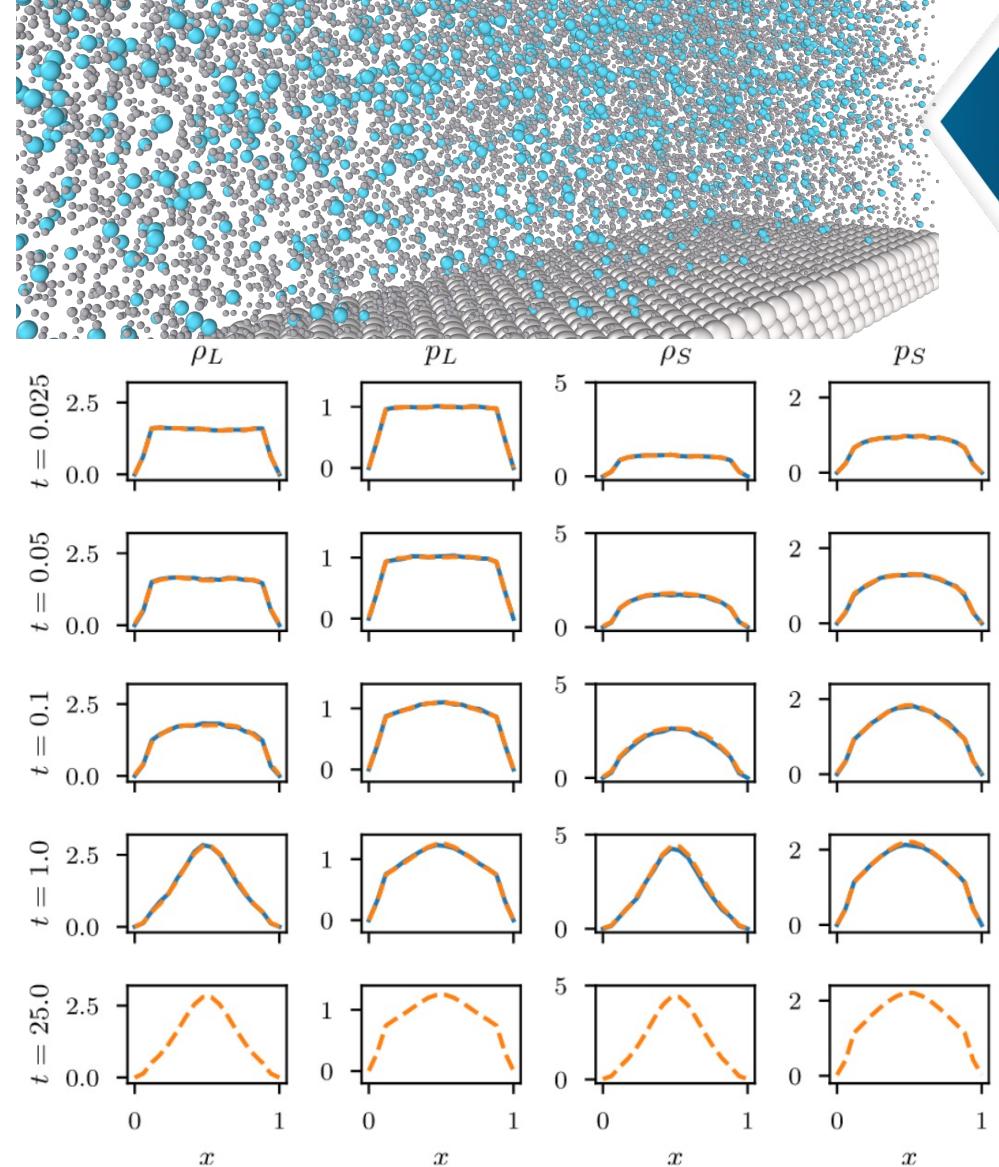
MOR-PHYSICS: EXAMPLE



MOR-Physics parameterization¹

¹R.G. Patel and Desjardins, *arxiv*: 1810.08552 (2018)

²R.G. Patel et al., *CMAME* (2021)



MOR-physics learns dynamics of colloidal system from molecular dynamics simulations. Generalizes to unseen concentration and colloid diameter²



Deep Operator Network (DeepONet)¹

- Given pairs of functions, $(u_i, v_i)^{i=1,2,\dots}$, let's find a Poisson-like PDE,

