Meta Learning of Interface Conditions for Multi-Domain PINNs

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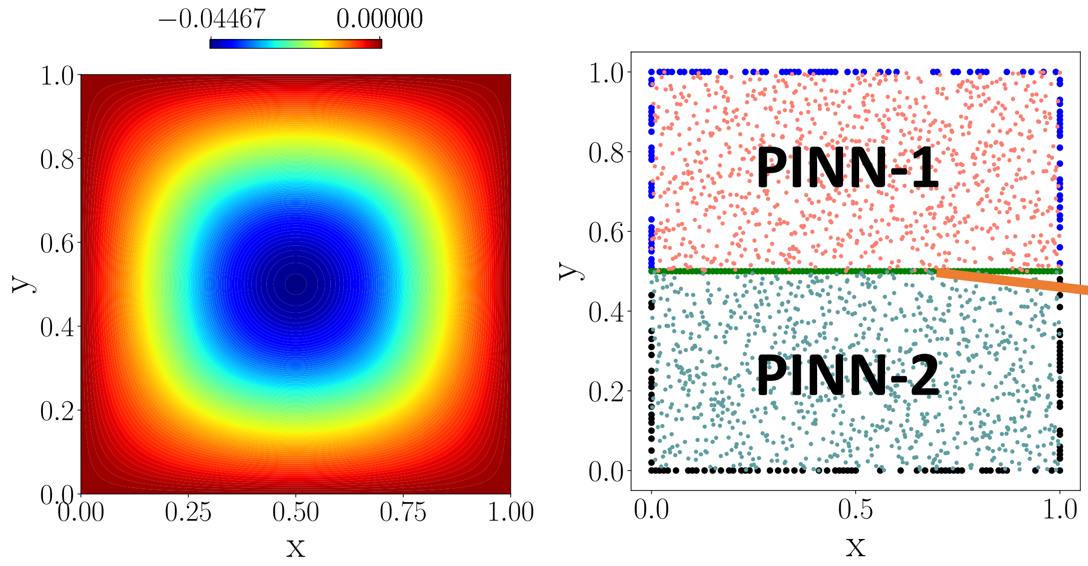
* equal contribution

PINNs with Domain Decomposition



(a) Solution at $s = 20$ (b) Subdomains

Some 2D Poisson Equation with an interior-square source parameterized by *s*

$$u_{xx} + u_{yy} = \tilde{f}(x, y; s)$$

where $(x, y) \in [0,1] \times [0,1]$, $\tilde{f}(x, y; s) = f(x, y; s)/\max_{x,y} f(x, y; s)$, and

$$f(x,y;s) = [\mathrm{erf}((x-0.25)s) - \mathrm{erf}((x-0.75)s)] \cdot [\mathrm{erf}((y-0.25)s) - \mathrm{erf}((y-0.75)s)], \quad s \in [0, 50]$$

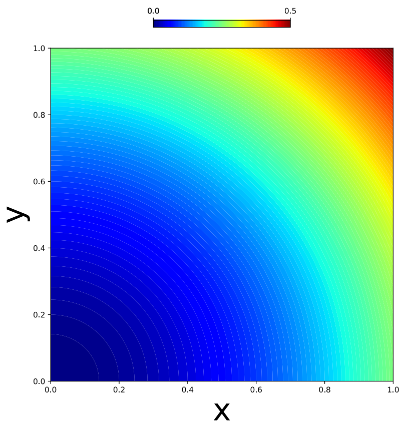
Advantages

- Reduce problem complexity
- Possibly use simpler NNs
- Allow parallelization

How to select problem-specific interface conditions?

- Each problem, according to its own properties, might demand a **different** set of conditions
- Adding inappropriate conditions can hurt the performance
- Naively adding *all* conditions increases the optimization challenge

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



$u_{xx} + u_{yy} = 1$

META Learning of Interface Conditions (METALIC)

