Learning Hidden Physics and System Parameters with Deep Operator Networks

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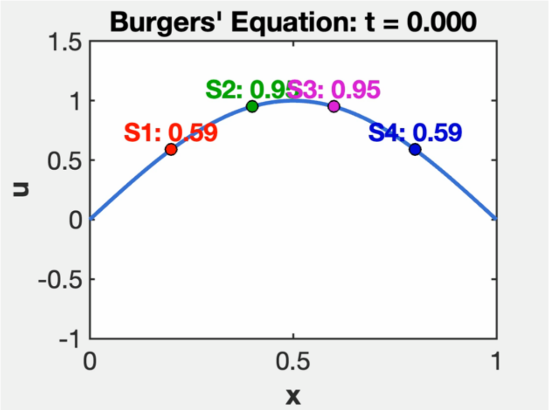
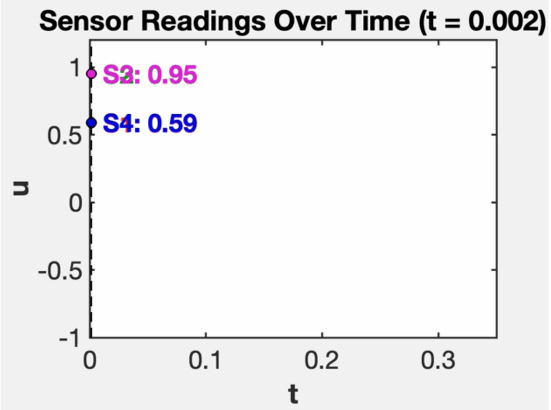
Outline

- The Challenge
- Proposed frameworks:
  - The Deep Hidden Physics Operator (DHPO) network Neural Operators
  - Neural Operator for System Parameter Identification
- Results
- Future work

The Challenge

Objective: Scientific Discovery from sparse data





- Data is spatiotemporally scattered
- Governing equations are partially unknown
- System parameters need identification

Current Method Limitations:

- **SINDy (Brunton et. al.):** requires well-structured, regularly sampled data.
- **DHPM (Raissi et. al.):** Cannot be used as a surrogate
- **PINNs (Raissi et. al.):** Require retraining for each variation

- **Neural Operator:** After training, infer the unknown physics and system parameters in real time.

Proposed Frameworks

Framework 1: DHPO (Deep Hidden Physics Operator)

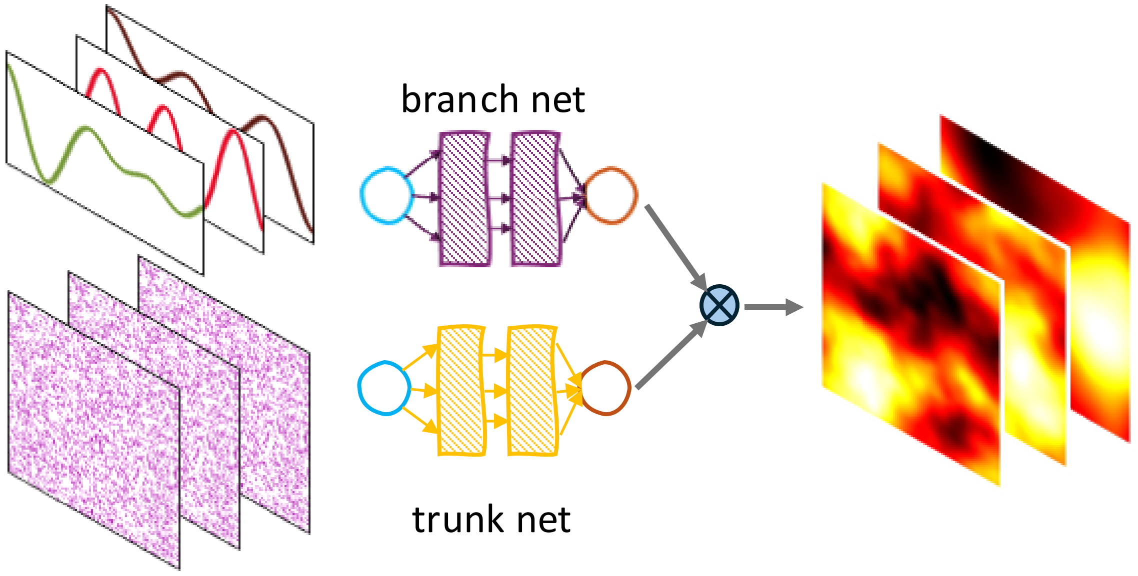
- Discovers unknown physics terms
- Built an operator using only primary variable data and physics (semi-supervised)
- Inspired from DeepONet, PINNs, DHPM.

Framework 2: Parameter Identification (Inverse Neural Operator)

- Discovers unknown system parameters.
- Built an operator using only primary variable data and physics (semi-supervised)
- Inspired from DeepONet, PINNs.

DeepONet (Lu et al., 2019): inspired by the universal approximation theorem of operators.

