



Domain Decomposition for Randomized Neural Networks

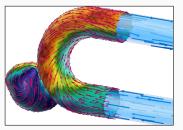
Alexander Heinlein¹

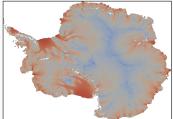
95th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2025), Poznan, Poland, April 7-11, 2025

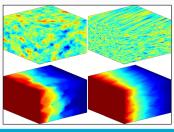
¹Delft University of Technology

Based on joint work with Siddhartha Mishra (ETH Zürich) and Yong Shang and Fei Wang (Xi'an Jiaotong University)

Scientific Computing and Machine Learning







Numerical methods

Based on physical models

- + Robust and generalizable
- Require availability of mathematical models

Machine learning models

Driven by data

- + Do not require mathematical models
- Sensitive to data, limited extrapolation capabilities

Scientific machine learning

Combining the strengths and compensating the weaknesses of the individual approaches:

numerical methods machine learning techniques

improve assist

machine learning techniques

numerical methods

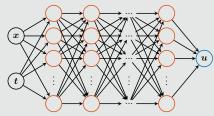
Randomized Neural Networks (RaNNs)

Neural networks

A standard multilayer perceptron (MLP) with *L* hidden layers is a parametric model of the form

$$u(x,\theta) = \mathbf{F}_{L+1}^{\mathbf{A}} \cdot \mathbf{F}_{L}^{\mathbf{W}_{L},\mathbf{b}_{L}} \circ \ldots \circ \mathbf{F}_{1}^{\mathbf{W}_{1},\mathbf{b}_{1}}(x),$$

where **A** is linear, and the *i*th hidden layer is nonlinear $F_i^{W_i,b_i}(x) = \sigma(W_i \cdot x + b_i)$.



In order to optimize the loss function

$$\min_{\theta} \mathcal{L}(\theta)$$
,

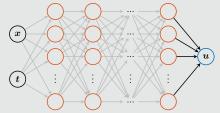
all parameters $\theta = (A, W_1, b_1, \dots, W_L, b_L)$ are trained.

Randomized neural networks

In randomized neural networks (RaNNs) as introduced by Pao and Takefuji (1992),

$$u(\mathbf{x},\mathbf{A})=\mathbf{F}_{L+1}^{\mathbf{A}}\cdot\mathbf{F}_{L}^{W_{L},b_{L}}\circ\ldots\circ\mathbf{F}_{1}^{W_{1},b_{1}}(\mathbf{x}),$$

the weights in the hidden layers are randomly initialized and **fixed**; only **A** is trainable.



The model is linear with respect to the trainable parameters \boldsymbol{A} , and the optimization problem reads

$$\min_{\mathbf{A}} \mathcal{L}(\mathbf{A}).$$

This can simplify the training process.

Physics-Informed Neural Networks (PINNs)

In the physics-informed neural network (PINN) approach introduced by Raissi et al. (2019), a neural network is employed to discretize a partial differential equation

$$\mathcal{N}[u] = f$$
, in Ω .

PINNs use a hybrid loss function:

$$\mathcal{L}(\boldsymbol{\theta}) = \omega_{\text{data}} \mathcal{L}_{\text{data}}(\boldsymbol{\theta}) + \omega_{\text{PDE}} \mathcal{L}_{\text{PDE}}(\boldsymbol{\theta}),$$

where ω_{data} and ω_{PDE} are weights and

$$egin{aligned} \mathcal{L}_{\mathsf{data}}(heta) &= rac{1}{N_{\mathsf{data}}} \sum_{i=1}^{N_{\mathsf{data}}} \left(u(\hat{oldsymbol{x}}_i, oldsymbol{ heta}) - u_i
ight)^2, \ \mathcal{L}_{\mathsf{PDE}}(heta) &= rac{1}{N_{\mathsf{PDF}}} \sum_{i=1}^{N_{\mathsf{PDE}}} \left(\mathcal{N}[u](oldsymbol{x}_i, oldsymbol{ heta}) - f(oldsymbol{x}_i)
ight)^2. \end{aligned}$$

See also Dissanayake and Phan-Thien (1994); Lagaris et al. (1998).