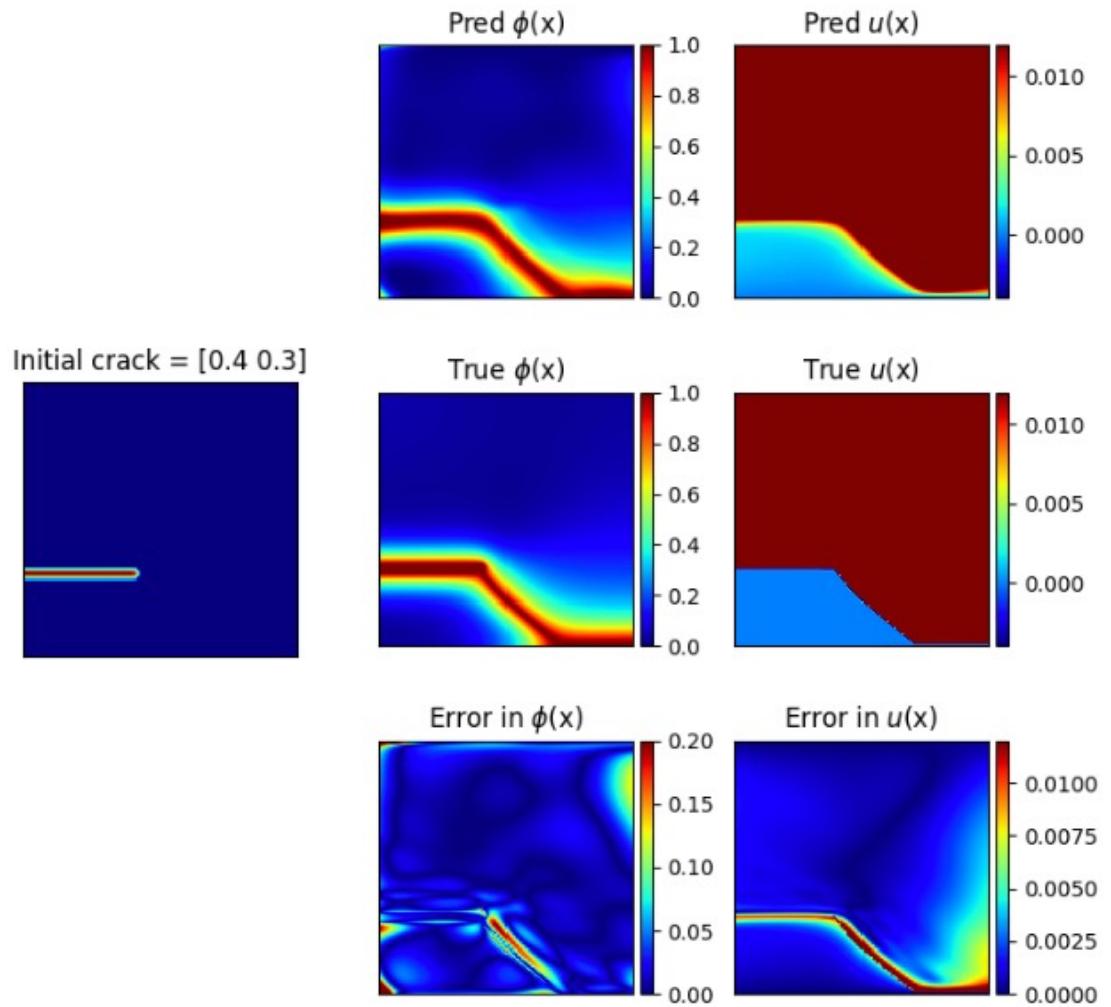
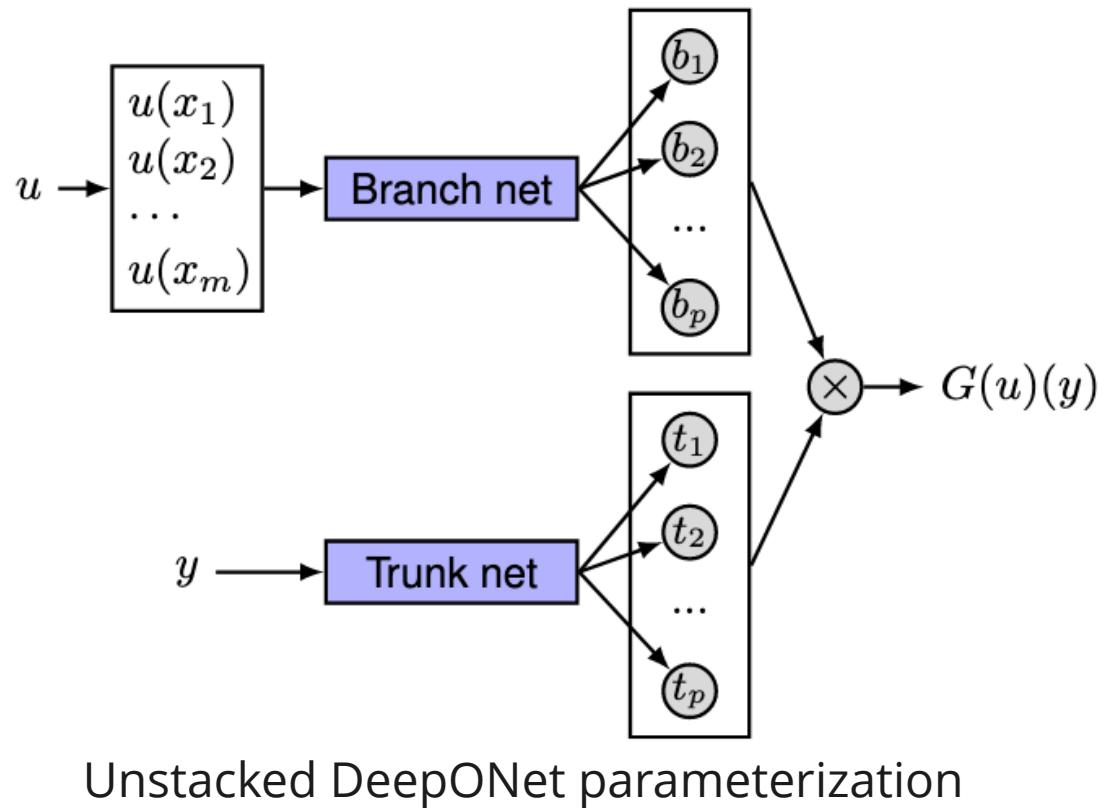
$$\mathcal{N}(u) = v$$

