Designing Next-Generation Numerical Methods with Physics-Informed Neural Networks

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Talk Outline

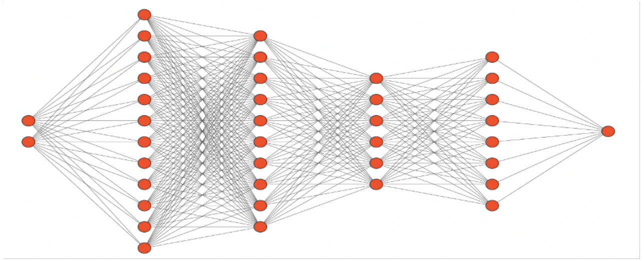
1. How does a Physics-Informed Neural Network (PINN) Solver Work?
2. Optimization of PINN Solvers
3. Integrating PINN into Traditional Solvers

1.1 Physics-Informed Neural Networks = PINN

- PINNs have many usages:
  - data assimilation
  - uncertainty quantification
  - solving ill-defined problems (e.g., no BC or EoS)
- In this talk, I focus on PINN for solving Partial Differential Equations (PDE)

1.2 Neural Network for Solving 2D Poisson Equation

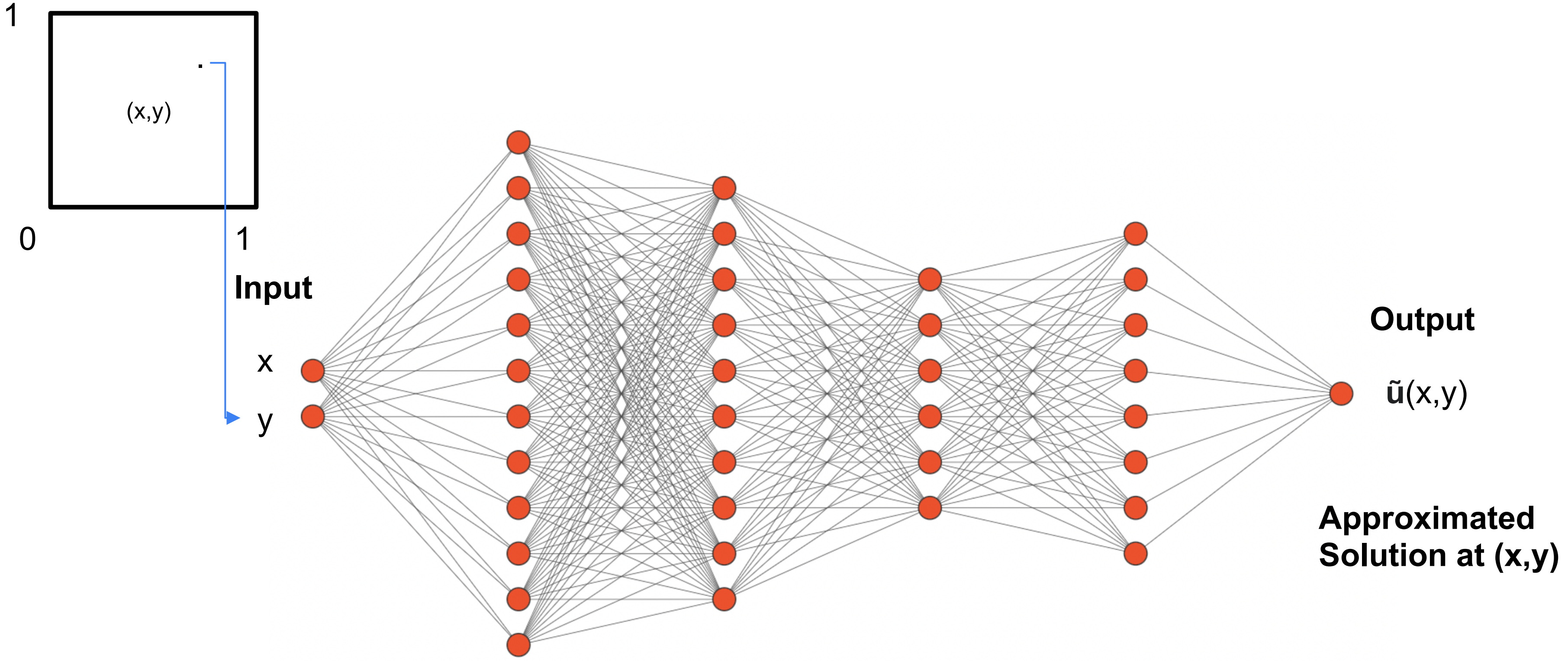
$$\nabla^2 u(x, y) = f(x, y), (x, y) \in [0, 1] \times [0, 1]$$



How would you do it?

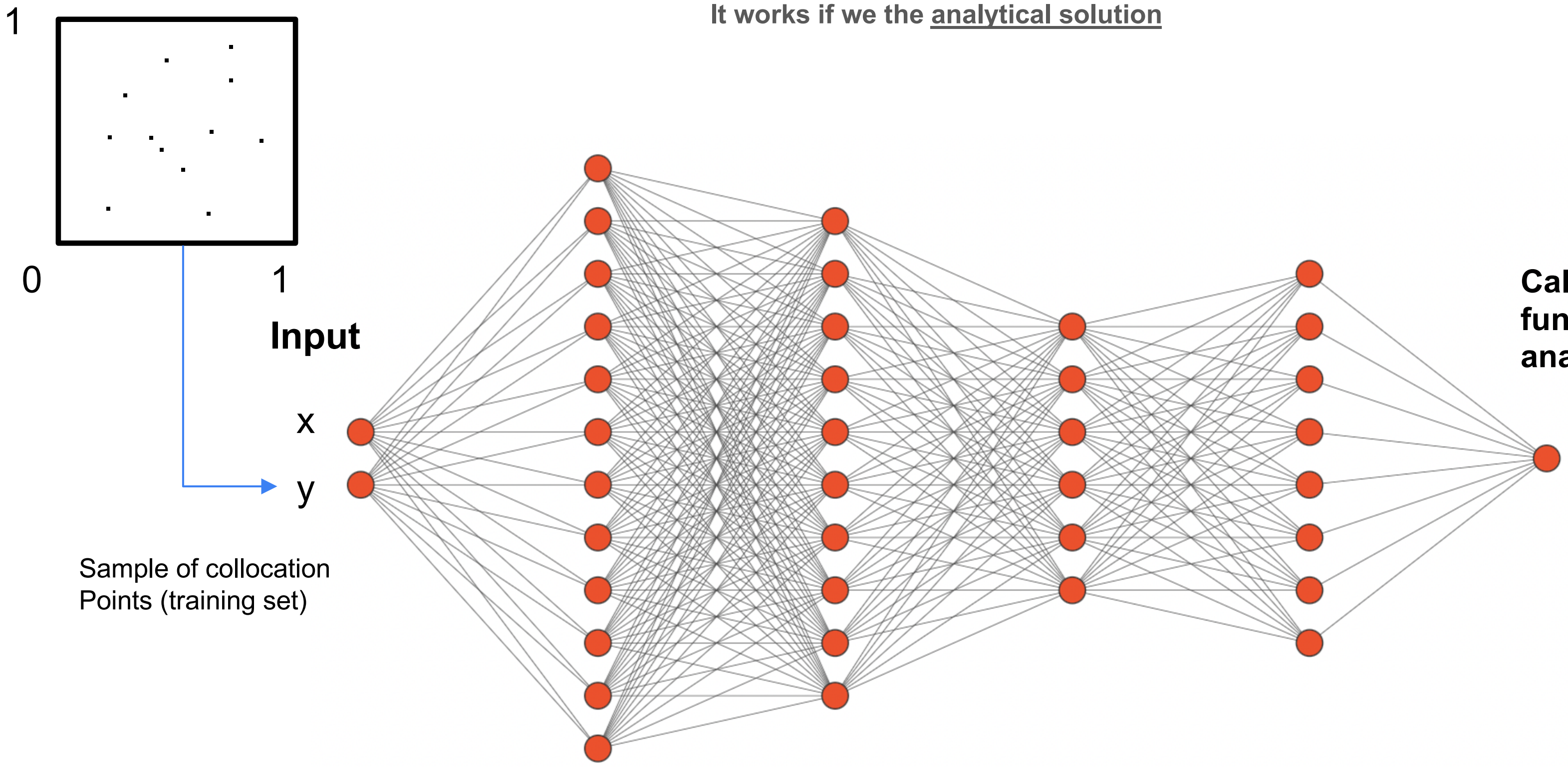
Let's assume you have the analytical or the numerical solution …

