

Report: Deep Ritz Method for Solving the Biharmonic Equation with Neumann-Type Boundary Conditions (Phase-2)

1. Introduction

The biharmonic equation is a fourth-order partial differential equation (PDE) that arises in various applications in physics and engineering.

The general biharmonic problem is stated as:

$$\Delta^2 u = f \text{ in } \Omega$$

where $\Delta^2 = \Delta(\Delta u)$ is the biharmonic operator, obtained by applying the Laplacian operator twice. For a two-dimensional domain $\Omega \subset \mathbb{R}^2$, this expands to:

$$\Delta^2 u = \frac{\partial^4 u}{\partial x_1^4} + 2 \frac{\partial^4 u}{\partial x_1^2 \partial x_2^2} + \frac{\partial^4 u}{\partial x_2^4}$$

The Deep Ritz Method:

The Deep Ritz Method (DRM) is a physics-informed machine learning technique that combines the classical Ritz variational method with deep neural networks. Instead of discretizing the domain and using finite-dimensional function spaces, DRM parameterizes the solution using a neural network and minimizes the energy functional directly.

Key advantages of DRM:

1. Automatic differentiation: Neural network frameworks provide derivatives automatically
2. Flexibility: Can handle complex geometries and high-dimensional problems
3. Universal approximation: Neural networks can approximate arbitrary smooth functions

2. Problem Formulation

2.1 The Biharmonic Problem (P2)

We consider the biharmonic equation in the unit square $\Omega = (0,1)^2$:

$$\Delta^2 u = f \text{ in } \Omega$$

with mixed boundary conditions:

- Essential (Dirichlet): $u = g_1$ on $\partial\Omega$
- Neumann-type: $\frac{\partial^2 u}{\partial n^2} = g_2$ on $\partial\Omega$

The second normal derivative is defined as:

$$\frac{\partial^2 u}{\partial n^2} = \mathbf{n}^T \cdot D^2 u \cdot \mathbf{n} = n_1^2 \frac{\partial^2 u}{\partial x_1^2} + 2n_1 n_2 \frac{\partial^2 u}{\partial x_1 \partial x_2} + n_2^2 \frac{\partial^2 u}{\partial x_2^2}$$

where $\mathbf{n} = (n_1, n_2)$ is the outward normal vector and $D^2 u$ is the Hessian matrix of second derivatives.

2.2 Ritz Variational Formulation

The classical Ritz method seeks the solution by minimizing an energy functional. For Problem (P2), the energy functional is:

$$\mathcal{L}(v) = \frac{1}{2} \int_{\Omega} \|D^2 v\|_F^2 dx - \int_{\Omega} f v dx - \int_{\partial\Omega} g_2 \frac{\partial v}{\partial n} ds$$

where:

- $\|D^2 v\|_F^2$ is the Frobenius norm squared of the Hessian matrix
- The last term incorporates the natural (Neumann-type) boundary condition

The Frobenius norm squared of the Hessian is:

$$\|D^2 v\|_F^2 = \left(\frac{\partial^2 v}{\partial x_1^2} \right)^2 + 2 \left(\frac{\partial^2 v}{\partial x_1 \partial x_2} \right)^2 + \left(\frac{\partial^2 v}{\partial x_2^2} \right)^2$$

Admissible space: Classically, we minimize over $K = \{v \in H^2(\Omega): v = g_1 \text{ on } \partial\Omega\}$, where $H^2(\Omega)$ is the Sobolev space of functions with square-integrable second derivatives.

Euler-Lagrange equation: The minimizer of $\mathcal{L}(v)$ satisfies the original PDE and boundary conditions.