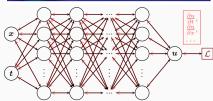
Advantages

- "Meshfree"
- Small data
- Generalization properties
- High-dimensional problems
- Inverse and parameterized problems

Drawbacks

- Training cost and robustness
- Convergence not well-understood
- Difficulties with scalability and multi-scale problems







- Known solution values can be included in \(\mathcal{L}_{\text{data}} \)
- Initial and boundary conditions are also included in £data

Error Estimate & Spectral Bias

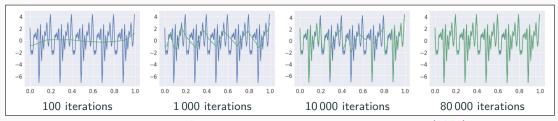
Estimate of the generalization error (Mishra and Molinaro (2022))

The generalization error (or total error) satisfies

$$\mathcal{E}_G \leq C_{PDE} \mathcal{E}_T + C_{PDE} C_{quad}^{1/p} N^{-\alpha/p}$$

- $\mathcal{E}_G = \mathcal{E}_G(X, \theta) := \|\mathbf{u} \mathbf{u}^*\|_V$ general. error (V Sobolev space, X training data set)
- &_T training error (I^p loss of the residual of the PDE)
- N number of the training points and α convergence rate of the quadrature
- ullet C_{PDE} and C_{quad} constants depending on the PDE, quadrature, and neural network

Rule of thumb: "As long as the PINN is trained well, it also generalizes well"



Rahaman et al., On the spectral bias of neural networks, ICML (2019)

Related works: Cao et al. (2021), Wang, et al. (2022), Hong et al. (arXiv 2022), Xu et al (2024), ...

Scaling of PINNs for a Simple ODE Problem

Solve

$$u' = \cos(\omega x),$$

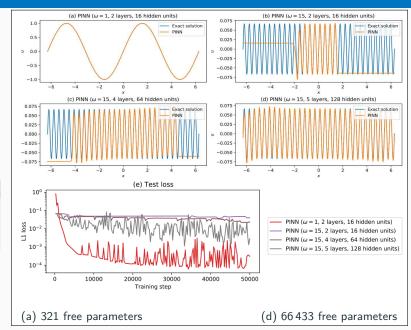
$$u(0) = 0,$$

for different values of ω using PINNs with varying network capacities.

Scaling issues

- Large computational domains
- Small frequencies

Cf. Moseley, Markham, and Nissen-Meyer (2023)



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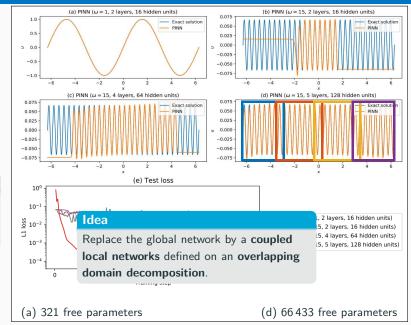
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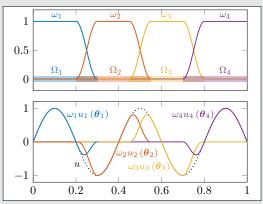
FBPINNs (Moseley, Markham, Nissen-Meyer (2023))

FBPINNs employ the network architecture

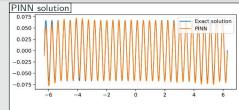
$$u(\theta_1,\ldots,\theta_J)=\sum\nolimits_{j=1}^J\omega_ju_j\left(\theta_j\right)$$

and the loss function

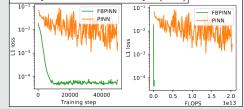
$$\mathcal{L} = \frac{1}{N} \sum_{i=1}^{N} \left(n \left[\sum_{\mathbf{x}_i \in \Omega_j} \omega_j u_j \right] (\mathbf{x}_i, \theta_j) - f(\mathbf{x}_i) \right)^2.$$



1D single-frequency problem



Moseley, Markham, Nissen-Meyer (2023)



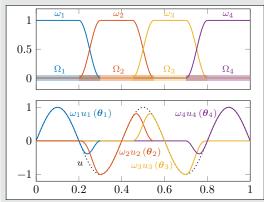
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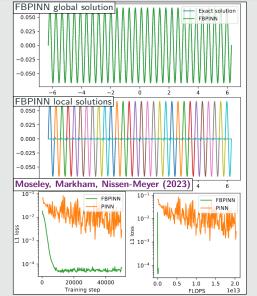
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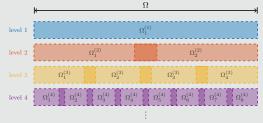
1D single-frequency problem



