PINNACLE: PINN Adaptive ColLocation and Experimental Points Selection

Gregory Kang Ruey Lau*[1,2] Apivich Hemachandra*[1] See-Kiong Ng[1] Bryan Kian Hsiang Low[1]

* Equal contribution [1] Department of Computer Science, National University of Singapore [2] CNRS@Create

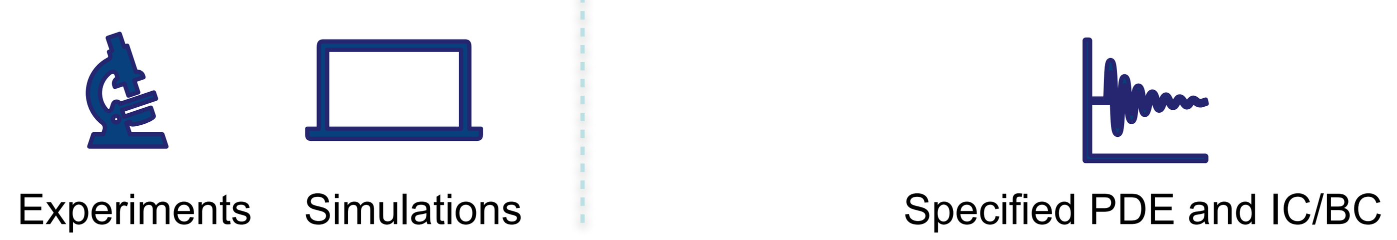
Scan me!

Training Point Selection in PINNs

- Physics-Informed Neural Networks (PINN) incorporate PDEs as soft constraints/regularization terms
- This makes PINNs hard to train, due to:
  - Different interacting training dynamics
  - A large number of training points needed

$$\mathcal{L}(\hat{u}_\theta; X) = \underbrace{\sum_{x \in X_s} \frac{(\hat{u}_\theta(x) - u(x))^2}{2N_s}}_{\text{EXP points}} + \lambda_p \underbrace{\sum_{x \in X_p} \frac{(\mathcal{N}[\hat{u}_\theta](x) - f(x))^2}{2N_p}}_{\text{PDE CL points}} + \lambda_b \underbrace{\sum_{x \in X_b} \frac{(\mathcal{B}[\hat{u}_\theta](x) - g(x))^2}{2N_b}}_{\text{IC/BC CL points}}$$

Experimental points (EXP points)	Collocation points (CL points)
From Data	Encodes Inductive Bias
Experiments, Simulations	Specified PDE and IC/BC



Can we jointly select all types of training points in order to improve the training of PINNs?

eNTK Eigenfunctions in Augmented Space

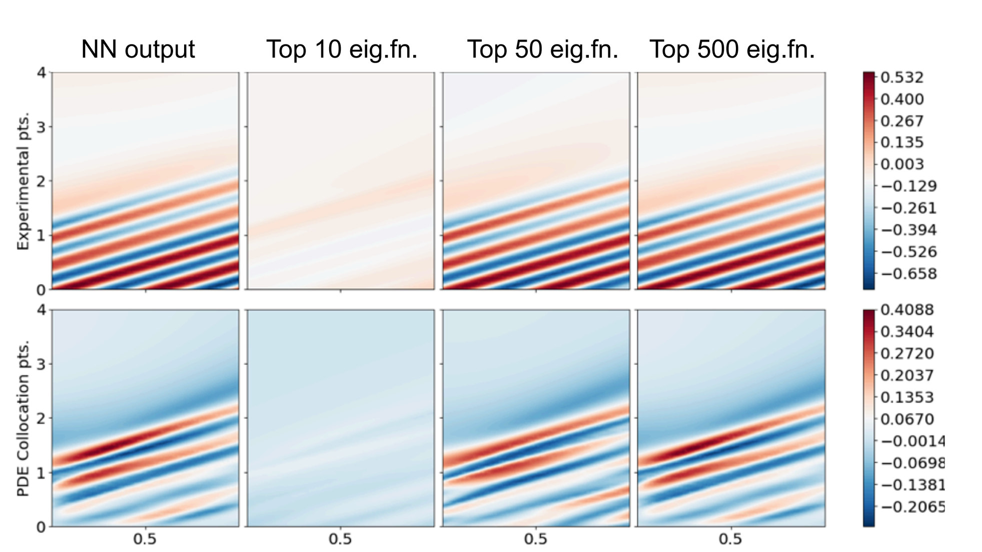
$$\mathcal{Z} = \underbrace{\{(x, \mathrm{s}) : x \in \mathcal{X}\}}_{\text{EXP points}} \cup \underbrace{\{(x, \mathrm{p}) : x \in \mathcal{X}\}}_{\text{PDE CL points}} \cup \underbrace{\{(x, \mathrm{b}) : x \in \partial\mathcal{X}\}}_{\text{IC/BC CL points}}$$

