A Unified Hard-Constraint Framework for Solving Geometrically Complex PDEs

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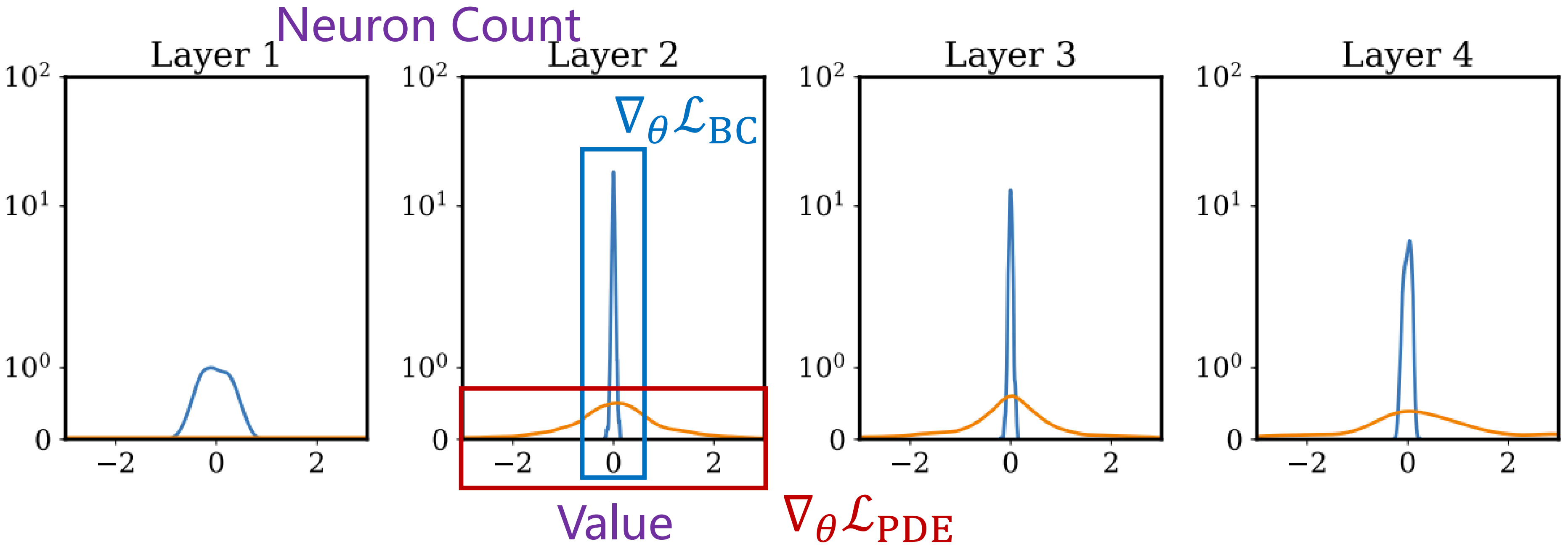
Background

Solving PDEs via Neural Networks

- **PINNs → PDEs with Boundary Conditions (BCs)**

$$\hat{u} \coloneqq \mathrm{NN}(\,\cdot\,;\boldsymbol{\theta}), \qquad \mathcal{L}(\boldsymbol{\theta}) \coloneqq \mathcal{L}_{\mathrm{PDE}}(\boldsymbol{\theta}) + \mathcal{L}_{\mathrm{BC}}(\boldsymbol{\theta})$$



Unbalanced Competition[1]: $|\nabla_\theta \mathcal{L}_{\mathrm{PDE}}| \gg |\nabla_\theta \mathcal{L}_{\mathrm{BC}}|$!