2.3 Penalized Deep Ritz Formulation

In the Deep Ritz Method, enforcing the essential boundary condition $u = g_1$ exactly is challenging when using neural networks. Instead, we use a penalty method by adding a penalty term to the energy functional:

$$\mathcal{L}_\lambda(v) = \frac{1}{2} \int_{\Omega} \|D^2 v\|_F^2 dx - \int_{\Omega} f v dx - \int_{\partial\Omega} g_2 \frac{\partial v}{\partial n} ds + \frac{\lambda}{2} \int_{\partial\Omega} (v - g_1)^2 ds$$

where:

- $\lambda > 0$ is the penalty parameter
- The penalty term $\frac{\lambda}{2} \int_{\partial\Omega} (v - g_1)^2 ds$ enforces $v \approx g_1$ on the boundary
- Larger λ enforces the boundary condition more strongly

Key insight: As $\lambda \rightarrow \infty$, the penalized solution converges to the constrained solution.

Admissible space: Now we minimize over $K_\lambda = H^2(\Omega)$ (no explicit boundary constraint).

2.4 Monte Carlo Approximation

The integrals in \mathcal{L}_λ cannot be computed analytically for neural networks. We approximate them using Monte Carlo sampling:

$$\begin{aligned}\int_{\Omega} h(x) dx &\approx \frac{|\Omega|}{N} \sum_{i=1}^N h(X_i), X_i \sim iid \mathcal{U}(\Omega) \\ \int_{\partial\Omega} h(x) ds &\approx \frac{|\partial\Omega|}{M} \sum_{j=1}^M h(Y_j), Y_j \sim iid \mathcal{U}(\partial\Omega)\end{aligned}$$

For the unit square: $|\Omega| = 1$, $|\partial\Omega| = 4$.

Empirical loss function:

$$\hat{\mathcal{L}}_\lambda(u_\theta) = \frac{1}{N} \sum_{i=1}^N \frac{1}{2} \| D^2 u_\theta(X_i) \|_F^2 - f(X_i) u_\theta(X_i) + \frac{4}{M} \sum_{j=1}^M [-g_2(Y_j) \frac{\partial u_\theta}{\partial n}(Y_j) + \frac{\lambda}{2} (u_\theta(Y_j) - g_1(Y_j))^2]$$

3. Neural Network Setup

3.1 Architecture

The solution $u(x_1, x_2)$ is approximated by a fully connected feed-forward neural network (multi-layer perceptron), implemented in the class U_FCN. The architecture used in this work consists of:

- Input layer: 2 neurons (coordinates x_1, x_2)
- Hidden layers: 6 layers with widths

$$[64, 128, 256, 512, 256, 128, 64]$$

- Activation function: hyperbolic tangent (\tanh) after each hidden layer

- Output layer: 1 neuron representing $u_\theta(x_1, x_2)$

Let $x = (x_1, x_2) \in \mathbb{R}^2$. If we denote the hidden layer widths by $(h_1, h_2, \dots, h_6) = (64, 128, 256, 512, 256, 128, 64)$ and the activation function by $\sigma(z) = \tanh(z)$, the network can be written as:

$$\begin{aligned} z_1 &= \sigma(W_1 x + b_1), \\ z_2 &= \sigma(W_2 z_1 + b_2), \\ z_3 &= \sigma(W_3 z_2 + b_3), \\ z_4 &= \sigma(W_4 z_3 + b_4), \\ z_5 &= \sigma(W_5 z_4 + b_5), \\ z_6 &= \sigma(W_6 z_5 + b_6), \\ u_\theta(x) &= W_7 z_6 + b_7, \end{aligned}$$

where

$$\theta = \{W_1, b_1, \dots, W_7, b_7\}$$

is the set of all trainable parameters.

Total number of parameters: **345665**

Choice of activation:

The activation function **tanh** is chosen because:

1. It is smooth and infinitely differentiable.
2. It allows stable computation of second-order and fourth-order derivatives using automatic differentiation.
3. ReLU is not suitable for high-order PDEs, as its second derivative vanishes almost everywhere.

3.2 Sampling Strategy

Training requires interior points to enforce the PDE and boundary points to enforce boundary conditions.

Interior sampling:

We draw N points uniformly inside the computational domain

$$\Omega = (0,1)^2,$$

as

$$X_i \sim \mathcal{U}([0,1]^2), i = 1, \dots, N.$$

Typical choice: $N = 1024$ interior points per training batch.