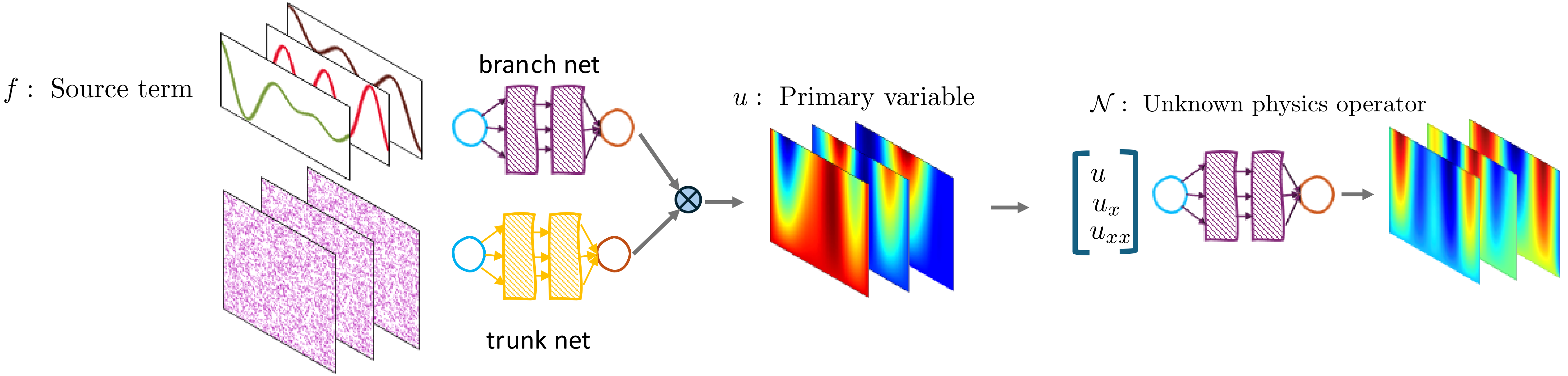
$$G_\theta(u)(y) = \sum_i^p \underbrace{b_i(u(x_1), u(x_2), \ldots, u(x_m))}_{\text{branch net}} \cdot \underbrace{tr_i(y)}_{\text{trunk net}}$$



#1: The Deep Hidden Physics Operator (DHPO) network

$$\frac{\partial u}{\partial t} = \mathcal{N}(t, x, u, u_x, u_{xx}, \ldots) + f(x)$$

$u:$ Primary variable
$f:$ Source term
$\mathcal{N}:$ Unknown physics



$$\text{Loss, } \mathcal{L} = \mathcal{L}_{\text{pde}} + \mathcal{L}_{\text{bc}} + \mathcal{L}_{\text{ic}} + \mathcal{L}_{\text{data}}$$

Consider Burger's equation

$$\mathcal{L}_{\text{pde}} = ||u_t^{\text{NO}} + \mathcal{N}^{\text{DHPO}} - f(x)||^2 \qquad \mathcal{L}_{\text{ic}} = ||u^{\text{NO}} - u^{\text{ic}}||^2$$

$$\mathcal{L}_{\text{bc}} = ||u^{\text{NO}} - u^{\text{bc}}||^2 \qquad \mathcal{L}_{\text{data}} = ||u^{\text{NO}} - u^{\text{data}}||^2$$

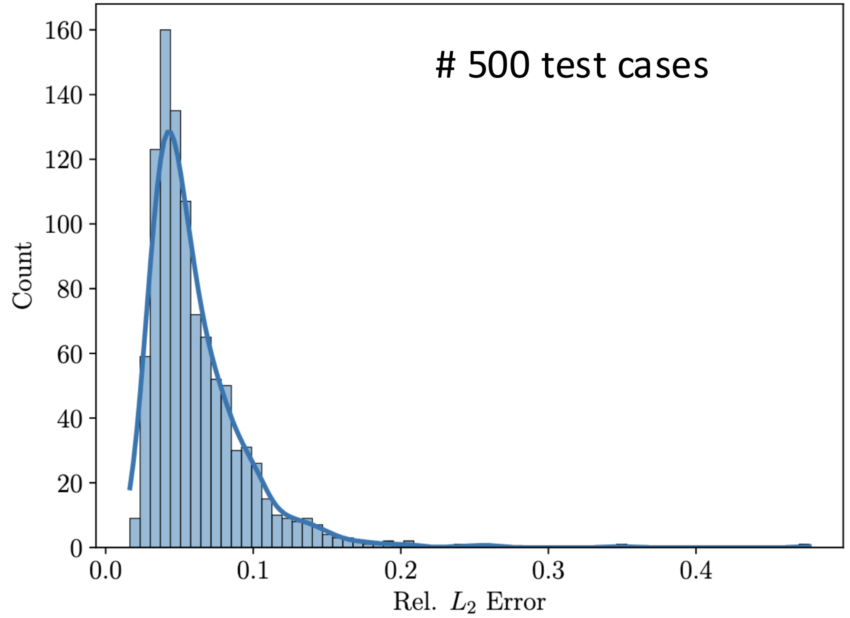
Results: Physics Discovery

Burger's problem:

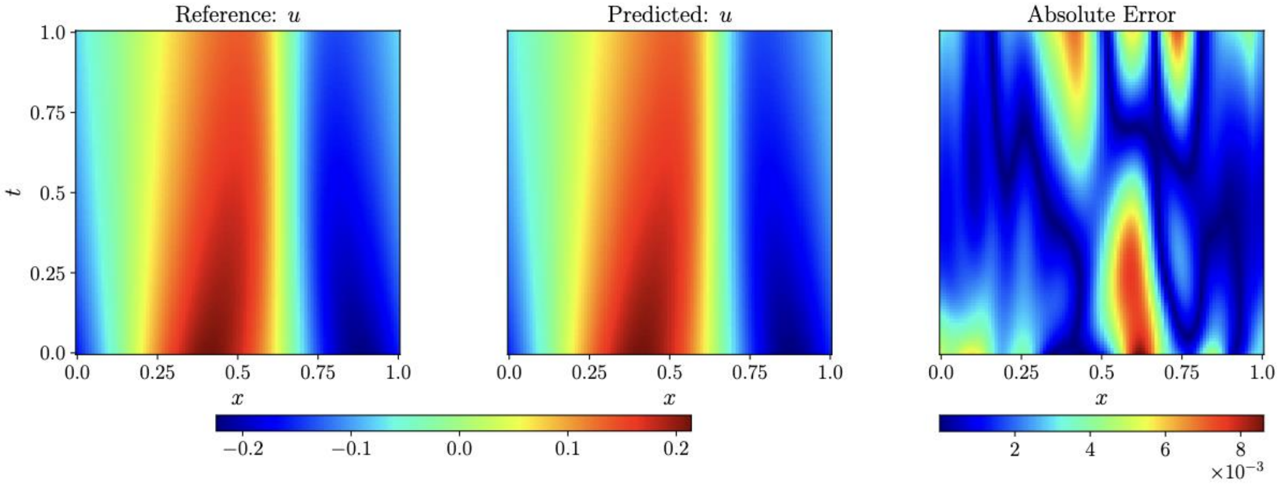
$$\frac{\partial u}{\partial t}(x,t) = \overbrace{\nu \frac{\partial^2 u}{\partial x^2}(x,t) - u\frac{\partial u}{\partial x}(x,t)}^{\mathcal{N}(u, u_x, u_{xx})} \text{ on } \Omega : (x,t) \in [0,1]^2,$$

$$\boxed{\text{IC: } u(x,0) = f(x),}$$

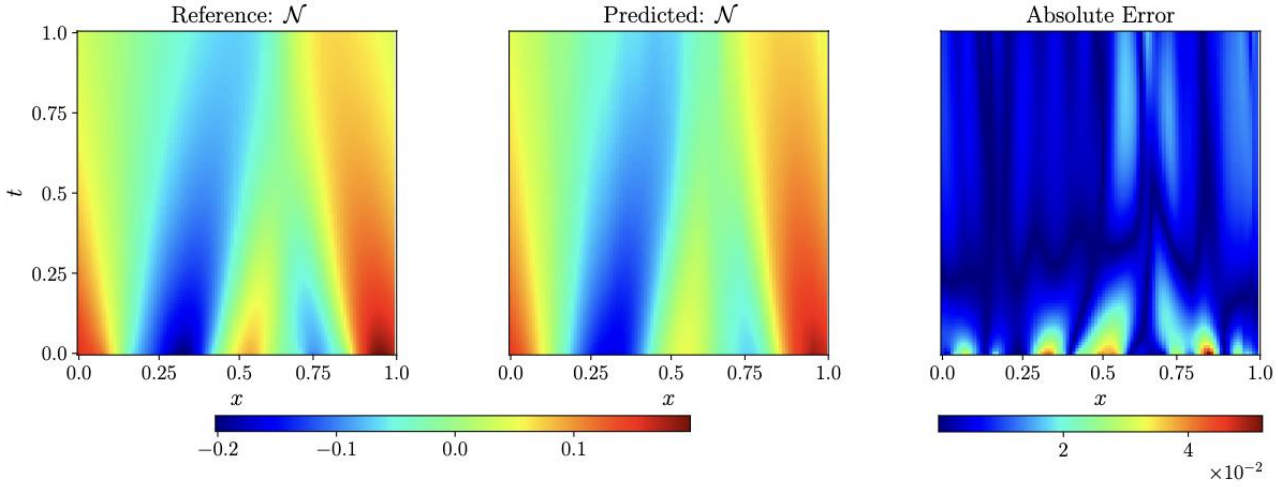
$$\text{BC: } u(0,t) = u(1,t) \text{ and } \frac{\partial u}{\partial x}(0,t) = \frac{\partial u}{\partial x}(1,t),$$



Average relative L_2 error of $\mathcal{N}(u, u_{\dot{x}}, u_{xx})$ $\mathcal{O}(10^{-2})$



(a) Sample 1: solution field accuracy comparison, relative L_2 error $= 0.02134$.