$$F[h](x, \mathrm{s}) = h(x), \quad F[h](x, \mathrm{p}) = \mathcal{N}[h](x), \quad F[h](x, \mathrm{b}) = \mathcal{B}[h](x)$$

Empirical NTK (eNTK)

$$\Theta_t(z, z') = \nabla_\theta F[\hat{u}_{\theta_t}](z) \, \nabla_\theta F[\hat{u}_{\theta_t}](z')^\top$$

Dominant eigenfunctions form basis of NN output in augmented space



Training Dynamics

- Residual component that aligns with dominant eigenfunctions will decay faster

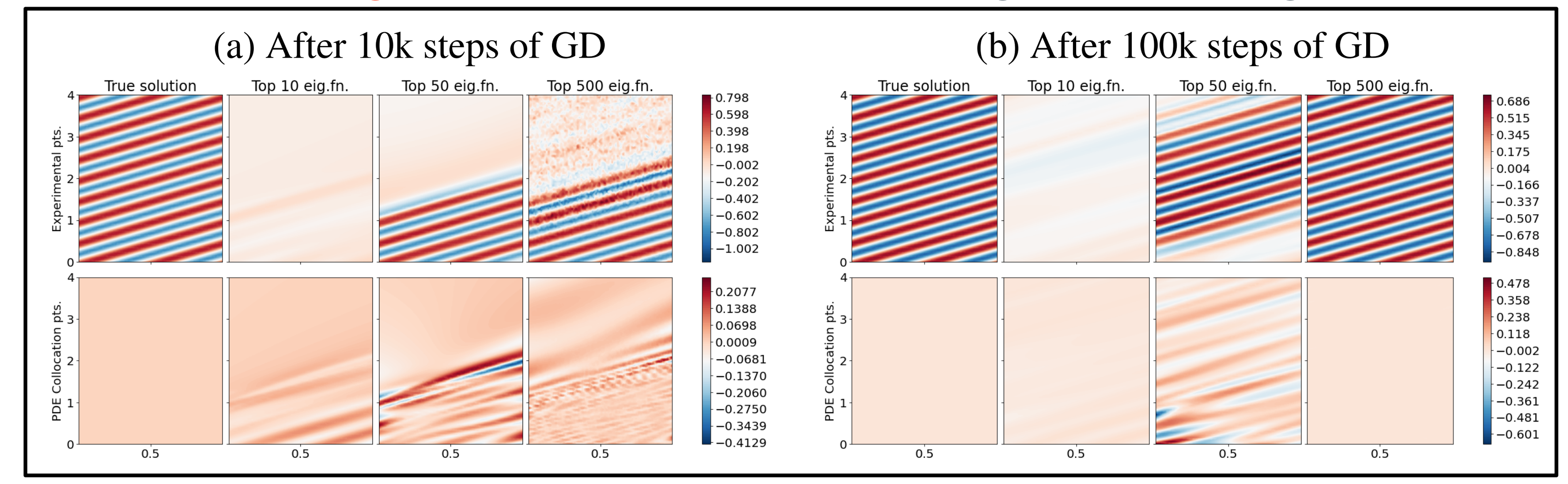
Convergence criterion

RKHS norm of residue change when trained on Z

$$\alpha(Z) \triangleq \|\Delta R_{\theta_t}(\cdot\,; Z)\|^2_{\mathcal{H}_{\Theta_t}} = \sum_{i=0}^{\infty} \lambda_{t,i}^{-1} \langle \Delta R_{\theta_t}(\cdot\,; Z), \psi_{t,i} \rangle^2_{\mathcal{H}_{\Theta_t}}$$

