Importance Sampling Methods to Accelerate PINN Calculations for *k*-Eigenvalue Neutron Diffusion Problems

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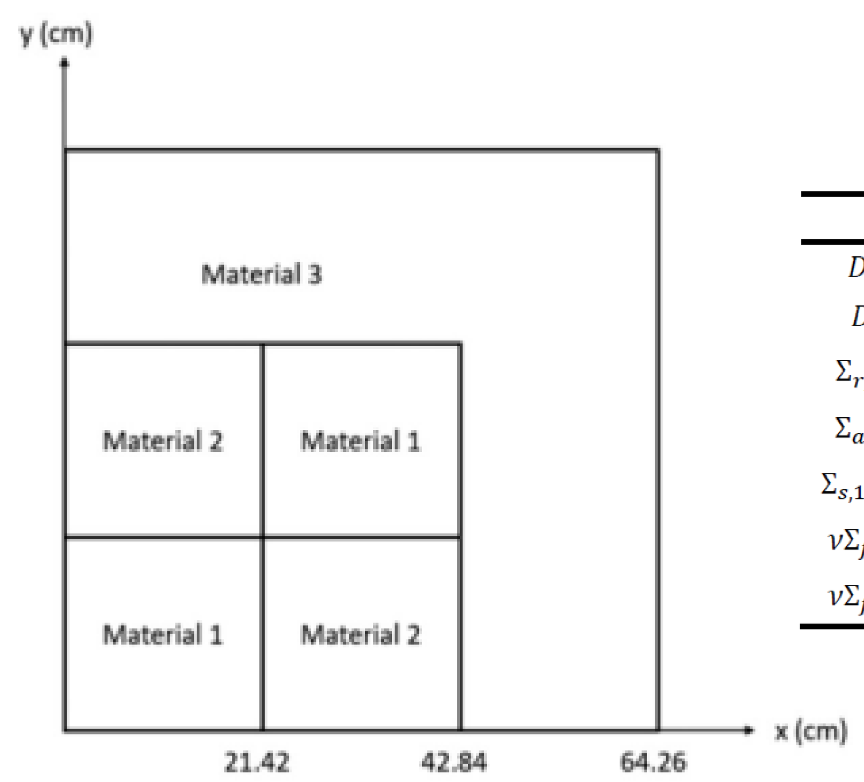
INTRODUCTION

Physics Informed Neural Networks (PINNs) have been successfully used to estimate the solution of partial differential equations [1]. In our previous development, the PINN approach was applied to two-dimensional (2D) two-energy group (2G) *k*-eigenvalue mode neutron diffusion models [2]. The PINN model was proved to be capable of predicting the solution to the eigenvalue 2G diffusion equations described by Eq.(1) for a problem given geometry and materials shown in Figure 1. In this work, we focus on improving the computational efficiency of the PINN approach by investigating and integrating advanced sampling methods into the PINN framework.

$$\begin{cases} -\nabla(D_1\nabla\phi_1) + \Sigma_{r,1}\phi_1 = \frac{1}{k}\left(\nu\Sigma_{f,1}\phi_1 + \nu\Sigma_{f,2}\phi_2\right) \\ -\nabla(D_2\nabla\phi_2) + \Sigma_{a,2}\phi_2 = \Sigma_{s,1\to2}\phi_1 \end{cases}, \qquad (1)$$