(b) Sample 1: hidden physics solution comparison, relative L_2 error $= 0.118278$.

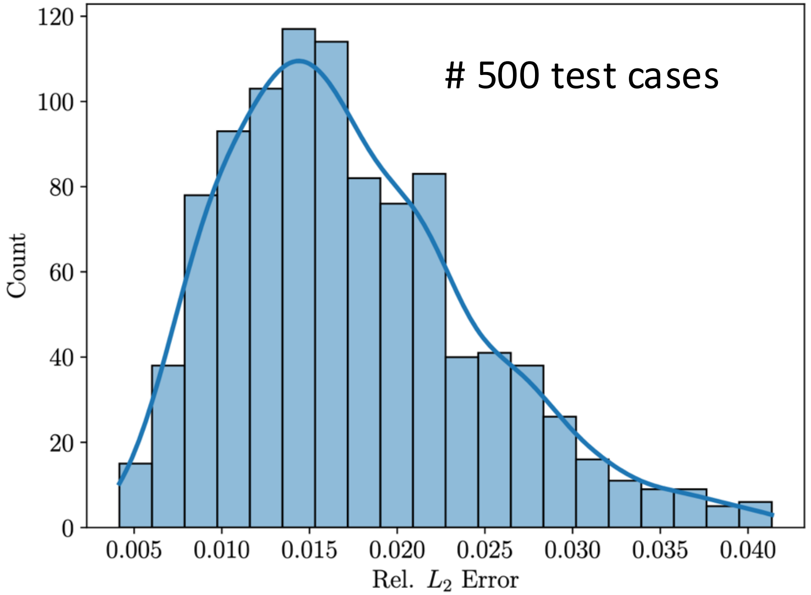
Results: Physics Discovery

Reaction diffusion problem:

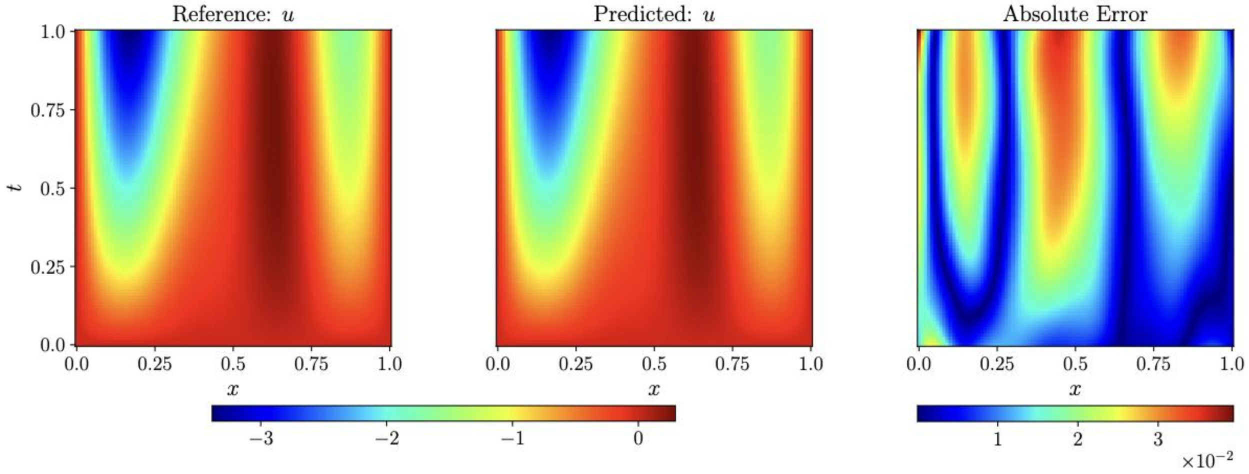
$$\frac{\partial u}{\partial t}(x,t) = \overbrace{D\frac{\partial^2 u}{\partial x^2}(x,t) + Ku^2(x,t)}^{\mathcal{N}(u, u_x, u_{xx})} + \boxed{f(x)} \text{ on } \Omega : (x,t) \in [0,1]^2,$$

