Meta Learning of Interface Conditions for Multi-Domain Physics-Informed Neural Networks

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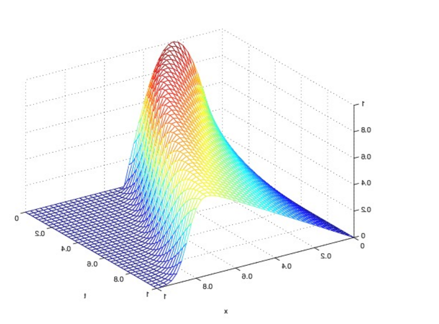
Abstract: Physics-informed neural networks (PINNs) are emerging as popular mesh-free solvers for partial differential equations (PDEs). Recent extensions decompose the domain, applying different PINNs to solve the problem in each subdomain and stitching the subdomains at the interface. Hence, they can further alleviate the problem complexity, reduce the computational cost, and allow parallelization. However, the performance of multi-domain PINNs is sensitive to the choice of the interface conditions. While quite a few conditions have been proposed, there is no suggestion about how to select the conditions according to specific problems. To address this gap, we propose META Learning of Interface Conditions (METALIC), a simple, efficient yet powerful approach to dynamically determine the optimal interface conditions for solving a family of parametric PDEs. Specifically, we develop two contextual multi-arm bandit (MAB) models. The first one applies to the entire training course, and online updates a Gaussian process (GP) reward that given the PDE parameters and interface conditions predicts the performance. We prove a sub-linear regret bound for both UCB and Thompson sampling, which in theory guarantees the effectiveness of our MAB. The second one partitions the training into two stages, one is the stochastic phase and the other deterministic phase; we update a GP reward for each phase to enable different condition selections at the two stages so as to further bolster the flexibility and performance. We have shown the advantage of METALIC on four bench-mark PDE families.

Introduction & Motivation

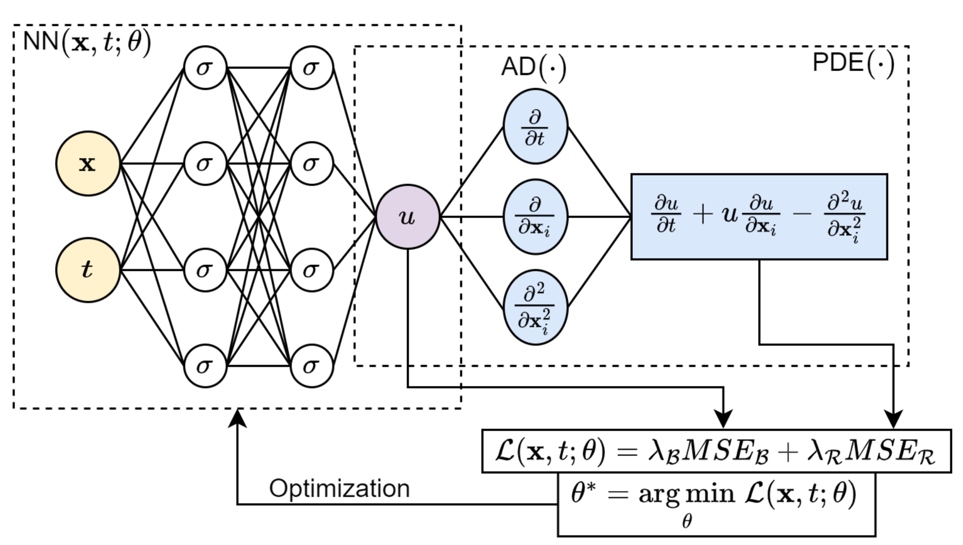
Physical-Informed Neural Networks (PINNs):

- Data-driven, Robust, Low-data availability, mesh-free, PDE solvers
- *A universal function approximator* that can embed physical laws