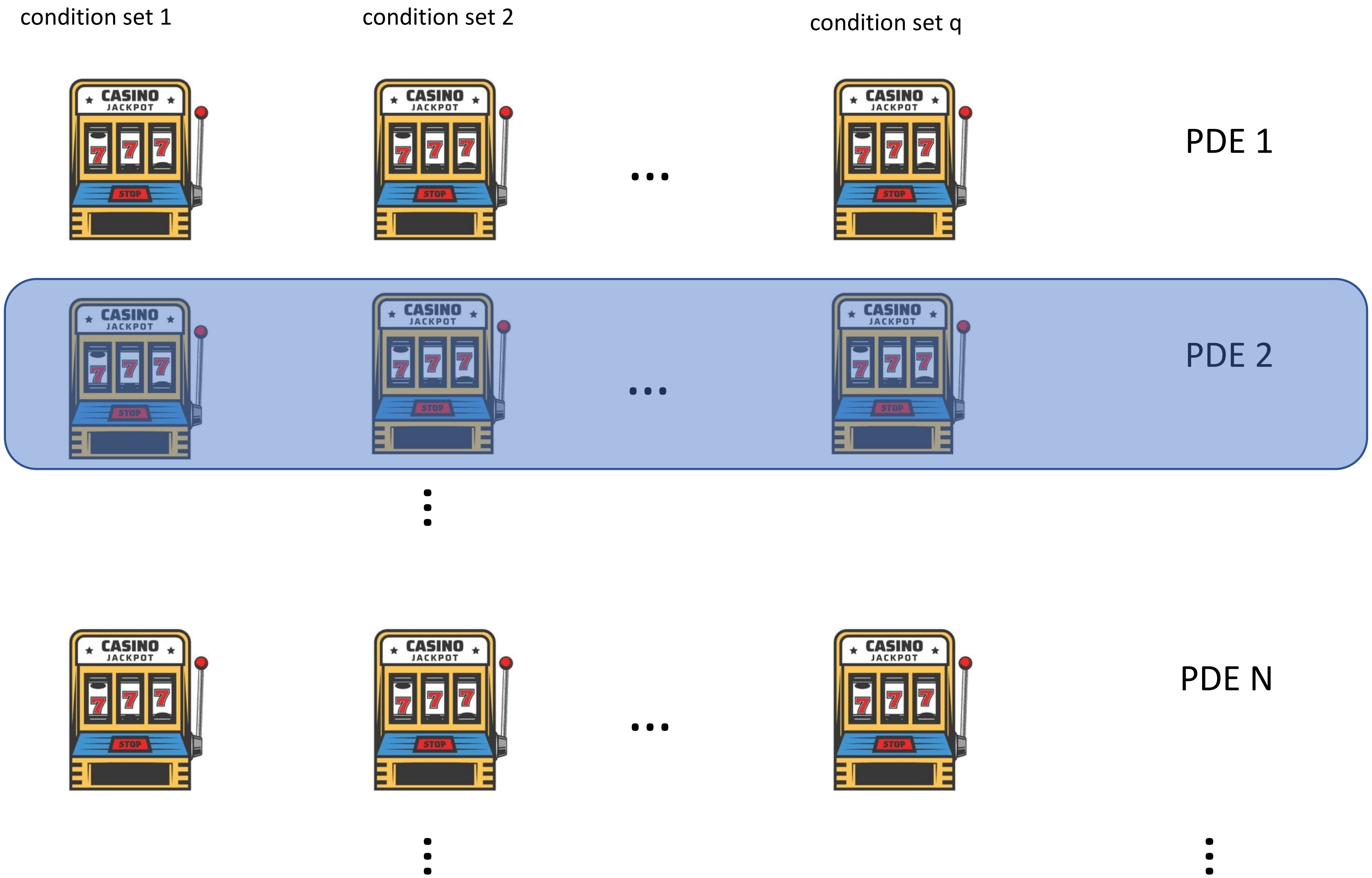
1. Given a parameterized PDE family *A* and domain decomposition: each PDE in *A* is parameterized by $\boldsymbol{\beta} \in \mathcal{X} \subset \mathbb{R}^d$

2. Given a set of interface conditions $\mathcal{S} = \{I_1, \ldots, I_s\}$

Goal: $\boldsymbol{\beta} \in \mathcal{X} \subset \mathbb{R}^d \longrightarrow I(\boldsymbol{\beta}) \subseteq \mathcal{S}$

The **best set of conditions** for the multi-domain PINNs to solve the PDE parameterized by $\boldsymbol{\beta}$

METALIC-Single: *contextual* MAB for the entire training course



- Payoffs varying across different PDEs
- Payoffs are correlated according to PDE parameters