Criterion related to PINN generalization error bound (Thm. 1), and can be approximated using Nystrom approximation (Prop. 1)

- The eNTK eigenspectrum evolves throughout training



Algorithm: *Iterative phases of (1) point selection to maximize convergence degree and (2) PINN training*

Algorithm 1 PINNACLE

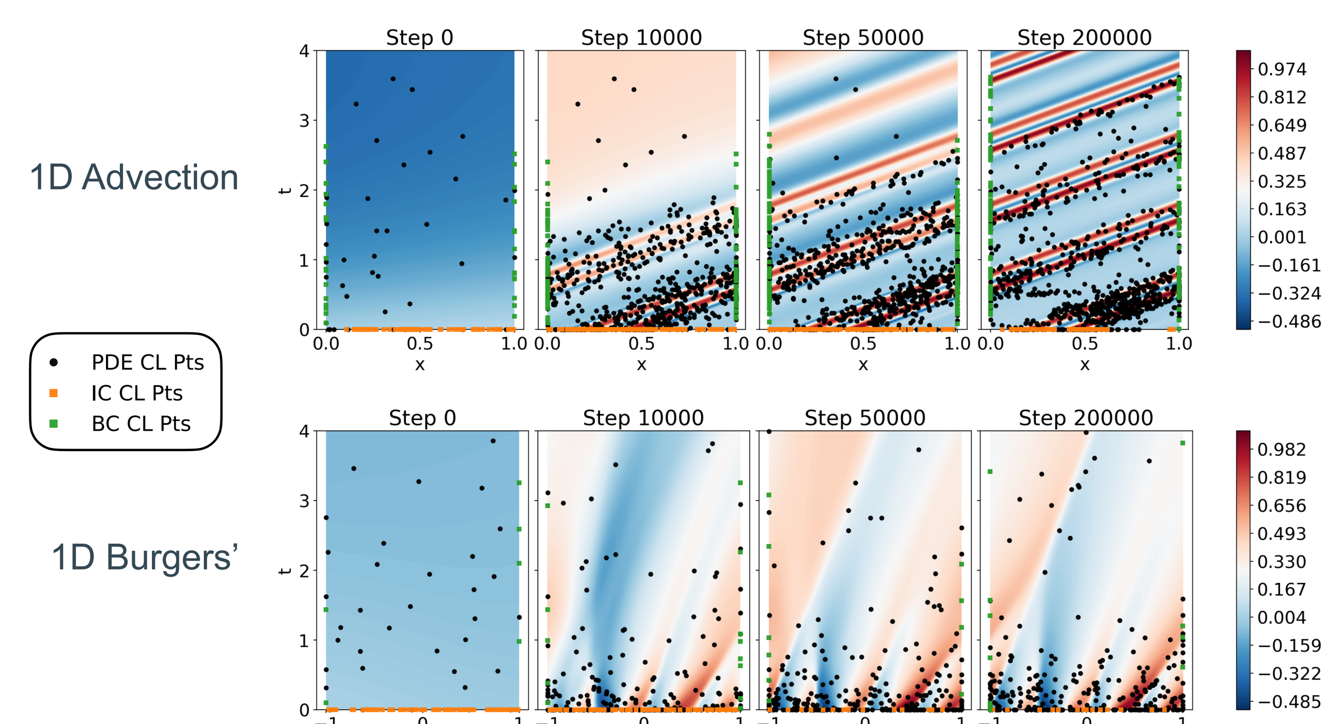
1. **Input:** PINN $\hat{u}_\theta$, learning rate η, number of iterations T, eNTK approx. error δ.
2. **repeat**
3. // Point selection phase
4. Randomly sample candidates Z_{pool} from $\mathcal{Z}$
5. Compute Θ_t using Nystrom approximation
6. Select subset $Z \subset Z_{\text{pool}}$ to fit constraint using SAMPLING or K-MEANS++
7. // Training phase
8. Compute $\bar{\Theta} = \Theta_t(Z_{\text{pool}})$
9. **for** $t' = t, \dots, t+T$ **do**
10. $\theta_{t'+1} \leftarrow \theta_{t'} - \eta \nabla_\theta \mathcal{L}(\hat{u}_{\theta_{t'}}; Z)$
11. Exit training if $\|\bar{\Theta} - \Theta_{t'}(Z_{\text{pool}})\| \geq \delta \|\bar{\Theta}\|$
12. **until** training converges or budget exhausted