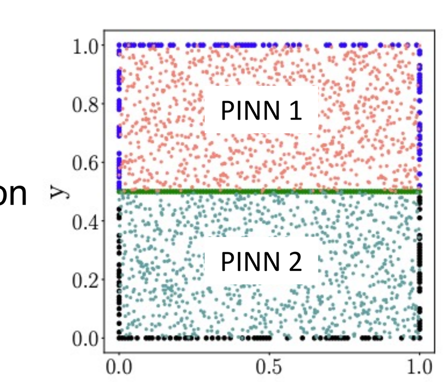
Viscous Burger's Equation

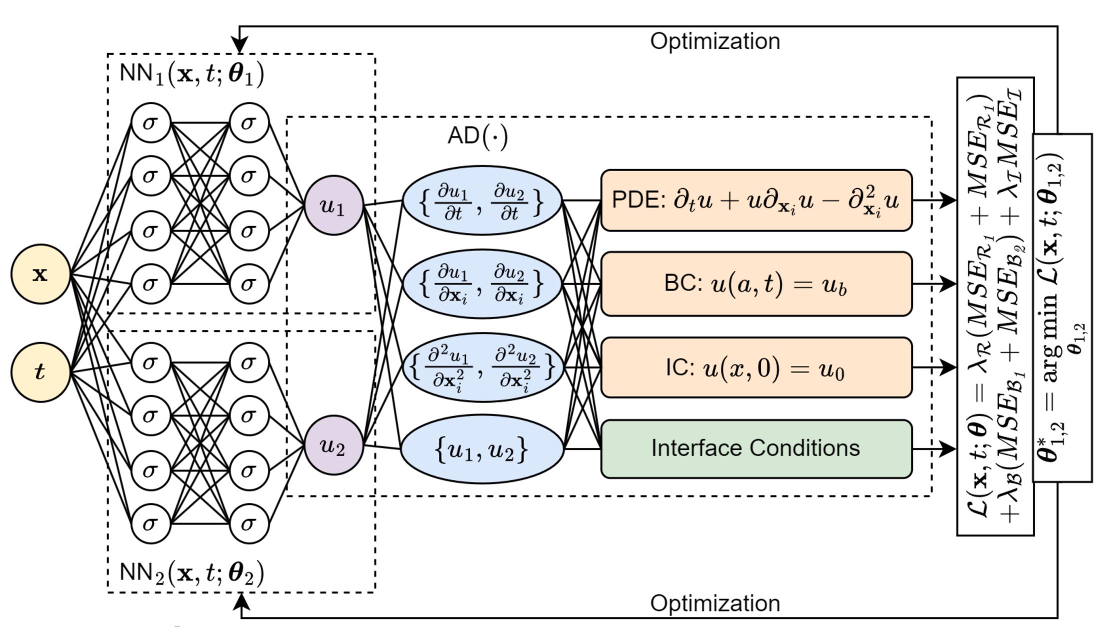
$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2}$$

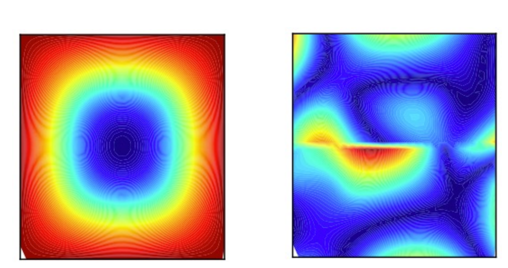


Multi-Domain Extensions of PINNs:

- Decompose into subdomains
- Divide-and-conquer
- Align the solutions at the interface with conditions
- *Simpler* subproblems, *reduced* training costs and *parallel* computation







Ground-truth Solution

Solutions with ***Bad choice*** of interface selection

Naive combinations of interface conditions could be WORSE!

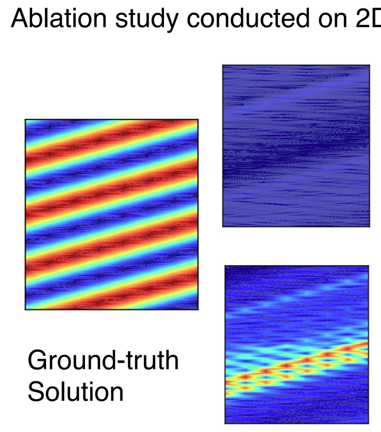
Model	L_2 Relative Error
PINN	1.05e-3 ± 4.38e-4
$I_{u_{avg}}$	4.28e-3 ± 2.63e-3
$I_{u_{avg}} + I_{rc}$	3.92e-3 ± 2.25e-3
$I_{u_{avg}} + I_c$	9.45e-4 ± 2.85e-4
$I_{u_{avg}} + I_{rc} + I_c$	9.77e-4 ± 3.45e-4
$I_{u_{avg}} + I_{rc} + I_{gr}$	4.57e-3 ± 3.18e-3
$I_{u_{avg}} + I_c + I_{yy}$	**5.26e-4 ± 1.97e-4**
$I_{u_{avg}} + I_{rc} + I_{gr} + I_c + I_{yy}$	9.34e-4 ± 3.18e-4

