SetPINNs: Set-based Physics-Informed Neural Networks

AISTATS 2026 Spotlight

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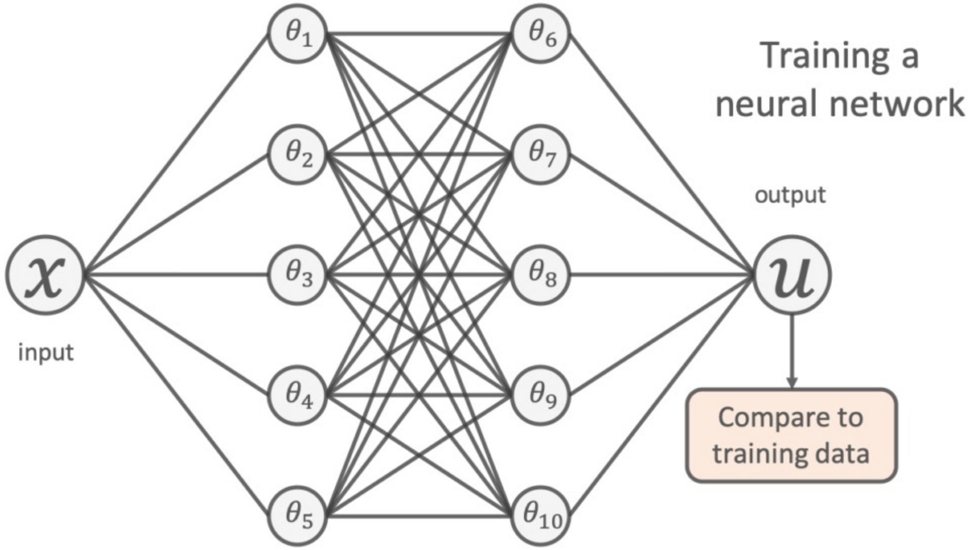
Setting for Machine Learning in Science

- Given some experimental data
- Train model to predict more data

➔ Common approach: Train Neural Network

$$\min \frac{1}{N} \sum_{\mathrm{i}}^{\mathrm{N}} (\mathrm{u}_{\mathrm{NN}}(\mathrm{x}_{\mathrm{i}}; \theta) - \mathrm{u}_{\mathrm{true}}(\mathrm{x}_{\mathrm{i}}))^2$$



https://benmoseley.blog/my-research/so-what-is-a-physics-informed-neural-network/