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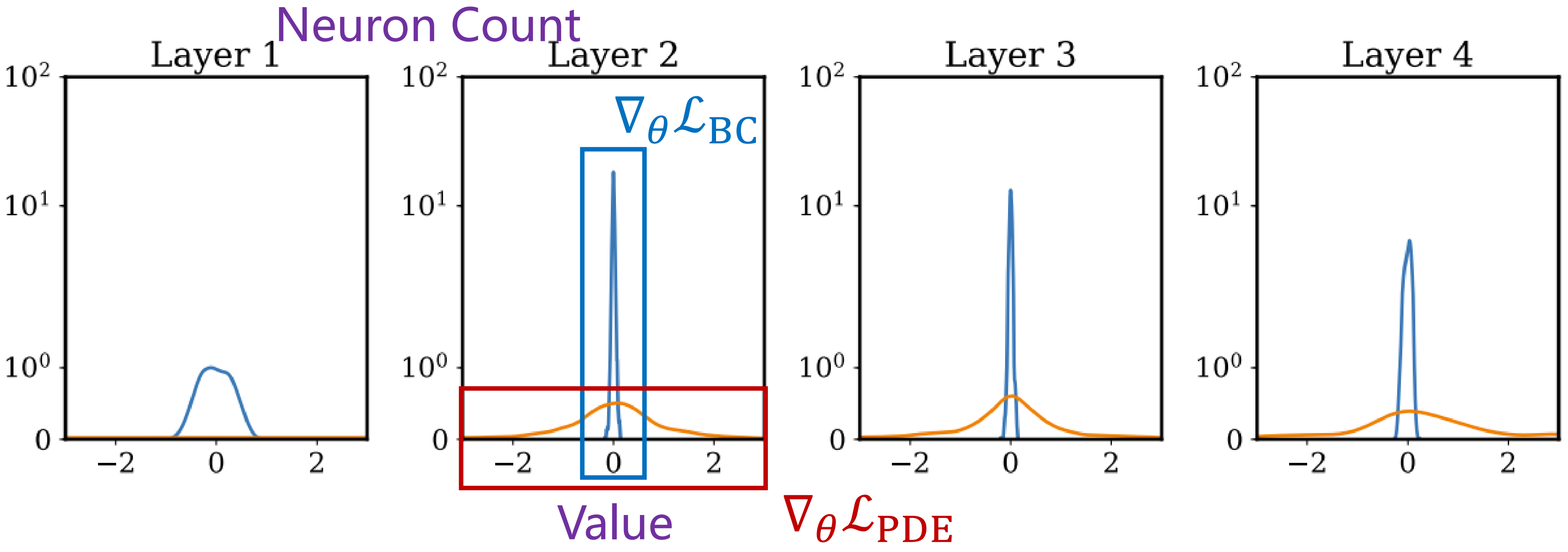