I_u	Solution continuity
$I_{u_{avg}}$	Average solution continuity
I_r	Residual
I_{rc}	Residual continuity
I_{gr}	Gradient-enhanced residual
I_c	Flux continuity
I_z	First-order spatial/temporal derivative continuity
I_{zz}	Second-order spatial/temporal derivative continuity

Ablation study conducted on 2D Poisson $u_{xx} + u_{yy} = 1$

Advection

$u_t + \beta u_x = 0$



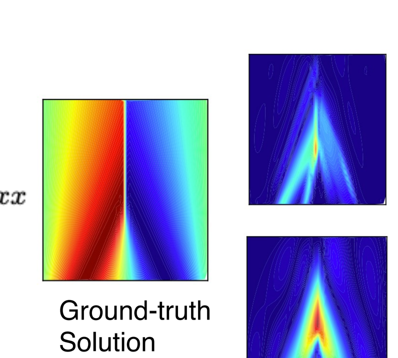
Ground-truth Solution

Errors by Single PINN

Errors by MD-PINNS with ***bad interfaces***

Burgers

$u_t + uu_x = \nu u_{xx}$



Ground-truth Solution

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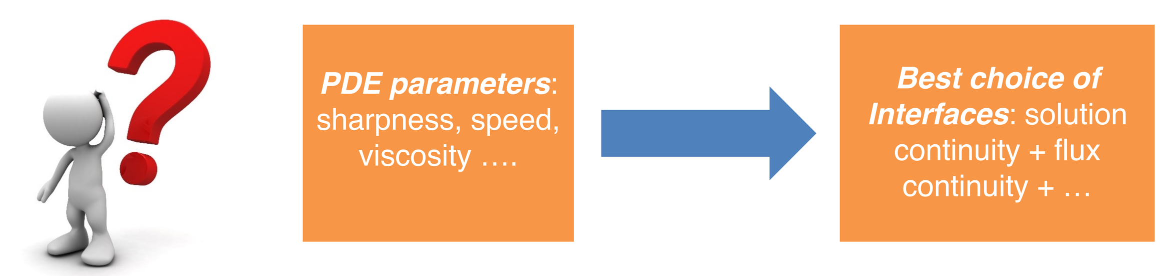
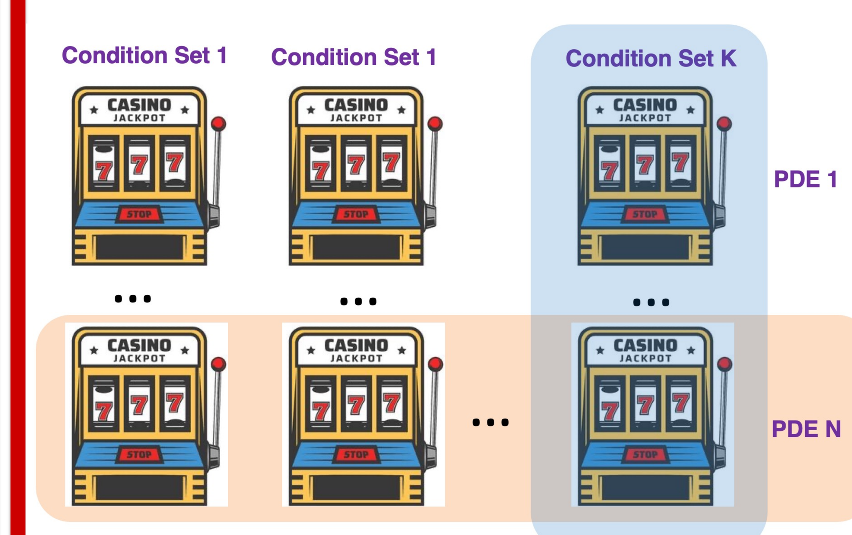