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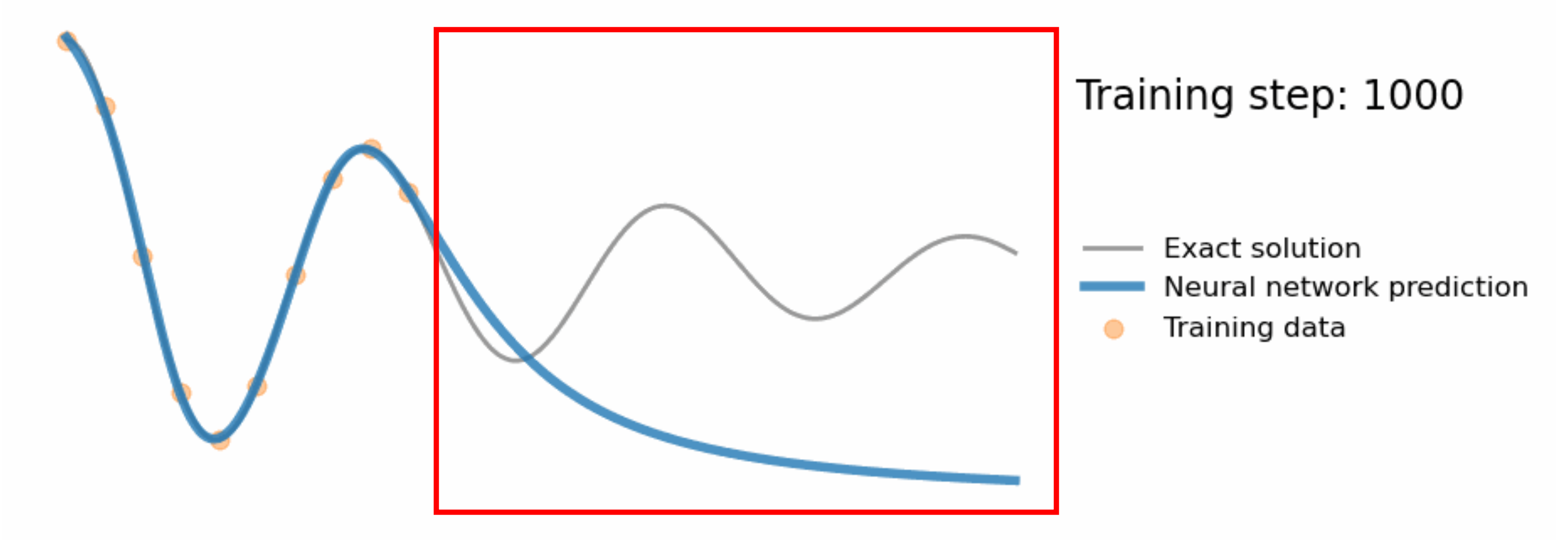
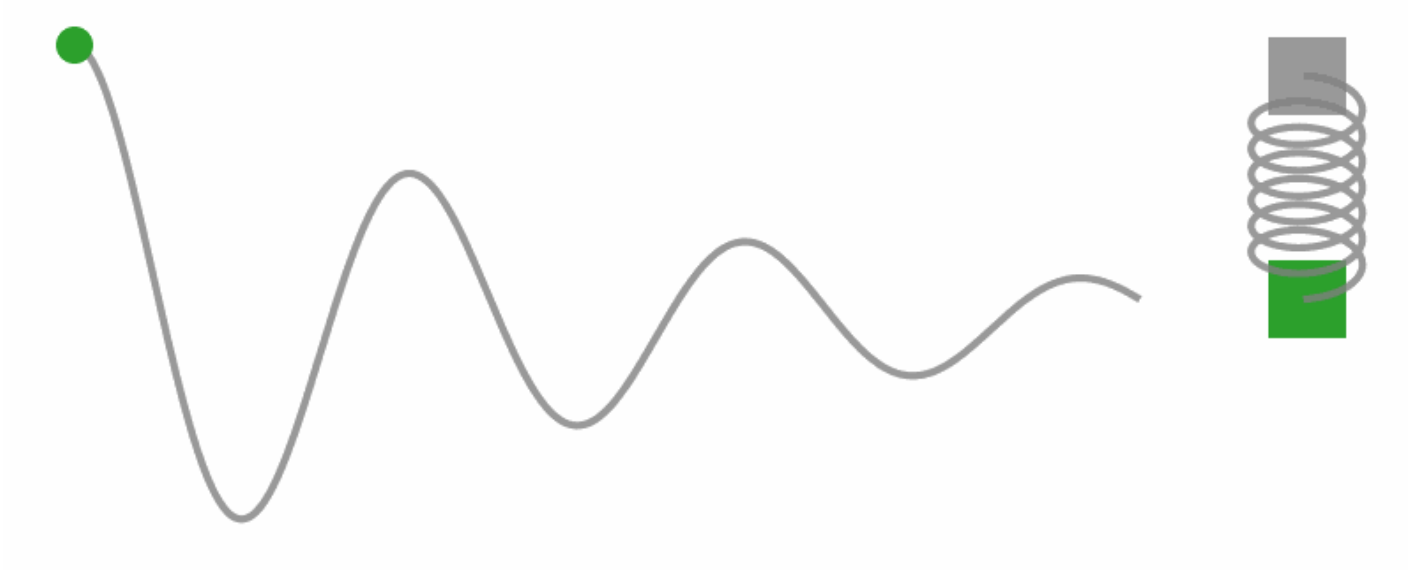
Why PINNs?