- PINNACLE-S: Sample z with probability proportional to $\hat{\alpha}(z)$
- PINNACLE-K: Perform K-Means++ initialization on the embedding $z \mapsto \left(\hat{\lambda}_{t,i}^{1/2} \hat{a}_{t,i}(z)\right)_{i=1}^{p}$

Re-compute training points when eNTK has evolved with eigenfunctions that are more aligned with labels/true solution

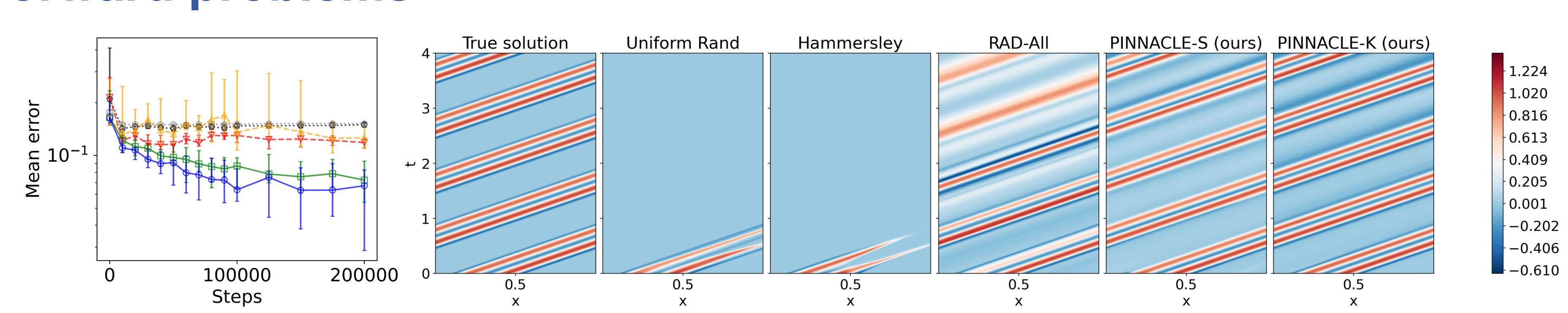
Empirical results: *PINNACLE outperforms benchmarks for various tasks with interpretable point selection*

