GUANGDONG AND HONG KONG UNIVERSITIES "1+1+1" Joint Research Collaboration Scheme

粵港高校「1+1+1」聯合資助計劃

Guangdong-Hong Kong "1+1+1" Joint Funding Programme

Data-driven scientific and engineering computing algorithms and software

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Introduction

- Scientific machine learning often becomes unreliable when the underlying problem has nontrivial geometry, strong oscillations, long-time dependence, or intrinsic physical laws that are not explicitly built into the model.
- The central theme here is to incorporate **problem-specific structure** into data-driven scientific computing.

Manifold

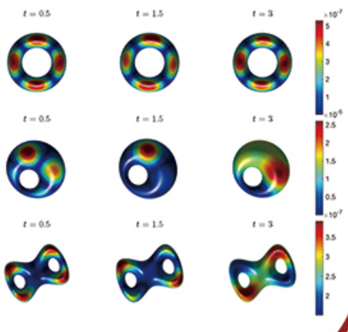
We consider PDE discovery on a **closed surface** $\mathcal{S} \subset \mathbb{R}^d$ from point-cloud data. The governing law is unknown and the operators are intrinsic to the surface, we express them in the **ambient space**:

$$\nabla_{\mathcal{S}} = (I - nn^T)\nabla, \qquad \Delta_{\mathcal{S}} = \nabla_{\mathcal{S}} \cdot \nabla_{\mathcal{S}}$$

A sparse feature library built from $u, \nabla_{\mathcal{S}} u$ and $\Delta_{\mathcal{S}}$ is then used to identify the PDE:

$$\arg\min_{\xi} \|\Lambda(X)\xi - f(X)\|_2^2 + \mu\|\xi\|_1$$

Here $\Lambda(X)$ is the library matrix, $\mu > 0$ is the sparsity parameter.

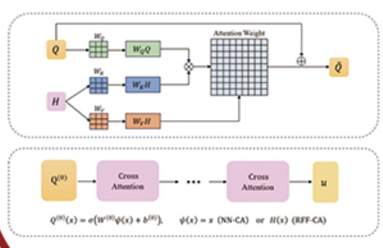


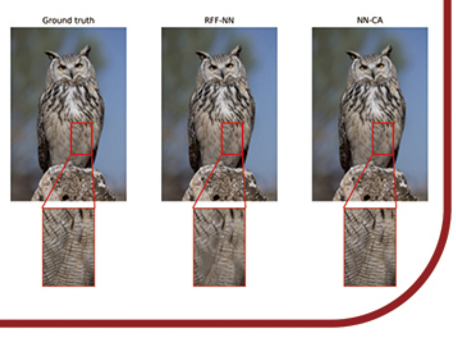
Frequency

We address the **spectral bias** of neural networks in oscillatory and multiscale problems. A multiscale random Fourier feature bank $H(x)$ is introduced.

$$\mathrm{CA}(Q(x), H(x)) = \mathrm{softmax}\left(\frac{Q(x)W_Q(H(x)W_K)^\top}{\sqrt{d_q}}\right) H(x)W_V$$

$$\widetilde{Q}^{(l)}(x) = Q^{(l)}(x) + \mathrm{CA}(Q^{(l)}(x), H(x)).$$





Temporal

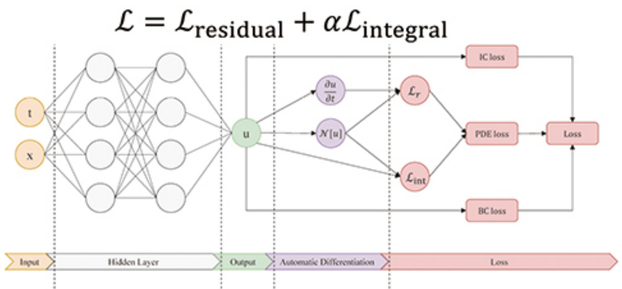
We consider **evolution equations** and long-time integration. Standard PINNs use pointwise residuals, which may lead to temporal error accumulation.

For
$$u_t + \mathcal{N}[u] = f$$

We introduce the interval residual

$$r_{\mathrm{int}}(a,b,x) = u(b,x) - u(a,x) - \frac{1}{b-a}\int_a^b \mathcal{N}[u](t,x) - f(t,x)\,dt$$

$$\mathcal{L} = \mathcal{L}_{\mathrm{residual}} + \alpha\mathcal{L}_{\mathrm{integral}}$$



Energy

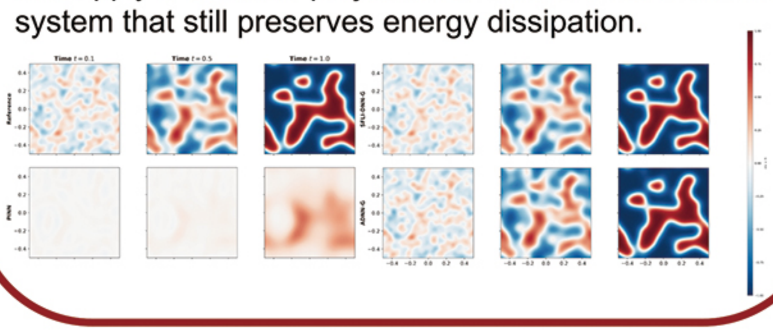
We consider dissipative systems, especially **gradient flows**, where preserving the energy law is essential.

$$\partial_t u = G\frac{\delta \mathcal{E}}{\delta u} \qquad \frac{d}{dt}E[u(t)] \le 0$$

We interpret the last layer as adaptive basis functions,

$$V_\theta = \mathrm{span}\{\phi_1(\cdot;\theta), \cdots, \phi_m(\cdot;\theta)\}$$

and apply a Galerkin projection to obtain a semi-discrete system that still preserves energy dissipation.



Conclusion

- These four directions show how mathematical structure can be built into scientific machine learning through geometry, frequency, time, and energy.
- The common goal is to improve reliability, robustness, and physical consistency beyond purely black-box learning.

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[2] **X. Feng**, **T. Tang**, X. Wan, and T. Zhou. Overcoming Spectral Bias via Cross-Attention. arXiv:2512.18586, 2025.

[3] **X. Feng**, H. Shangguan, **T. Tang**, and X. Wan. Integral Regularization PINNs for Evolution Equations. Commun. Comput. Phys., 39(2):356–386, 2026.

[4] **T. Tang**, J. Yang, Y. Zhao, and Q. Zhu. Energy Dissipation Preserving Feature-based DNN Galerkin Methods for Gradient Flows. arXiv:2603.14029, 2026.