Multi-Level FBPINNs

Multi-level FBPINNs (ML-FBPINNs)

ML-FBPINNs (Dolean, Heinlein, Mishra, Moseley (2024)) are based on a hierarchy of domain decompositions:



This yields the **network architecture**

$$u(\theta_1^{(1)},\ldots,\theta_{J^{(L)}}^{(L)}) = \sum_{l=1}^{L} \sum_{i=1}^{N^{(l)}} \omega_j^{(l)} u_j^{(l)}(\theta_j^{(l)})$$

and the loss function

$$\mathcal{L} = \frac{1}{N} \sum\nolimits_{i=1}^{N} \left(n[\sum\nolimits_{\mathbf{x}_i \in \Omega_i^{(l)}} \omega_j^{(l)} u_j^{(l)}](\mathbf{x}_i, \boldsymbol{\theta}_j^{(l)}) - f(\mathbf{x}_i) \right)_{.}^{2}$$

Multi-Frequency Problem

Let us now consider the two-dimensional multi-frequency Laplace boundary value problem

$$-\Delta u = 2\sum_{i=1}^{\infty} (\omega_i \pi)^2 \sin(\omega_i \pi x) \sin(\omega_i \pi y) \quad \text{in } \Omega,$$

with
$$\omega_i = 2^i$$
.

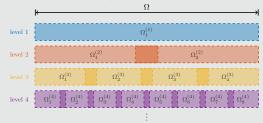
For increasing values of *n*, we obtain the **analytical** solutions:



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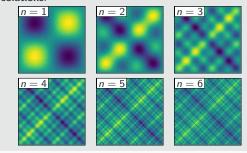
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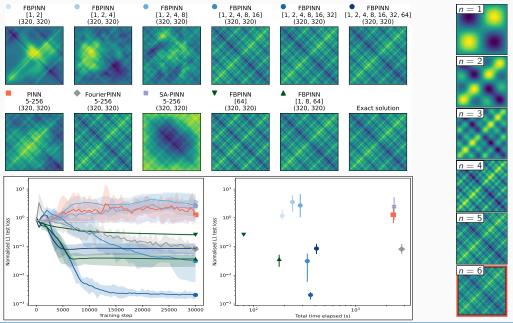
$$-\Delta u = 2\sum_{i=1}^{n} (\omega_i \pi)^2 \sin(\omega_i \pi x) \sin(\omega_i \pi y)$$
 in Ω ,
$$u = 0$$
 on $\partial \Omega$,

with $\omega_i = 2^i$.

For increasing values of *n*, we obtain the **analytical solutions**:

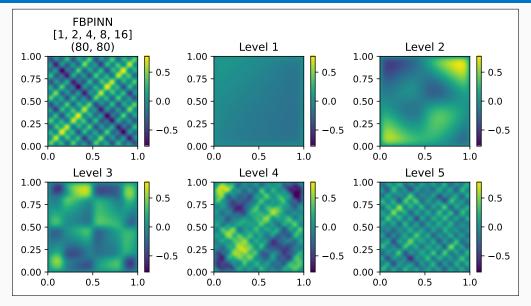


Multi-Level FBPINNs for a Multi-Frequency Problem – Strong Scaling



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Multi-Frequency Problem – What the FBPINN Learns



Cf. Dolean, Heinlein, Mishra, Moseley (2024).

Multi-Level FBPINNs for a Multi-Frequency Problem – Weak Scaling

n=1

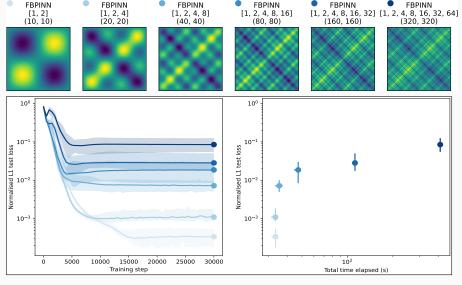
n=2

n = 3

n = 4

n = 5

n = 6



 \rightarrow Details and results for the Helmholtz equation can be found in **Dolean**, **Heinlein**, **Mishra**, **Moseley** (2024).

Physics-Informed Randomized Neural Networks (PIRaNNs)

Physics-informed randomized neural networks (PIRaNNs) make use of the aforementioned linearization of the model with respect to the trainable parameters as well as the fact that RaNNs retain universal approximation properties, as shown in Igelnik and Pao (1995).