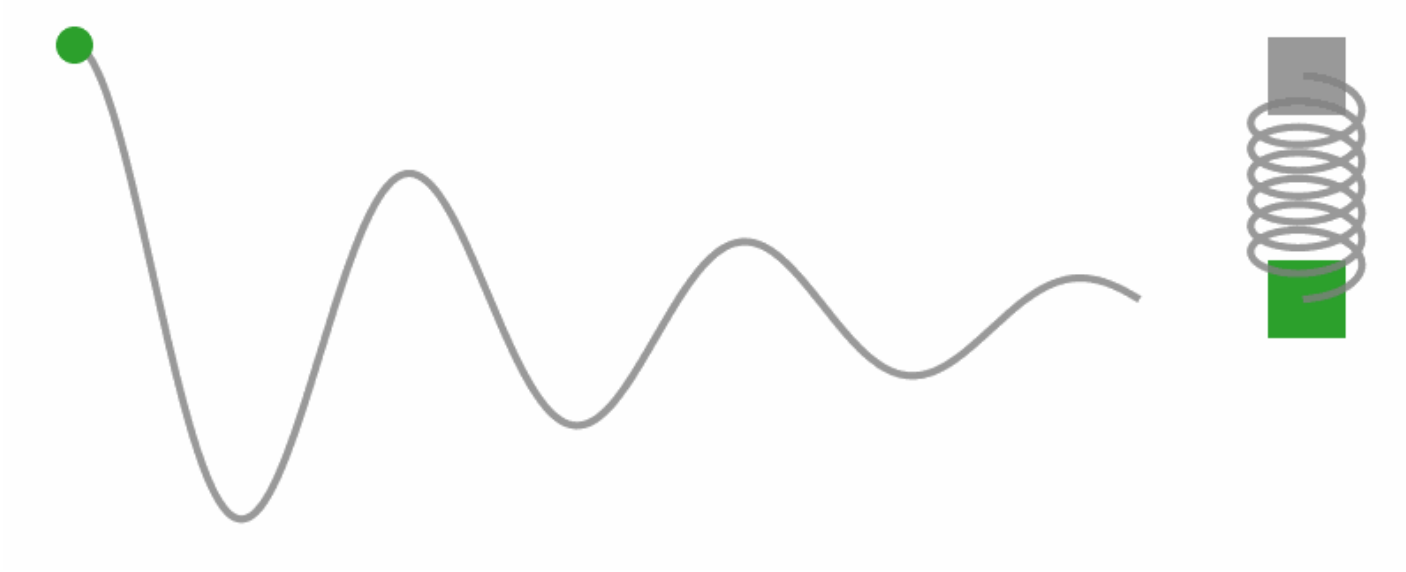
Neural Network generalizes poorly!

PINNs Use Data and the Underlying Physics



$$m\frac{d^2u}{dx^2}+\mu\frac{du}{dx}+ku=0$$

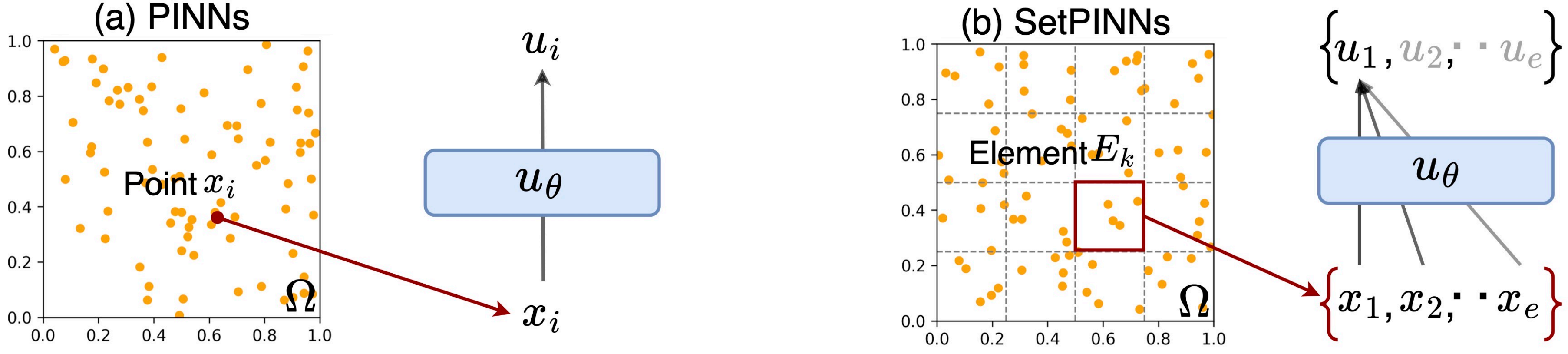
PINNs Use Data and the Underlying Physics