METALIC-Single: *contextual* MAB for the entire training course

- State/context space: PDE parameter space $\mathcal{X} \subset \mathbb{R}^d$
- Action space *P*: the power set of $\mathcal{S} = \{I_1, \ldots, I_s\}$, i.e., all subsets of *S*. Each action means pulling the lever of one slot machine
- Reward: the negative L_2 relative solution error
- Reward function:

$$(\mathcal{X}, \mathcal{P}, r(\cdot, \cdot))$$

$$r : \mathcal{X} \times \mathcal{P} \to \mathbb{R}$$

$$vec = [0, 1, 1, 0, 1, 0, 1, 0, 0]$$

PDE parameters

Interface condition set

Negative solution error of the entire training of multi-domain PINN

METALIC-Single

- Use GP to online estimate the reward function

Gaussian noise model for the observed reward

$$r \sim \mathcal{GP}\left(0, \kappa\left([\boldsymbol{\beta}, \mathbf{a}], [\boldsymbol{\beta}', \mathbf{a}']\right)\right) \quad y \sim \mathcal{N}(y|r, \sigma_0^2)$$

PDE parameters

Binary encodings of the action: e.g., 1001100

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

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

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

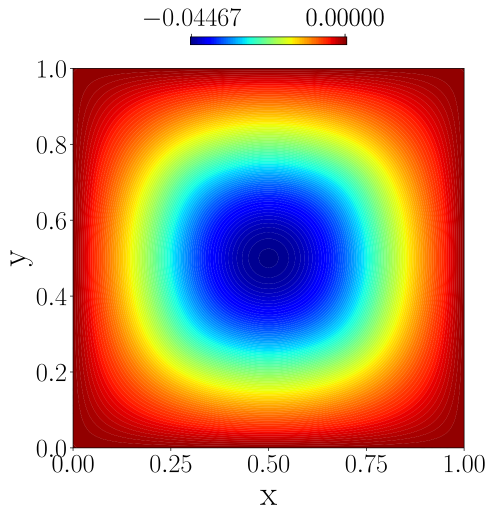
Experiments

2D Poisson Equation

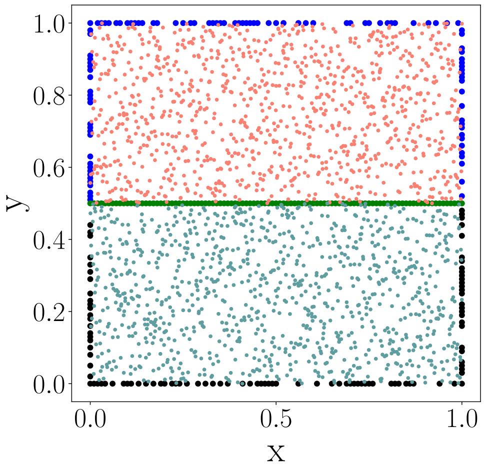
$$u_{xx} + u_{yy} = \widetilde{f}(x, y; s) \quad (x, y) \in [0, 1] \times [0, 1]$$

$$\widetilde{f}(x, y; s) = \frac{f(x, y; s)}{\max_{x,y} f(x, y; s)}$$

$$f(x, y; s) = [\mathrm{erf}((x - 0.25)s) - \mathrm{erf}((x - 0.75)s)] \cdot [\mathrm{erf}((y - 0.25)s) - \mathrm{erf}((y - 0.75)s)],$$