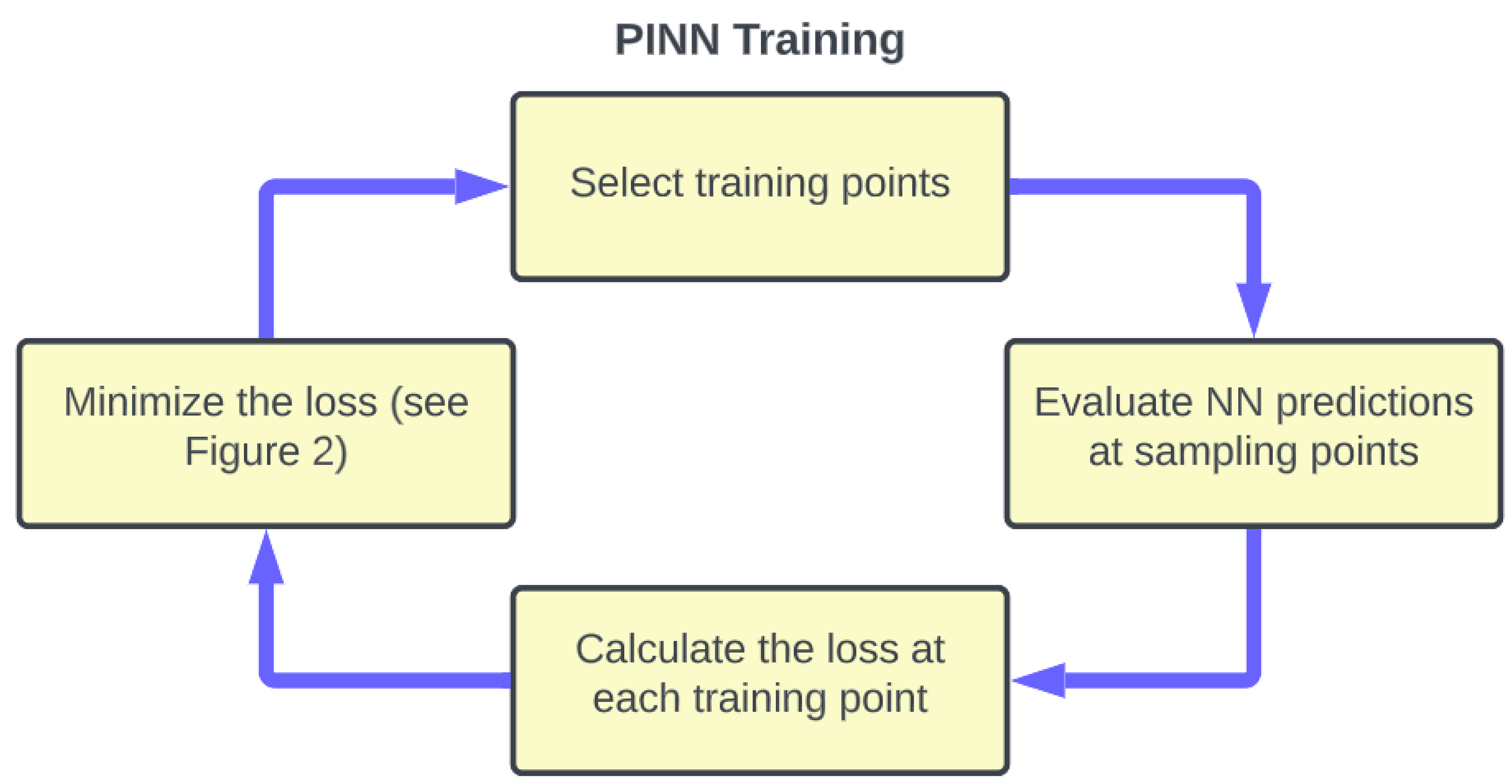
	Material 1	Material 2	Material 3
D_1 (cm)	1.2	1.2	1.2
D_2 (cm)	0.4	0.4	0.2
$\Sigma_{r,1}$ (cm^{-1})	0.03	0.03	0.051
$\Sigma_{a,2}$ (cm^{-1})	0.3	0.25	0.04
$\Sigma_{s,1\to2}$ (cm^{-1})	0.015	0.015	0.05
$\nu\Sigma_{f,1}$ (cm^{-1})	0.0075	0.0075	0
$\nu\Sigma_{f,2}$ (cm^{-1})	0.45	0.375	0