$$m\frac{d^2u}{dx^2}+\mu\frac{du}{dx}+ku=0$$

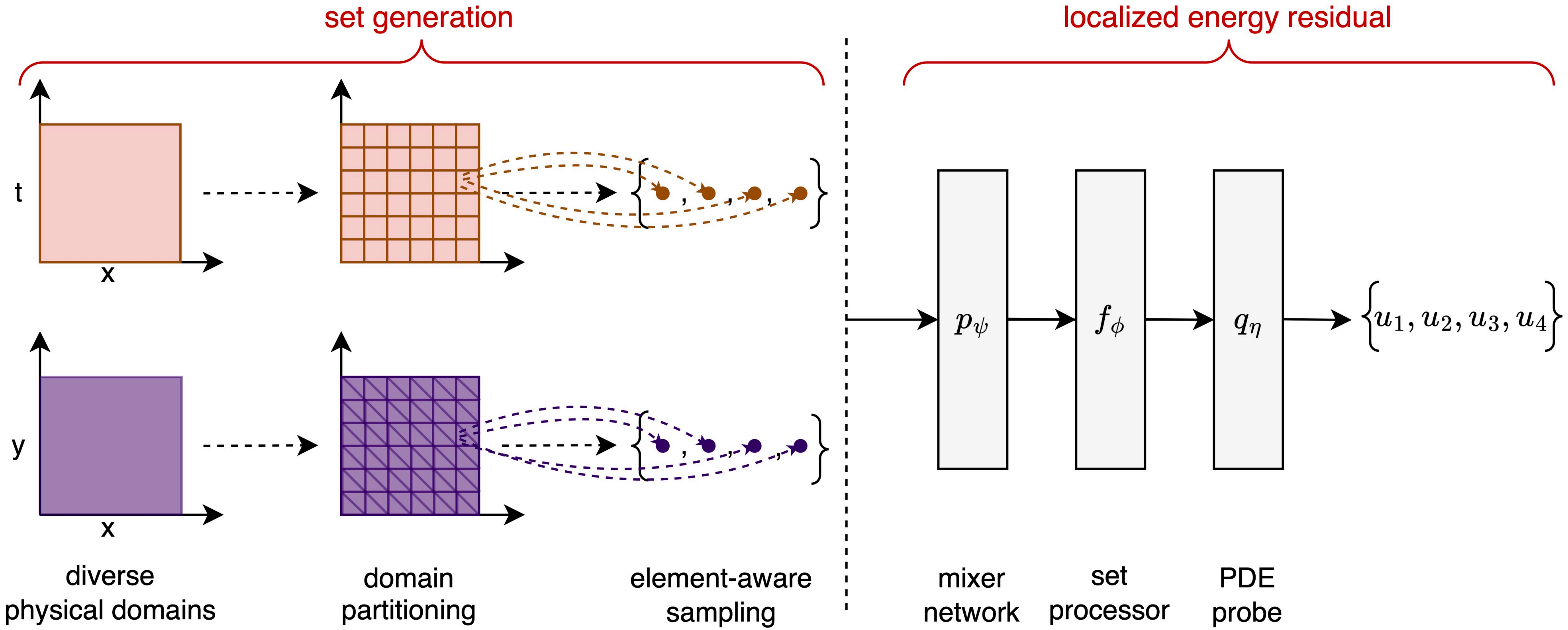
$$\min\frac{1}{N}\sum_{\mathrm{i}}^{\mathrm{N}}\left(\mathrm{u}_{\mathrm{NN}}(\mathrm{x}_{\mathrm{i}};\theta)-\mathrm{u}_{\mathrm{true}}(\mathrm{x}_{\mathrm{i}})\right)^2+\frac{1}{\mathrm{M}}\sum_{\mathrm{i}}^{\mathrm{N}}\left(\left[m\frac{d^2}{dx^2}+\mu\frac{d}{dx}+k\right]\mathrm{u}_{\mathrm{NN}}(\mathrm{x}_{\mathrm{i}};\theta)\right)^2$$