- Let's assume they're given as point-wise evaluations on two (possibly different) sets of collocation points
- We parameterize the unknown operator as,
$$\mathcal{N}(u, \xi_b, \xi_t)(y) = \sum_i b_i(u, \xi_b) t_i(y, \xi_t)$$
Where b and t are neural networks
- Optimization problem becomes,

$$\xi_b, \xi_t = \operatorname{argmin}_{\hat{\xi}_b, \hat{\xi}_t} \sum_i \left\| v_i - \mathcal{N}(u_i; \hat{\xi}_b, \hat{\xi}_t) \right\|_2^2$$

¹Lu, Jin and Karniadakis, *Nature*, 2021

DEEPONET EXAMPLE



Variational DeepONet learns crack path under shear loading. Generalizes to unseen crack tip locations.²

¹Lu, Jin and Karniadakis, *Nature*, 2021

²Goswami et al., *CMAME*, 2022

INCLUDING A PRIORI KNOWLEDGE

- Operator learning is flexible
 - Can learn several operators simultaneously
 - Can combine a partially known PDE with unknown operators
- Often, we'll know more about a system than just the data
 - Theoretical results
 - Symmetries
 - Conservation principles



- 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,

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

- More generally,

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

TIME EVOLVING SYSTEMS



- Alternatively, parameterize your operator with time

$$u(\cdot, t) = \mathcal{N}(u^0; t)$$

Lu, Jin and Karniadakis, *Nature*, 2021

Li et al., *ICLR* (2021)

OTHER OPERATOR LEARNING FRAMEWORKS AND RELATED METHODS



- Fourier Neural Operator
 - Li et al., *ICLR* (2021)
- Nonlocal operator regression
 - H. You et al., *CMAME* (2020)
- Operator Inference
 - B. Peherstorfer and K. Willcox, *CMAME* (2016)
- Function-to-function regression
 - J.S. Morris, *Annu. Rev. Stat. Appl.* (2015)