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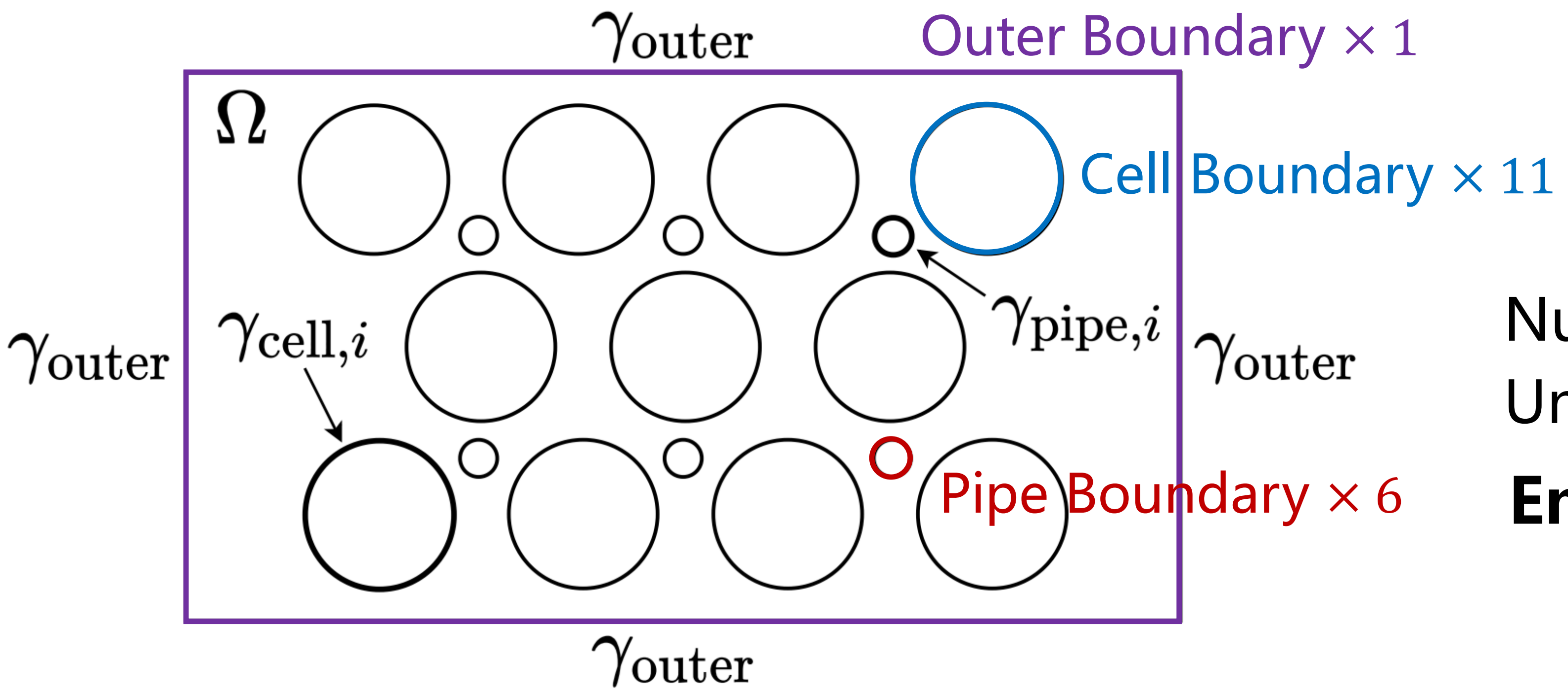
Geometrically Complex PDEs

- **Example:** a 2D battery pack



Number of BCs ↑

Unbalance Competition↑

Embed BCs into Ansatz!

Previous Work

Methods	Neumann BCs	Robin BCs	Complex Geometries	High Dimension	Meshless
Variational PINNs[2]	✗*	✗	✗	✓	✓
Hard-Constraint PINNs[3]	✗	✗	✗	✓	✓
Deep TFCs[4]	✓	✓	✗	✗	✓
Hard-Constraint CNNs[5]	✓	✓	✓	✗	✗
Our Proposed Method	✓	✓	✓	✓	✓

*Only applicable to homogeneous Neumann BCs

Method

Problem Formulation

- **PDE:**

$$\mathcal{F}[u(\boldsymbol{x})] = 0, \qquad \boldsymbol{x} = (x_1, \ldots, x_d) \in \Omega$$

with Dirichlet, Neumann, Robin BCs:

$$a_i(\boldsymbol{x})u + b_i(\boldsymbol{x})(\boldsymbol{n}(\boldsymbol{x}) \cdot \nabla u) = g_i(\boldsymbol{x}), \qquad \boldsymbol{x} \in \gamma_i, \qquad i = 1, \ldots, m,$$

where $\cup_{i=1}^{m} \gamma_i = \partial\Omega$, $\boldsymbol{n}$ is the (outward facing) unit normal.