Consider a linear differential operator $\mathcal{A}.$ Then, solving the PDE

$$\mathcal{A}[u] = f$$
, in Ω .

using PIRaNNs yields the \mbox{linear} equation \mbox{system}

$$\mathcal{A}[u](\mathbf{x}_i) = f(\mathbf{x}_i), \quad i = 1, \ldots, N_{PDE},$$

where \textit{N}_{PDE} is the number of collocation points.

The resulting linear equation system

We construct u to explicitly satisfy BCs:

$$u(x, \mathbf{A}) = G(x) + L(x)\mathcal{N}(x, \mathbf{A})$$

- N is a feedforward neural network with trainable parameters A
- *G* and *L* are **fixed functions**, chosen such that *u* satisfies the boundary conditions

$$HA = f$$

generally does **not have a unique solution**. In fact, **H** is typically **rectangular**, **dense**, and **ill-conditioned**.

Solving the system using least squares corresponds to applying the classical PINN loss function to the RaNN model u. As we will see, this approach offers a potentially efficient alternative.

Randomized Neural Networks - (Non-Exhaustive) Literature Overview

Randomized neural networks

- RaNNs: Pao, Takefuji (1992); Pao Park, Sobajic (1994); Igelnik, Pao (1995)
- Extreme Learning Machines (ELMs): Huang, Zhu, Siew (2006); Liu, Lin, Fang, Xu (2014); Gallicchio, Scardapane (2020); Calabrò, Fabiani, Siettos (2021); Ni, Dong (2023); Wang, Dong (2024)

Domain decomposition for neural networks and randomized neural networks

- cPINNs, XPINNs: Jagtap, Kharazmi, Karniadakis (2020); Jagtap, Karniadakis (2020)
- Schwarz it. for PINNs or DeepRitz (D3M, DeepDDM, etc):: Li, Tang, Wu, Liao (2019); Li, Xiang, Xu (2020); Mercier, Gratton, Boudier (arXiv 2021); Dolean, H., Mercier, Gratton (arXiv 2024); Li, Wang, Cui, Xiang, Xu (2023); Sun, Xu, Yi (arXiv 2023, 2024); Kim, Yang (2023, 2024, 2024)
- FBPINNs, FBKANs: Moseley, Markham, Nissen-Meyer (2023); Dolean, H., Mishra, Moseley (2024, 2024); H., Howard, Beecroft, Stinis (acc. 2024); Howard, Jacob, Murphy, H., Stinis (arXiv 2024)
- DD for RaNNs, ELMS, Random Feature Method: Dong, Li (2021); Dang, Wang (2024); Sun, Dong, Wang (2024); Sun, Wang (2024); Chen, Chi, E, Yang (2022); Shang, H., Mishra, Wang (acc. 2025)

An overview of the state-of-the-art in 2024:



A. Klawonn, M. Lanser, J. Weber

Machine learning, domain decomposition methods – a survey

Computational Science and Engineering. 2024

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Domain Decomposition-Based PIRaNNs

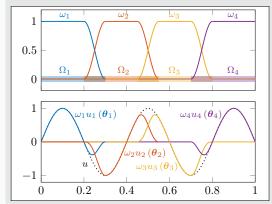
FBPINNs (Moseley, Markham, Nissen-Meyer (2023))

FBPINNs employ the network architecture

$$u(\theta_1,\ldots,\theta_J)=\sum_{j=1}^J \omega_j u_j(\theta_j)$$

and the loss function

$$\mathcal{L} = \frac{1}{N} \sum_{i=1}^{N} \left(n \left[\sum_{\mathbf{x}_i \in \Omega_j} \omega_j u_j \right] (\mathbf{x}_i, \theta_j) - f(\mathbf{x}_i) \right)^2$$

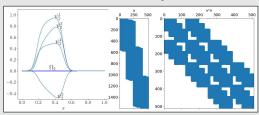


Domain decomposition for RaNNs

We employ the FBPINNs approach; cf. Shang, Heinlein, Mishra, Wang (acc. 2025). This is closely related to the random feature method (RFM) by Chen, Chi, E, Yang (2022). In particular, we solve

$$\mathcal{A}\left[\sum_{i=1}^{J}\omega_{j}u_{j}\left(\mathbf{A}_{j}\right)\right]\left(\mathbf{x}_{i}\right)=f(\mathbf{x}_{i}),$$

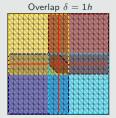
for $i=1,\ldots,N_{\text{PDE}}$; the boundary condtions are incorporated directly into the u_i .