1.3 Replace a Solver with a Neural Network



1.4 Training with Analytical Solution

It works if we the analytical solution

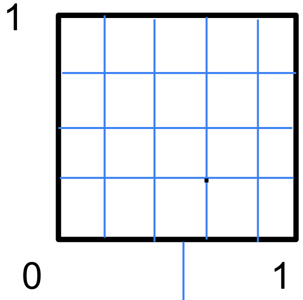


Calculate the loss function knowing the analytical solution

L = 1/n SUM $(\tilde{u}(x,y) - u(x,y))^2$

1.5 Training with a Numerical Solution

It works if we the numerical solution

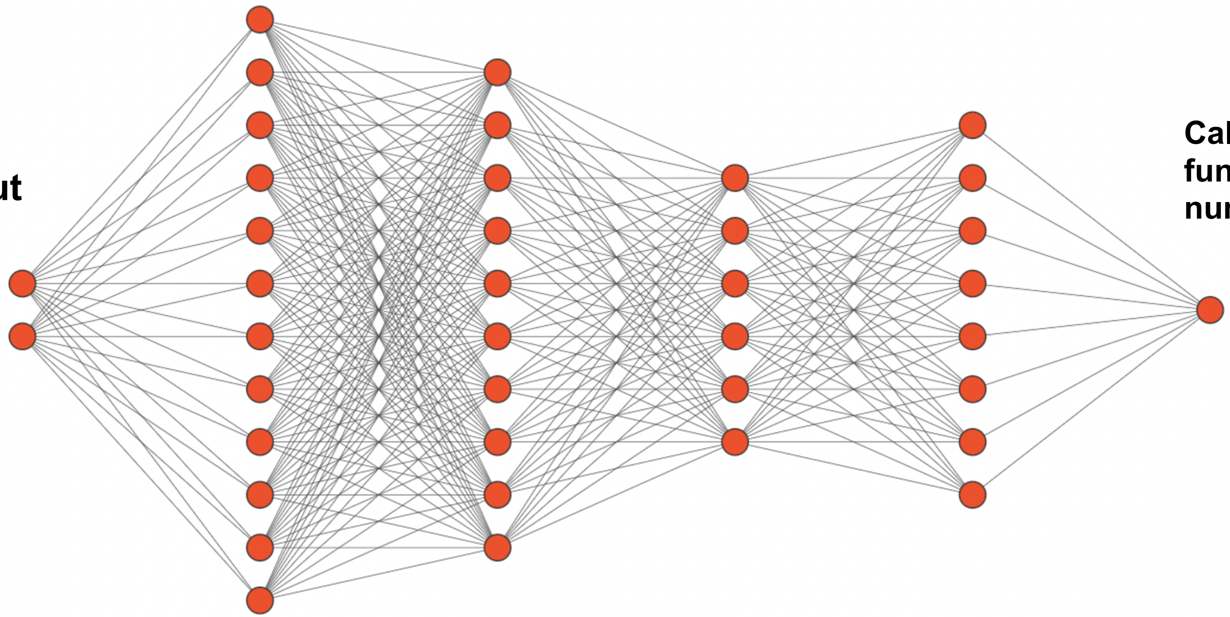


Input

x

y

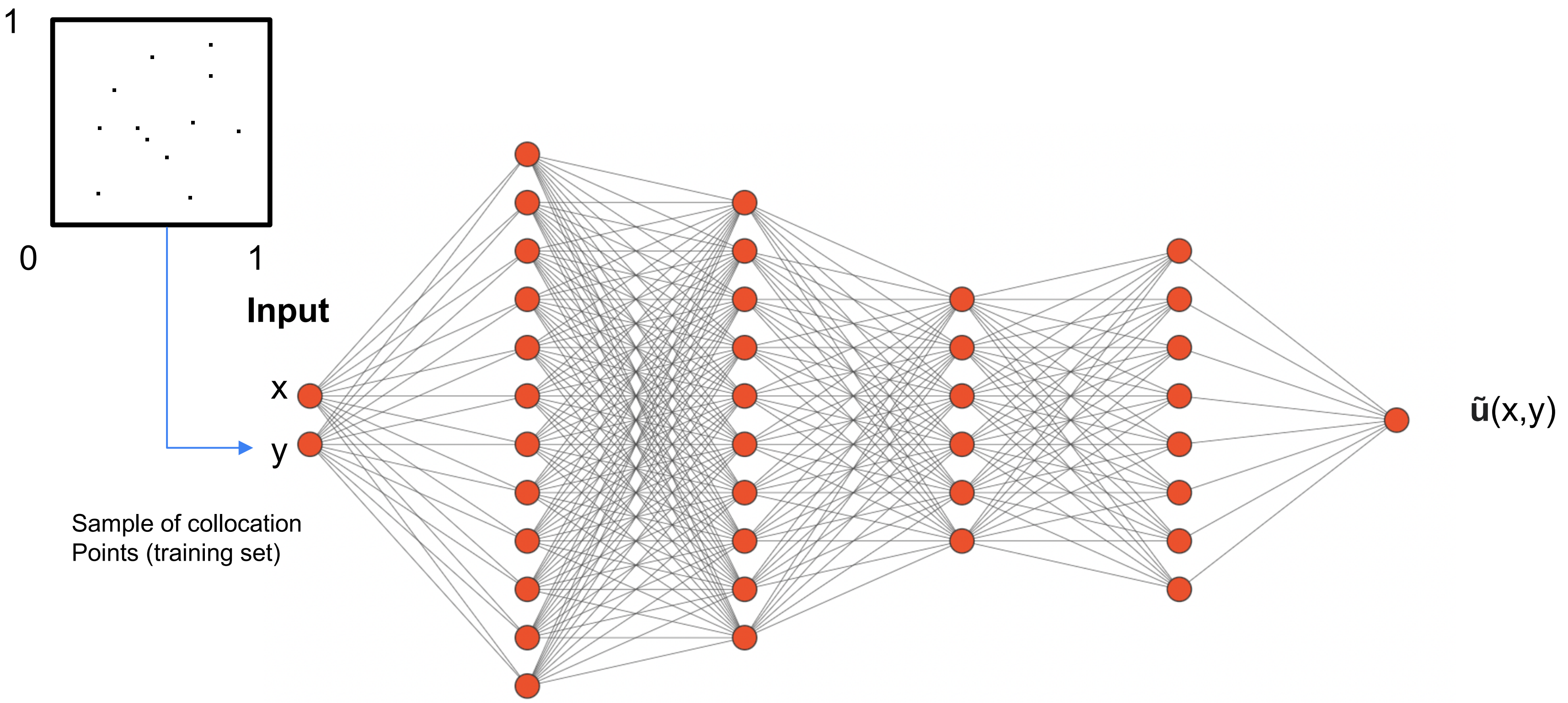
Sample of collocation
Points (training set)