Our Contribution:

- ***METALIC***: META Learning of Interface Conditions
- A systematic method that select ***optimal interface*** conditions for ***a family of PDEs***
- Also considers the **training stages** characterized by PINNs

Methods

Contextual MAB for Interface Selection (*METALIC-Single*):



Payoffs varying across different PDEs

Payoffs are correlated according to PDE parameters

- *State / context space*: PDE parameters $\mathcal{X} \subset \mathbb{R}^d$
- *Action space P*: the power set of
  $$\mathcal{S} = \{I_1, \ldots, I_s\}$$
  $e.g.\ a = [0, 1, 1, 0, 1, 0, 1, 0, 0]$
- *Reward*: negative L2 relative error
- *Reward function*:
  $$r : \mathcal{X} \times \mathcal{P} \to \mathbb{R}$$

Reward modeling: Gaussian Process $r \sim \mathcal{GP}\left(0, \kappa\left([\boldsymbol{\beta}, \mathbf{a}], [\boldsymbol{\beta}', \mathbf{a}']\right)\right)$

Product kernel $\kappa\left([\boldsymbol{\beta}, \mathbf{a}], [\boldsymbol{\beta}', \mathbf{a}']\right) = \kappa_1(\boldsymbol{\beta}, \boldsymbol{\beta}')\kappa_2(\mathbf{a}, \mathbf{a}')$

(Continuous) PDE parameters

$$\kappa_1(\boldsymbol{\beta}, \boldsymbol{\beta}') = \exp(-\tau_1 \|\boldsymbol{\beta} - \boldsymbol{\beta}'\|^2)$$

(Binary Encodings) interface selection

$$\kappa_2(\mathbf{a}, \mathbf{a}') = \exp\left(\tau_2 \cdot \frac{1}{q}\sum_{i=1}^{q} \mathbb{1}(a_i = a_i')\right)$$

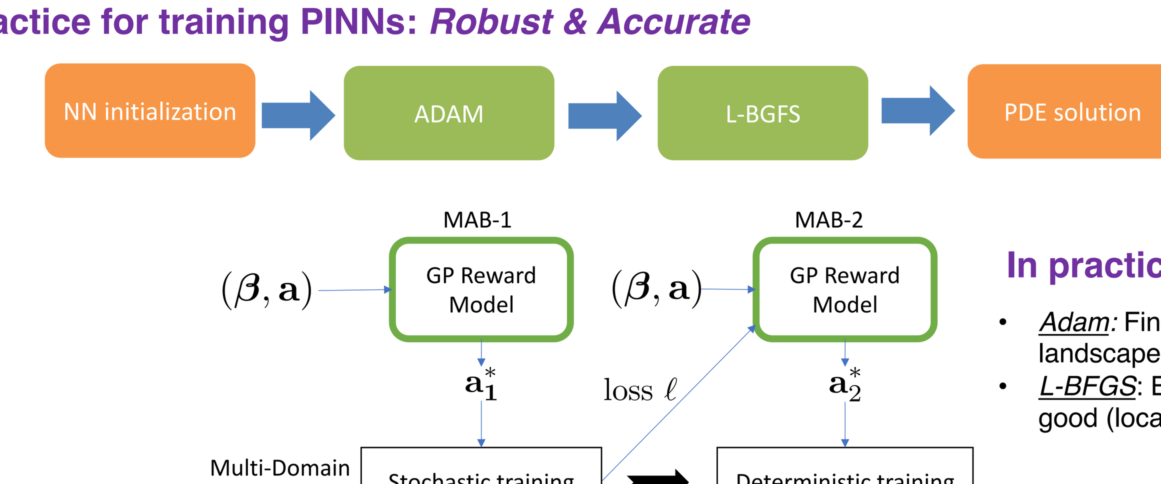
Predictive distribution of reward $p(\widehat{r}|\mathcal{D}, \boldsymbol{\beta}, \mathbf{a}) = \mathcal{N}\left(\widehat{r}|\mu(\mathbf{a}, \boldsymbol{\beta}), \sigma^2(\mathbf{a}, \boldsymbol{\beta})\right)$