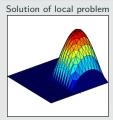


The hidden weights are randomly initialized, the resulting matrices \mathbf{H} and $\mathbf{H}^{\top}\mathbf{H}$ are block-sparse.

Preconditioning for Domain Decomposition-Based PIRaNNs

One-level Schwarz preconditioner





Based on an **overlapping domain decomposition**, we define a **one-level Schwarz operator** for

$$K := H^{\top}H$$

$$\mathbf{M}_{\mathrm{OS-1}}^{-1}\mathbf{K} = \sum_{i=1}^{N} \mathbf{R}_{i}^{\top} \mathbf{K}_{i}^{-1} \mathbf{R}_{i} \mathbf{K},$$

where \mathbf{R}_i and \mathbf{R}_i^{\top} are restriction and prolongation operators corresponding to Ω_i' , and $\mathbf{K}_i := \mathbf{R}_i \mathbf{K} \mathbf{R}_i^{\top}$.

Here, the matrix K_i could be singular in which case we use a **pseudo inverse** K_i^+ instead of K_i^{-1} .

We also consider restricted and scaled additive Schwarz preconditioners; cf. Cai, Sarkis (1999).

Singular Value Decomposition

As discussed before, on each subdomain Ω_j , the RaNN is

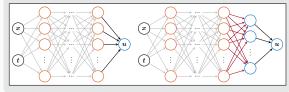
$$u_{j}(x, \mathbf{A}_{j}) = \mathbf{F}_{L+1}^{\mathbf{A}} \cdot \mathbf{F}_{L}^{W_{L}, b_{L}} \circ \dots \circ \mathbf{F}_{1}^{W_{1}, b_{1}}(x)$$
$$= \mathbf{A}_{j} \begin{bmatrix} \Phi_{1}(x) & \cdots & \Phi_{k}(x) \end{bmatrix}^{\top},$$

where k is the width of the last hidden layer and the Φ_l are the randomized basis functions.

Consider a **reduced SVD** $\Phi = U\Sigma V^{\top}$, where the entries of the matrix are $\Phi_{i,l} = \Phi_l(x_l)$. Then, we consider

$$\hat{u}_j(\mathbf{x}, \mathbf{A}_j) = \mathbf{A}_j \hat{\mathbf{V}}^{\top} \begin{bmatrix} \Phi_1(\mathbf{x}) & \cdots & \Phi_k(\mathbf{x}) \end{bmatrix}^{\top},$$

where $\hat{\mathbf{V}}^{\top}$ is obtained by omitting the right singular vectors corresponding to small singular values.



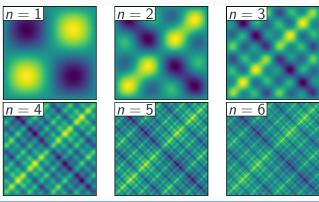
Let us now consider the two-dimensional multi-frequency Laplace boundary value problem

$$-\Delta u = 2 \sum_{i=1}^{n} (\omega_i \pi)^2 \sin(\omega_i \pi x) \sin(\omega_i \pi y) \quad \text{in } \Omega = [0, 1]^2,$$

$$u = 0 \quad \text{on } \partial \Omega,$$

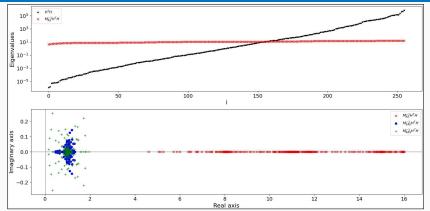
with $\omega_i = 2^i$.