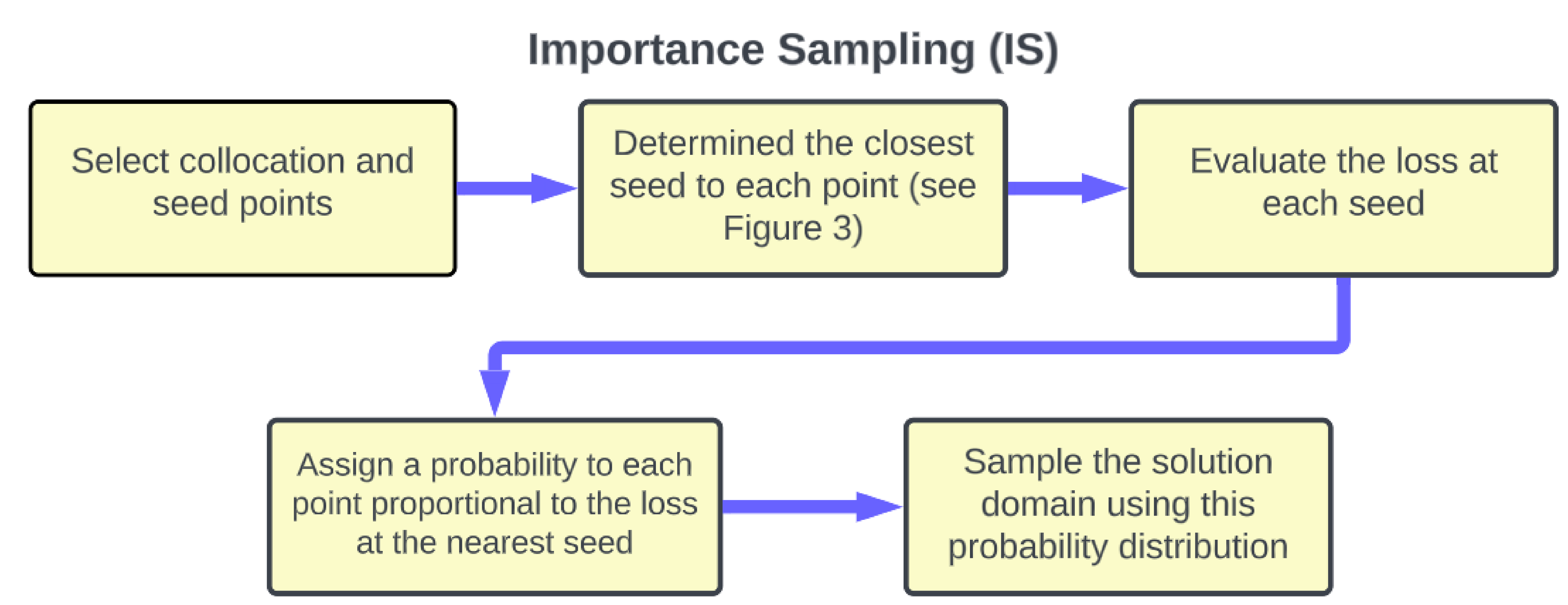
Figure 1. Problem geometry and material properties.

BACKGROUND

Applying a technique known as automatic differentiation (AD) to evaluate the partial derivative of the neural network function allows PINN to be trained to follow physical laws without the use of a traditional dataset [3]. Instead, by applying AD the PINN can be trained by sampling the solution domain and minimizing the residual form of the PDE also known as the residual loss. Previously, the PINN model was trained with semi-random fixed points in the solution domain generated by Latin hypercube sampling (LHS) to ensure the sampling points were evenly spaced [2]. The importance sampling (IS) method investigated in this work enables new sampling points to be selected for each iteration based on some prior sampling distribution. In the IS method, the new sampling distribution is weighted based on relative contribution to the PDE residual after each training iteration. IS has been demonstrated to accelerate the convergence of similar PINN models in the application of elasticity, diffusion, and plane stress problems [4].