Calculate the loss function knowing the numerical solution

$$L = 1/n \text{ SUM } (\tilde{u}(x_i,y_i) - u(x_i,y_i))^2$$

1.6 Prediction with the Surrogate Model = PDE Solver

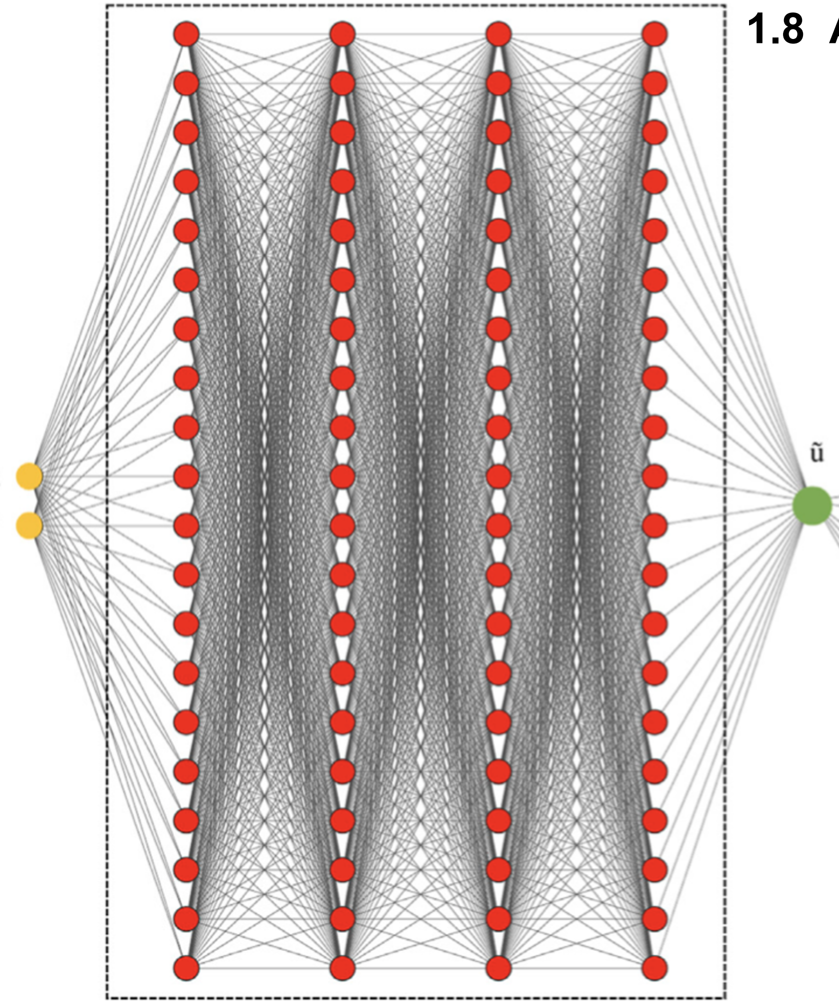


This PDE solver is <u>gridless</u>

1.7 Entering PINNs!

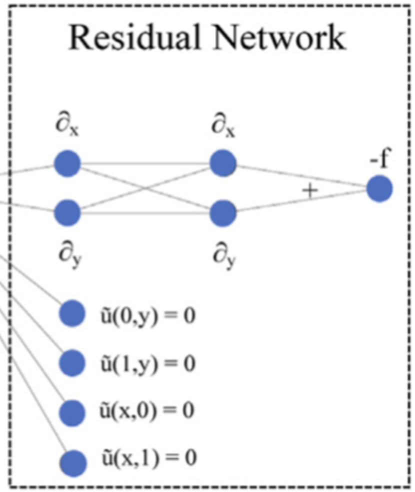
- PINNs are neural networks that encode the partial differential equations into a part of neural network, exclusively to calculate the loss function
    - We still use the surrogate to evaluate the solution!
- Two major innovations:
    1. Add a part of the network / graph to calculate the residual.
        1. This part encodes the PDE into the NN.
    2. Leverage automatic differentiation to calculate the derivatives on the network.

Raissi, M., Perdikaris, P., & Karniadakis, G. E. (2019). Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *Journal of Computational physics*, *378*, 686-707.
https://github.com/maziarraissi/PINNs



1.8 Adding a Residual Network to Calculate a Residual

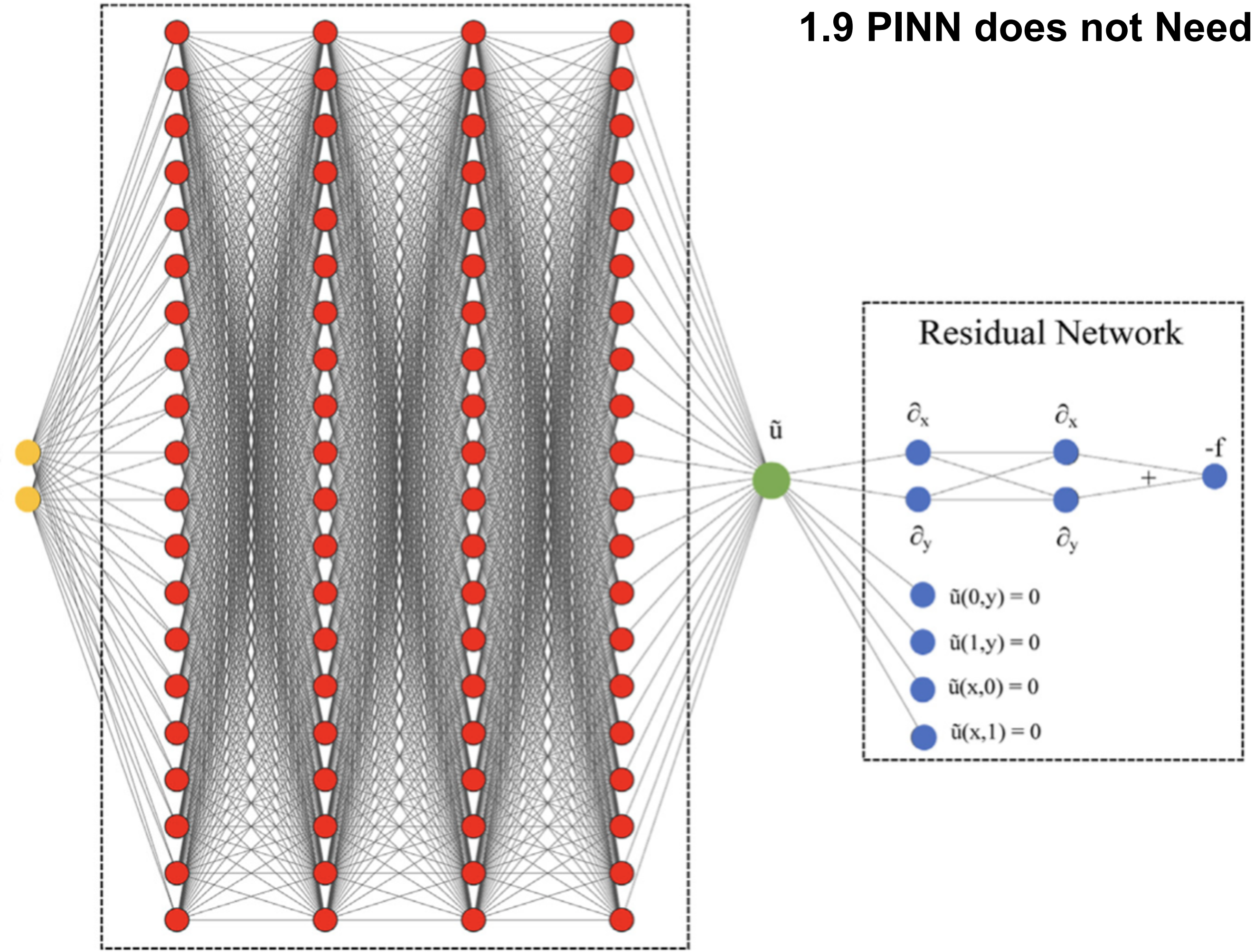
$$r = \nabla^2 \tilde{u}(x, y) - f(x, y)$$ *Residual function*