For increasing values of n, we obtain the **analytical solutions**:



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Results for the Multi-Frequency Problem (n=2)



	$M^{-1} = I$		$M^{-1} = M_{AS}^{-1}$		$M^{-1} = M_{RAS}^{-1}$		$M^{-1} = M_{SAS}^{-1}$	
	iter	e_{L^2}	iter	e_{L^2}	iter	e_{L^2}	iter	e_{L^2}
CG	> 2000	$1.95 \cdot 10^{-2}$	8	$5.03 \cdot 10^{-3}$	_		_	_
CGS	> 2000	$2.63 \cdot 10^{-2}$	4	$5.04 \cdot 10^{-3}$	24	$5.03 \cdot 10^{-3}$	6	$5.04 \cdot 10^{-3}$
BICG	> 2000	$1.03 \cdot 10^{-2}$	8	$5.08 \cdot 10^{-3}$	32	$5.05 \cdot 10^{-3}$	11	$5.09 \cdot 10^{-3}$
GMRES	> 2000	$8.68 \cdot 10^{-2}$	13	$5.07 \cdot 10^{-3}$	31	$5.06 \cdot 10^{-3}$	11	$5.08 \cdot 10^{-3}$

 $4 \times 4 \text{ subdomains; DoF} = 256; \ \textit{N} = 1600; \ \theta^0 \in \mathcal{U}(-1,1); \ \text{stop.:} \ \|\textit{\textit{M}}^{-1}\textit{\textit{r}}^k\|_{L^2}/\|\textit{\textit{M}}^{-1}\textit{\textit{r}}^0\|_{L^2} \leq 10^{-5}$

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Results for the Multi-Frequency Problem (n=2) – Initialization & Activation

Now, we inverstigate the effect of different sampling strategies for the 40×40 collocation points:

- uniformly-spaced points in the domain,
- Gauss-Legendre quadrature points, and
- random sampling from a uniform distribution $\mathcal{U}(0,1)$.

as well as tanh and sigmoid activation functions:

collocation points	activation		$M^{-1} =$	= 1	$M^{-1} = M_{AS}^{-1}$		
conocation points		κ	iter	e_{L^2}	κ	iter	<i>e</i> _{L²}
:6	tanh	10 ¹¹	> 2000	$1.15 \cdot 10^{-2}$	3.5	8	$5.02 \cdot 10^{-3}$
uniformly-spaced	sigmoid	10^{15}	> 2000	$4.29 \cdot 10^{-2}$	3.6	8	$3.38 \cdot 10^{-3}$
and destroy a sinte	tanh	10 ¹²	> 2000	$2.51 \cdot 10^{-2}$	28.3	21	$9.03 \cdot 10^{-3}$
quadrature points	sigmoid	10^{15}	> 2000	$4.55 \cdot 10^{-2}$	49.6	22	$5.86 \cdot 10^{-3}$
random samples	tanh	10 ¹²	> 2000	$5.67 \cdot 10^{-2}$	38.3	22	$3.18 \cdot 10^{-2}$
random samples	sigmoid	10^{15}	> 2000	$7.17 \cdot 10^{-2}$	46.7	25	$1.68 \cdot 10^{-2}$

 $^{4 \}times 4$ subdomains; N = 1600; $\theta^0 \in \mathcal{U}(-1,1)$; stop.: $\|\mathbf{M}^{-1}\mathbf{r}^k\|_{L^2}/\|\mathbf{M}^{-1}\mathbf{r}^0\|_{L^2} \leq 10^{-5}$

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Results for the Multi-Frequency Problem (n=2) – Effect of the SVD

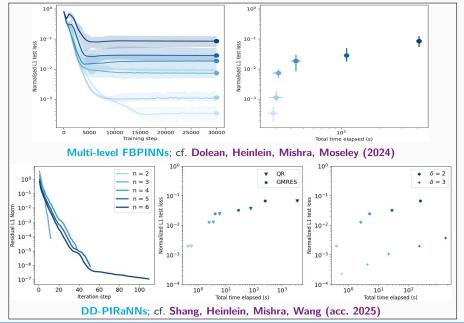
We now investigate the effect of omitting right singular vectors associated with singular values below a varying tolerance τ .