$$IC : u(x,0) = 0,$$

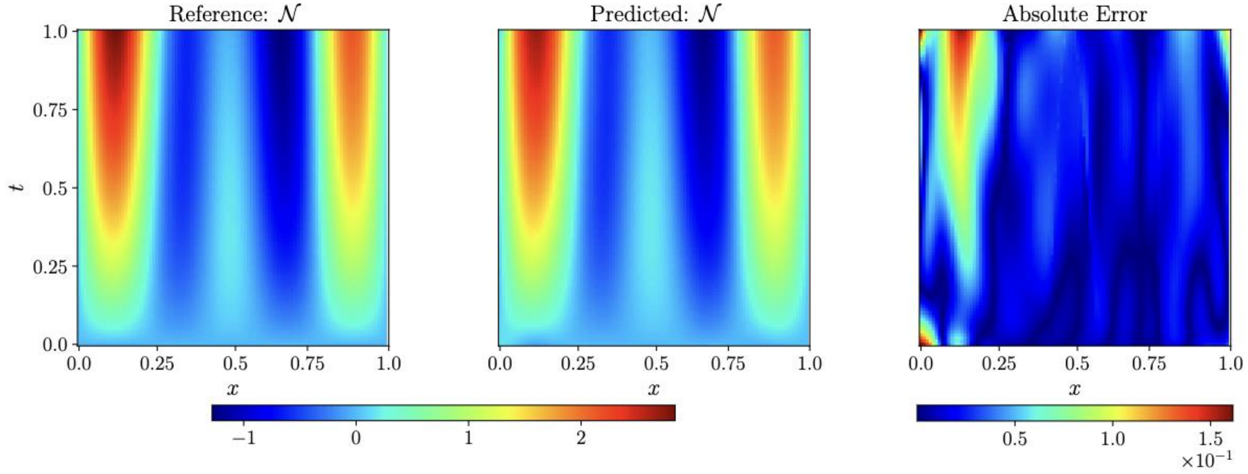
$$BC : u(0,t) = u(1,t) = 0,$$



Average relative L_2 error of $\mathcal{N}(u, u_{\dot{x}}, u_{xx})$ $\mathcal{O}(10^{-2})$



(a) Sample 1: solution field accuracy comparison, relative L_2 error = 0.01639.



(b) Sample 1: hidden physics solution comparison, relative L_2 error = 0.03949.

#2: Neural Operator for System Parameter Identification

Consider Burger's equation

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2}$$

u : Primary variable

ν : Viscosity

Step 2: Learn parameter operator and fine tune the solution operator

Step 1: Learn solution operator

Loss, $\mathcal{L} = \mathcal{L}_{\text{pde}} + \mathcal{L}_{\text{sensor data}}$

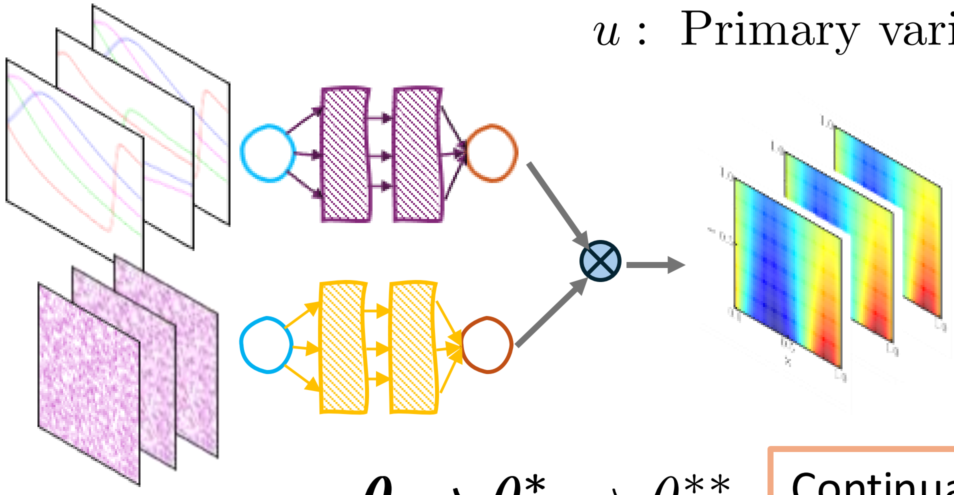
Loss, $\mathcal{L} = \mathcal{L}_{\text{sensor data}}$

$$\mathcal{L}_{\text{pde}} = ||u_t^{\text{NO}} + u^{\text{NO}} u_x^{\text{NO}} - \nu^{\text{INO}} u_{xx}^{\text{NO}}||^2$$