Loss function

$$MSE_r = \frac{1}{N_{x_i,y_i}} \sum |r(x_i, y_i)|^2$$

1.9 PINN does not Need Solutions for Training

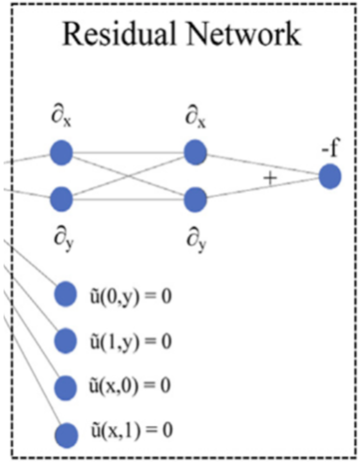


Loss function

$$MSE_r = \frac{1}{N_{x_i,y_i}} \sum |r(x_i, y_i)|^2$$

No need for prior data (solutions)
→ **<u>unsupervised training</u>**

1.10 How do we Calculate the Derivative on the Network?

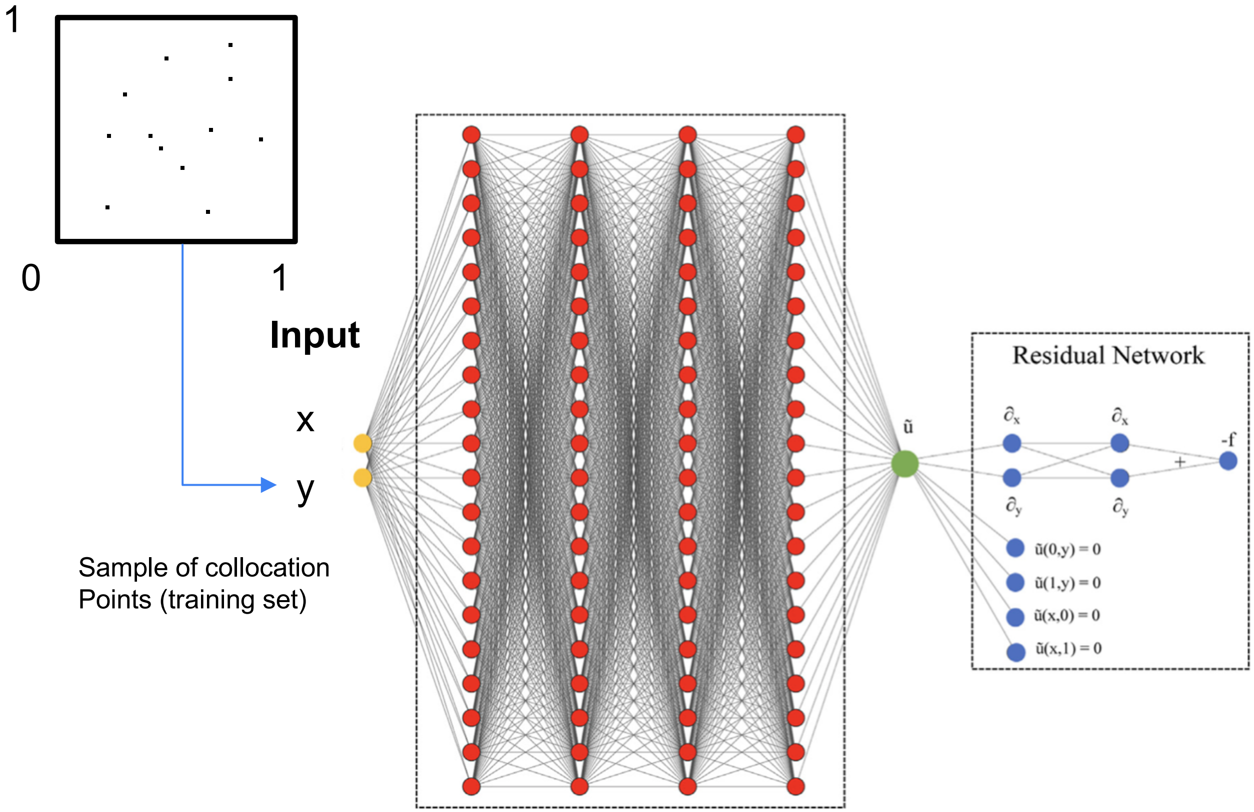



```python
# Creating the parameters
w1 , w2 = tf.Variable(5.0) , tf.Variable(3.)

# Using automatic differentiation
with tf.GradientTape() as tape:
        # Forward pass
        z = f(w1 ,w2)

# Getting the gradients
gradients = tape.gradient(z , [w1 , w2])
print(gradients)
```


- We use a critical ML technology used in backpropagation
  - **Automatic differentiation**
  - Available in the TensorFlow and PyTorch

Baydin, A. G., Pearlmutter, B. A., Radul, A. A., & Siskind, J. M. (2018). Automatic differentiation in machine learning: a survey. *Journal of Marchine Learning Research*, *18*, 1-43.

1.11 PINN Training Iteration



Sample of collocation
Points (training set)

1. We train network first via iterations / epochs
2. We make a prediction/inference step on a grid or any point of interest
   - Remember that PINN are gridless