$$\mathrm{UCB}(\mathbf{a}) = \mu(\mathbf{a}, \boldsymbol{\beta}) + c_t \cdot \sigma(\mathbf{a}, \boldsymbol{\beta})$$

$$\mathrm{TS}(\mathbf{a}) \sim p(\widehat{r}|\mathcal{D}, \boldsymbol{\beta}, \mathbf{a})$$

Two-Stages Interface Selection (*METALIC-Sequential*):

Best practice for training PINNs: *Robust & Accurate*



In practice to train PINNs

- *Adam:* Find a nice valley of loss landscape
- *L-BFGS*: Ensure convergence to good (local) minimum

(Discounted) Two-stages reward $r_1 = -\xi_1 + \gamma \cdot (-\xi_2) \quad r_2 = -\xi_2$

Theoretical guarantees (METALIC-Single):

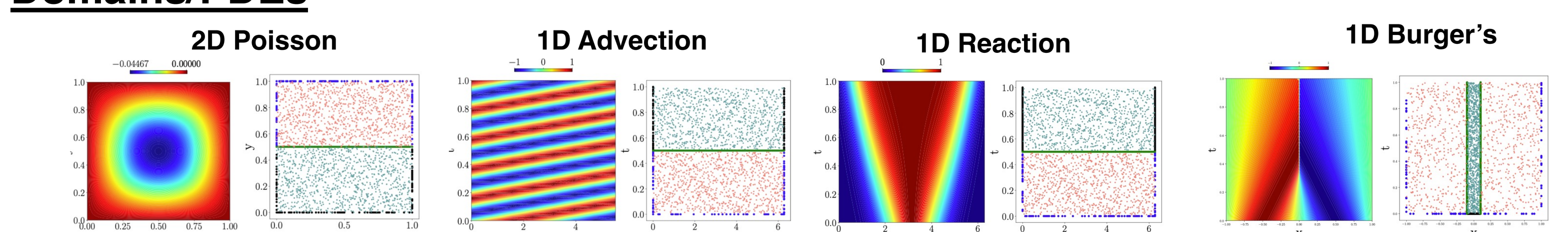
- Consider a sequence of PDEs: $\{\beta_t\}$
- Instantaneous regret: $\zeta_t = \xi(\beta_t, \mathbf{a}_t) - \xi(\beta_t, \mathbf{a}_t^*)$
- Accumulated regret: $R_T = \sum_{t=1}^{T} \zeta_t$

$$\lim_{T\to\infty} \frac{\mathbb{E}[R_T]}{T} = 0$$

Roughly speaking, for enough long run, our MAB guarantees to find the optimal conditions for every sequence of PDEs

Experimental Results

Domains/PDEs



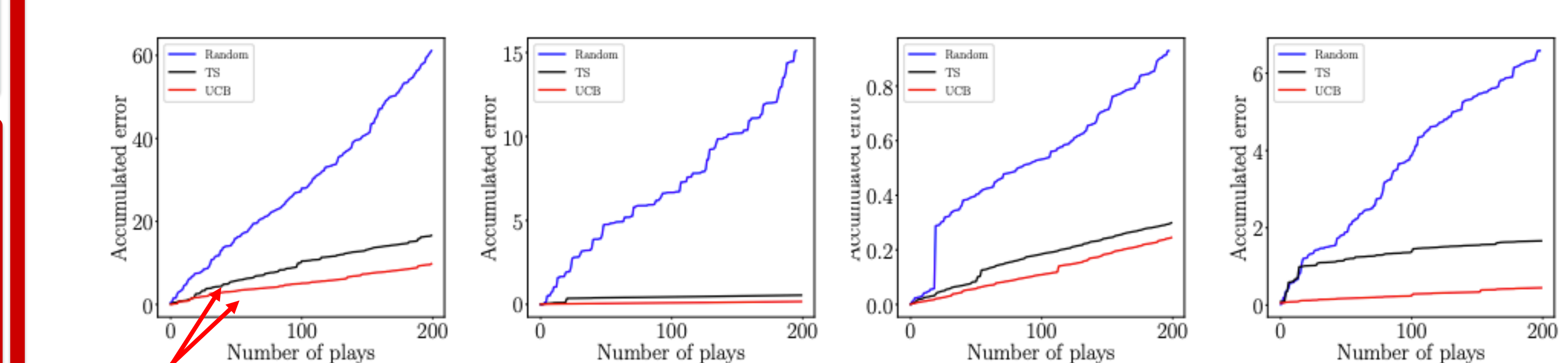
2D Poisson: $u_{xx} + u_{yy} = \widetilde{f}(x, y; s)$, $\widetilde{f}(x, y; s) = \frac{f(x, y; s)}{\max_{x,y} f(x, y; s)}$