$$\mathcal{L}_{\text{sensor data}} = ||u^{\text{NO}} - u^{\text{data}}||^2$$

u_{data} : Sensor data

u : Primary variable

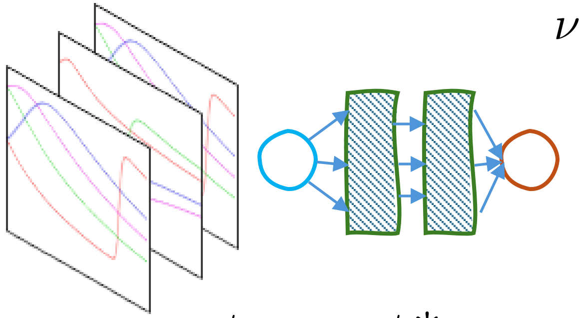


$\boldsymbol{\theta} \rightarrow \theta^* \rightarrow \theta^{**}$

Continual learning

u_{data} : Sensor data

ν : Viscosity



ν

$\phi \rightarrow \phi^*$

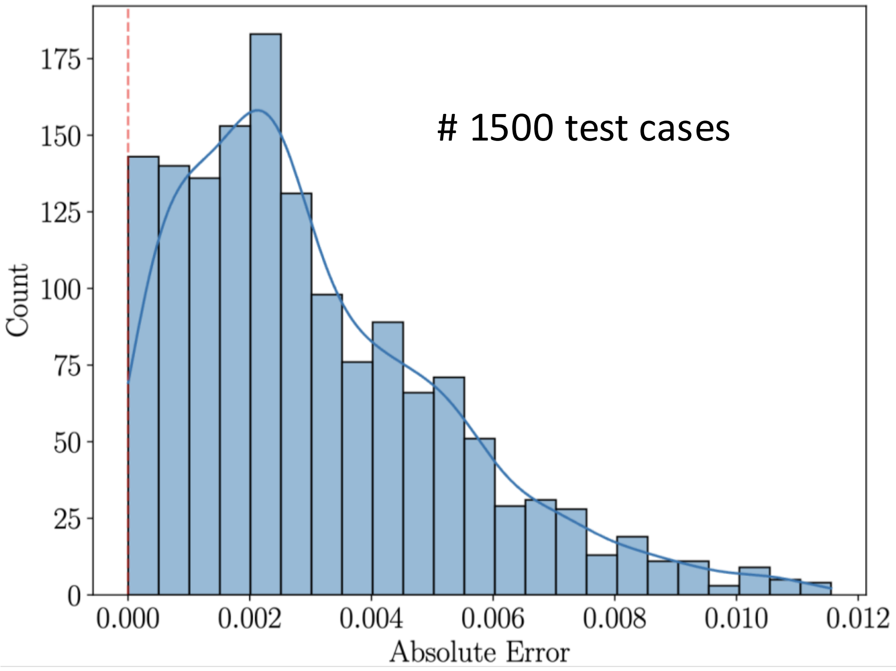
Results: Parameter Identification

Burger's problem:

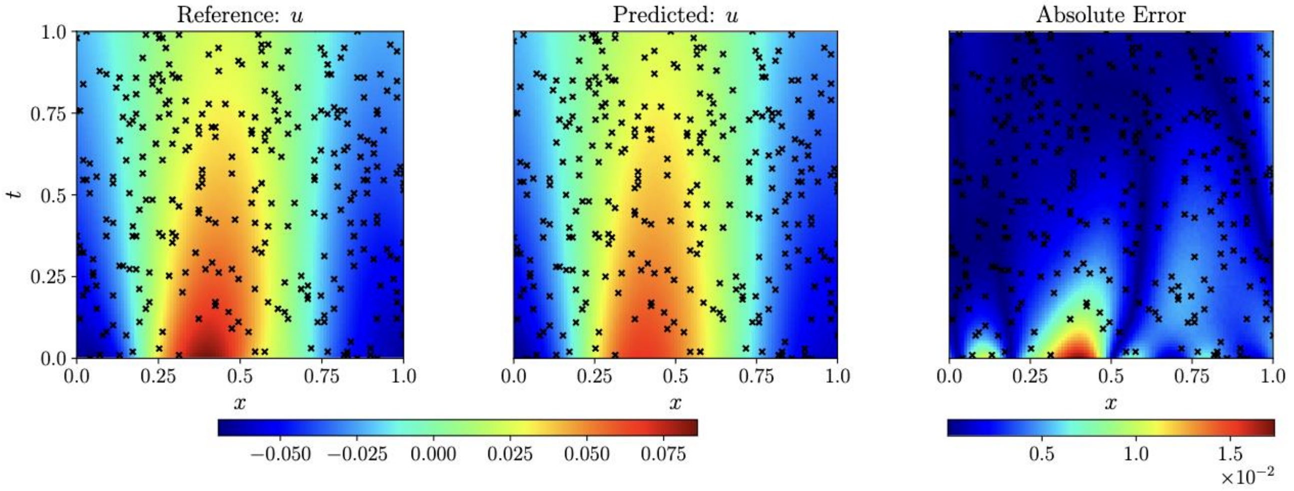
$$\frac{\partial u}{\partial t}(x,t) = \boxed{\nu}\frac{\partial^2 u}{\partial x^2}(x,t) - u\frac{\partial u}{\partial x}(x,t) \text{ on } \Omega : (x,t) \in [0,1]^2,$$