$$MSE_r = \frac{1}{N_{x_i,y_i}} \sum |r(x_i, y_i)|^2$$

1.12 PINN As an Iterative Solver – Convergence / Stability

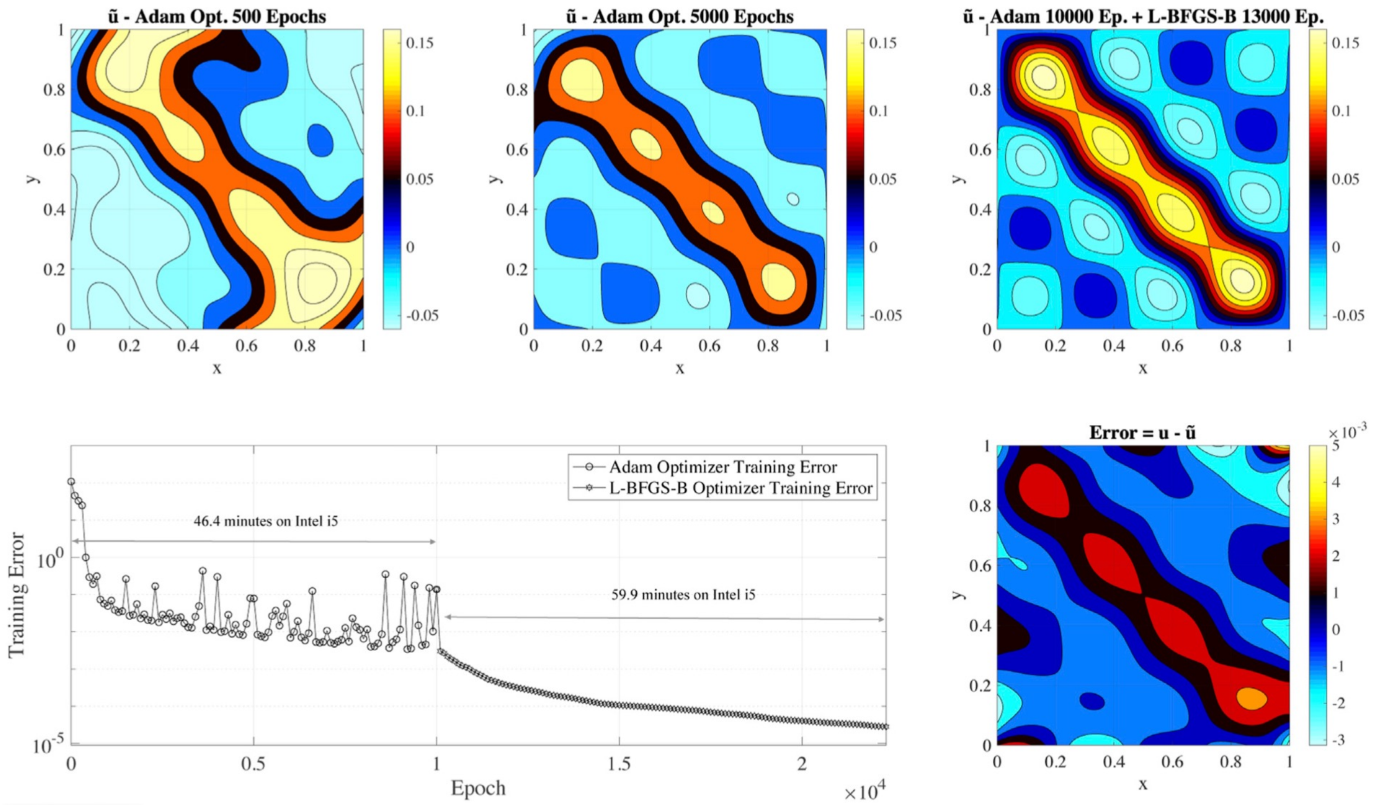
- For stability and convergence studies, we need to study how error changes
- Possible to define errors (generalization, training, …) and do an analytical study
- It has shown that PINNs requires sufficiently smooth activation functions for convergence:
    - PINNs with ReLU, ELU and SELU do not converge

Shin, Y., Darbon, J., & Karniadakis, G. E. (2020). On the convergence of physics informed neural networks for linear second-order elliptic and parabolic type PDEs. arXiv preprint arXiv:2004.01806.

Mishra, S., & Molinaro, R. (2022). Estimates on the generalization error of physics-informed neural networks for approximating PDEs. *IMA Journal of Numerical Analysis*.

1.13 What is the Performance of a Simple PINN?

$$\nabla^2 u(x, y) = f(x, y) \qquad f(x, y) = \frac{1}{4}\sum_{k=1}^{4}(-1)^{k+1}2k\sin(k\pi x)\sin(k\pi y)$$



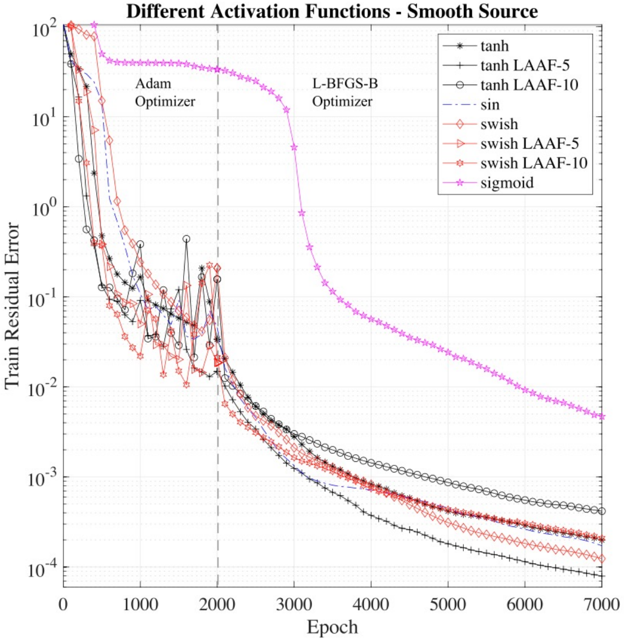
- Python and DeepXDE
- Fully Connected
- 4 layers
- 50 units per layer
- tanh act. function
- 10,000 coll. points
- Adam + L-BFGS.B Optimizers
- PETSc CG took 92 seconds for full convergence on 128x128 grid!

2.1 Optimization of PINN Solvers

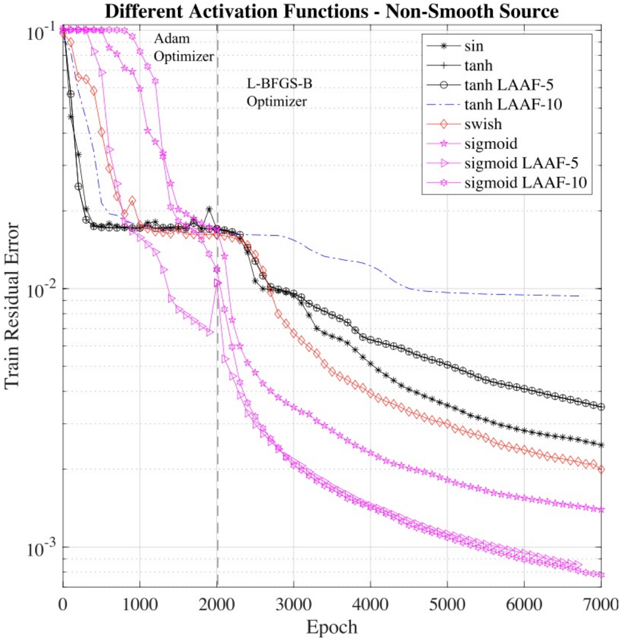
1. Activation functions / Adaptive Functions
2. Optimizers
3. Transfer-Learning