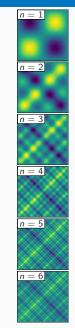
τ	DoF	\mathcal{M}^{-1}	σ_{min}	σ_{max}	iter	e _{L2}
		1	10^{-10}	10^{6}	> 2000	$3.72 \cdot 10^{-2}$
10^{-4}	512	M_{AS}^{-1}	10^{-6}	10^{6}	27	$5.46 \cdot 10^{-5}$
		M_{SAS}^{-1}	10^{-7}	10^{5}	30	$5.49 \cdot 10^{-5}$
		1	10^{-8}	10 ⁵	> 2000	$3.75 \cdot 10^{-2}$
10^{-3}	436	M_{AS}^{-1}	10^{-5}	10^{5}	16	$1.28 \cdot 10^{-4}$
		M_{SAS}^{-1}	10^{-6}	10^{4}	18	$1.28 \cdot 10^{-4}$
		1	10^{-5}	10 ⁵	> 2000	$4.51 \cdot 10^{-2}$
10^{-2}	335	M_{AS}^{-1}	10^{-3}	10^{4}	14	$7.14 \cdot 10^{-4}$
		M_{SAS}^{-1}	10^{-4}	10^{3}	13	$7.11 \cdot 10^{-4}$
		1	10^{-3}	10 ⁶	> 2000	$5.01 \cdot 10^{-2}$
10^{-1}	212	M_{AS}^{-1}	10^{-2}	10^{3}	12	$7.13 \cdot 10^{-3}$
		M_{SAS}^{-1}	10^{-3}	10 ²	11	$7.10 \cdot 10^{-3}$

 $^{4 \}times 4$ subdomains; N = 1600; $\theta^0 \in \mathcal{U}(-1,1)$; stop.: $\|\mathbf{M}^{-1}\mathbf{r}^k\|_{L^2}/\|\mathbf{M}^{-1}\mathbf{r}^0\|_{L^2} \leq 10^{-5}$

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Results for the Multi-Frequency Problem





Numerical Results for 1D Advection-Diffusion Problem

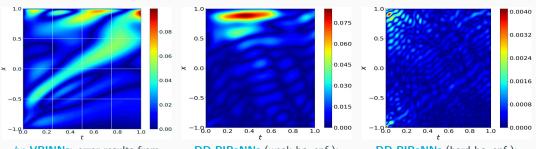
Given $\Omega = (-1, 1)$, we consider a **one-dimensional advection-diffusion equation**

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = \kappa \frac{\partial u^2}{\partial x^2} \qquad \text{in } \Omega \times I,$$

$$u(-1, t) = u(1, t) = 0 \qquad \text{in } I,$$

$$u(x, 0) = -\sin(\pi x) \qquad \text{in } \Omega,$$

with I=(0,1). Here, $\kappa=0.1/\pi$ is the diffusivity coefficient, complicating the solution near x=1 due to the no-slip boundary; see **Kharazmi, Zhang, Karniadakis (2021)**.



hp-VPINNs: error results from Kharazmi, Zhang, Karniadakis (2021)

DD-PIRaNNs (weak bc. enf.): error; relative L^2 error of 2.88×10^{-2} ; $0.12 \, \mathrm{s}$

DD-PIRaNNs (hard bc. enf.): error; relative L^2 error of 7.40×10^{-4} ; 0.08 s

CWI Research Semester Programme:

Bridging Numerical Analysis and Scientific Machine Learning: Advances and Applications

Co-organizers: Victorita Dolean (TU/e), Alexander Heinlein (TU Delft), Benjamin Sanderse (CWI), Jemima Tabbeart (TU/e), Tristan van Leeuwen (CWI)

- Autumn School (October 27–31, 2025):
 - Chris Budd (University of Bath)
 - Ben Moseley (Imperial College London)
 - Gabriele Steidl (Technische Universität Berlin)
 - Andrew Stuart (California Institute of Technology)
 - Andrea Walther (Humboldt-Universität zu Berlin)
 - Ricardo Baptista (University of Toronto)
- **Workshop** (December 1–3, 2025):
 - 3 days with plenary talks (academia & industry) and an industry panel
 - Confirmed plenary speakers:
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 - Benjamin Peherstorfer (New York University)
 - Andreas Roskopf (Fraunhofer Institute)





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Summary

Physics-informed neural networks and randomized neural networks

- PINNs incorporate physics the loss, improving accuracy and generalization. RaNNs use random weights and biases, while only training the last layer. This can simplify the training and reduce computational cost.
- Both approaches suffer from ill-conditioning leading to a challenging training process.
- Not in this talk: extension to Kolmogorov–Arnold networks (KANs) and neural operators

Domain decomposition architectures and preconditioning

- Domain decomposition-based architectures improve the scalability of PINNs to large domains / high frequencies, keeping the complexity of the local networks low.
- Preconditioning, using a combination of Schwarz preconditioning and SVD, can improve the conditioning of the RaNN problem and significantly reduce the number of iterations needed for convergence.

Thank you for your attention!