$$\boxed{\text{IC: } u(x,0) = f(x),}$$

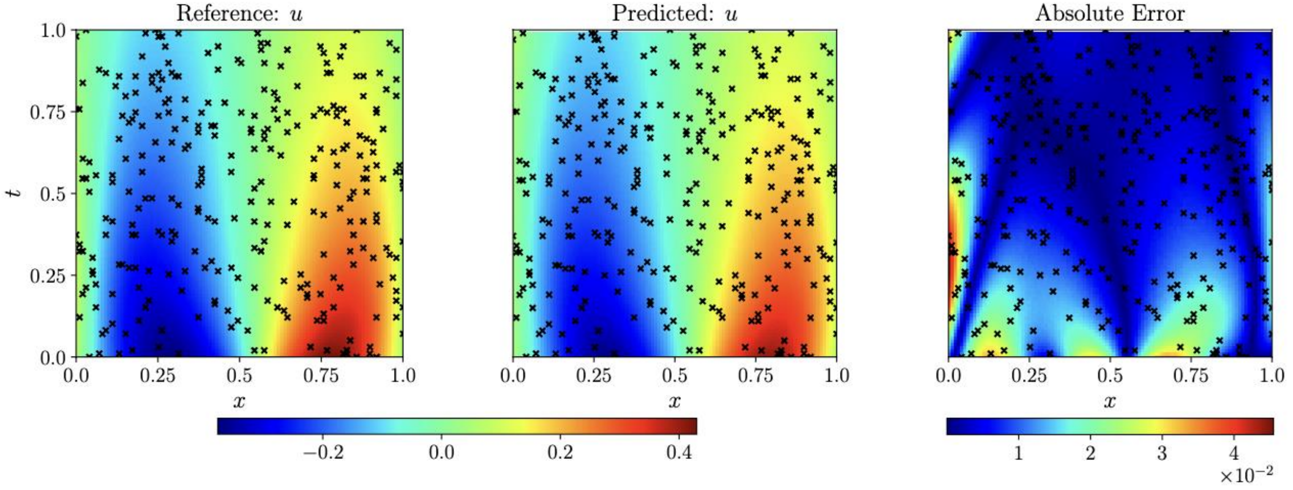
$$\text{BC: } u(0,t) = u(1,t) \text{ and } \frac{\partial u}{\partial x}(0,t) = \frac{\partial u}{\partial x}(1,t),$$



Average absolute error of viscosity, : ν $\mathcal{O}(10^{-3})$



(a) Sample 1: Relative L_2 error of $u(x,t) = 0.092$. For this case, $\boxed{\nu_{\text{true}} = 0.028 \text{ while } \nu_{\text{predicted}} = 0.025.}$



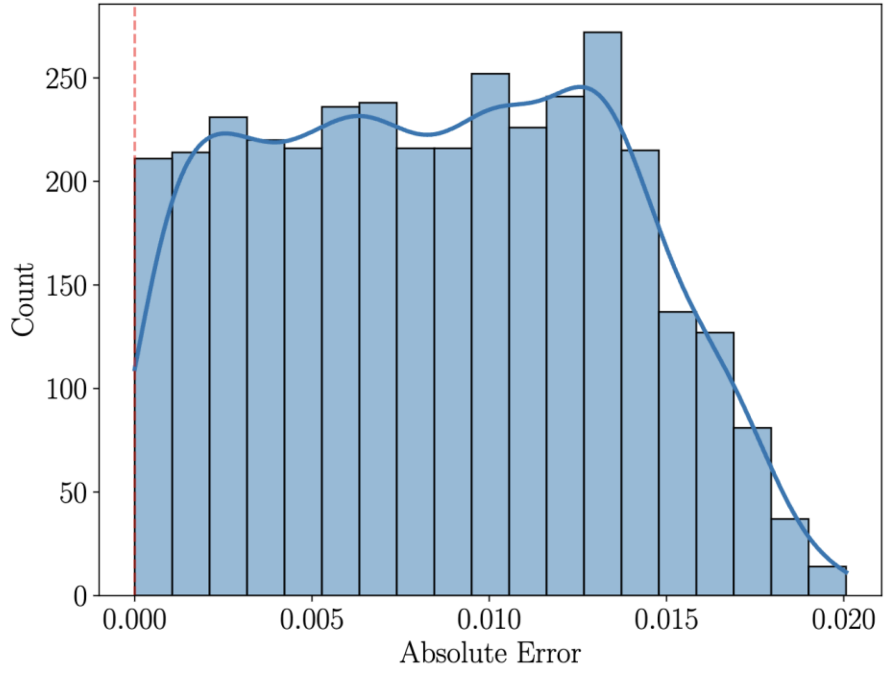
(b) Sample 2: Relative L_2 error of $u(x,t) = 0.061$. For this case, $\boxed{\nu_{\text{true}} = 0.032 \text{ while } \nu_{\text{predicted}} = 0.032.}$