1D Advection: $u_t + \beta u_x = 0$, $u(x, t) = h(x - \beta t)$, $h(x) = \sin(x)$

1D Reaction: $u_t - \rho u(1 - u) = 0$, $u(x, 0) = e^{-\frac{(x-\pi)^2}{2(\pi/4)^2}}$

1D Burger's: $u_t + uu_x = \nu u_{xx}$, $u(x, 0) = -\sin(\pi x)$

Online Performance (*Trial and Error*)

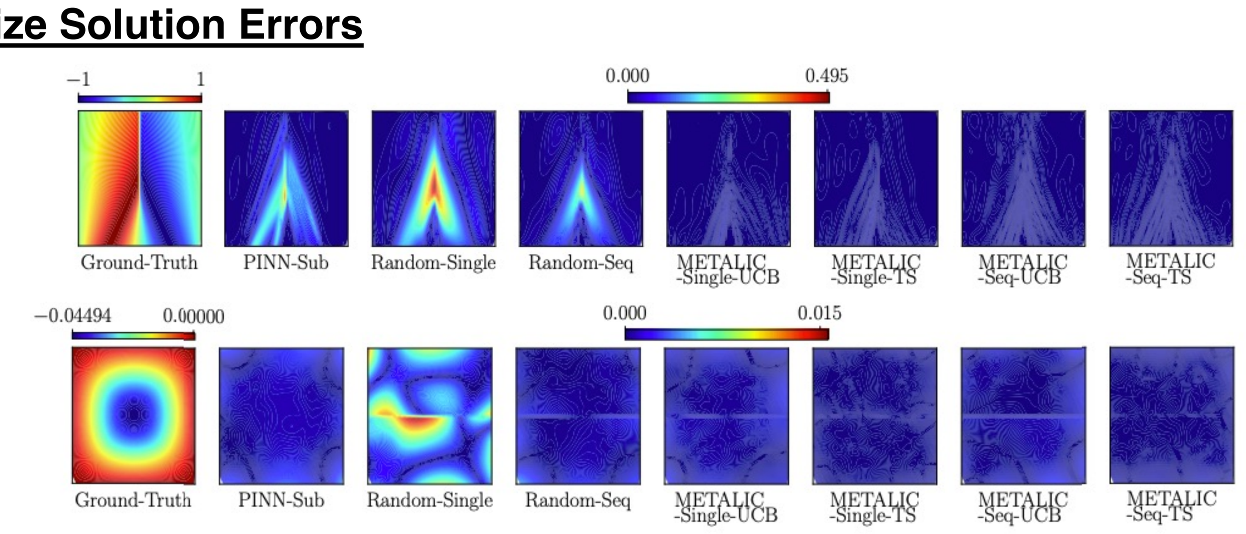


(a) Poisson equation (b) Advection equation (c) Reaction equation (d) Burgers' equation