(a) Solution at $s = 20$



(b) Subdomains

Experiments

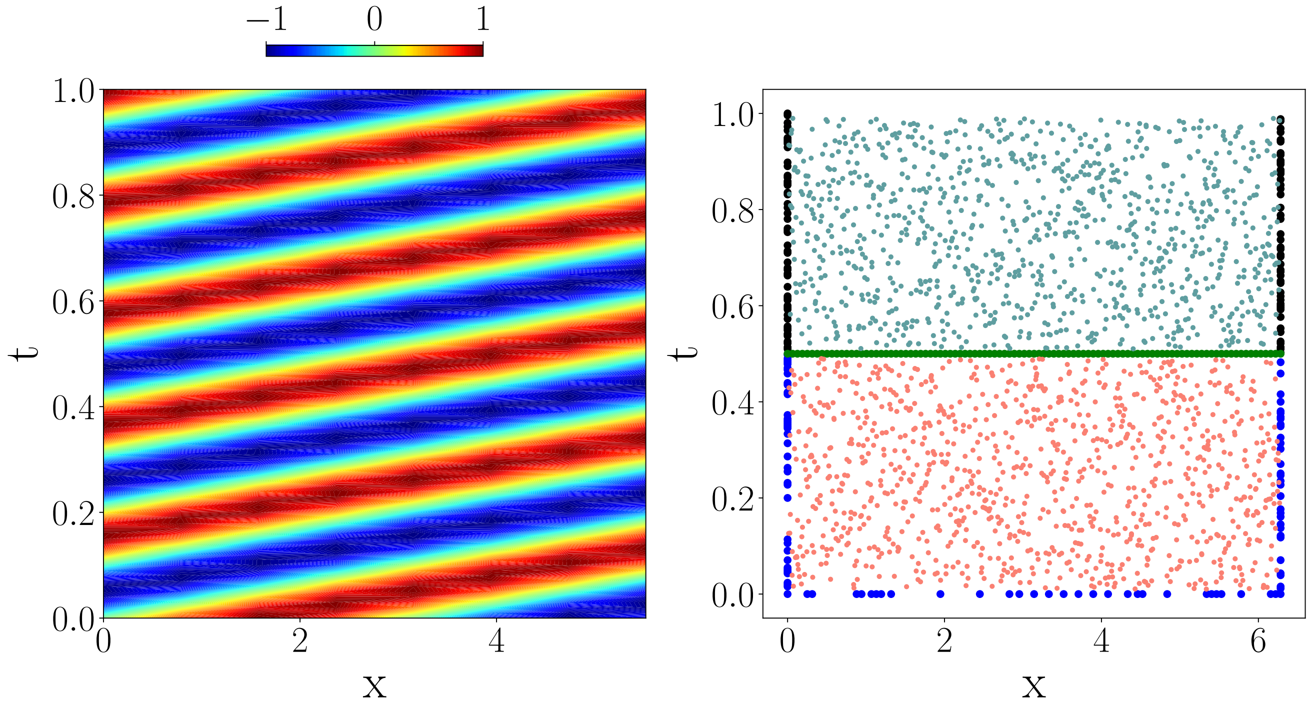
1D Advection Equation

$$u_t + \beta u_x = 0$$

$$x \in [0, 2\pi],\ t \in [0, 1]$$

$$u(x,t) = h(x - \beta t)$$

$$h(x) = \sin(x)$$



(a) Solution at $\beta = 30$ (b) Subdomains

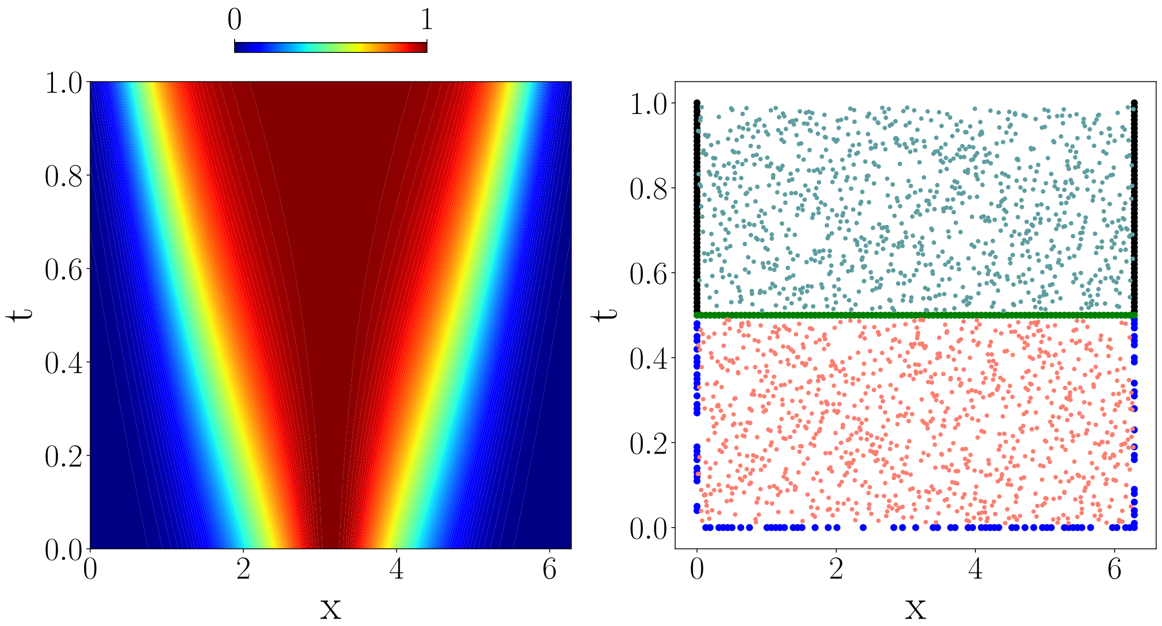
Experiments

1D Reaction Equation