Results: Parameter Identification

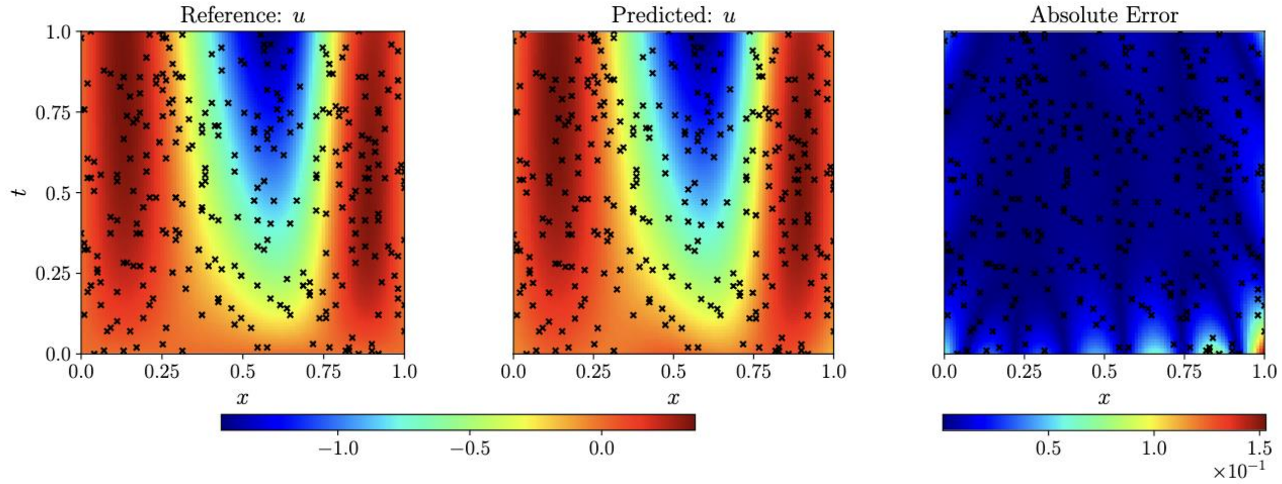
Reaction diffusion problem:

$$\frac{\partial u}{\partial t}(x,t) = \boxed{D}\frac{\partial^2 u}{\partial x^2}(x,t) + Ku^2(x,t) + \boxed{f(x)} \text{ on } \Omega : (x,t) \in [0,1]^2,$$
$$IC : u(x,0) = 0,$$
$$BC : u(0,t) = u(1,t) = 0,$$

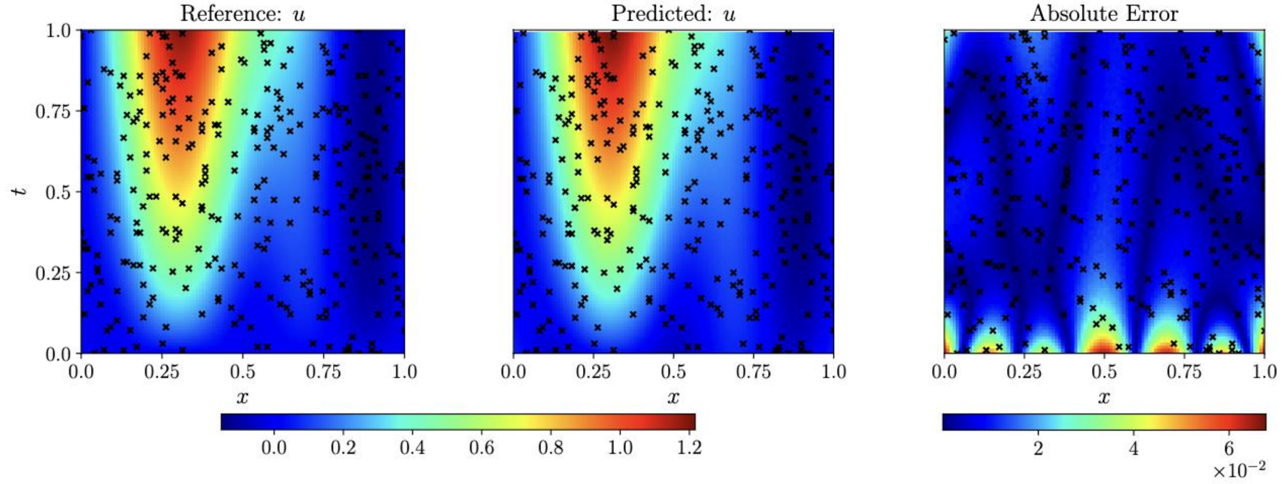
1500 test cases



Average absolute error of diffusion coefficient, : D $\mathcal{O}(10^{-3})$



(a) Sample 1: Relative L_2 error of $u(x,t) = 0.027$. For this case, $D_{\text{true}} = 0.027$ while $D_{\text{predicted}} = 0.027$.



(b) Sample 2: Relative L_2 error of $u(x,t) = 0.029$. For this case, $D_{\text{true}} = 0.036$ while $D_{\text{predicted}} = 0.034$.

Conclusions and Future Directions

- We built operator frameworks that can discover the hidden physics and the system parameters.

- These operators are trained using physics informed loss functions which allow them to learn without labelled data of input and output functions.

- Both frameworks are utilized for Burger's and Reaction-Diffusion Equation

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Thank you