2.2 PINN Optimization – Activation Functions

$$f(x,y) = \frac{1}{4}\sum_{k=1}^{4}(-1)^{k+1}2k\sin(k\pi x)\sin(k\pi y)$$



$$f(x,y) = 1 \text{ for } \sqrt{(x-0.5)^2 + (y-0.5)^2} \le 0.2$$



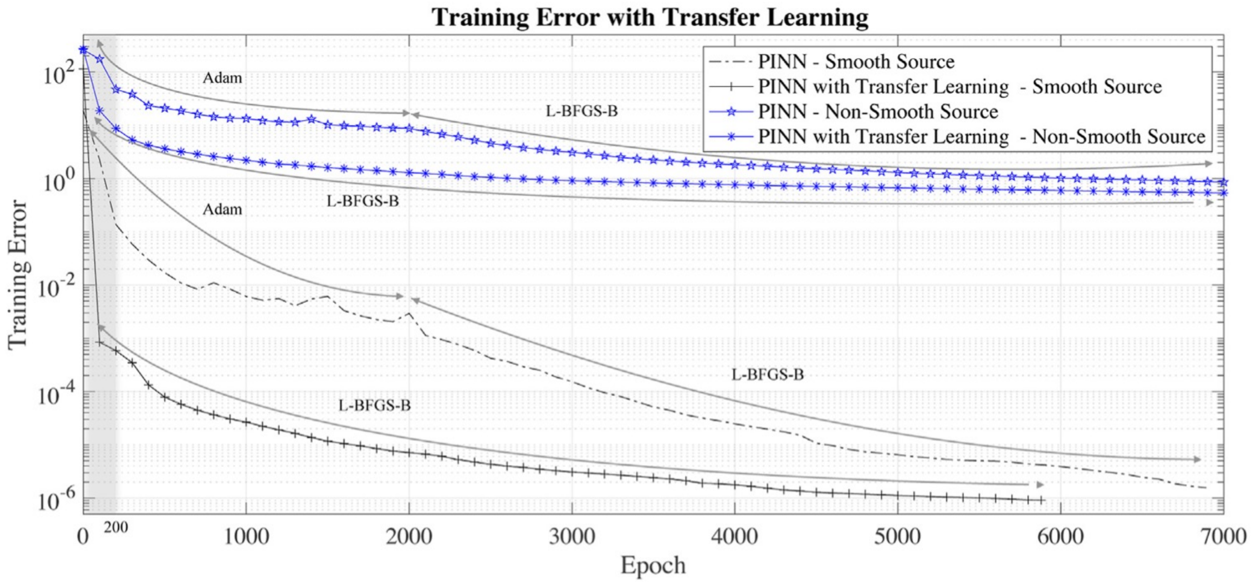
- Activation functions largely impacts the performance
- Best activation function depends on the problem
- LAAF activation functions introducing adaptive local scaling are best
  - Deal better with BCs

Jagtap, A. D., Kawaguchi, K., & Em Karniadakis, G. (2020). Locally adaptive activation functions with slope recovery for deep and physics-informed neural networks. *Proceedings of the Royal Society A*, *476*(2239), 20200334.

2.3 PINN Optimization – BFGS Optimizer

- In PINN two optimizers in succession
  1. Adam optimizer
  2. Broyden- Fletcher-Goldfarb-Shanno (BFGS) optimizer
     - Higher-order: BFGS uses the Hessian matrix (curvature in highly dimensional space)
     - Without using the Adam optimizer can rapidly converge to a local minimum!
       - For this reason, the Adam optimizer is used first to avoid local minima, and then the solution is refined by BFGS.
- BFGS is currently the most critical technology for PINNs as it provides much higher accuracy than available DL optimizers.
  - L-BFGS-B from in SciPy. Not available on GPUs.
  - New L-BFGS-B available in Google's Tensorflow Probability Framework
    - Built on the top of TensorFlow

2.4 PINN Optimization – Transfer Learning



The transfer learning technique = training a network solving the Poisson equation with a <u>different source term</u>.

- Initialize the PINN network we intend to solve with the first fully trained network weights and biases → first PINN transfers the learned information

3.1 Integration of PINNs into Traditional Solvers

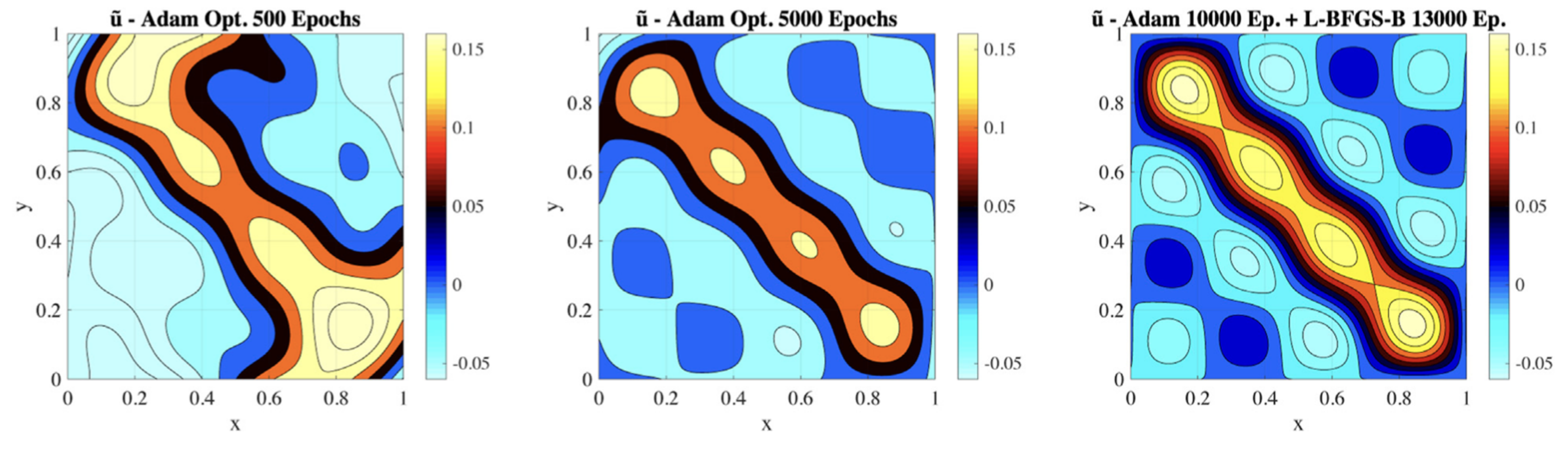
- Even after these optimizations, PINN performance is not as good as traditional iterative solvers!
  - Especially when it comes to accuracy
- **Idea:** combine two approaches to get the best from the two world
  - What PINNs are good at?

3.2 DLN F-principle: Convergence of PINN on Large Scale Structures First!

Frequency-principle (F-principle): DNNs often fit target functions from low to high frequencies during the training process

The F-principle implies that in PINNs, the low frequency/large scale features of the solution emerge first, while it will take several training epochs to recover high frequency/small-scale features.

$$f(x,y) = \frac{1}{4}\sum_{k=1}^{4}(-1)^{k+1}2k\sin(k\pi x)\sin(k\pi y)$$



Xu, Z. Q. J., Zhang, Y., Luo, T., Xiao, Y., & Ma, Z. (2019). *Frequency principle: Fourier analysis sheds light on deep neural networks. arXiv preprint arXiv:1901.06523.*

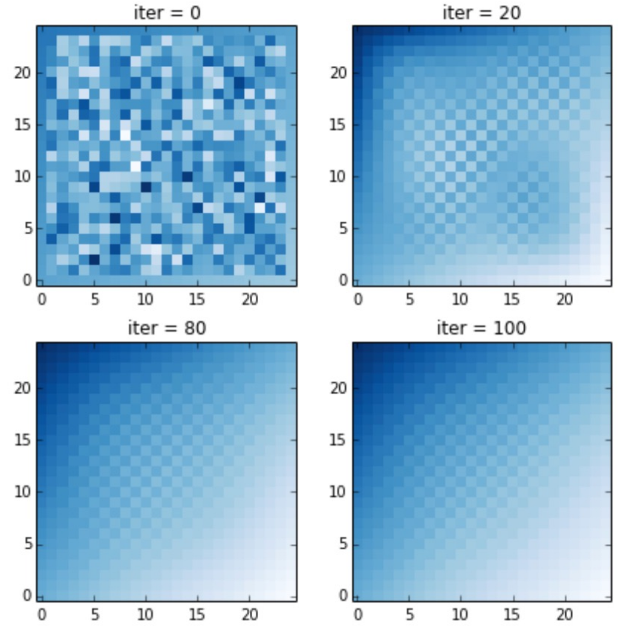
3.3 Traditional Jacobi and GS Solvers: Convergence on Small Scales First!

