Multilevel Physics Informed Neural Networks (MPINNs)

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Joint work with:
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The context

The problem: numerical approximation of PDE's solutions.

- *Classical approaches*: discretization and multigrid methods (MG)
- *New advances in machine learning*: Physics Informed Neural Networks (PINNs)

Our objective:
Transfer the advantages of the first approach to the second.

Outline

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Multigrid methods (MG)

Physics Informed Neural Networks (PINNs)

Multilevel PINNs (MPINNs)

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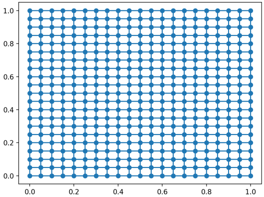
The numerical solution of PDEs

- Classically PDEs are discretized on a grid using finite differences or finite elements
- The resulting linear system $Au = f$ is solved using a fixed point iterative method (Gauss-Siedel or Jacobi)
- The size of the grids impacts the size of the system and the accuracy of the solution approximation



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The intuition behind multigrid methods

- Example: $\Delta u = 0$, $v_k(j) = \sin(\frac{kj\pi}{n})$, k-th Fourier mode
- The smoothing property: hard for fixed point iterative methods to reduce the low frequency components of the error

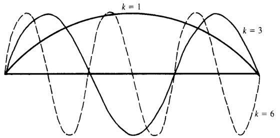
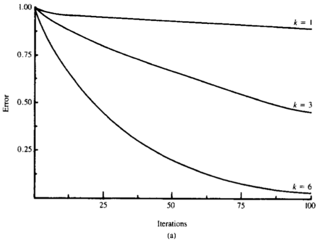


Figure 2.2: *The modes* $v_j = \sin\left(\frac{jk\pi}{n}\right)$, $0 \le j \le n$, *with wavenumbers* $k = 1, 3, 6$. *The* k*th mode consists of* $\frac{k}{2}$ *full sine waves on the interval.*



The intuition behind multigrid methods

- How does a smooth component look like on a coarser grid?

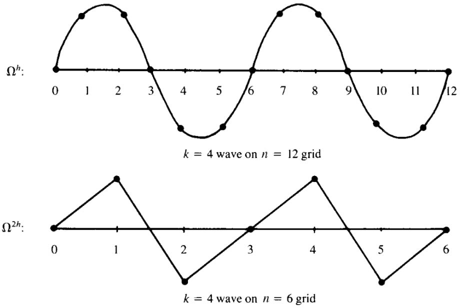
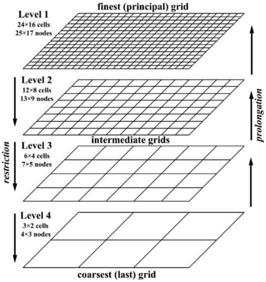


Figure 3.1: *Wave with wavenumber $k = 4$ on Ω^h ($n = 12$ points) projected onto Ω^{2h} ($n = 6$ points). The coarse grid "sees" a wave that is more oscillatory on the coarse grid than on the fine grid.*

Multigrid methods for PDEs

State-of-the-art methods for PDEs: exploit representation of the problem at different scales



- Fine scales: eliminate high frequency components of the error
- Coarse scales: eliminate low frequency components of the error

Two-level multigrid methods

Consider a linear PDE:

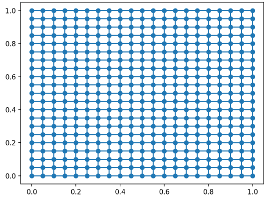
$$Au = f.$$

Consider two discretizations of the same system:

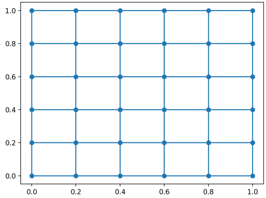
- Fine grid: $A_h u_h = f_h$
- Coarse grid: $A_H u_H = f_H$

Idea: write the solution u as the sum of a fine and a coarse term:

$$u \sim \underbrace{v_h}_{\in \mathbb{R}^h} + P(\underbrace{e_H}_{\in \mathbb{R}^H}),\ H < h.$$



$R \Downarrow \qquad P \Uparrow$



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Two-level multigrid methods

Update the two components in an alternate fashion:

$$u \sim v + e$$
$$r = f - Av$$
$$Ae = r \text{ residual equation}$$

- *Fine level*: get v_h by iterating on $A_h u = f_h$
- Compute $r_h = f - Av_h$ and project $r_H = Rr_h$
- *Coarse level*: compute correction: $A_H e_H = r_H$
- Correct: $v_h \leftarrow v_h + P(e_H)$

