Scientific machine learning for inverse problems and model order reduction

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Abstract

The application of scientific machine learning for engineering applications has grown rapidly in recent years. We introduce two interesting applications of scientific machine learning: inverse problem in electromagnetics and model order reduction. We discuss two cases related to inverse problem in electromagnetics. First, we introduce a Physics Informed Neural Network (PINN)-based deep learning approach to reconstruct one-dimensional rough surfaces from field data illuminated by an electromagnetic incident wave. Next, we discuss application of DeepONet for inverse rough surface scattering problem, which seeks to recover the profile of rough surfaces from the measured scattered electromagnetic field and finds extensive applications across diverse domains including non-destructive testing, geophysical radar, ocean optics. In the case of model order reduction of parametric partial differential equations, deep learning based methods have gained traction in recent years. On exascale systems, such approaches require more careful numerical implementation. We introduce a framework, DLRBniCSx, for deep learning based model order reduction for large scale problems.
Keywords: Inverse problems, Electromagnetics, Exascale computing, Model order reduction

1 Scientific machine learning for inverse problems in electromagnetics

The inverse problem of rough surface scattering aims to recover the profile of rough surface provided the information of scattered data. The traditional methods to solve the problem are generally based on physical equations of surface scattering, and their robustness is contingent upon certain conditions on surface and incident wave (e.g. the convergence of iterative method in Chen et al. [2018] is based on low grazing angle approximation).

In order to maintain the physics of rough surface scattering, while improving the robustness of the method, it motivates us to employ two machine learning type methods: the Physics Informed Neural Networks (PINN) Raissi et al. [2019] and the DeepONet operator learning method Lu et al. [2021].

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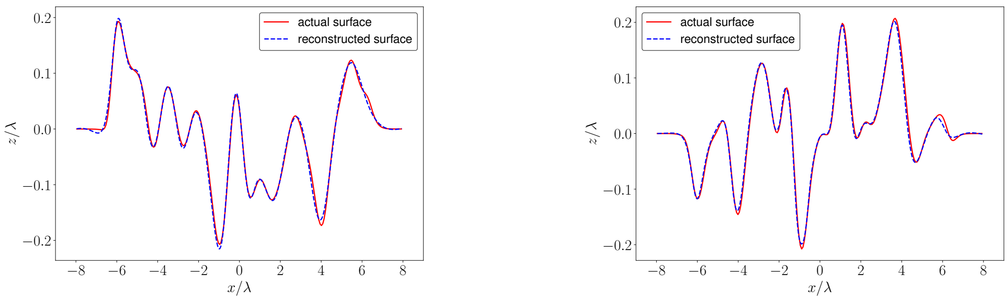
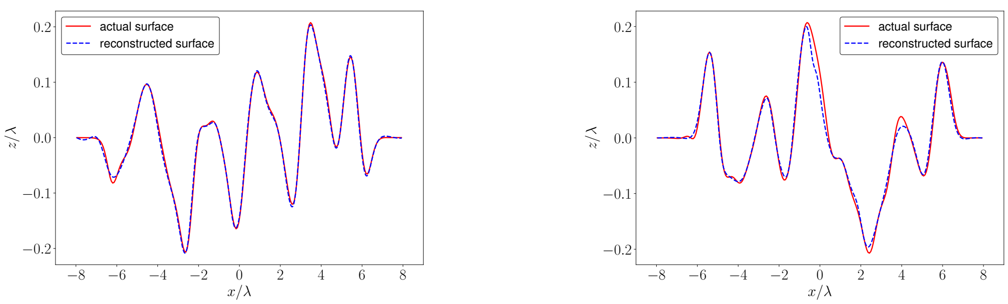


(a) (b)

Figure 1: Reconstruction of rough surfaces against the actual surfaces using PINN for (**a**) known full scattered data (left), (**b**) known phaseless total field data (right).



(a) (b)

Figure 2: Reconstruction of rough surfaces against the actual surfaces using DeepONet for (**a**) known full scattered data (left), (**b**) known phaseless total field data (right).

Both methods are developed to numerically solve the partial differential equations. It is found that the two methods can be adapted to solve the inverse surface scattering problem with great accuracy and strong robustness with respect to different problem settings (Figures 1 and 2).

The PINN-based approach is an unsupervised approach, independent of any surface data, rather only the field data is used. In the case of DeepONet based approach, the reconstructed surface agrees closely with the exact surface. A small height discrepancy can be seen between the reconstruction and exact surface, but all key features are well-captured and correctly located horizontally.

2 Deep learning based model order reduction of parametrised partial differential equations

Model order reduction methods aim to identify a low-dimensional model that can reduce dependence on large-scale problems. Deep learning-based methods are used extensively to identify such a low-dimensional model Hesthaven and Ubbiali [2018], Meneghetti et al. [2022]. Deep learning based methods can be non-intrusive in nature and may not require access to source code used to solve high-fidelity model. In the case of offline-online two stage procedure, deep learning methods are quicker in the online phase. However during the offline phase, they suffer from severe computational cost associated to generation of training data and training of artificial neural network. On exascale systems, such approaches require more careful numerical implementation. In this context, a PyTorch-RBniCSx-MDFEniCSx-FEniCSx based framework for the deep learning-based model order reduction, DLRBniCSx, has been developed Shah et al. [2024b], Shah et al. [2024a] . DLRBniCSx focuses on the efficient execution of model order reduction operations on High Performance Computing (HPC) systems. This includes identification and decoupling of CPU-based and GPU-based operations, implementation of data-parallel distributed neural network training routines, and data management routines.

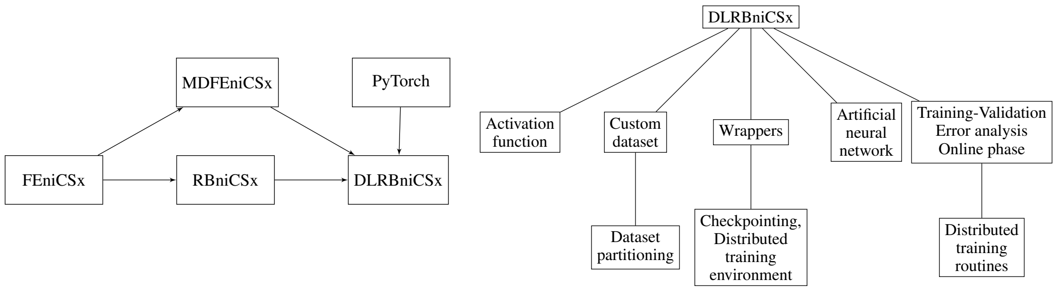


Figure 3: DLRBniCSx dependencies (left) and DLRBniCSx modules (right)

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