METHODOLOGY





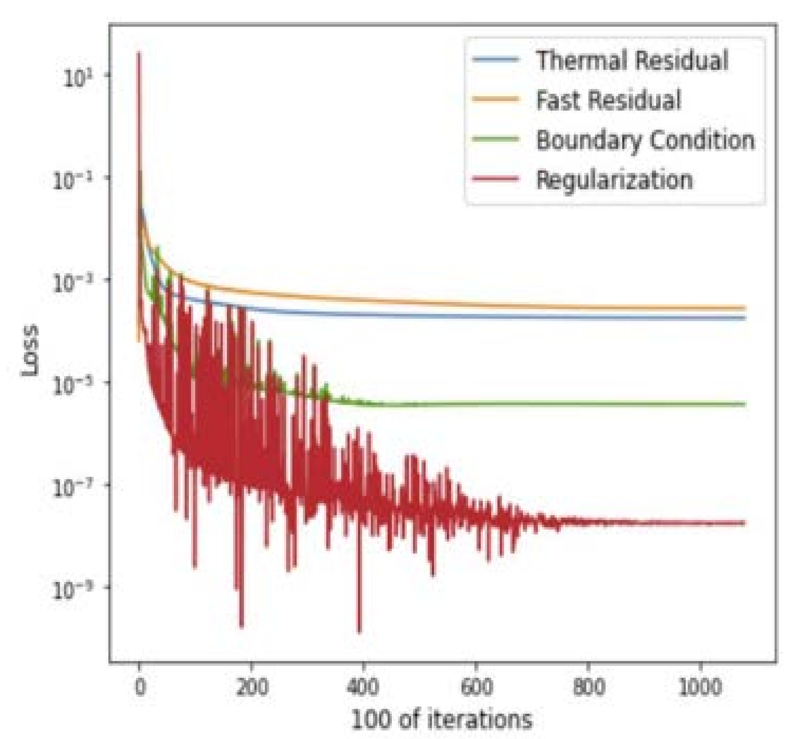


Figure 2. Loss minimization.

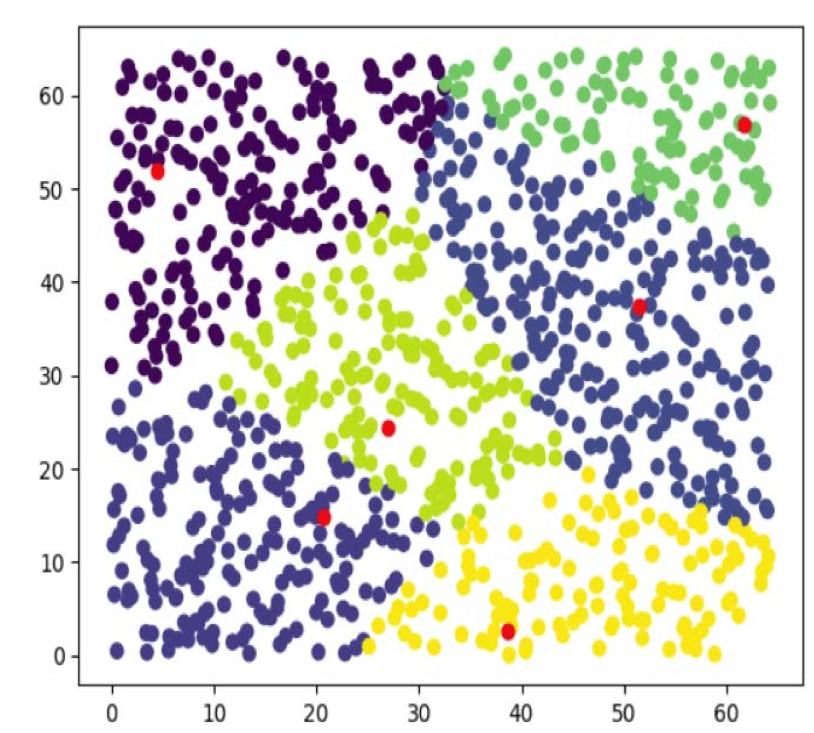


Figure 3. Sampling discretization.

RESULTS

For the LHS case, the relative error of the k-eff value was 0.733%. The total runtime to obtain this solution was 107 minutes. For the importance sampling case, the relative error of the k-value was 0.622%. The total runtime to obtain this solution was 62 minutes, which is considerably reduced compared to the LHS method. The convergence of the k-eff value is shown in Figure 4 and Figure 5 for the LHS and IS methods, respectively.