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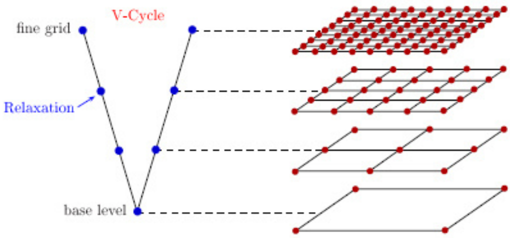
General multigrid methods



W. Briggs, V. Henson, S. McCormick. A Multigrid Tutorial, SIAM, 2000.

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A new approach for PDEs

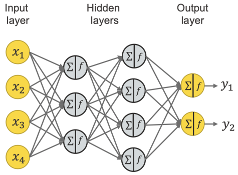
A recent development: use neural networks to approximate the solution of a PDE

M. Raissi, P. Perdikaris, G. Karniadakis, Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations, 2019.

Why this approach ?

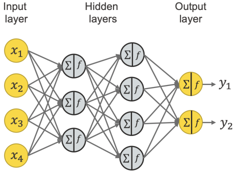
- Natural approach for nonlinear equations
- Provides analytic and continuously differentiable expression of the approximate solution
- The solution is meshless, well suited for problems with complex geometries
- The training is highly parallelizable on GPU
- Allows to alleviate the effect of the curse of dimensionality

General NN strategy for learning problems



- Dataset composed of input/output couples (x_i, y_i), $i = 1, \dots, m$.
- Loss function $L(\theta; x, y) = \frac{1}{m} \sum_{i=1}^{m} (NN(x_i, \theta) - y_i)^2 = MSE$
- The associated minimization problem : $\underset{\theta \in \Theta}{min} L(\theta; x, y)$
- Optimize by SGD

General NN strategy for learning problems



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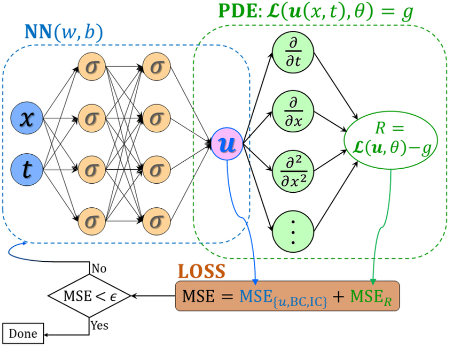
How to integrate the physical knowledge in the model?

Physics Informed Neural Networks (PINNs)

$\mathcal{L}(u(x,t),\theta) = g(x,t)$
$+$ BC $+$ IC
in $\Omega \times [0,T]$

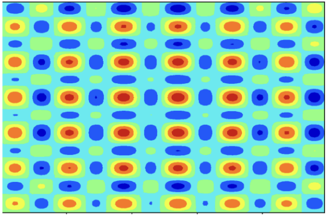


Given x_i, t_i sampled randomly, and $y_i = u^*(x_i,t_i)$,

$$MSE_{\{u,BC,IC\}} = \frac{1}{N_m} \sum_{x_i \in \Omega \cup \partial\Omega, t_i \in [0,T]} (NN(x_i,t_i) - y_i)^2,$$

$$MSE_R = \frac{1}{N_r} \sum_{x_i \in \Omega, t_i \in [0,T]} R(x_i,t_i)^2$$

On the spectral bias of neural networks



On the Spectral Bias of Neural Networks

Nasim Rahaman [*1 2] Aristide Baratin [*1] Devansh Arpit [1] Felix Draxler [2] Min Lin [1] Fred A. Hamprecht [2]
Yoshua Bengio [1] Aaron Courville [1]

WHEN AND WHY PINNS FAIL TO TRAIN: A NEURAL TANGENT KERNEL PERSPECTIVE

A PREPRINT

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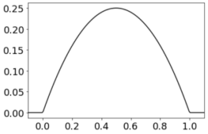
⇒ PINNs are not effective in approximating highly oscillatory solutions

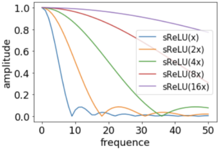
Mscale networks

Z.Q. Liu, W. Cai, and Z.Q. John Xu, Multi-scale Deep Neural Network (MscaleDNN) forSolving Poisson-Boltzmann Equation in Complex Domains, 2020

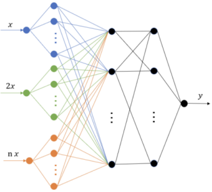
Idea: simultaneous training of frequency-selective subnetworks