$$u_t - \rho u(1-u) = 0$$

$$x \in [0, 2\pi],\ t \in [0, 1]$$

$$u(x, 0) = e^{-\frac{(x-\pi)^2}{2(\pi/4)^2}}$$



(a) Solution at $\rho = 5.0$ (b) Subdomains

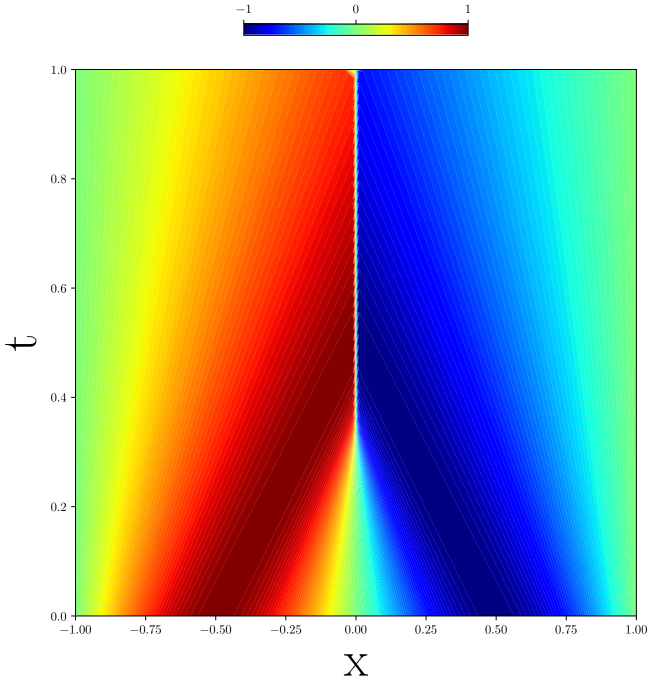
Experiments

Burger's equation

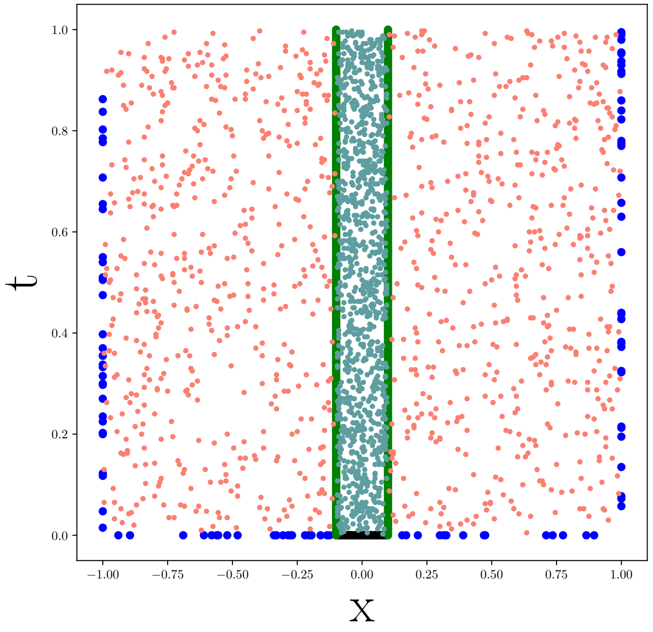
$$u_t + uu_x = \nu u_{xx}$$

$$x \in [-1, 1], t \in [0, 1]$$

$$u(x, 0) = -\sin(\pi x)$$