PINNs Miss Implicit Dependencies

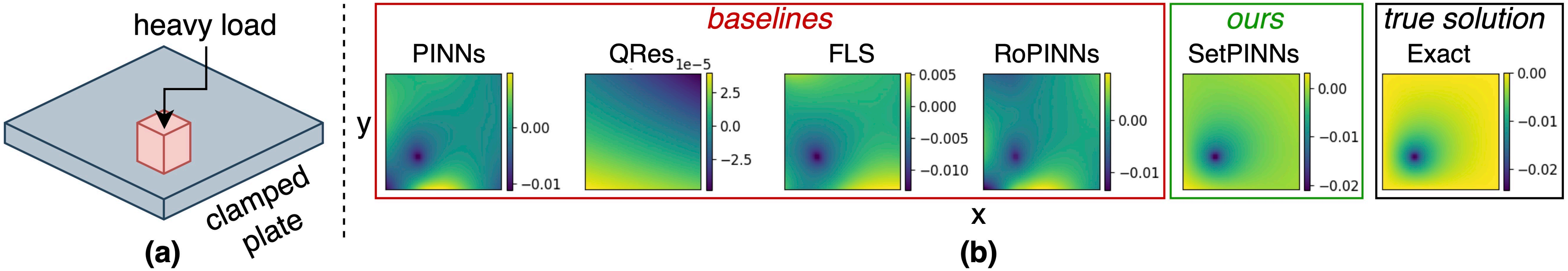


➔ SetPINNs model local depencies & provide better domain coverage

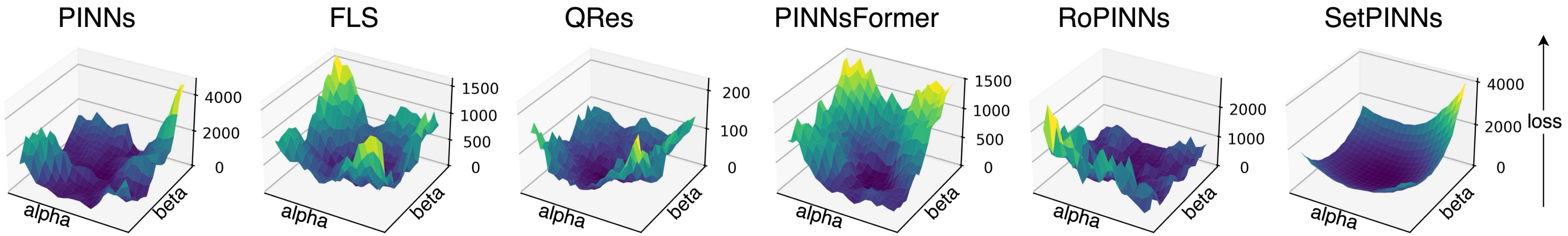
How Do SetPINNs Model Local Dependencies?