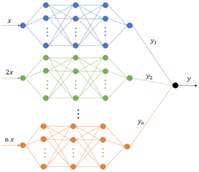
(b) sReLU



(a) sReLU



(a) MscaleDNN-1



(b) MscaleDNN-2

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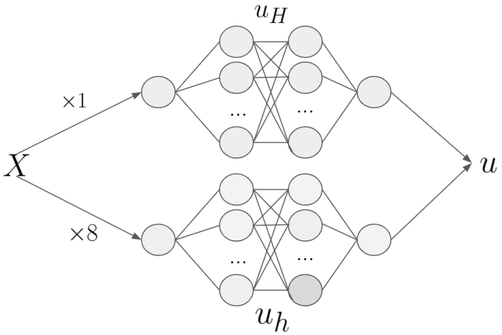
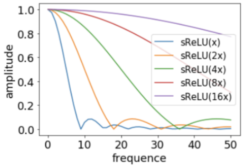
Multilevel PINNs: the architecture

Idea: $u_{sol}(x) \sim u_h(\theta_h, x) + u_H(\theta_H, x)$
Also exploit frequency-selective subnetworks





(a) sReLU

Multilevel PINNs: the loss

Problem definition

$$\mathcal{L}(u(x)) = g(x),\ x \in \Omega,$$
$$u_{sol}(x) \sim u_h(\theta_h, x) + u_H(\theta_H, x)$$

Fine problem	**Coarse problem**
$MSE_h(\theta_h) = MSE_{R,h}(\theta_h) + MSE_{B,h}(\theta_h)$	$MSE_H(\theta_H) = MSE_{R,H}(\theta_H) + MSE_{B,H}(\theta_H)$
$MSE_{R,h}(\theta_h) = \|\|\mathcal{L}(\hat{u}_h(\theta_h) + u_H) - g\|\|^2$	$MSE_{R,H}(\theta_H) = \|\|\mathcal{L}(\hat{u}_H(\theta_H) + u_h) - g\|\|^2$
$MSE_{B,h}(\theta_h) = \|\|\hat{u}_h(\theta_h) + u_H - u\|\|^2$	$MSE_{B,H}(\theta_H) = \|\|\hat{u}_H(\theta_H) + u_h - u\|\|^2$
Computed on z_h the fine sampling	Computed on z_H the coarse sampling

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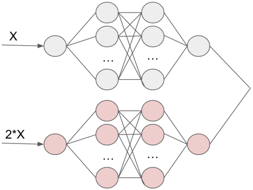
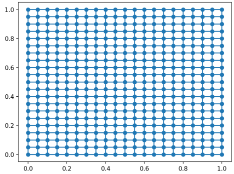
Multilevel PINNs: the training

Algorithm 1 2-level training of PINNs

1: Freeze coarse-network parameters, unfreeze fine-network parameters
2: **for** i=1,2,... **do**
3: Perform ν_1 epochs for the minimization of the fine problem
4: Freeze fine-network parameters, unfreeze coarse-network parameters
5: Perform ν_2 epochs for the minimization of the coarse problem
6: **end for**
7: Return : $u_H + u_h$

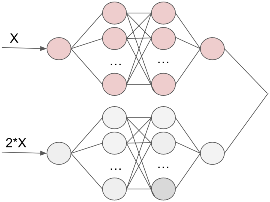


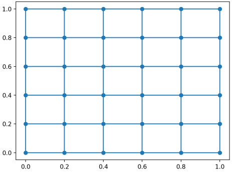


Multilevel PINNs: the training

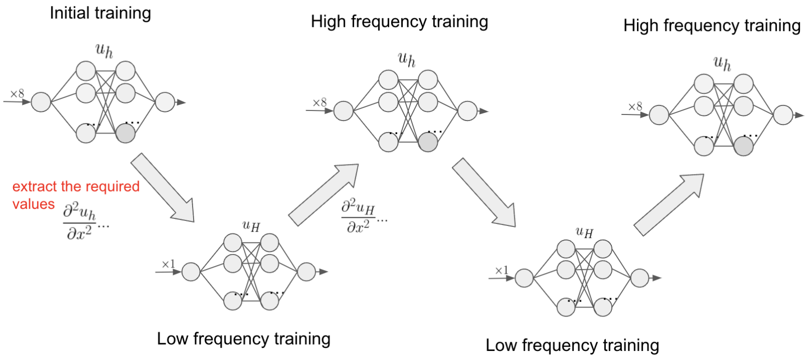
Algorithm 2 2-level training of PINNs

Freeze coarse-network parameters, unfreeze fine-network parameters
for i=1,2,... **do**
    Perform ν_1 epochs for the minimization of the fine problem
    Freeze fine-network parameters, unfreeze coarse-network parameters
    Perform ν_2 epochs for the minimization of the coarse problem
end for
Return : $u_H + u_h$