- Both the Jacobi and Gauss-Seidel methods show fast convergence for small-scale features
    - Update of unknown values involves only the values of the neighbor points

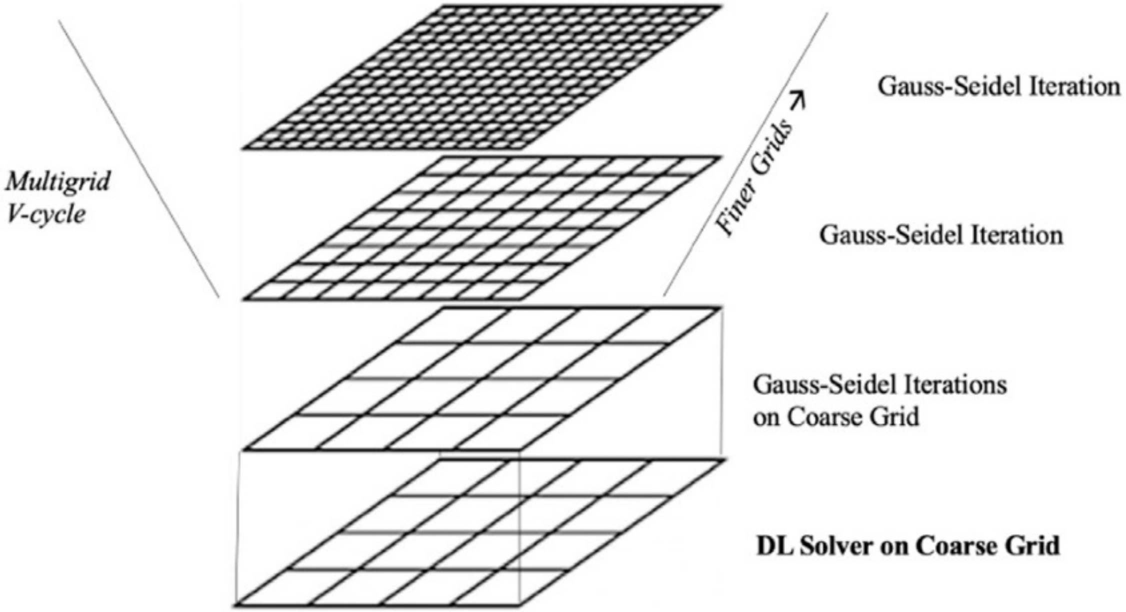
$$u_{i,j}^{n+1} = \frac{1}{4}(u_{i+1,j}^n + u_{i-1,j}^n + u_{i,j+1}^n + u_{i,j-1}^n)$$

- Between two different iterations, the information can only propagate to neighbour cells

Jacobi Iteration



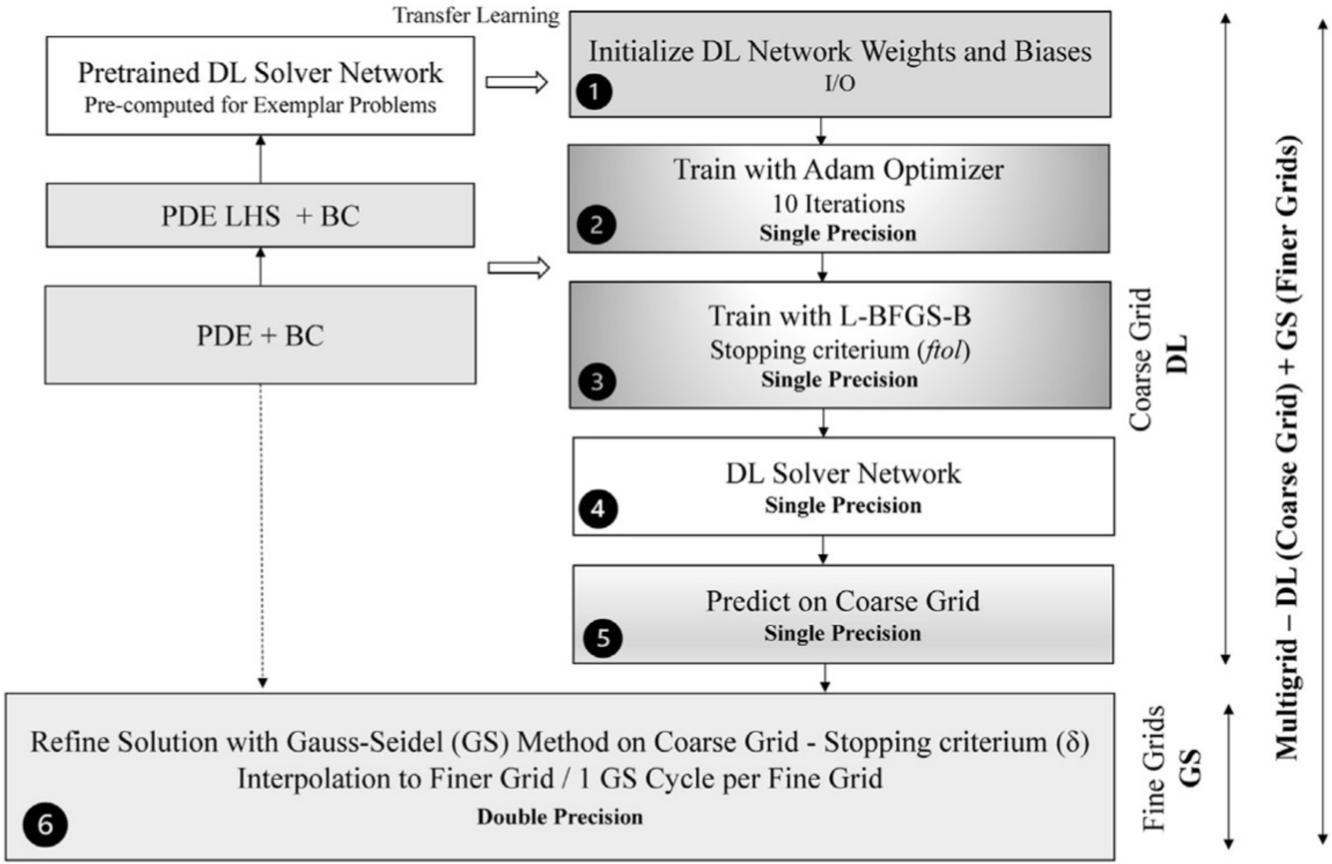
3.4 Combining Low Frequency and High Frequency Solvers in a Multigrid Solver



Basic Idea: optimized PINN for a coarse grid then use a MG solvers

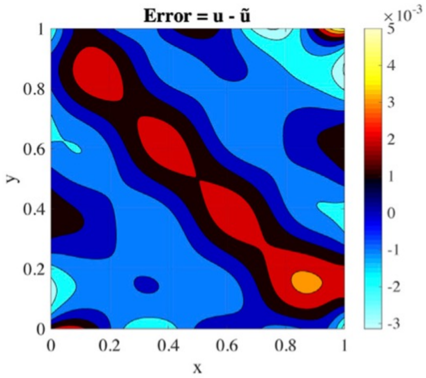
Markidis, S. (2021). The old and the new: Can physics-informed deep-learning replace traditional linear solvers? *Frontiers in big Data*, 92.