Boundary sampling:

The boundary $\partial\Omega$ consists of four edges. We draw $M/4$ points uniformly on each edge (with total boundary points $M = 256$). For each edge, we associate the outward unit normal vector:

- Bottom edge ($x_2 = 0$): $n = (0, -1)$
- Right edge ($x_1 = 1$): $n = (1, 0)$
- Top edge ($x_2 = 1$): $n = (0, 1)$
- Left edge ($x_1 = 0$): $n = (-1, 0)$

Resampling:

- During Adam optimization, interior and boundary points are resampled every iteration.
This reduces overfitting and improves generalization.
- During L-BFGS optimization, a fixed set of points is used for stability.

3.3 Automatic Differentiation

PyTorch's automatic differentiation (`torch.autograd.grad`) is used to compute all derivatives of the neural network output $u_\theta(x)$ with respect to the spatial coordinates.

First derivatives (gradient)

$$\nabla u_\theta(x) = \left(\frac{\partial u_\theta}{\partial x_1}(x), \frac{\partial u_\theta}{\partial x_2}(x) \right).$$

Second derivatives (Hessian)

The Hessian matrix is:

$$H(u_\theta)(x) = \begin{bmatrix} u_{x_1 x_1} & u_{x_1 x_2} \\ u_{x_2 x_1} & u_{x_2 x_2} \end{bmatrix}.$$

u_{x_1} and u_{x_2} again with respect to x .

Biharmonic operator

The biharmonic operator required in problem (P2) is

$$\Delta^2 u_\theta = \frac{\partial^2}{\partial x_1^2} (\Delta u_\theta) + \frac{\partial^2}{\partial x_2^2} (\Delta u_\theta),$$

and is computed using repeated applications of `torch.autograd.grad` in the function `biharmonic_operator`.

Normal derivatives:

For Neumann-type boundary conditions, we require:

- First normal derivative:

$$\frac{\partial u_\theta}{\partial n} = \nabla u_\theta \cdot n$$

- Second normal derivative:

$$\frac{\partial^2 u_\theta}{\partial n^2} = \nabla \left(\frac{\partial u_\theta}{\partial n} \right) \cdot n$$

All derivative computations use `create_graph=True` so that higher-order derivatives remain part of the computational graph.

4. Loss Function and Deep Ritz Formulation for Problem (P2)

For the biharmonic equation

$$\Delta^2 u = f \text{ in } \Omega = (0,1)^2,$$

with boundary conditions

$$u = g_1 \text{ on } \partial\Omega, \quad \frac{\partial^2 u}{\partial n^2} = g_2 \text{ on } \partial\Omega,$$

we adopt a penalized Deep Ritz formulation.

The total loss consists of:

$$\mathcal{L}_\theta = \mathcal{L}_{\text{interior}} + \mathcal{L}_{\text{boundary}},$$

and in our implementation, we additionally apply uncertainty-based weighting through learnable log-variances.

4.1 Interior Loss

In the Deep Ritz Method, the biharmonic equation is obtained as the Euler–Lagrange equation of the energy functional

$$E(u) = \int_{\Omega} \left(\frac{1}{2} \|\nabla^2 u\|^2 - fu \right) dx.$$

The discrete interior loss implemented in the code is:

$$\mathcal{L}_{\text{interior}} = \frac{1}{|\Omega|} \sum_{i=1}^N \left(\frac{1}{2} \|H(u_{\theta}(x_i))\|_F^2 - f(x_i)u_{\theta}(x_i) \right),$$

where:

- $H(u_{\theta})$ is the Hessian matrix,
- $\|\cdot\|_F$ is the Frobenius norm,
- $f(x)$ is the source term,
- $u_{\theta}(x)$ is the neural network prediction.