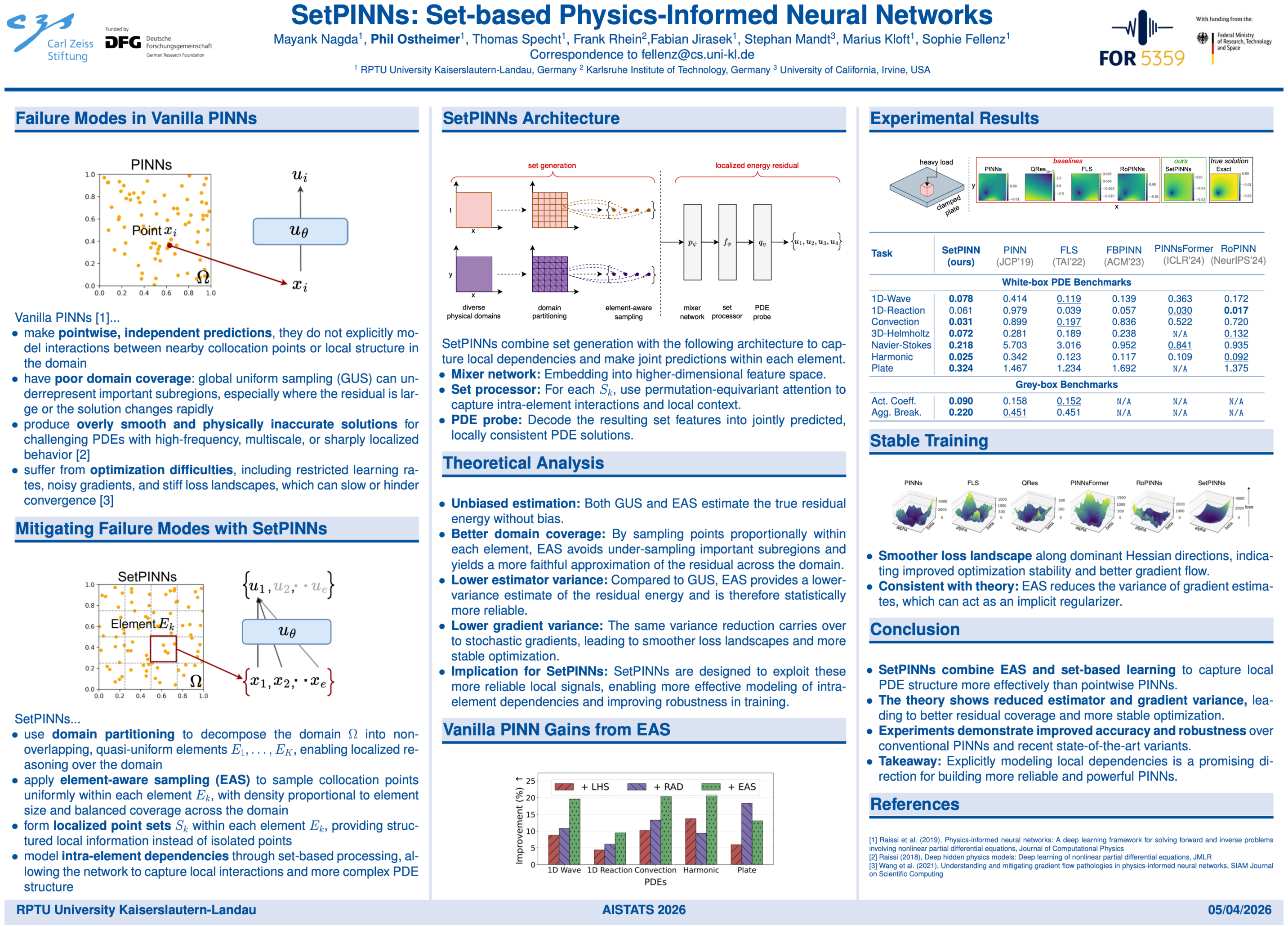
SetPINNs Have Superior Accuracy



…and Training Stability



Meet You at the Poster Session! #190



SetPINNs: Set-based Physics-Informed Neural Networks

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Failure Modes in Vanilla PINNs

Vanilla PINNs [1]...