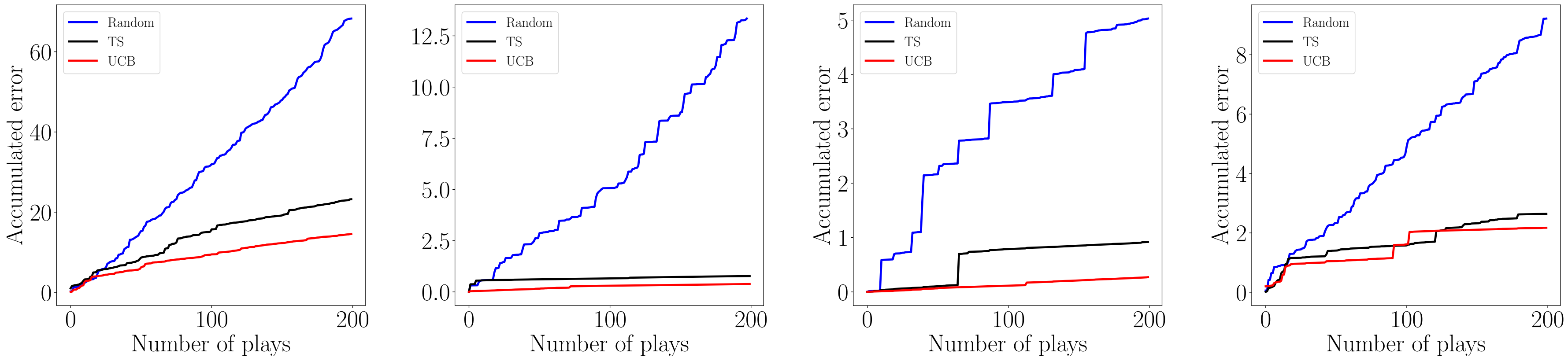


(a) Solution at $\nu = 0.001$



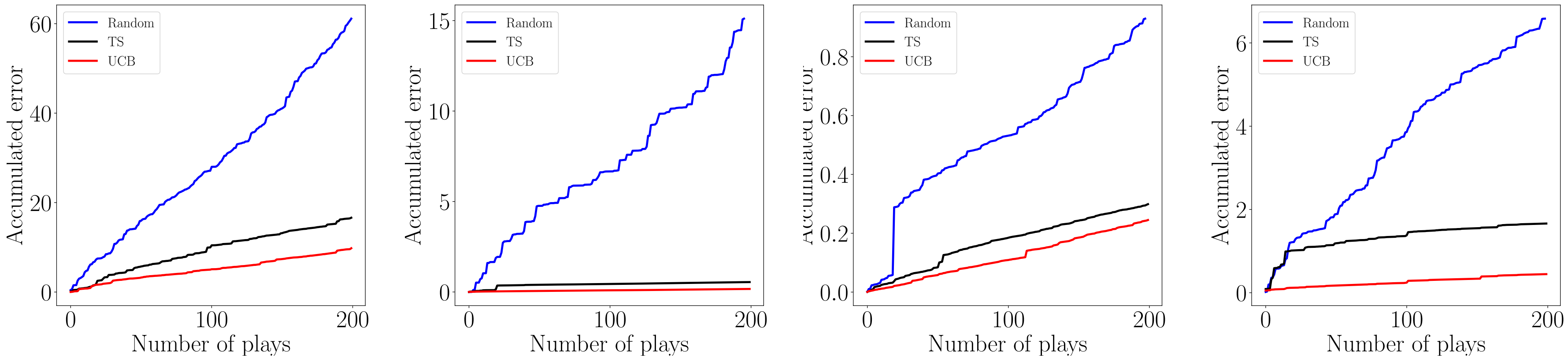
(b) Subdomains

Online performance: #plays vs. accumulated solution error



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

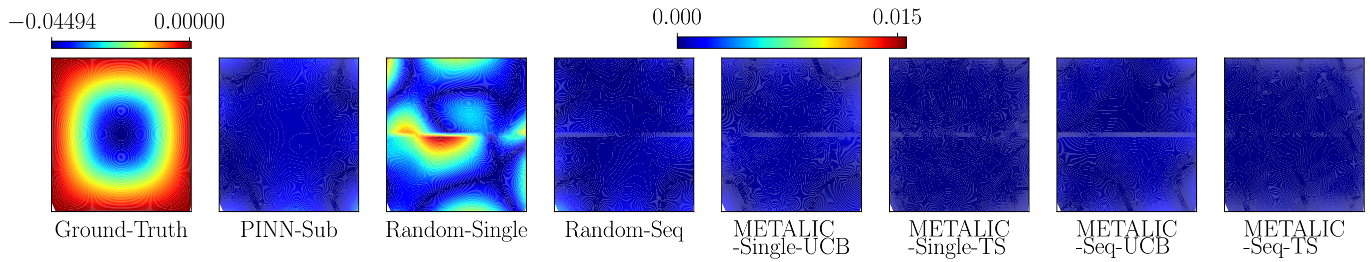
Figure 6: Online performance of METALIC-single.