3.5 Combining Low Frequency and High Frequency Solvers in a Multigrid Solver

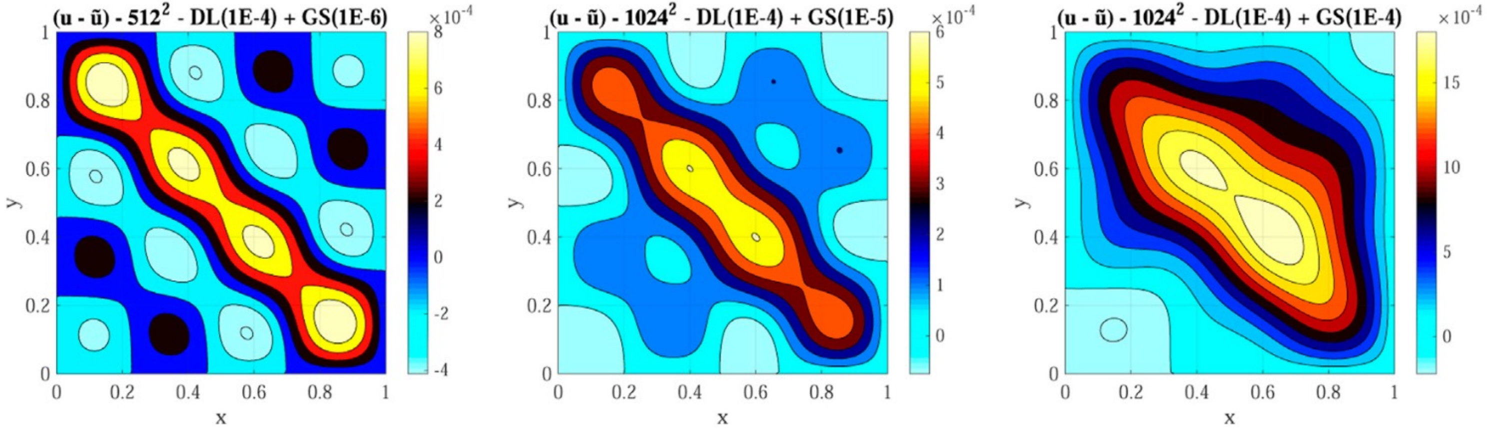


3.6 Hybrid Solver - Accuracy

Direct PINN Error

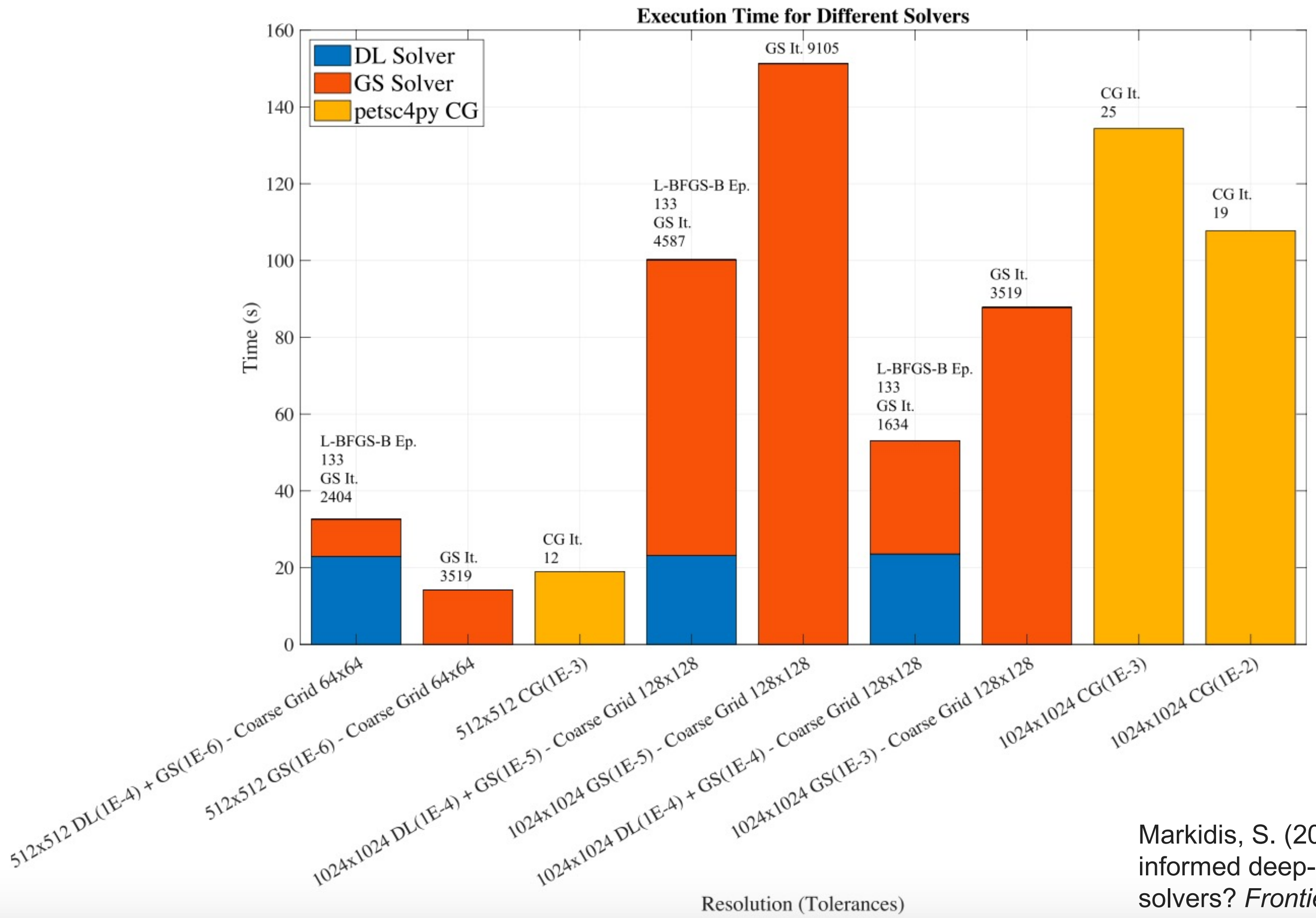


Hybrid DL-solver



Markidis, S. (2021). The old and the new: Can physics-informed deep-learning replace traditional linear solvers? *Frontiers in big Data*, 92.

3.7 Hybrid Solver – Computational Performance



- Different resolutions, tolerances for hybrid, pure GS and PETSc CG
- Python implementations (CG step developed in Cython)

Markidis, S. (2021). The old and the new: Can physics-informed deep-learning replace traditional linear solvers? *Frontiers in big Data*, 92.

Conclusions

1. PINN are neural networks encoding PDEs in the network and they can be used for solving PDEs in an unsupervised fashion
2. The PINN performance (both computational and accuracy) is still far from performance of traditional approaches, but optimization are possible: activation function tuning, high-order optimizers and transfer learning
3. Combine traditional and PINN solver technology is a realistic approach for developing the next-generation Solvers
    - We are still in the infancy of these method: lot of work to do!