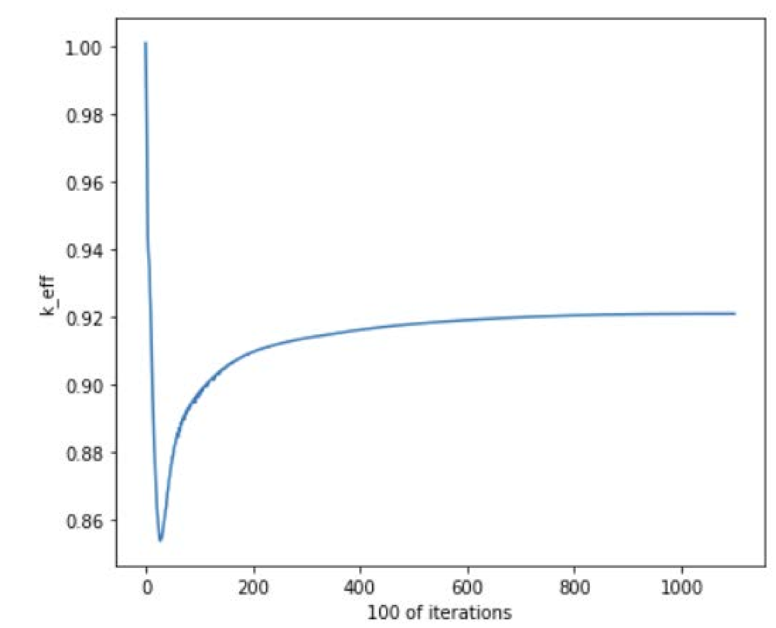


Figure 4. K-eff convergence for LHS.

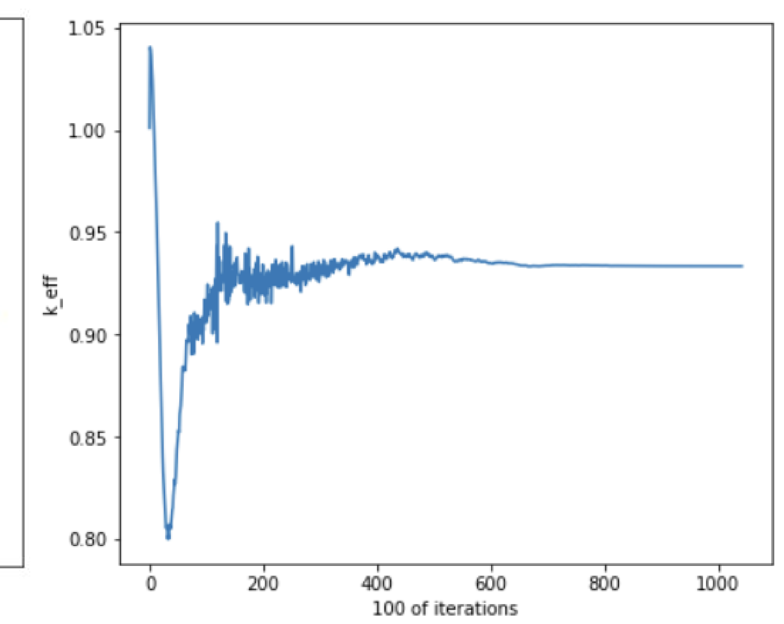


Figure 5. K-eff convergence for IS.

CONCLUSIONS

While the IS method did not significantly decrease the required number of training iterations, the total runtime required to obtain a solution with similar accuracy was reduced by 42%. This represents a significant decrease in the computational cost of training the neural networks (NN). This decrease can be attributed to the significantly smaller required sample size since the NN had to be evaluated at an order of magnitude fewer sampling points during each training iteration. However, no significant increase in model accuracy was achieved by implementing this sampling method.

REFERENCES

1. M. RAISSI et al., "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 (2019).
2. M. H. Elhareef and Z. WU, "Physics-Informed Neural Network Method and Application to Nuclear Reactor Calculations: A Pilot Study," *Nuclear Science and Engineering*, **174**(4), 601-622, (2023).
3. A. GRIEWANK and A. WALTHER, *Evaluating Derivatives, Principles and Techniques of Algorithmic Differentiation*, 2nd Edition, Society for Industrial and Applied Mathematics, Philadelphia, PA (2008).
4. M. A. NABIAN, R. J. GLADSTONEG, and H. MEIDANI, "Efficient training of physics-informed neural networks via importance sampling," *Computer Aided Civ Inf.*, **36**, 962–977 (2021).