- make **pointwise, independent predictions**, they do not explicitly model interactions between nearby collocation points or local structure in the domain
- have **poor domain coverage**: global uniform sampling (GUS) can underrepresent important subregions, especially where the residual is large or the solution changes rapidly
- produce **overly smooth and physically inaccurate solutions** for challenging PDEs with high-frequency, multiscale, or sharply localized behavior [2]
- suffer from **optimization difficulties**, including restricted learning rates, noisy gradients, and stiff loss landscapes, which can slow or hinder convergence [3]

Mitigating Failure Modes with SetPINNs

SetPINNs...

- use **domain partitioning** to decompose the domain Ω into non-overlapping, quasi-uniform elements $E_1, \dots, E_K$, enabling localized reasoning over the domain
- apply **element-aware sampling (EAS)** to sample collocation points uniformly within each element E_k, with density proportional to element size and balanced coverage across the domain
- form **localized point sets** S_k within each element E_k, providing structured local information instead of isolated points
- model **intra-element dependencies** through set-based processing, allowing the network to capture local interactions and more complex PDE structure

SetPINNs Architecture

SetPINNs combine set generation with the following architecture to capture local dependencies and make joint predictions within each element.

- **Mixer network:** Embedding into higher-dimensional feature space.
- **Set processor:** For each S_k, use permutation-equivariant attention to capture intra-element interactions and local context.
- **PDE probe:** Decode the resulting set features into jointly predicted, locally consistent PDE solutions.

Theoretical Analysis

- **Unbiased estimation:** Both GUS and EAS estimate the true residual energy without bias.
- **Better domain coverage:** By sampling points proportionally within each element, EAS avoids under-sampling important subregions and yields a more faithful approximation of the residual across the domain.
- **Lower estimator variance:** Compared to GUS, EAS provides a lower-variance estimate of the residual energy and is therefore statistically more reliable.
- **Lower gradient variance:** The same variance reduction carries over to stochastic gradients, leading to smoother loss landscapes and more stable optimization.
- **Implication for SetPINNs:** SetPINNs are designed to exploit these more reliable local signals, enabling more effective modeling of intra-element dependencies and improving robustness in training.

Vanilla PINN Gains from EAS

Experimental Results

Task	**SetPINN (ours)**	PINN (JCP'19)	FLS (TAI'22)	FBPINN (ACM'23)	PINNsFormer (ICLR'24)	RoPINN (NeurIPS'24)
White-box PDE Benchmarks						
1D-Wave	**0.078**	0.414	0.119	0.139	0.363	0.172
1D-Reaction	0.061	0.979	0.039	0.057	0.030	**0.017**
Convection	**0.031**	0.899	0.197	0.836	0.522	0.720
3D-Helmholtz	**0.072**	0.281	0.189	0.238	N/A	0.132
Navier-Stokes	**0.218**	5.703	3.016	0.952	0.841	0.935
Harmonic	**0.025**	0.342	0.123	0.117	0.109	0.092
Plate	**0.324**	1.467	1.234	1.692	N/A	1.375
Grey-box Benchmarks						
Act. Coeff.	**0.090**	0.158	0.152	N/A	N/A	N/A
Agg. Break.	**0.220**	0.451	0.451	N/A	N/A	N/A

Stable Training

- **Smoother loss landscape** along dominant Hessian directions, indicating improved optimization stability and better gradient flow.
- **Consistent with theory:** EAS reduces the variance of gradient estimates, which can act as an implicit regularizer.

Conclusion

- **SetPINNs combine EAS and set-based learning** to capture local PDE structure more effectively than pointwise PINNs.
- **The theory shows reduced estimator and gradient variance,** leading to better residual coverage and more stable optimization.
- **Experiments demonstrate improved accuracy and robustness** over conventional PINNs and recent state-of-the-art variants.
- **Takeaway:** Explicitly modeling local dependencies is a promising direction for building more reliable and powerful PINNs.

References

[1] Raissi et al. (2019), Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations, Journal of Computational Physics
[2] Raissi (2018), Deep hidden physics models: Deep learning of nonlinear partial differential equations, JMLR
[3] Wang et al. (2021), Understanding and mitigating gradient flow pathologies in physics-informed neural networks, SIAM Journal on Scientific Computing

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