- **Extra Fields:** $\boldsymbol{p} = \nabla u, \quad x \in \Omega \cup \partial\Omega$

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General Solution at Boundaries

- **Reformulated BC:**

$$a_i(\boldsymbol{x})u + b_i(\boldsymbol{x})(\boldsymbol{n}(\boldsymbol{x}) \cdot \boldsymbol{p}) = g_i(\boldsymbol{x}), \qquad \boldsymbol{x} \in \gamma_i,$$

- **The General Solutions Go With:**

$$(u^{\gamma_i}, \boldsymbol{p}^{\gamma_i}) = \boldsymbol{B}(\boldsymbol{x})\mathrm{NN}^{\gamma_i}(\boldsymbol{x}; \boldsymbol{\theta}^{\gamma_i}) + \tilde{\boldsymbol{n}}(\boldsymbol{x})\tilde{g}_i(\boldsymbol{x}),$$

where $\tilde{\boldsymbol{n}} = (a_i, b_i\boldsymbol{n})/\left(a_i^2 + b_i^2\right)^{1/2}$, $\tilde{g}_i = g_i/\left(a_i^2 + b_i^2\right)^{1/2}$,
$\mathrm{NN}^{\gamma_i}: \mathbb{R}^d \to \mathbb{R}^{d+1}$, $\boldsymbol{B}(\boldsymbol{x}) = \boldsymbol{I}_{d+1} - \tilde{\boldsymbol{n}}(\boldsymbol{x})\tilde{\boldsymbol{n}}(\boldsymbol{x})^{\top}$.

- It strictly **satisfies BC** and retains **expressive power**.

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- Gather the general solution at γ_i

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- **Our Final Ansatz:**

$$(\hat{u}, \widehat{\boldsymbol{p}}) = l^{\partial\Omega}(\boldsymbol{x})\mathrm{NN}(\boldsymbol{x}, \boldsymbol{\theta}) + \sum_{i=1}^{m} \exp[-\alpha_i l^{\gamma_i}(\boldsymbol{x})](u^{\gamma_i}, \boldsymbol{p}^{\gamma_i})$$

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Freedom Term

where $l^{\partial\Omega}, l^{\gamma_i}: \mathbb{R}^d \to \mathbb{R}$ are the distance function to $\partial\Omega$, γ_i, $\mathrm{NN}: \mathbb{R}^d \to \mathbb{R}^{d+1}$.

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Freedom Term — General Solution at γ_i

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Experiments

Experimental Results

- **Evaluation Metrics:**
  - Mean Absolute Error (**MAE**), Mean Absolute Percentage Error (**MAPE**)
  - Weighted Mean Absolute Percentage Error (**WMAPE**):

$$\text{WMAPE} = \Sigma|\text{error}_i| \,/\, \Sigma|\text{truth}_i|$$

- **Baselines:**
  - **PINN**[6]**:** vanilla PINN
  - **PINN-LA**[7] **& PINN-LA-2:** PINN with learning rate annealing
  - **xPINN**[8] **& FBPINN**[9]**:** PINN with domain decomposition for geometrically complex PDEs
  - **PFNN**[10] **& PFNN-2**[11]**:** hard-constraint methods based on the variational formulation of PDEs

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Experimental Results

Result:

- Error $\downarrow > 70\%$
- Convergence $\uparrow$

Methods	Real-world Problems					
	2D Battery Pack		Airfoil (u_1)		High Dimension	
	MAE	MAPE	MAE	WMAPE	MAE	MAPE
PINN	0.0539	24.82%	0.4682	0.5924	0.0582	1.99%
PINN-LA	0.0661	27.06%	0.4018	0.5084	0.0235	0.78%
PINN-LA-2	0.0402	19.76%	0.5047	0.6385	0.0466	1.49%
FBPINN	0.0343	14.74%	0.4058	0.5134	-	-
xPINN	0.1454	54.70%	0.7188	0.9095	-	-
PFNN	0.2758	68.29%	-	-	0.1425	4.64%
PFNN-2	0.3215	59.62%	-	-	-	-
HC (**Ours**)	**0.0221**	**5.10%**	**0.2689**	**0.3402**	**0.0026**	**0.10%**