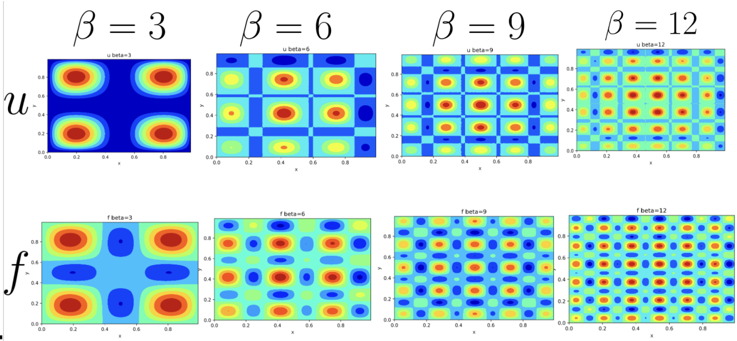


Multilevel PINNs: V-cycles



A simple Poisson problem

- $\Omega = [0, 1] \times [0, 1]$
- $\Delta u = f \ \forall x \in \Omega$
- $u = 0 \ \forall x \in \partial\Omega$
- $u(x, y) = (sin(\pi x) + sin(\beta\pi x)) * (sin(\pi y) + sin(\beta\pi y))$

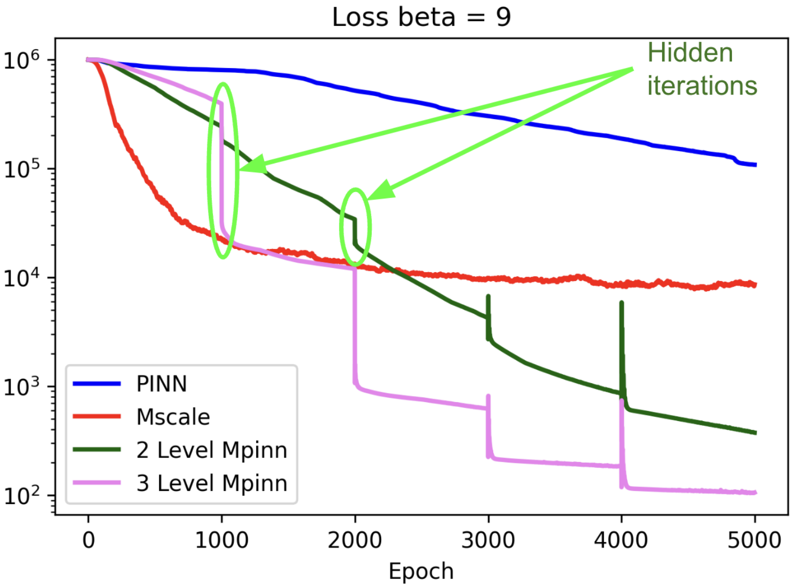


Experimental settings

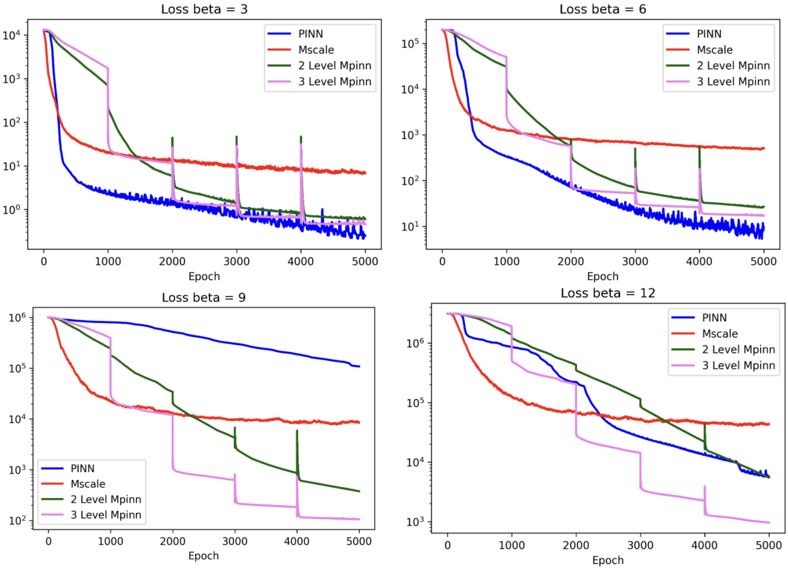
In what follows:

- The PINNs have two hidden layers of 300 neurons each.
- The Mscale have four subnetworks of two hidden layers of 150 neurons each, the input scaling used are 1,2,4 and 8.
- The two-level MPINN is composed of two networks of two hidden layers of 210 neurons each and trained in a V-cycle with 1 and 8 input scalings ($\nu_1 = \nu_2 = 1000$).
- The three-level MPINN is composed of three networks of two hidden layers of 150 neurons each and trained in a V-cycle with 1,4 and 8 input scalings ($\nu_1 = \nu_2 = \nu_3 = 1000$).
- The input of all networks is a regular grid sample of 80×80 points
- In all cases, we plot the median for ten random runs.

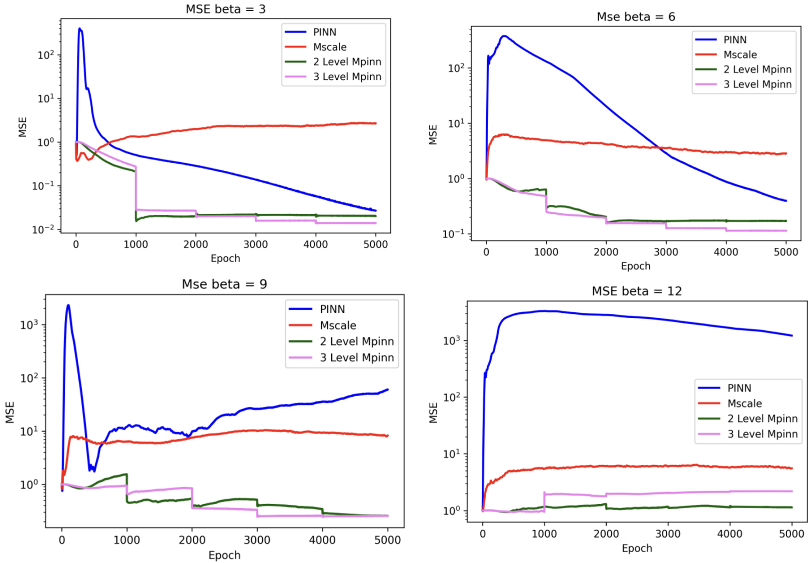
Experimental results



Varying β (the frequency content)

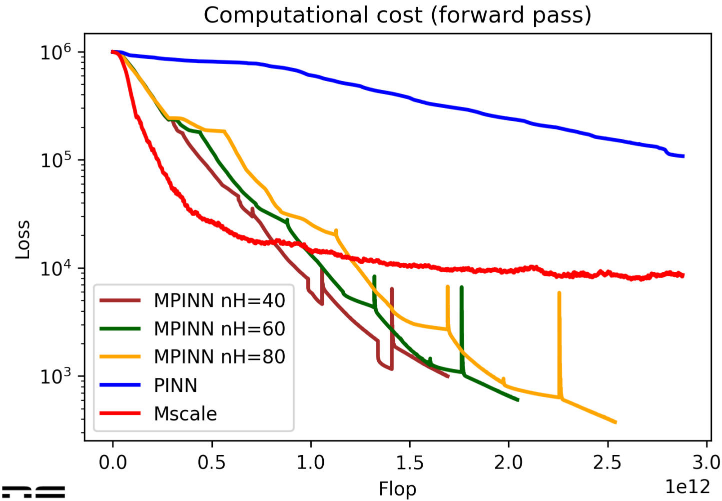


Convergence of MSE (extrapolation)



Computational cost for two levels...

...as a function of coarse grid size (nH)



Conclusions

- We have presented a new multigrid-inspired training framework using recent advances in NN to efficiently solve PINN-type problems.
- We have proposed an algorithm which works without prior knowledge of frequency content and which is promising.
- We have demonstrated that exploiting spectral complementarity using our framework may bring significant computational benefits (faster convergence).

Perspectives

- Perform further extensive testing, including more complex problems.
- Pursue the sensitivity analysis for
  - the relative sizes of the grids,
  - the relative sizes of the networks.
- Investigate theoretical aspects:
  - convergence of the iterates from an optimization point of view,
  - convergence to the solution in functional space.

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Thank you for your attention!

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