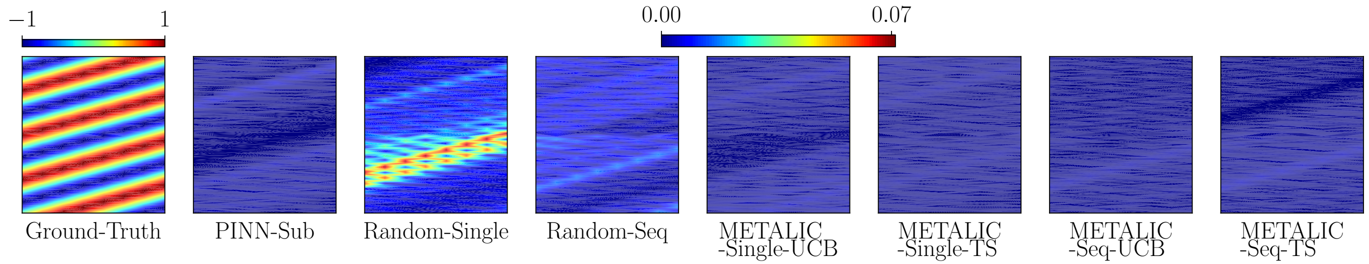
(a) Poisson equation (b) Advection equation (c) Reaction equation (d) Burgers' equation

Figure 7: Online performance of METALIC-seq.

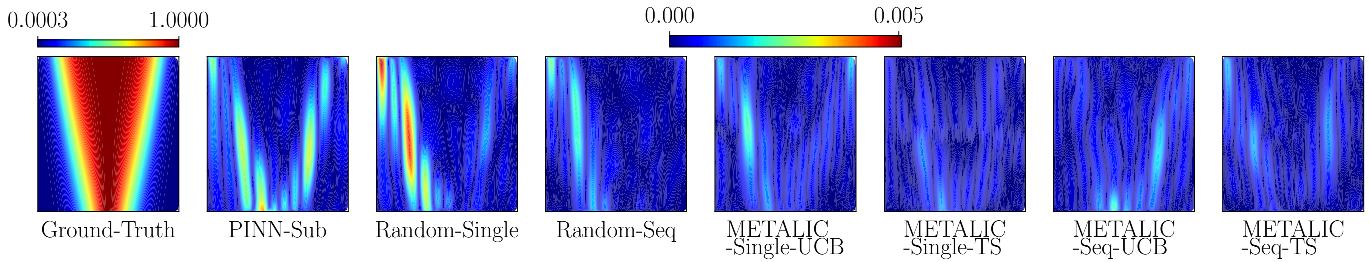
Point-wise error



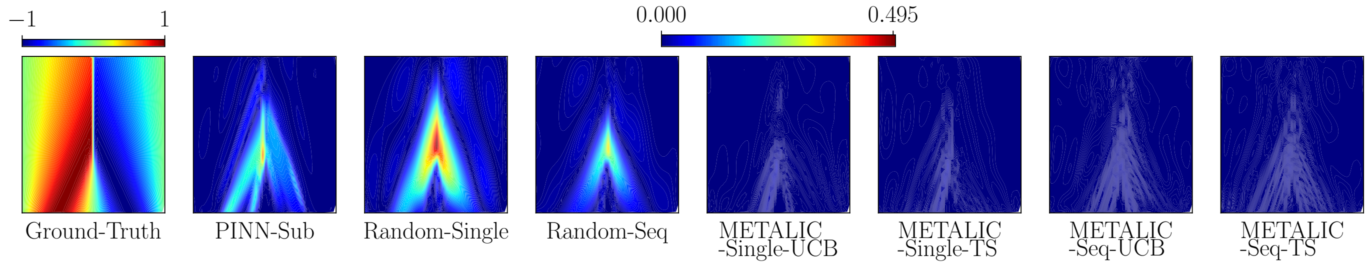
(a) Poisson equation ($s = 46.1$)



(b) Advection equation ($\beta = 24.02$)



(c) Reaction equation ($\rho = 4.1$)



(d) Burgers’ equation ($\nu = 0.0036$)

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