4.2 Boundary Loss

For problem (P2), the boundary conditions are:

1. **Dirichlet:**

$$u_{\theta}(x) = g_1(x),$$

2. **Second normal derivative (Neumann-type):**

$$\frac{\partial^2 u_{\theta}}{\partial n^2} = g_2(x).$$

The penalty-based boundary loss is:

$$\mathcal{L}_{\text{boundary}} = \lambda_D \|u_{\theta} - g_1\|_{\partial\Omega}^2 - \int_{\partial\Omega} g_2(x) \frac{\partial u_{\theta}}{\partial n}(x) ds.$$

4.3 Uncertainty-Based Loss Weighting

We introduce learnable log-variances:

- `log_var_interior`

- `log_var_boundary`

and define the total loss as:

$$\mathcal{L}_\theta = \frac{1}{2} [e^{-s_1} \mathcal{L}_{\text{interior}} + s_1 + e^{-s_2} \mathcal{L}_{\text{boundary}} + s_2],$$

where $s_1 = \text{log_var_interior}$ and $s_2 = \text{log_var_boundary}$.

5. Training Procedure

5.1 Adam Training (Stochastic)

For epochs $1 \rightarrow E_{\text{switch}}$:

- At every epoch, new interior and boundary samples are drawn.
- Adam optimizer updates the parameters.
- Uncertainty parameters (`log_var_*`) are updated together with the network.
- Losses and validation errors are logged.

6. Error Computation and Validation

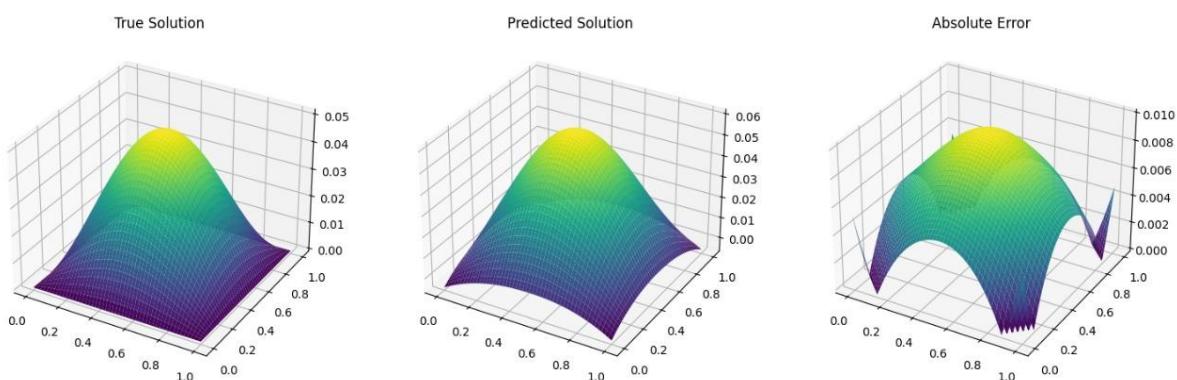
To evaluate accuracy, we compute the **L² error** over a dense set of points:

$$\| u_\theta - u \|_{L^2} \approx \sqrt{\frac{1}{N} \sum_{i=1}^N (u_\theta(x_i) - u(x_i))^2}$$

7. Visualization of Results

We visualize:

Results Example 3.1



10000 Epochs

Total Loss = -0.198

Interior Loss=-0.183

Boundary Loss=0.0251

pinns loss=4.08e-5

boundary loss=1.25e-5

Validation L2 error at Epoch 10000: 0.00591528182849288

L2: 0.02367546326942574

L2 relative 0.141109406148341

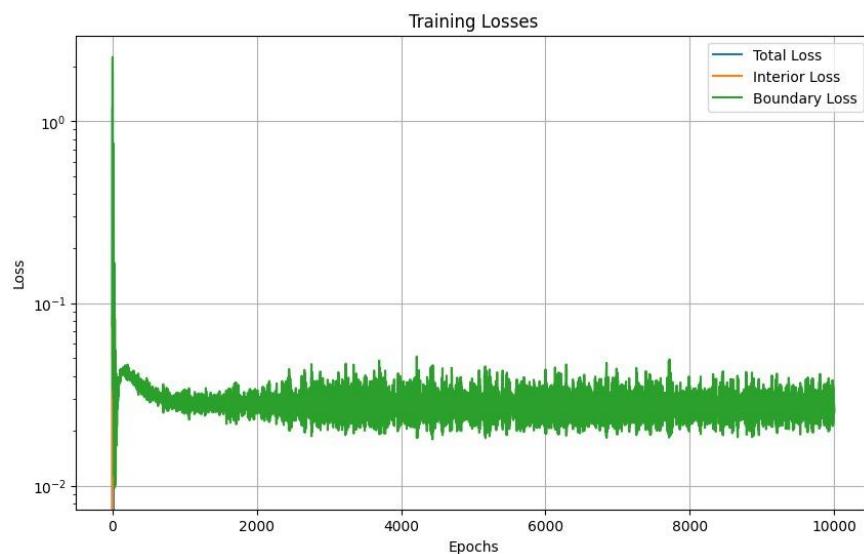
H1: 0.04473904672464288

H1 Relative: 0.3251126548132155

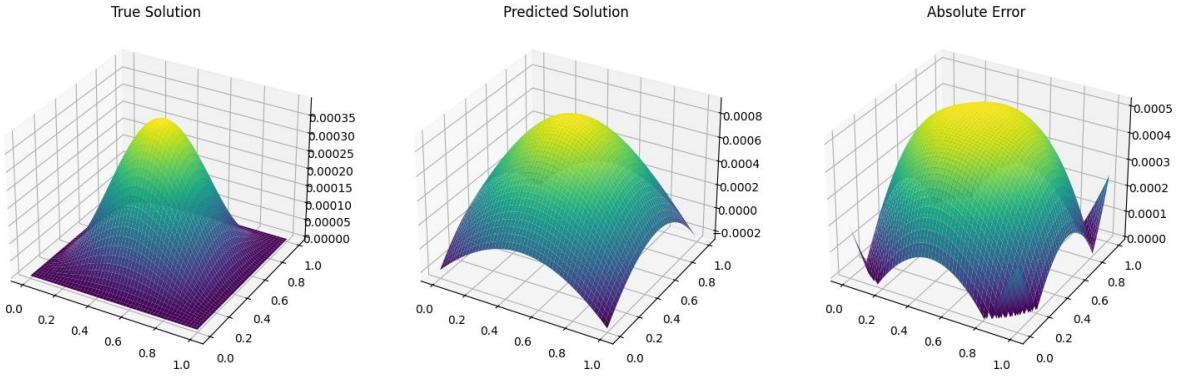
H2: 0.05807589850740585

H2 Relative: 0.11614920776104432

Loss Curve of 3.1



Results Example 3.2



Epoch 6000

Total Loss=-0.101

Interior Loss=-0.12,

Boundary Loss=0.0428

pinns loss=0.00995

boundary loss=0.00013

Validation L2 Error at epoch 6000: 0.004631813615560532

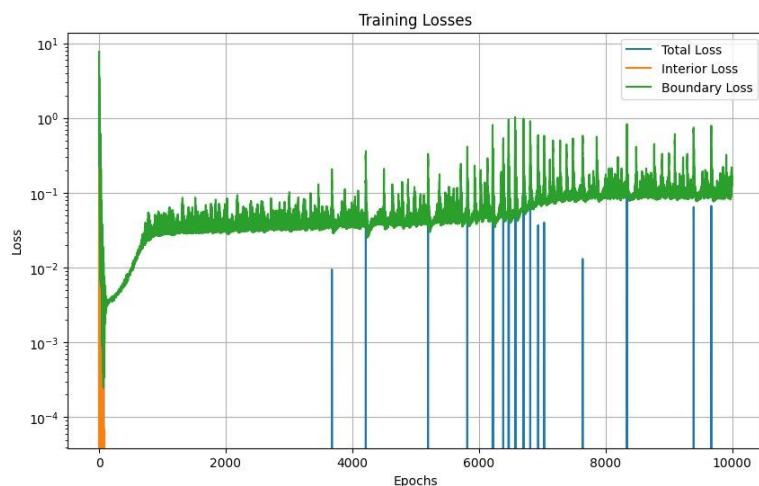
L2 relative: 0.18

H1 : 0.25

H2: 0.03

H2 relative: 0.45

Loss Curve of 3.2



Contributions

Every One in team has equally Contributed to this Project Completion.