Point selection behavior of PINNACLE



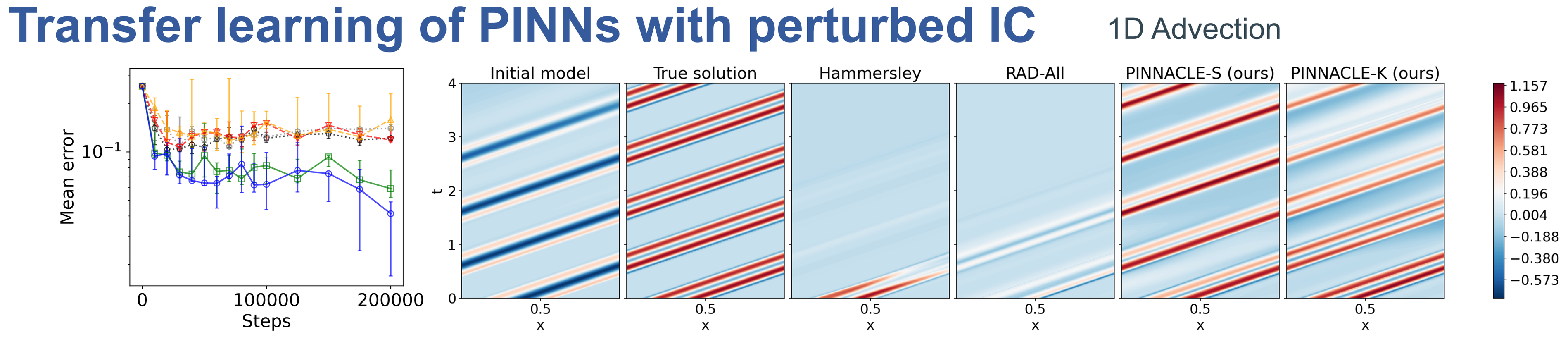
Forward problems

1D Advection

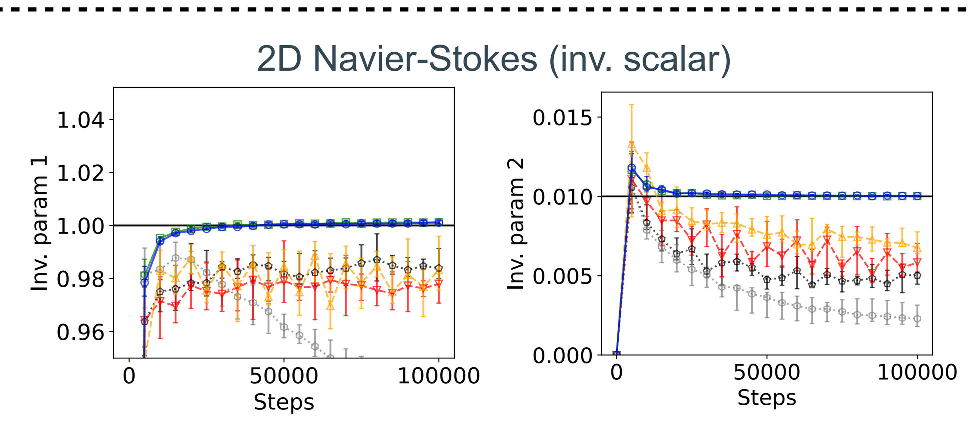


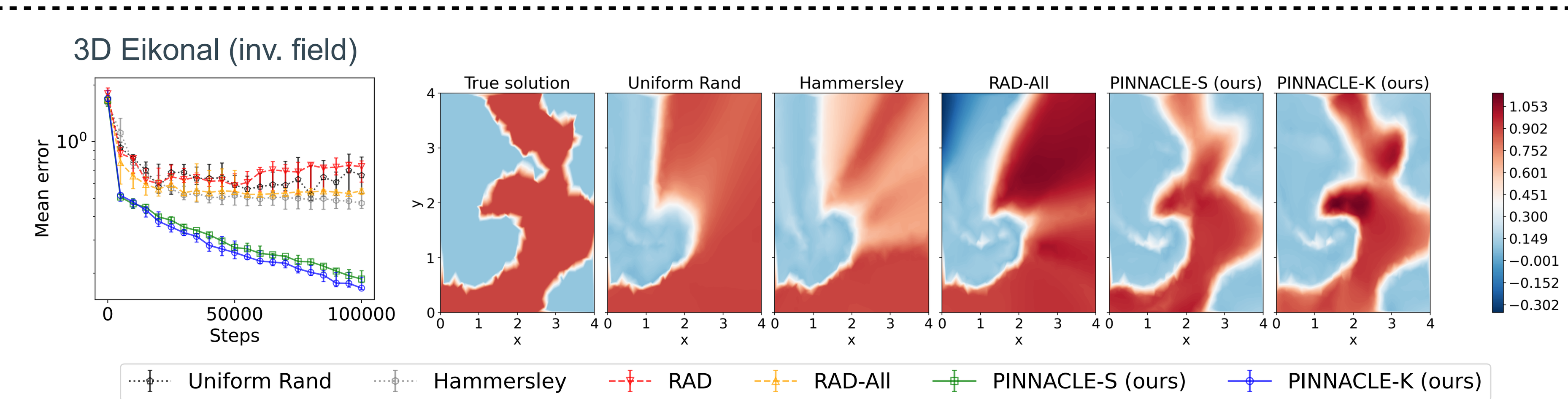
Transfer learning of PINNs with perturbed IC

1D Advection



Inverse problems





This research/project is supported by the National Research Foundation, Singapore under its AI Singapore Programme (AISG Award No: AISG-PhD/2023-01-039J).
This research is part of the programme DesCartes and is supported by the National Research Foundation, Prime Minister's Office, Singapore under its Campus for Research Excellence and Technological Enterprise (CREATE) programme.