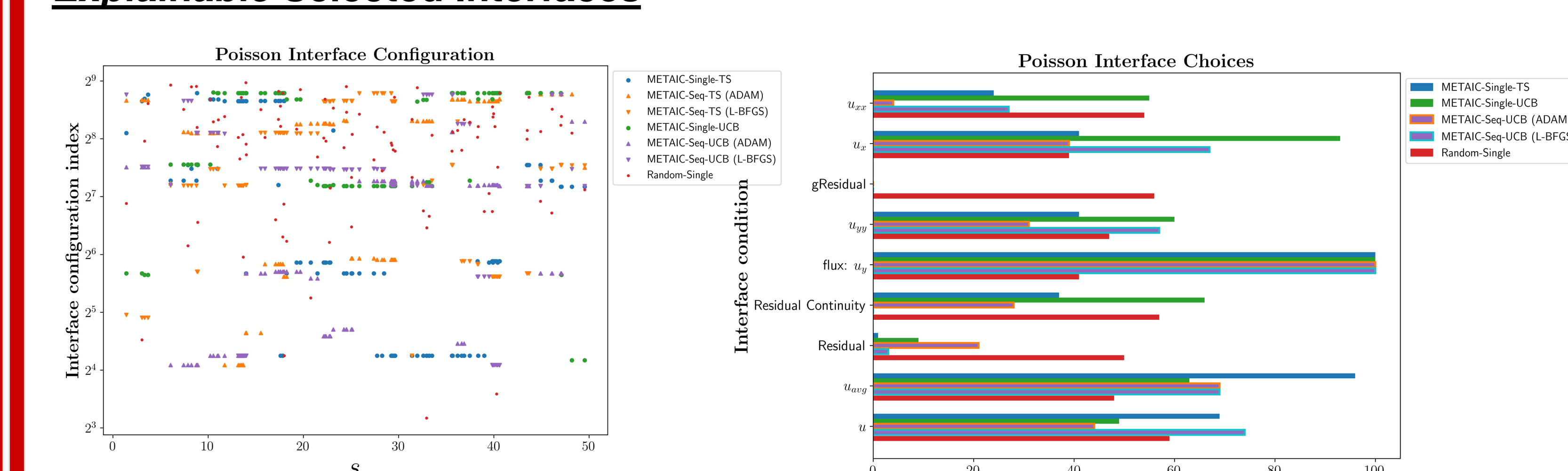
Offline Performance

	Method	Poisson	Advection	Reaction	Burger's
	Random-Single	0.3992 ± 0.0037	0.07042 ± 0.01575	0.00612 ± 0.000278	0.04021 ± 0.00057
	Random-Seq	0.3004 ± 0.0032	0.03922 ± 0.00919	0.01284± 0.000707	0.03486 ± 0.00066
	PINN-Sub	0.03078 ± 0.00177	0.00130 ± 8.108e-5	0.00213 ± 0.00021	0.00738 ± 0.00313
Double Volumed PINNs	PINN-Merge-H	0.02398 ± 0.00144	0.00098 ± 5.038e-5	0.00223 ± 0.00026	0.00951 ± 0.00390
Double Volumed PINNs	PINN-Merge-V	0.02184 ± 0.00211	0.00079 ± 3.391e-5	**0.00099 ± 0.00013**	0.00276 ± 0.00041
Our methods	METALIC-Single-TS	0.02503 ± 0.0002	0.00079 ± 4.5897e-5	0.00204 ± 1.013e-4	**0.00109 ± 1.306e-5**
Our methods	METALIC-Single-UCB	0.0245± 0.0002	0.00078 ± 3.6771e-5	0.00102 ± 8.945e-6	0.00161 ± 2.939e-5
Our methods	METALIC-Seq-TS	0.01639± 9.5384e-5	0.00078 ± 3.6473e-5	**0.00099 ± 8.4704e-6**	0.00152 ± 5.571e-5
Our methods	METALIC-Seq-UCB	**0.01406 ± 9.1099e-5**	**0.00070 ± 3.2790e-5**	**0.00099 ± 5.999e-6**	0.00139 ± 3.948e-5

Visualize Solution Errors



Explainable Selected Interfaces



- Predicts in groupings vs. random
- METALIC-Single differs from METALIC-Seq
- Start of training requires different conditions than the end of training

- Gradient-enhanced Residual never chosen
- Robust METALIC able to distinguish valid and invalid terms
- Agrees with preliminary Poisson study that flux is necessary