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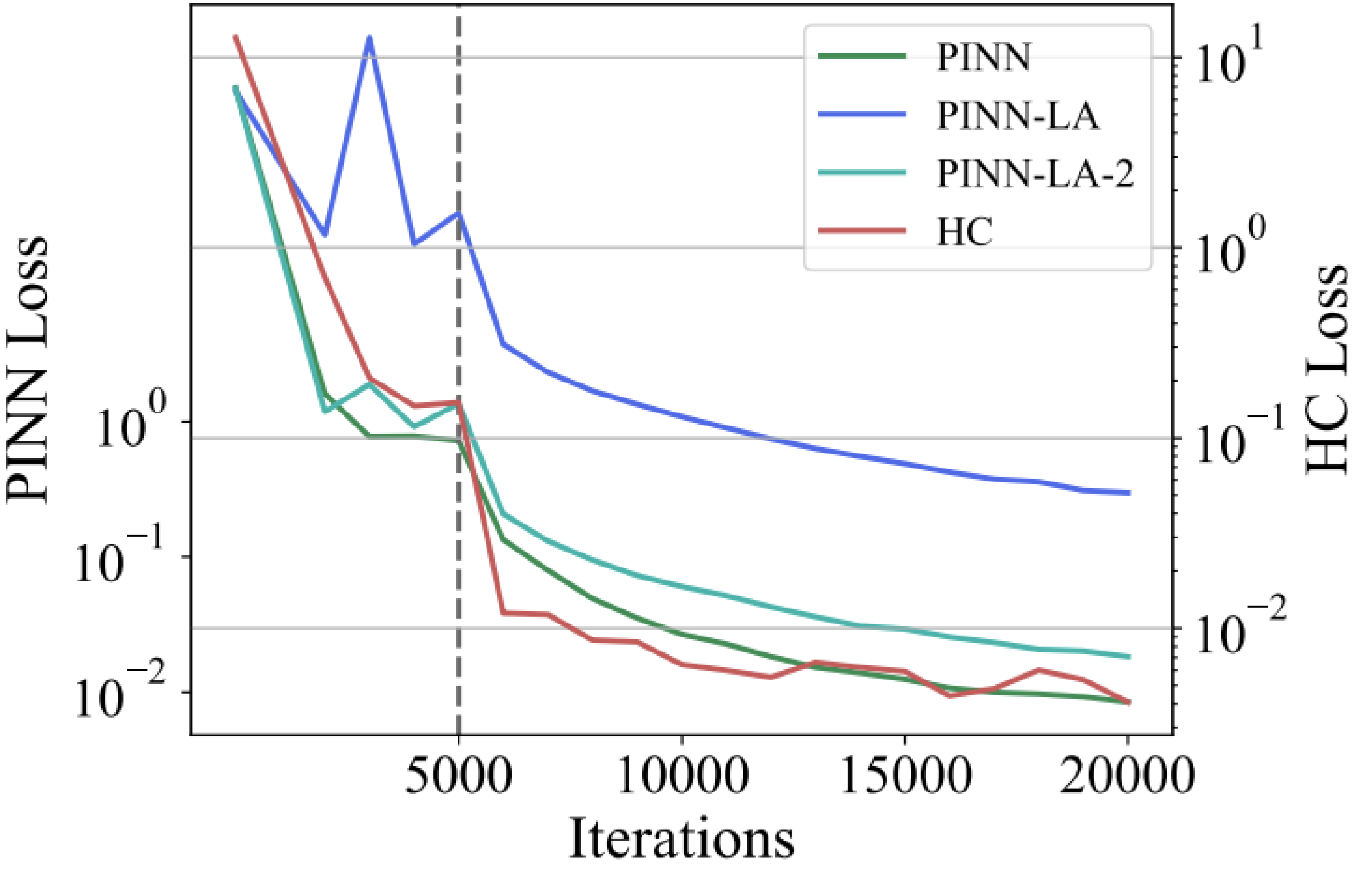

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Thank You!

Paper Link: https://arxiv.org/pdf/2210.03526.pdf

Code Link: https://github.com/csuastt/HardConstraint